

# checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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: 3

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|                 |                    |                    |              |
|-----------------|--------------------|--------------------|--------------|
| Bond precision: | C-C = 0.0120 Å     | Wavelength=0.71073 |              |
| Cell:           | a=24.1332(9)       | b=13.5042(6)       | c=20.4034(9) |
|                 | alpha=90           | beta=96.462(4)     | gamma=90     |
| Temperature:    | 150 K              |                    |              |
|                 | Calculated         | Reported           |              |
| Volume          | 6607.2(5)          | 6607.2(5)          |              |
| Space group     | C 2/m              | C 2/m              |              |
| Hall group      | -C 2y              | ?                  |              |
| Moiety formula  | C48 H108 O16 Si4 U | ?                  |              |
| Sum formula     | C48 H108 O16 Si4 U | C48 H108 O16 Si4 U |              |
| Mr              | 1291.74            | 1291.73            |              |
| Dx, g cm-3      | 1.299              | 1.299              |              |
| Z               | 4                  | 4                  |              |
| Mu (mm-1)       | 2.584              | 2.584              |              |
| F000            | 2688.0             | 2688.0             |              |
| F000'           | 2651.85            |                    |              |
| h, k, lmax      | 32, 18, 27         | 32, 17, 27         |              |
| Nref            | 8547               | 8461               |              |
| Tmin, Tmax      | 0.211, 0.538       | 0.289, 0.580       |              |
| Tmin'           | 0.176              |                    |              |

Correction method= MULTI-SCAN

Data completeness= 0.990      Theta(max)= 28.280

R(reflections)= 0.0459( 7113)      wR2(reflections)= 0.1070( 8461)

S = 1.098      Npar= 604

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The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level**.  
Click on the hyperlinks for more details of the test.

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### 🟡 Alert level B

|                   |                   |                             |           |
|-------------------|-------------------|-----------------------------|-----------|
| PLAT215_ALERT_3_B | Disordered C70    | has ADP max/min Ratio ..... | 4.4       |
| PLAT220_ALERT_2_B | Large Non-Solvent | C Ueq(max)/Ueq(min) ...     | 5.9 Ratio |

### 🟡 Alert level C

|                   |                            |                                     |             |
|-------------------|----------------------------|-------------------------------------|-------------|
| PLAT215_ALERT_3_C | Disordered C10             | has ADP max/min Ratio .....         | 3.7         |
| PLAT215_ALERT_3_C | Disordered C11             | has ADP max/min Ratio .....         | 3.4         |
| PLAT215_ALERT_3_C | Disordered C12             | has ADP max/min Ratio .....         | 3.9         |
| PLAT222_ALERT_3_C | Large Non-Solvent          | H Uiso(max)/Uiso(min) ..            | 4.1 Ratio   |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C5 -- C6 ..                         | 0.19 Ang.   |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for C5 |             |
| PLAT342_ALERT_3_C | Low Bond Precision on      | C-C Bonds .....                     | 0.0120 Ang. |
| PLAT722_ALERT_1_C | Angle Calc                 | 128.00, Rep 129.30 Dev...           | 1.30 Deg.   |
|                   | C63 -C4 -H4C               | 6.565 1.555 1.555 #                 | 144         |

### 🟡 Alert level G

|                   |                                                  |                                      |
|-------------------|--------------------------------------------------|--------------------------------------|
| PLAT004_ALERT_5_G | Info: Polymeric Structure Found with Dimension . | 1                                    |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  | ? Do !                               |
| PLAT063_ALERT_4_G | Crystal Size Likely too Large for Beam Size .... | 0.64 mm                              |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large. | 7.59                                 |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for Si4 |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for C1  |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for C9  |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for C29 |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for C61 |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for C65 |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for C69 |
| PLAT301_ALERT_3_G | Note: Main Residue Disorder .....                | 89 %                                 |
| PLAT764_ALERT_4_G | Overcomplete CIF Bond List Detected (Rep/Expd) . | 2.28 Ratio                           |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C3 -- C67 .          | 1.84 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C4 -- C1 .           | 1.74 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C21 -- C30 .         | 1.98 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C22 -- C30 .         | 1.87 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C25 -- C32 .         | 1.85 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C27 -- C69 .         | 1.79 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C30 -- C22 .         | 1.87 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C30 -- C21 .         | 1.98 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C31 -- C31 .         | 1.81 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C32 -- C25 .         | 1.85 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C41 -- C44 .         | 1.89 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C42 -- C51 .         | 1.72 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C44 -- C41 .         | 1.89 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C49 -- C72 .         | 1.82 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C51 -- C42 .         | 1.72 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C67 -- C3 .          | 1.84 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C69 -- C27 .         | 1.79 Ang.                            |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF: C72 -- C49 .         | 1.82 Ang.                            |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 68                                   |
|                   | 01 -SI1 -01 6.565 1.555 1.555                    | 42.70 Deg.                           |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 69                                   |
|                   | SI1 -SI1 -01 6.565 1.555 1.555                   | 36.70 Deg.                           |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 85                                   |
|                   | 03 -SI1 -03 1.555 1.555 6.565                    | 38.20 Deg.                           |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 88                                   |
|                   | 01 -SI1 -U1 6.565 1.555 1.555                    | 14.20 Deg.                           |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 90                                   |
|                   | 01 -SI1 -U1 1.555 1.555 1.555                    | 41.50 Deg.                           |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 99                                   |
|                   | 01 -01 -SI1 6.565 1.555 1.555                    | 36.70 Deg.                           |

|                   |                       |                     |        |            |
|-------------------|-----------------------|---------------------|--------|------------|
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 106        |
| 01 -02 -SI1       | 6.565 1.555 1.555     |                     |        | 35.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 120        |
| SI1 -03 -SI1      | 1.555 1.555 6.565     |                     |        | 43.10 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 121        |
| C9 -04 -C12       | 1.555 1.555 6.565     |                     |        | 6.00 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 138        |
| C61 -C4 -H4A      | 6.565 1.555 1.555     |                     |        | 39.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 219        |
| C12 -C9 -C9       | 1.555 1.555 6.565     |                     |        | 5.00 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 221        |
| C9 -C10 -C12      | 1.555 1.555 6.565     |                     |        | 3.20 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 231        |
| C12 -C11 -C9      | 6.565 1.555 1.555     |                     |        | 6.00 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 245        |
| C12 -C12 -C9      | 6.565 1.555 1.555     |                     |        | 5.00 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 251        |
| C9 -C12 -C10      | 6.565 1.555 6.565     |                     |        | 32.00 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 256        |
| C9 -C12 -H12A     | 6.565 1.555 1.555     |                     |        | 36.80 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 261        |
| C10 -C12 -H12A    | 6.565 1.555 1.555     |                     |        | 18.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 266        |
| 04 -C12 -H12B     | 6.565 1.555 1.555     |                     |        | 7.80 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 271        |
| C11 -C12 -H12C    | 6.565 1.555 1.555     |                     |        | 16.40 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 311        |
| 024 -SI2 -C29     | 1.555 1.555 6.565     |                     |        | 15.60 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 331        |
| 024 -024 -C29     | 6.565 1.555 1.555     |                     |        | 15.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 342        |
| C29 -024 -C31     | 6.565 1.555 6.565     |                     |        | 41.00 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 349        |
| C68 -C23 -H23A    | 6.565 1.555 1.555     |                     |        | 41.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 364        |
| C24 -C24 -H24C    | 2.656 1.555 1.555     |                     |        | 39.90 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 396        |
| 064 -C27 -H27A    | 6.565 1.555 1.555     |                     |        | 19.90 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 397        |
| C69 -C27 -H27A    | 6.565 1.555 1.555     |                     |        | 34.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 403        |
| C70 -C27 -H27C    | 6.565 1.555 1.555     |                     |        | 36.60 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 415        |
| 024 -C29 -024     | 6.565 1.555 1.555     |                     |        | 39.00 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 426        |
| 024 -C29 -C29     | 1.555 1.555 6.565     |                     |        | 15.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 437        |
| C29 -C30 -024     | 1.555 1.555 6.565     |                     |        | 13.60 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 458        |
| 022 -C30 -H30B    | 6.565 1.555 1.555     |                     |        | 26.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 468        |
| C22 -C30 -H30C    | 6.565 1.555 1.555     |                     |        | 15.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 469        |
| C21 -C30 -H30C    | 6.565 1.555 1.555     |                     |        | 42.30 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 473        |
| C29 -C31 -024     | 1.555 1.555 6.565     |                     |        | 11.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 488        |
| 024 -C32 -C29     | 6.565 1.555 1.555     |                     |        | 18.40 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 500        |
| SI2 -C32 -H32A    | 6.565 1.555 1.555     |                     |        | 42.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant | (Bond) Angle in CIF | .... # | 524        |
| C44 -C41 -C44     | 1.555 1.555 6.565     |                     |        | 4.00 Deg.  |

|                   |                                             |                     |        |            |
|-------------------|---------------------------------------------|---------------------|--------|------------|
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 527        |
| C51 -C42 -H42A    | 7.557                                       | 1.555               | 1.555  | 10.90 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 541        |
| C47 -SI3 -O43     | 6.565                                       | 1.555               | 1.555  | 37.10 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 567        |
| C44 -C44 -C41     | 6.565                                       | 1.555               | 6.565  | 20.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 574        |
| C41 -C44 -H44B    | 6.565                                       | 1.555               | 1.555  | 44.00 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 588        |
| O43 -C45 -C47     | 1.555                                       | 1.555               | 6.565  | 37.40 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 591        |
| O43 -C45 -C47     | 6.565                                       | 1.555               | 1.555  | 37.40 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 609        |
| SI3 -C47 -H47A    | 6.565                                       | 1.555               | 1.555  | 31.00 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 638        |
| C63 -C1 -C4       | 6.565                                       | 1.555               | 1.555  | 6.00 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 641        |
| C2 -C1 -SI4       | 1.555                                       | 1.555               | 6.565  | 13.90 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 651        |
| O63 -C2 -H2A      | 6.565                                       | 1.555               | 1.555  | 40.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 654        |
| SI4 -C2 -H2B      | 6.565                                       | 1.555               | 1.555  | 35.10 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 657        |
| O62 -C2 -H2B      | 6.565                                       | 1.555               | 1.555  | 43.80 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 674        |
| C52 -C49 -C72     | 1.555                                       | 1.555               | 6.565  | 40.60 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 688        |
| C42 -C51 -H51C    | 7.557                                       | 1.555               | 1.555  | 9.90 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 692        |
| C72 -C52 -H52A    | 6.565                                       | 1.555               | 1.555  | 29.10 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 704        |
| C2 -SI4 -O63      | 6.565                                       | 1.555               | 1.555  | 35.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 711        |
| C2 -SI4 -C1       | 6.565                                       | 1.555               | 6.565  | 23.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 719        |
| SI4 -O62 -C2      | 1.555                                       | 1.555               | 6.565  | 32.00 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 721        |
| C2 -O63 -SI4      | 6.565                                       | 1.555               | 1.555  | 32.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 732        |
| C63 -C61 -C4      | 1.555                                       | 1.555               | 6.565  | 8.00 Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 750        |
| C1 -C63 -H63B     | 6.565                                       | 1.555               | 1.555  | 32.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 779        |
| C66 -C66 -H66C    | 6.575                                       | 1.555               | 1.555  | 43.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 787        |
| C3 -C67 -H67B     | 6.565                                       | 1.555               | 1.555  | 16.10 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 796        |
| C23 -C68 -H68B    | 6.565                                       | 1.555               | 1.555  | 31.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 814        |
| C27 -C70 -H70A    | 6.565                                       | 1.555               | 1.555  | 29.40 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 826        |
| C26 -C71 -H71B    | 6.565                                       | 1.555               | 1.555  | 41.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 841        |
| C49 -C72 -H72B    | 6.565                                       | 1.555               | 1.555  | 27.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant                       | (Bond) Angle in CIF | .... # | 843        |
| C52 -C72 -H72C    | 6.565                                       | 1.555               | 1.555  | 36.00 Deg. |
| PLAT811_ALERT_5_G | No ADDSYM Analysis: Too Many Excluded Atoms | ....                |        | ! 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  
 8 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight

97 **ALERT level G** = General information/check it is not something unexpected

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

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## Datablock: 3-py

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Bond precision: C-C = 0.0052 A

Wavelength=0.71073

Cell: a=24.5649(8) b=13.2630(3) c=25.9619(8)  
alpha=90 beta=118.606(4) gamma=90  
Temperature: 150 K

|                | Calculated            | Reported              |
|----------------|-----------------------|-----------------------|
| Volume         | 7426.0(5)             | 7426.0(4)             |
| Space group    | C 2/c                 | C 2/c                 |
| Hall group     | -C 2yc                | ?                     |
| Moiety formula | C58 H118 N2 O16 Si4 U | ?                     |
| Sum formula    | C58 H118 N2 O16 Si4 U | C58 H118 N2 O16 Si4 U |
| Mr             | 1449.93               | 1449.93               |
| Dx, g cm-3     | 1.297                 | 1.297                 |
| Z              | 4                     | 4                     |
| Mu (mm-1)      | 2.308                 | 2.308                 |
| F000           | 3024.0                | 3024.0                |
| F000'          | 2987.92               |                       |
| h, k, lmax     | 30, 16, 32            | 30, 16, 32            |
| Nref           | 7605                  | 7590                  |
| Tmin, Tmax     | 0.667, 0.812          | 0.592, 0.812          |
| Tmin'          | 0.556                 |                       |

Correction method= MULTI-SCAN

Data completeness= 0.998

Theta(max)= 26.370

R(reflections)= 0.0234( 7026)

wR2(reflections)= 0.0542( 7590)

S = 1.049

Npar= 564

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.



### Alert level B

|                   |                         |                  |       |     |    |     |      |
|-------------------|-------------------------|------------------|-------|-----|----|-----|------|
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | Si2              | --    | 024 | .. | 7.2 | su   |
| PLAT391_ALERT_3_B | Deviating Methyl C7     | H-C-H Bond Angle | ..... |     |    | 99  | Deg. |

PLAT391\_ALERT\_3\_B Deviating Methyl C7      H-C-H Bond Angle      119 Deg.

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● **Alert level C**

|                   |                                                  |             |
|-------------------|--------------------------------------------------|-------------|
| PLAT094_ALERT_2_C | Ratio of Maximum / Minimum Residual Density .... | 3.44        |
| PLAT213_ALERT_2_C | Atom C26 has ADP max/min Ratio .....             | 3.6 prola   |
| PLAT220_ALERT_2_C | Large Non-Solvent C Ueq(max)/Ueq(min) ...        | 3.6 Ratio   |
| PLAT222_ALERT_3_C | Large Non-Solvent H Uiso(max)/Uiso(min) ..       | 5.7 Ratio   |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for Si2 -- O22 ..            | 5.4 su      |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C21         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C25         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C29         |
| PLAT245_ALERT_2_C | U(iso) H2A Smaller than U(eq) C2 by ...          | 0.012 AngSq |
| PLAT245_ALERT_2_C | U(iso) H2C Smaller than U(eq) C2 by ...          | 0.013 AngSq |
| PLAT350_ALERT_3_C | Short C-H (X0.96,N1.08A) C43 - H43 ...           | 0.79 Ang.   |
| PLAT390_ALERT_3_C | Deviating Methyl C2 X-C-H Bond Angle .....       | 103 Deg.    |
| PLAT391_ALERT_3_C | Deviating Methyl C12 H-C-H Bond Angle .....      | 102 Deg.    |

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● **Alert level G**

|                   |                                                  |            |
|-------------------|--------------------------------------------------|------------|
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  | ? Do !     |
| PLAT164_ALERT_4_G | Nr. of Refined C-H H-Atoms in Heavy-Atom Struct. | 32         |
| PLAT301_ALERT_3_G | Note: Main Residue Disorder .....                | 15 %       |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 169        |
|                   | C23B -C21 -C23 1.555 1.555 1.555                 | 12.00 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 190        |
|                   | C27 -C25 -C27B 1.555 1.555 1.555                 | 26.90 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 195        |
|                   | C26B -C25 -C26 1.555 1.555 1.555                 | 24.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 213        |
|                   | C32 -C29 -C32B 1.555 1.555 1.555                 | 22.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 218        |
|                   | C31 -C29 -C31B 1.555 1.555 1.555                 | 40.70 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 221        |
|                   | C30B -C29 -C30 1.555 1.555 1.555                 | 36.00 Deg. |
| PLAT811_ALERT_5_G | No ADDSYM Analysis: Too Many Excluded Atoms .... | ! Info     |

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

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

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## Datablock: 2

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|                 |                |                                  |
|-----------------|----------------|----------------------------------|
| Bond precision: | C-C = 0.0186 A | Wavelength=0.71073               |
| Cell:           | a=18.2032(12)  | b=25.9028(11)      c=36.9447(18) |
|                 | alpha=90       | beta=90      gamma=90            |
| Temperature:    | 150 K          |                                  |

|                | Calculated                                 | Reported             |
|----------------|--------------------------------------------|----------------------|
| Volume         | 17419.9(16)                                | 17420.0(16)          |
| Space group    | P b c a                                    | P b c a              |
| Hall group     | -P 2ac 2ab                                 | ?                    |
| Moiety formula | C48 H108 O16 Si4 U, C12<br>H24 K O6, C7 H8 | ?                    |
| Sum formula    | C67 H140 K O22 Si4 U                       | C67 H140 K O22 Si4 U |
| Mr             | 1687.29                                    | 1687.28              |
| Dx, g cm-3     | 1.287                                      | 1.287                |
| Z              | 8                                          | 8                    |
| Mu (mm-1)      | 2.028                                      | 2.028                |
| F000           | 7080.0                                     | 7080.0               |
| F000'          | 7010.02                                    |                      |
| h, k, lmax     | 21, 30, 43                                 | 21, 30, 43           |
| Nref           | 14859                                      | 14742                |
| Tmin, Tmax     | 0.864, 0.960                               | 0.642, 0.968         |
| Tmin'          | 0.615                                      |                      |

Correction method= ANALYTICAL

Data completeness= 0.992

Theta(max)= 24.710

R(reflections)= 0.0729( 6866)

wR2(reflections)= 0.1384( 14742)

S = 0.980

Npar= 955

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

|                                                                    |                                      |           |
|--------------------------------------------------------------------|--------------------------------------|-----------|
| PLAT213_ALERT_2_B Atom C86                                         | has ADP max/min Ratio .....          | 4.6 prola |
| PLAT220_ALERT_2_B Large Non-Solvent C                              | Ueq(max)/Ueq(min) ...                | 6.3 Ratio |
| PLAT234_ALERT_4_B Large Hirshfeld Difference C49                   | -- C50B ..                           | 0.28 Ang. |
| PLAT234_ALERT_4_B Large Hirshfeld Difference 084                   | -- C86 ..                            | 0.26 Ang. |
| PLAT234_ALERT_4_B Large Hirshfeld Difference 085                   | -- C88 ..                            | 0.28 Ang. |
| PLAT241_ALERT_2_B Check High                                       | Ueq as Compared to Neighbors for C86 |           |
| PLAT241_ALERT_2_B Check High                                       | Ueq as Compared to Neighbors for C88 |           |
| PLAT250_ALERT_2_B Large U3/U1 Ratio for Average U(i,j) Tensor .... |                                      | 4.2       |

### Alert level C

|                                                                              |                             |           |
|------------------------------------------------------------------------------|-----------------------------|-----------|
| RINTA01_ALERT_3_C The value of Rint is greater than 0.12                     |                             |           |
| Rint given                                                                   | 0.153                       |           |
| THETM01_ALERT_3_C The value of sine(theta_max)/wavelength is less than 0.590 |                             |           |
| Calculated sin(theta_max)/wavelength =                                       | 0.5882                      |           |
| PLAT020_ALERT_3_C The value of Rint is greater than 0.12 .....               |                             | 0.153     |
| PLAT026_ALERT_3_C Ratio Observed / Unique Reflections too Low ....           |                             | 47 %      |
| PLAT213_ALERT_2_C Atom C22                                                   | has ADP max/min Ratio ..... | 3.3 prola |
| PLAT213_ALERT_2_C Atom C24                                                   | has ADP max/min Ratio ..... | 3.3 prola |
| PLAT213_ALERT_2_C Atom C52B                                                  | has ADP max/min Ratio ..... | 4.0 prola |
| PLAT213_ALERT_2_C Atom C66                                                   | has ADP max/min Ratio ..... | 3.1 prola |

|                   |                            |                                  |                     |        |           |
|-------------------|----------------------------|----------------------------------|---------------------|--------|-----------|
| PLAT213_ALERT_2_C | Atom C88                   | has ADP max/min Ratio            | .....               | 4.0    | prola     |
| PLAT213_ALERT_2_C | Atom C91                   | has ADP max/min Ratio            | .....               | 3.2    | prola     |
| PLAT222_ALERT_3_C | Large Non-Solvent          | H                                | Uiso(max)/Uiso(min) | ..     | 4.8 Ratio |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for    | 083                              | -- C84              | ..     | 5.1 su    |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for    | 085                              | -- C89              | ..     | 6.3 su    |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for    | 086                              | -- C90              | ..     | 6.7 su    |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C9                               | -- C11              | ..     | 0.17 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C49                              | -- C52              | ..     | 0.24 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C69                              | -- C71              | ..     | 0.18 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 081                              | -- C81              | ..     | 0.20 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 081                              | -- C92              | ..     | 0.21 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 082                              | -- C82              | ..     | 0.17 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 082                              | -- C83              | ..     | 0.23 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 084                              | -- C87              | ..     | 0.21 Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 086                              | -- C91              | ..     | 0.21 Ang. |
| PLAT241_ALERT_2_C | Check High                 | Ueq as Compared to Neighbors for |                     | 081    |           |
| PLAT241_ALERT_2_C | Check High                 | Ueq as Compared to Neighbors for |                     | 082    |           |
| PLAT241_ALERT_2_C | Check High                 | Ueq as Compared to Neighbors for |                     | 083    |           |
| PLAT241_ALERT_2_C | Check High                 | Ueq as Compared to Neighbors for |                     | 084    |           |
| PLAT241_ALERT_2_C | Check High                 | Ueq as Compared to Neighbors for |                     | 086    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C1     |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C5     |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C21    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C41    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C49    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C65    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C69    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | K1     |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C81    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C83    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C85    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C87    |           |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for |                     | C89    |           |
| PLAT243_ALERT_4_C | High 'Solvent'             | Ueq as Compared to Neighbors of  |                     | C105   |           |
| PLAT244_ALERT_4_C | Low 'Solvent'              | Ueq as Compared to Neighbors of  |                     | C106   |           |
| PLAT342_ALERT_3_C | Low Bond Precision on      | C-C Bonds                        | .....               | 0.0186 | Ang.      |
| PLAT362_ALERT_2_C | Short C(sp3)-C(sp2) Bond   | C101 - C107                      | ...                 | 1.41   | Ang.      |
| PLAT722_ALERT_1_C | Angle Calc                 | 108.00, Rep                      | 109.50 Dev...       | 1.50   | Deg.      |
|                   | C49 -C52B -H52E            | 1.555 1.555 1.555                | #                   | 296    |           |
| PLAT722_ALERT_1_C | Angle Calc                 | 111.00, Rep                      | 109.50 Dev...       | 1.50   | Deg.      |
|                   | H52D -C52B -H52F           | 1.555 1.555 1.555                | #                   | 299    |           |

### ● Alert level G

|                   |                                                  |            |
|-------------------|--------------------------------------------------|------------|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 10         |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  | ? Do !     |
| PLAT301_ALERT_3_G | Note: Main Residue Disorder .....                | 7 %        |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 259        |
|                   | C50B -C49 -C51 1.555 1.555 1.555                 | 40.00 Deg. |
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints .....   | 60         |

0 ALERT level A = Most likely a serious problem - resolve or explain

8 ALERT level B = A potentially serious problem, consider carefully

47 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

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

34 ALERT type 2 Indicator that the structure model may be wrong or deficient

8 ALERT type 3 Indicator that the structure quality may be low

15 ALERT type 4 Improvement, methodology, query or suggestion

1 ALERT type 5 Informative message, check



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## Datablock: 4

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Bond precision: C-C = 0.0210 Å

Wavelength=0.71073

Cell: a=15.5600(7) b=28.0501(11) c=25.1711(11)  
alpha=90 beta=97.154(5) gamma=90

Temperature: 150 K

|                        | Calculated             | Reported            |
|------------------------|------------------------|---------------------|
| Volume                 | 10900.6(8)             | 10900.6(8)          |
| Space group            | P 21/n                 | P 21/n              |
| Hall group             | -P 2yn                 | ?                   |
| Moiety formula         | C88 H168 N4 O16 Si4 U2 | ?                   |
| Sum formula            | C88 H168 N4 O16 Si4 U2 | C44 H84 N2 O8 Si2 U |
| Mr                     | 2126.69                | 1063.34             |
| Dx, g cm <sup>-3</sup> | 1.296                  | 1.296               |
| Z                      | 4                      | 8                   |
| Mu (mm <sup>-1</sup> ) | 3.066                  | 3.066               |
| F000                   | 4368.0                 | 4368.0              |
| F000'                  | 4293.84                |                     |
| h, k, lmax             | 19, 35, 31             | 19, 35, 31          |
| Nref                   | 22289                  | 22210               |
| Tmin, Tmax             | 0.743, 0.941           | 0.753, 0.938        |
| Tmin'                  | 0.729                  |                     |

Correction method= ANALYTICAL

Data completeness= 0.996

Theta(max)= 26.370

R(reflections)= 0.0822( 10507)

wR2(reflections)= 0.2252( 22210)

S = 0.983

Npar= 1063

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

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### Alert level A

PLAT602\_ALERT\_2\_A VERY LARGE Solvent Accessible VOID(S) in Structure

[! Info](#)

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### Alert level B

|                                         |                             |             |
|-----------------------------------------|-----------------------------|-------------|
| PLAT213_ALERT_2_B Atom C26              | has ADP max/min Ratio ..... | 4.7 prola   |
| PLAT213_ALERT_2_B Atom C113             | has ADP max/min Ratio ..... | 4.3 oblat   |
| PLAT220_ALERT_2_B Large Non-Solvent     | C Ueq(max)/Ueq(min) ...     | 7.6 Ratio   |
| PLAT222_ALERT_3_B Large Non-Solvent     | H Uiso(max)/Uiso(min) ..    | 8.9 Ratio   |
| PLAT342_ALERT_3_B Low Bond Precision on | C-C Bonds .....             | 0.0210 Ang. |

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### ● Alert level C

RINTA01\_ALERT\_3\_C The value of Rint is greater than 0.12  
Rint given 0.159

PLAT020\_ALERT\_3\_C The value of Rint is greater than 0.12 ..... 0.159

PLAT026\_ALERT\_3\_C Ratio Observed / Unique Reflections too Low .... 47 %

PLAT213\_ALERT\_2\_C Atom C6 has ADP max/min Ratio ..... 3.3 oblat

PLAT213\_ALERT\_2\_C Atom C12 has ADP max/min Ratio ..... 3.7 prola

PLAT213\_ALERT\_2\_C Atom C21 has ADP max/min Ratio ..... 3.4 prola

PLAT213\_ALERT\_2\_C Atom C28 has ADP max/min Ratio ..... 3.2 oblat

PLAT213\_ALERT\_2\_C Atom C41 has ADP max/min Ratio ..... 3.8 prola

PLAT213\_ALERT\_2\_C Atom C42 has ADP max/min Ratio ..... 3.2 prola

PLAT213\_ALERT\_2\_C Atom C69 has ADP max/min Ratio ..... 3.3 prola

PLAT213\_ALERT\_2\_C Atom C93 has ADP max/min Ratio ..... 3.2 oblat

PLAT213\_ALERT\_2\_C Atom C94 has ADP max/min Ratio ..... 3.8 prola

PLAT213\_ALERT\_2\_C Atom C99 has ADP max/min Ratio ..... 3.5 oblat

PLAT213\_ALERT\_2\_C Atom C102 has ADP max/min Ratio ..... 3.1 prola

PLAT213\_ALERT\_2\_C Atom C105 has ADP max/min Ratio ..... 3.2 prola

PLAT213\_ALERT\_2\_C Atom C115 has ADP max/min Ratio ..... 3.1 prola

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C03 -- C5 .. 0.17 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C1 -- C4 .. 0.18 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C21 -- C22 .. 0.19 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C21 -- C23 .. 0.18 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C25 -- C27 .. 0.24 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C49 -- C52 .. 0.21 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C95 -- C100 .. 0.18 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C105 -- C106 .. 0.19 Ang.

PLAT234\_ALERT\_4\_C Large Hirshfeld Difference C117 -- C118 .. 0.19 Ang.

PLAT241\_ALERT\_2\_C Check High Ueq as Compared to Neighbors for C102

PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C25

PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C45

PLAT242\_ALERT\_2\_C Check Low Ueq as Compared to Neighbors for C101

PLAT395\_ALERT\_2\_C Deviating X-O-Y Angle from 120 Deg for 03 143.8 Deg.

PLAT395\_ALERT\_2\_C Deviating X-O-Y Angle from 120 Deg for 063 142.3 Deg.

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### ● Alert level G

PLAT003\_ALERT\_2\_G Number of Uiso or Uij Restrained non-H Atoms ... 13

PLAT005\_ALERT\_5\_G No \_iucr\_refine\_instructions\_details in the CIF ? Do !

PLAT045\_ALERT\_1\_G Calculated and Reported Z Differ by ..... 0.50 Ratio

PLAT128\_ALERT\_4\_G Note: Alternate Setting of Space-group P21/c . P21/n

PLAT774\_ALERT\_1\_G Suspect X-Y Bond in CIF: U1 -- U2 .. 3.77 Ang.

PLAT860\_ALERT\_3\_G Note: Number of Least-Squares Restraints ..... 78

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- 1 **ALERT level A** = Most likely a serious problem - resolve or explain
- 5 **ALERT level B** = A potentially serious problem, consider carefully
- 31 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
- 6 **ALERT level G** = General information/check it is not something unexpected
- 
- 2 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
- 10 ALERT type 4 Improvement, methodology, query or suggestion
- 1 ALERT type 5 Informative message, check
- 

## Datablock: 5-Ad

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Bond precision: C-C = 0.0159 A

Wavelength=0.71073

Cell: a=14.4543(8) b=14.5344(8) c=25.4464(12)  
 alpha=94.358(4) beta=91.810(4) gamma=118.909(5)  
 Temperature: 150 K

|                        | Calculated                                         | Reported                     |
|------------------------|----------------------------------------------------|------------------------------|
| Volume                 | 4651.9(5)                                          | 4651.9(4)                    |
| Space group            | P -1                                               | P -1                         |
| Hall group             | -P 1                                               | ?                            |
| Moiety formula         | 2(C58 H123 N 016 Si4 U),<br>2(C12 H24 K 06), C3 H7 | ?                            |
| Sum formula            | C143 H301 K2 N2 O44 Si8 U2                         | C71.50 H150.50 K N 022 Si4 U |
| Mr                     | 3531.85                                            | 1765.92                      |
| Dx, g cm <sup>-3</sup> | 1.261                                              | 1.261                        |
| Z                      | 1                                                  | 2                            |
| Mu (mm <sup>-1</sup> ) | 1.902                                              | 1.902                        |
| F000                   | 1859.0                                             | 1859.0                       |
| F000'                  | 1841.52                                            |                              |
| h, k, lmax             | 18, 18, 31                                         | 18, 18, 31                   |
| Nref                   | 19016                                              | 18800                        |
| Tmin, Tmax             | 0.833, 0.945                                       | 0.820, 0.949                 |
| Tmin'                  | 0.811                                              |                              |

Correction method= ANALYTICAL

Data completeness= 0.989 Theta(max)= 26.370

R(reflections)= 0.0785( 11498) wR2(reflections)= 0.1325( 18800)

S = 0.986 Npar= 978

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

|                                     |   |                        |            |
|-------------------------------------|---|------------------------|------------|
| PLAT222_ALERT_3_A Large Non-Solvent | H | Uiso(max)/Uiso(min) .. | 10.0 Ratio |
|-------------------------------------|---|------------------------|------------|

#### Alert level B

|                                     |   |                                  |            |
|-------------------------------------|---|----------------------------------|------------|
| PLAT220_ALERT_2_B Large Non-Solvent | C | Ueq(max)/Ueq(min) ...            | 10.0 Ratio |
| PLAT242_ALERT_2_B Check Low         |   | Ueq as Compared to Neighbors for | C41        |
| PLAT242_ALERT_2_B Check Low         |   | Ueq as Compared to Neighbors for | C69        |

#### Alert level C

|                            |                             |           |
|----------------------------|-----------------------------|-----------|
| PLAT213_ALERT_2_C Atom C30 | has ADP max/min Ratio ..... | 3.8 prola |
| PLAT213_ALERT_2_C Atom C42 | has ADP max/min Ratio ..... | 3.3 prola |
| PLAT213_ALERT_2_C Atom C43 | has ADP max/min Ratio ..... | 3.6 prola |
| PLAT213_ALERT_2_C Atom C44 | has ADP max/min Ratio ..... | 3.9 prola |
| PLAT213_ALERT_2_C Atom C45 | has ADP max/min Ratio ..... | 3.5 prola |

|                   |                            |                                  |        |       |
|-------------------|----------------------------|----------------------------------|--------|-------|
| PLAT213_ALERT_2_C | Atom C48                   | has ADP max/min Ratio .....      | 4.0    | prola |
| PLAT213_ALERT_2_C | Atom C63                   | has ADP max/min Ratio .....      | 3.1    | prola |
| PLAT213_ALERT_2_C | Atom C64                   | has ADP max/min Ratio .....      | 3.6    | prola |
| PLAT213_ALERT_2_C | Atom C70                   | has ADP max/min Ratio .....      | 3.3    | prola |
| PLAT213_ALERT_2_C | Atom C71                   | has ADP max/min Ratio .....      | 3.3    | prola |
| PLAT213_ALERT_2_C | Atom C95                   | has ADP max/min Ratio .....      | 3.6    | prola |
| PLAT216_ALERT_3_C | Disordered C113            | (An/Solv) ADP max/min Ratio      | 5.6    |       |
| PLAT230_ALERT_2_C | Hirshfeld Test Diff for    | 093 -- C95 ..                    | 5.7    | su    |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 043 -- C45 ..                    | 0.16   | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C5 -- C6 ..                      | 0.16   | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C41 -- C43 ..                    | 0.16   | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C45 -- C47 ..                    | 0.17   | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | 092 -- C93 ..                    | 0.20   | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C93 -- C94 ..                    | 0.17   | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference | C101 -- C102 ..                  | 0.21   | Ang.  |
| PLAT241_ALERT_2_C | Check High                 | Ueq as Compared to Neighbors for | 044    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | Si3    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C1     |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C5     |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C9     |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C21    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C25    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C29    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C45    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C49    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C61    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C65    |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | K1     |       |
| PLAT242_ALERT_2_C | Check Low                  | Ueq as Compared to Neighbors for | C95    |       |
| PLAT342_ALERT_3_C | Low Bond Precision on      | C-C Bonds .....                  | 0.0159 | Ang.  |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond   | C49 - C50 ...                    | 1.41   | Ang.  |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond   | C95 - C96 ...                    | 1.42   | Ang.  |

### ● Alert level G

|                   |                                                  |        |       |
|-------------------|--------------------------------------------------|--------|-------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 3      |       |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 15     |       |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  | ? Do ! |       |
| PLAT045_ALERT_1_G | Calculated and Reported Z Differ by .....        | 0.50   | Ratio |
| PLAT301_ALERT_3_G | Note: Main Residue Disorder .....                | 2      | %     |
| PLAT302_ALERT_4_G | Note: Anion/Solvent Disorder .....               | 100    | %     |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 263    |       |
|                   | 064B -SI4 -064 1.555 1.555 1.555                 | 37.70  | Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 268    |       |
|                   | 062 -SI4 -062B 1.555 1.555 1.555                 | 38.60  | Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 333    |       |
|                   | 064 -C69 -064B 1.555 1.555 1.555                 | 43.20  | Deg.  |
| PLAT793_ALERT_4_G | The Model has Chirality at C90 (Verify) ....     | R      |       |
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints .....   | 88     |       |

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

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

# Datablock: 5-TMS

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Bond precision: C-C = 0.0217 Å

Wavelength=0.71073

Cell: a=14.0470(8) b=14.0470(8) c=43.104(3)  
alpha=90 beta=90 gamma=120

Temperature: 150 K

|                        | Calculated                                   | Reported               |
|------------------------|----------------------------------------------|------------------------|
| Volume                 | 7365.7(11)                                   | 7365.7(8)              |
| Space group            | P 32                                         | P 32                   |
| Hall group             | P 32                                         | ?                      |
| Moiety formula         | C51 H117 N 016 Si5 U, C12 H24 K 06, 2(C7 H8) | ?                      |
| Sum formula            | C77 H157 K N 022 Si5 U                       | C77 H157 K N 022 Si5 U |
| Mr                     | 1866.62                                      | 1866.62                |
| Dx, g cm <sup>-3</sup> | 1.263                                        | 1.262                  |
| Z                      | 3                                            | 3                      |
| Mu (mm <sup>-1</sup> ) | 1.817                                        | 1.817                  |
| F000                   | 2949.0                                       | 2949.0                 |
| F000'                  | 2923.05                                      |                        |
| h, k, lmax             | 18, 18, 57                                   | 18, 18, 57             |
| Nref                   | 24424[ 12212]                                | 15296                  |
| Tmin, Tmax             | 0.586, 0.865                                 | 0.422, 0.867           |
| Tmin'                  | 0.351                                        |                        |

Correction method= MULTI-SCAN

Data completeness= 1.25/0.63 Theta(max)= 28.280

R(reflections)= 0.0640( 11084) wR2(reflections)= 0.1232( 15296)

S = 1.022 Npar= 1074

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The following ALERTS were generated. Each ALERT has the format

**test-name\_ALERT\_alert-type\_alert-level.**

Click on the hyperlinks for more details of the test.

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## Alert level B

|                   |                            |                                  |                   |      |     |             |
|-------------------|----------------------------|----------------------------------|-------------------|------|-----|-------------|
| PLAT220_ALERT_2_B | Large Non-Solvent          | C                                | Ueq(max)/Ueq(min) | ...  | 7.8 | Ratio       |
| PLAT234_ALERT_4_B | Large Hirshfeld Difference | C69                              | --                | C71  | ..  | 0.26 Ang.   |
| PLAT241_ALERT_2_B | Check High                 | Ueq as Compared to Neighbors for |                   |      |     | C100        |
| PLAT242_ALERT_2_B | Check Low                  | Ueq as Compared to Neighbors for |                   |      |     | C9          |
| PLAT242_ALERT_2_B | Check Low                  | Ueq as Compared to Neighbors for |                   |      |     | C29         |
| PLAT242_ALERT_2_B | Check Low                  | Ueq as Compared to Neighbors for |                   |      |     | C49         |
| PLAT242_ALERT_2_B | Check Low                  | Ueq as Compared to Neighbors for |                   |      |     | C69         |
| PLAT342_ALERT_3_B | Low Bond Precision on      | C-C Bonds                        | .....             |      |     | 0.0217 Ang. |
| PLAT413_ALERT_2_B | Short Inter XH3 .. XHn     | H71A                             | ..                | H92A | ..  | 2.09 Ang.   |

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### ● Alert level C

|                   |                                             |                                  |      |       |
|-------------------|---------------------------------------------|----------------------------------|------|-------|
| PLAT213_ALERT_2_C | Atom C3                                     | has ADP max/min Ratio .....      | 3.7  | prola |
| PLAT213_ALERT_2_C | Atom C32                                    | has ADP max/min Ratio .....      | 3.6  | prola |
| PLAT213_ALERT_2_C | Atom C50                                    | has ADP max/min Ratio .....      | 3.7  | prola |
| PLAT213_ALERT_2_C | Atom C47B                                   | has ADP max/min Ratio .....      | 3.1  | prola |
| PLAT213_ALERT_2_C | Atom C70B                                   | has ADP max/min Ratio .....      | 3.8  | prola |
| PLAT213_ALERT_2_C | Atom C93                                    | has ADP max/min Ratio .....      | 3.2  | prola |
| PLAT213_ALERT_2_C | Atom C94                                    | has ADP max/min Ratio .....      | 3.4  | prola |
| PLAT213_ALERT_2_C | Atom C99                                    | has ADP max/min Ratio .....      | 3.6  | prola |
| PLAT213_ALERT_2_C | Atom C100                                   | has ADP max/min Ratio .....      | 3.4  | prola |
| PLAT222_ALERT_3_C | Large Non-Solvent                           | H Uiso(max)/Uiso(min) ..         | 5.7  | Ratio |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | Si3 -- 044B ..                   | 0.16 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | Si4 -- 063 ..                    | 0.16 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | 043 -- C45 ..                    | 0.19 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | 044 -- C49 ..                    | 0.17 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C1 -- C4 ..                      | 0.23 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C9 -- C11 ..                     | 0.21 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C65 -- C68 ..                    | 0.22 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C69 -- C71B ..                   | 0.19 | Ang.  |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C97 -- C98 ..                    | 0.22 | Ang.  |
| PLAT241_ALERT_2_C | Check High                                  | Ueq as Compared to Neighbors for | C91  |       |
| PLAT241_ALERT_2_C | Check High                                  | Ueq as Compared to Neighbors for | C92  |       |
| PLAT241_ALERT_2_C | Check High                                  | Ueq as Compared to Neighbors for | C93  |       |
| PLAT241_ALERT_2_C | Check High                                  | Ueq as Compared to Neighbors for | C97  |       |
| PLAT241_ALERT_2_C | Check High                                  | Ueq as Compared to Neighbors for | C102 |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | Si1  |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | C1   |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | C5   |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | C21  |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | C25  |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | C41  |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | C61  |       |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for | K1   |       |
| PLAT244_ALERT_4_C | Low 'Solvent'                               | Ueq as Compared to Neighbors of  | C111 |       |
| PLAT244_ALERT_4_C | Low 'Solvent'                               | Ueq as Compared to Neighbors of  | C121 |       |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor | ....                             | 2.3  |       |
| PLAT331_ALERT_2_C | Small Average Phenyl C-C Dist.              | C111 -C116                       | 1.37 | Ang.  |
| PLAT331_ALERT_2_C | Small Average Phenyl C-C Dist.              | C121 -C126                       | 1.36 | Ang.  |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond                    | C9 - C10 ...                     | 1.43 | Ang.  |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond                    | C9 - C11 ...                     | 1.43 | Ang.  |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond                    | C65 - C67 ...                    | 1.43 | Ang.  |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond                    | C100 - C99 ...                   | 1.41 | Ang.  |

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### ● Alert level G

|                   |                                                  |                                  |       |       |
|-------------------|--------------------------------------------------|----------------------------------|-------|-------|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms     | ...                              | 7     |       |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details             | in the CIF                       | ?     | Do !  |
| PLAT104_ALERT_1_G | The Reported Crystal System is Inconsistent with |                                  | P32   |       |
| PLAT152_ALERT_1_G | The Supplied and Calc. Volume s.u. Differ by     | ...                              | 3     | Units |
| PLAT230_ALERT_2_G | Hirshfeld Test Diff for                          | C49 -- C52 ..                    | 9.5   | su    |
| PLAT232_ALERT_2_G | Hirshfeld Test Diff (M-X)                        | U1 -- N1 ..                      | 7.8   | su    |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for | 063   |       |
| PLAT242_ALERT_2_G | Check Low                                        | Ueq as Compared to Neighbors for | 063B  |       |
| PLAT301_ALERT_3_G | Note: Main Residue Disorder                      | .....                            | 14    | %     |
| PLAT380_ALERT_4_G | Check Incorrectly? Oriented X(sp2)-Methyl Moiety |                                  | C117  |       |
| PLAT773_ALERT_2_G | Check long C-C Bond in CIF:                      | C70B -- C71B .                   | 2.04  | Ang.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF        | .... #                           | 181   |       |
|                   | 043B -SI3 -043                                   | 1.555 1.555 1.555                | 36.00 | Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF        | .... #                           | 187   |       |
|                   | 044 -SI3 -044B                                   | 1.555 1.555 1.555                | 37.80 | Deg.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF        | .... #                           | 227   |       |

|                   |                                                  |       |       |       |       |       |            |
|-------------------|--------------------------------------------------|-------|-------|-------|-------|-------|------------|
| 043               | -C45                                             | -043B | 1.555 | 1.555 | 1.555 | 39.40 | Deg.       |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # |       |       |       |       | 230   |            |
|                   | C46B                                             | -C45  | -C46  | 1.555 | 1.555 | 1.555 | 27.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # |       |       |       |       | 237   |            |
|                   | C47B                                             | -C45  | -C47  | 1.555 | 1.555 | 1.555 | 39.50 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # |       |       |       |       | 328   |            |
|                   | 063B                                             | -SI4  | -063  | 1.555 | 1.555 | 1.555 | 40.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # |       |       |       |       | 334   |            |
|                   | 064                                              | -SI4  | -064B | 1.555 | 1.555 | 1.555 | 41.50 Deg. |
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints .....   |       |       |       |       | 37    |            |

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

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

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## Datablock: 6

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Bond precision: C-C = 0.0083 A

Wavelength=0.71073

|              |              |                |              |
|--------------|--------------|----------------|--------------|
| Cell:        | a=13.7947(3) | b=26.1912(7)   | c=25.0278(5) |
|              | alpha=90     | beta=93.479(2) | gamma=90     |
| Temperature: | 150 K        |                |              |

|                        | Calculated                           | Reported                |
|------------------------|--------------------------------------|-------------------------|
| Volume                 | 9025.9(4)                            | 9025.9(4)               |
| Space group            | P 21/n                               | P 21/n                  |
| Hall group             | -P 2yn                               | ?                       |
| Moiety formula         | C54 H123 K N4 O18 Si5 U,<br>2(C7 H8) | ?                       |
| Sum formula            | C68 H139 K N4 O18 Si5 U              | C68 H139 K N4 O18 Si5 U |
| Mr                     | 1718.42                              | 1718.41                 |
| Dx, g cm <sup>-3</sup> | 1.265                                | 1.265                   |
| Z                      | 4                                    | 4                       |
| Mu (mm <sup>-1</sup> ) | 1.969                                | 1.969                   |
| F000                   | 3600.0                               | 3600.0                  |
| F000'                  | 3565.19                              |                         |
| h, k, lmax             | 18, 34, 33                           | 18, 34, 33              |
| Nref                   | 22406                                | 22368                   |
| Tmin, Tmax             | 0.431, 0.790                         | 0.322, 0.802            |
| Tmin'                  | 0.226                                |                         |

Correction method= ANALYTICAL

Data completeness= 0.998

Theta(max)= 28.280

R(reflections)= 0.0449( 16407)

wR2(reflections)= 0.1074( 22368)

S = 1.052

Npar= 932

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

|                   |                                                  |             |                       |      |       |
|-------------------|--------------------------------------------------|-------------|-----------------------|------|-------|
| PLAT220_ALERT_2_B | Large Non-Solvent                                | C           | Ueq(max)/Ueq(min) ... | 4.2  | Ratio |
| PLAT250_ALERT_2_B | Large U3/U1 Ratio for Average U(i,j) Tensor .... |             |                       | 4.2  |       |
| PLAT250_ALERT_2_B | Large U3/U1 Ratio for Average U(i,j) Tensor .... |             |                       | 4.2  |       |
| PLAT362_ALERT_2_B | Short C(sp3)-C(sp2) Bond                         | C101 - C107 | ...                   | 1.29 | Ang.  |

### Alert level C

|                   |                                                  |                                  |    |        |       |
|-------------------|--------------------------------------------------|----------------------------------|----|--------|-------|
| PLAT165_ALERT_3_C | Nr. of Status R Flagged Non-Hydrogen Atoms ..... |                                  |    | 18     |       |
| PLAT213_ALERT_2_C | Atom C30                                         | has ADP max/min Ratio .....      |    | 3.5    | prola |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                       | C9 -- C10                        | .. | 0.16   | Ang.  |
| PLAT241_ALERT_2_C | Check High                                       | Ueq as Compared to Neighbors for |    | N3     |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | Si1    |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | Si5    |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | C1     |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | C5     |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | C9     |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | C21    |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | C29    |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | C41    |       |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for |    | C45    |       |
| PLAT243_ALERT_4_C | High 'Solvent'                                   | Ueq as Compared to Neighbors of  |    | C103   |       |
| PLAT243_ALERT_4_C | High 'Solvent'                                   | Ueq as Compared to Neighbors of  |    | C105   |       |
| PLAT244_ALERT_4_C | Low 'Solvent'                                    | Ueq as Compared to Neighbors of  |    | C102   |       |
| PLAT244_ALERT_4_C | Low 'Solvent'                                    | Ueq as Compared to Neighbors of  |    | C104   |       |
| PLAT244_ALERT_4_C | Low 'Solvent'                                    | Ueq as Compared to Neighbors of  |    | C106   |       |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor .... |                                  |    | 2.4    |       |
| PLAT342_ALERT_3_C | Low Bond Precision on                            | C-C Bonds .....                  |    | 0.0083 | Ang.  |

### Alert level G

|                   |                                                  |                                 |  |       |      |
|-------------------|--------------------------------------------------|---------------------------------|--|-------|------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite |                                 |  | 17    |      |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... |                                 |  | 21    |      |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  |                                 |  | ?     | Do ! |
| PLAT063_ALERT_4_G | Crystal Size Likely too Large for Beam Size .... |                                 |  | 0.75  | mm   |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large. |                                 |  | 22.28 |      |
| PLAT128_ALERT_4_G | Note: Alternate Setting of Space-group P21/c     |                                 |  | P21/n |      |
| PLAT244_ALERT_4_G | Low 'Solvent'                                    | Ueq as Compared to Neighbors of |  | C112  |      |
| PLAT244_ALERT_4_G | Low 'Solvent'                                    | Ueq as Compared to Neighbors of |  | C114  |      |
| PLAT244_ALERT_4_G | Low 'Solvent'                                    | Ueq as Compared to Neighbors of |  | C126  |      |
| PLAT302_ALERT_4_G | Note: Anion/Solvent Disorder .....               |                                 |  | 50    | %    |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # |                                 |  | 292   |      |
|                   | N61 -Si4 -U1                                     | 1.555 1.555 1.555               |  | 38.14 | Deg. |
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints .....   |                                 |  | 226   |      |

0 ALERT level A = Most likely a serious problem - resolve or explain

4 ALERT level B = A potentially serious problem, consider carefully



20 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 12 **ALERT level G** = General information/check it is not something unexpected

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

## Datablock: 7

Bond precision: C-C = 0.0181 Å Wavelength=0.71073

Cell: a=14.0305(5) b=24.7215(7) c=26.3108(9)  
 alpha=90 beta=98.009(3) gamma=90

Temperature: 150 K

|                        | Calculated                        | Reported                |
|------------------------|-----------------------------------|-------------------------|
| Volume                 | 9037.0(5)                         | 9037.0(5)               |
| Space group            | C c                               | C 1 c 1                 |
| Hall group             | C -2yc                            | ?                       |
| Moiety formula         | C60 H132 K N3 O22 Si4 U,<br>C7 H8 | ?                       |
| Sum formula            | C67 H140 K N3 O22 Si4 U           | C67 H140 K N3 O22 Si4 U |
| Mr                     | 1729.32                           | 1729.31                 |
| Dx, g cm <sup>-3</sup> | 1.271                             | 1.271                   |
| Z                      | 4                                 | 4                       |
| Mu (mm <sup>-1</sup> ) | 1.957                             | 1.957                   |
| F000                   | 3624.0                            | 3624.0                  |
| F000'                  | 3589.01                           |                         |
| h, k, lmax             | 18, 32, 35                        | 18, 32, 35              |
| Nref                   | 22402[ 11209]                     | 21805                   |
| Tmin, Tmax             | 0.242, 0.440                      | 0.280, 0.491            |
| Tmin'                  | 0.175                             |                         |

Correction method= MULTI-SCAN

Data completeness= 1.95/0.97 Theta(max)= 28.280

R(reflections)= 0.0580( 18236) wR2(reflections)= 0.1287( 21805)

S = 1.070 Npar= 880

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**

|                   |                                                  |                                  |                       |     |       |
|-------------------|--------------------------------------------------|----------------------------------|-----------------------|-----|-------|
| PLAT220_ALERT_2_B | Large Non-Solvent                                | C                                | Ueq(max)/Ueq(min) ... | 5.5 | Ratio |
| PLAT241_ALERT_2_B | Check High                                       | Ueq as Compared to Neighbors for |                       | 043 |       |
| PLAT241_ALERT_2_B | Check High                                       | Ueq as Compared to Neighbors for |                       | 063 |       |
| PLAT241_ALERT_2_B | Check High                                       | Ueq as Compared to Neighbors for |                       | N3  |       |
| PLAT241_ALERT_2_B | Check High                                       | Ueq as Compared to Neighbors for |                       | C82 |       |
| PLAT241_ALERT_2_B | Check High                                       | Ueq as Compared to Neighbors for |                       | C88 |       |
| PLAT241_ALERT_2_B | Check High                                       | Ueq as Compared to Neighbors for |                       | C92 |       |
| PLAT242_ALERT_2_B | Check Low                                        | Ueq as Compared to Neighbors for |                       | K3  |       |
| PLAT242_ALERT_2_B | Check Low                                        | Ueq as Compared to Neighbors for |                       | C41 |       |
| PLAT242_ALERT_2_B | Check Low                                        | Ueq as Compared to Neighbors for |                       | C45 |       |
| PLAT242_ALERT_2_B | Check Low                                        | Ueq as Compared to Neighbors for |                       | C61 |       |
| PLAT242_ALERT_2_B | Check Low                                        | Ueq as Compared to Neighbors for |                       | C65 |       |
| PLAT242_ALERT_2_B | Check Low                                        | Ueq as Compared to Neighbors for |                       | C69 |       |
| PLAT250_ALERT_2_B | Large U3/U1 Ratio for Average U(i,j) Tensor .... |                                  |                       | 4.1 |       |

### ● Alert level C

SHFSU01\_ALERT\_2\_C The absolute value of parameter shift to su ratio > 0.05  
 Absolute value of the parameter shift to su ratio given 0.052  
 Additional refinement cycles may be required.

|                   |                                                  |             |
|-------------------|--------------------------------------------------|-------------|
| PLAT165_ALERT_3_C | Nr. of Status R Flagged Non-Hydrogen Atoms ..... | 6           |
| PLAT213_ALERT_2_C | Atom C2 has ADP max/min Ratio .....              | 3.7 prola   |
| PLAT213_ALERT_2_C | Atom C4 has ADP max/min Ratio .....              | 3.1 prola   |
| PLAT213_ALERT_2_C | Atom C10 has ADP max/min Ratio .....             | 3.4 prola   |
| PLAT213_ALERT_2_C | Atom C11 has ADP max/min Ratio .....             | 3.4 prola   |
| PLAT213_ALERT_2_C | Atom C68 has ADP max/min Ratio .....             | 3.4 prola   |
| PLAT213_ALERT_2_C | Atom C72 has ADP max/min Ratio .....             | 3.5 prola   |
| PLAT213_ALERT_2_C | Atom C84 has ADP max/min Ratio .....             | 3.3 prola   |
| PLAT213_ALERT_2_C | Atom C85 has ADP max/min Ratio .....             | 3.3 oblat   |
| PLAT220_ALERT_2_C | Large Non-Solvent 0 Ueq(max)/Ueq(min) ...        | 4.0 Ratio   |
| PLAT222_ALERT_3_C | Large Non-Solvent H Uiso(max)/Uiso(min) ..       | 4.7 Ratio   |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference 083 -- C85 ..         | 0.22 Ang.   |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference N2 -- N3 ..           | 0.19 Ang.   |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C5 -- C8 ..           | 0.20 Ang.   |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C65 -- C67 ..         | 0.21 Ang.   |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C69 -- C71 ..         | 0.25 Ang.   |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | 042         |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | 064         |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | C84         |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | C85         |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | C86         |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | C87         |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | C89         |
| PLAT241_ALERT_2_C | Check High Ueq as Compared to Neighbors for      | C90         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | Si3         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | Si4         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | N2          |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C1          |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C5          |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C9          |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C21         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C25         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C29         |
| PLAT242_ALERT_2_C | Check Low Ueq as Compared to Neighbors for       | C49         |
| PLAT243_ALERT_4_C | High 'Solvent' Ueq as Compared to Neighbors of   | C103        |
| PLAT243_ALERT_4_C | High 'Solvent' Ueq as Compared to Neighbors of   | C106        |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of    | C101        |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of    | C102        |
| PLAT244_ALERT_4_C | Low 'Solvent' Ueq as Compared to Neighbors of    | C104        |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds .....            | 0.0181 Ang. |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond C41 - C42 ...           | 1.42 Ang.   |

|                   |       |                    |      |    |      |     |      |      |
|-------------------|-------|--------------------|------|----|------|-----|------|------|
| PLAT360_ALERT_2_C | Short | C(sp3)-C(sp3) Bond | C65  | -  | C66  | ... | 1.41 | Ang. |
| PLAT360_ALERT_2_C | Short | C(sp3)-C(sp3) Bond | C65  | -  | C68  | ... | 1.42 | Ang. |
| PLAT362_ALERT_2_C | Short | C(sp3)-C(sp2) Bond | C101 | -  | C107 | ... | 1.38 | Ang. |
| PLAT412_ALERT_2_C | Short | Intra XH3 .. XHn   | H10D | .. | H106 | ..  | 1.81 | Ang. |
| PLAT413_ALERT_2_C | Short | Inter XH3 .. XHn   | H44C | .. | H89B | ..  | 2.10 | Ang. |

### ● Alert level G

|                   |                                                  |            |
|-------------------|--------------------------------------------------|------------|
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 11         |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  | ? Do !     |
| PLAT063_ALERT_4_G | Crystal Size Likely too Large for Beam Size .... | 0.87 mm    |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large. | 9.56       |
| PLAT301_ALERT_3_G | Note: Main Residue Disorder .....                | 1 %        |
| PLAT380_ALERT_4_G | Check Incorrectly? Oriented X(sp2)-Methyl Moiety | C107       |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF: K3 -- C85 ..            | 3.51 Ang.  |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF: K3 -- C89 ..            | 3.53 Ang.  |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 135        |
|                   | K3 -C10 -H10A 4.465 1.555 1.555                  | 31.80 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 325        |
|                   | 062B -SI4 -062 1.555 1.555 1.555                 | 31.90 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 337        |
|                   | 062 -C61 -062B 1.555 1.555 1.555                 | 39.20 Deg. |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 463        |
|                   | 084 -C86 -K3 1.555 1.555 1.555                   | 44.50 Deg. |
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints .....   | 26         |

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 14 **ALERT level B** = A potentially serious problem, consider carefully  
 47 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
 13 **ALERT level G** = General information/check it is not something unexpected

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

## Datablock: 8

|                 |                |                    |              |  |
|-----------------|----------------|--------------------|--------------|--|
| Bond precision: | C-C = 0.0126 A | Wavelength=0.71073 |              |  |
| Cell:           | a=26.8752(7)   | b=14.2770(5)       | c=22.8128(5) |  |
|                 | alpha=90       | beta=90            | gamma=90     |  |
| Temperature:    | 150 K          |                    |              |  |

|                | Calculated                            | Reported                 |
|----------------|---------------------------------------|--------------------------|
| Volume         | 8753.2(4)                             | 8753.2(4)                |
| Space group    | P n a 21                              | P n a 21                 |
| Hall group     | P 2c -2n                              | ?                        |
| Moiety formula | C51 H114 K2 N7 O18 Si4 U,<br>2(C7 H8) | ?                        |
| Sum formula    | C65 H130 K2 N7 O18 Si4 U              | C65 H130 K2 N7 O18 Si4 U |
| Mr             | 1726.36                               | 1726.35                  |
| Dx,g cm-3      | 1.310                                 | 1.310                    |
| Z              | 4                                     | 4                        |
| Mu (mm-1)      | 2.065                                 | 2.065                    |
| F000           | 3596.0                                | 3596.0                   |
| F000'          | 3561.66                               |                          |
| h,k,lmax       | 35,19,30                              | 35,18,30                 |
| Nref           | 21696[ 11116]                         | 20519                    |
| Tmin,Tmax      | 0.250,0.723                           | 0.742,0.924              |
| Tmin'          | 0.210                                 |                          |

Correction method= ANALYTICAL

Data completeness= 1.85/0.95      Theta(max)= 28.280

R(reflections)= 0.0543( 16010)      wR2(reflections)= 0.1086( 20519)

S = 1.112      Npar= 881

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

|                                     |                                  |           |
|-------------------------------------|----------------------------------|-----------|
| PLAT213_ALERT_2_B Atom C2           | has ADP max/min Ratio .....      | 4.2 prola |
| PLAT220_ALERT_2_B Large Non-Solvent | C      Ueq(max)/Ueq(min) ...     | 6.2 Ratio |
| PLAT241_ALERT_2_B Check High        | Ueq as Compared to Neighbors for | N3        |
| PLAT242_ALERT_2_B Check Low         | Ueq as Compared to Neighbors for | Si4       |
| PLAT242_ALERT_2_B Check Low         | Ueq as Compared to Neighbors for | C1        |

### Alert level C

|                                     |                                                          |           |
|-------------------------------------|----------------------------------------------------------|-----------|
| SHFSU01_ALERT_2_C                   | The absolute value of parameter shift to su ratio > 0.05 |           |
|                                     | Absolute value of the parameter shift to su ratio given  | 0.073     |
|                                     | Additional refinement cycles may be required.            |           |
| STRVA01_ALERT_4_C                   | Flack test results are ambiguous.                        |           |
|                                     | From the CIF: _refine_ls_abs_structure_Flack             | 0.513     |
|                                     | From the CIF: _refine_ls_abs_structure_Flack_su          | 0.006     |
| PLAT080_ALERT_2_C                   | Maximum Shift/Error .....                                | 0.07      |
| PLAT165_ALERT_3_C                   | Nr. of Status R Flagged Non-Hydrogen Atoms .....         | 12        |
| PLAT213_ALERT_2_C Atom C3           | has ADP max/min Ratio .....                              | 3.2 oblat |
| PLAT213_ALERT_2_C Atom C23          | has ADP max/min Ratio .....                              | 3.9 prola |
| PLAT213_ALERT_2_C Atom C48          | has ADP max/min Ratio .....                              | 3.5 prola |
| PLAT213_ALERT_2_C Atom C62          | has ADP max/min Ratio .....                              | 3.5 prola |
| PLAT222_ALERT_3_C Large Non-Solvent | H      Uiso(max)/Uiso(min) ..                            | 5.3 Ratio |

|                   |                                             |                                  |     |     |    |        |      |
|-------------------|---------------------------------------------|----------------------------------|-----|-----|----|--------|------|
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | Si4                              | --  | C61 | .. | 0.25   | Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C1                               | --  | C2  | .. | 0.18   | Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C1                               | --  | C4  | .. | 0.16   | Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C21                              | --  | C22 | .. | 0.16   | Ang. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference                  | C79                              | --  | C80 | .. | 0.18   | Ang. |
| PLAT241_ALERT_2_C | Check High                                  | Ueq as Compared to Neighbors for |     |     |    |        | N6   |
| PLAT241_ALERT_2_C | Check High                                  | Ueq as Compared to Neighbors for |     |     |    |        | C82  |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for |     |     |    |        | K2   |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for |     |     |    |        | N5   |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for |     |     |    |        | C5   |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for |     |     |    |        | C21  |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for |     |     |    |        | C25  |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for |     |     |    |        | C29  |
| PLAT242_ALERT_2_C | Check Low                                   | Ueq as Compared to Neighbors for |     |     |    |        | C49  |
| PLAT244_ALERT_4_C | Low 'Solvent'                               | Ueq as Compared to Neighbors of  |     |     |    |        | C101 |
| PLAT250_ALERT_2_C | Large U3/U1 Ratio for Average U(i,j) Tensor | ....                             |     |     |    | 3.1    |      |
| PLAT342_ALERT_3_C | Low Bond Precision on C-C Bonds             | .....                            |     |     |    | 0.0126 | Ang. |
| PLAT360_ALERT_2_C | Short C(sp3)-C(sp3) Bond                    | C81 - C82                        | ... |     |    | 1.40   | Ang. |
| PLAT362_ALERT_2_C | Short C(sp3)-C(sp2) Bond                    | C101 - C107                      | ... |     |    | 1.37   | Ang. |

### ● Alert level G

|                   |                                                  |  |           |
|-------------------|--------------------------------------------------|--|-----------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite |  | 2         |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... |  | 21        |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  |  | ? Do !    |
| PLAT063_ALERT_4_G | Crystal Size Likely too Large for Beam Size .... |  | 0.71 mm   |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large. |  | 28.27     |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF: U1 -- K1 ..             |  | 3.60 Ang. |
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints .....   |  | 128       |

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7 **ALERT level G** = General information/check it is not something unexpected

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

## Datablock: 9

Bond precision: C-C = 0.0118 A

Wavelength=0.71073

|              |                 |                |                 |
|--------------|-----------------|----------------|-----------------|
| Cell:        | a=15.3369(5)    | b=17.9607(7)   | c=19.2055(6)    |
|              | alpha=78.456(3) | beta=84.822(3) | gamma=86.879(3) |
| Temperature: | 150 K           |                |                 |

|                                     | Calculated               | Reported                 |
|-------------------------------------|--------------------------|--------------------------|
| Volume                              | 5158.6(3)                | 5158.6(3)                |
| Space group                         | P -1                     | P -1                     |
| Hall group                          | -P 1                     | ?                        |
| Moiety formula                      | C72 H162 Cs N 024 Si6 U2 | ?                        |
| Sum formula                         | C72 H162 Cs N 024 Si6 U2 | C72 H162 Cs N 024 Si6 U2 |
| Mr                                  | 2203.55                  | 2203.54                  |
| Dx, g cm <sup>-3</sup>              | 1.419                    | 1.419                    |
| Z                                   | 2                        | 2                        |
| Mu (mm <sup>-1</sup> )              | 3.612                    | 3.612                    |
| F000                                | 2232.0                   | 2232.0                   |
| F000'                               | 2194.63                  |                          |
| h, k, l <sub>max</sub>              | 20, 23, 25               | 20, 23, 25               |
| N <sub>ref</sub>                    | 25618                    | 25447                    |
| T <sub>min</sub> , T <sub>max</sub> | 0.437, 0.777             | 0.479, 0.791             |
| T <sub>min</sub> '                  | 0.404                    |                          |

Correction method= MULTI-SCAN

Data completeness= 0.993

Theta(max)= 28.280

R(reflections)= 0.0456( 16847)

wR2(reflections)= 0.1145( 25447)

S = 0.929

N<sub>par</sub>= 1009

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

|                   |                         |                                  |                       |     |       |
|-------------------|-------------------------|----------------------------------|-----------------------|-----|-------|
| PLAT220_ALERT_2_B | Large Non-Solvent       | C                                | Ueq(max)/Ueq(min) ... | 5.7 | Ratio |
| PLAT230_ALERT_2_B | Hirshfeld Test Diff for | Si1                              | -- 03 ..              | 7.7 | su    |
| PLAT241_ALERT_2_B | Check High              | Ueq as Compared to Neighbors for |                       | 04  |       |
| PLAT242_ALERT_2_B | Check Low               | Ueq as Compared to Neighbors for |                       | C9  |       |

#### 🟢 Alert level C

|                   |                                                  |                                  |                        |
|-------------------|--------------------------------------------------|----------------------------------|------------------------|
| PLAT094_ALERT_2_C | Ratio of Maximum / Minimum Residual Density .... | 2.01                             |                        |
| PLAT213_ALERT_2_C | Atom C42 has ADP max/min Ratio .....             | 3.2                              | prola                  |
| PLAT220_ALERT_2_C | Large Non-Solvent                                | 0                                | Ueq(max)/Ueq(min) ...  |
| PLAT222_ALERT_3_C | Large Non-Solvent                                | H                                | Uiso(max)/Uiso(min) .. |
| PLAT234_ALERT_4_C | Large Hirshfeld Difference C49                   | -- C52 ..                        | 0.17 Ang.              |
| PLAT241_ALERT_2_C | Check High                                       | Ueq as Compared to Neighbors for | 01                     |
| PLAT241_ALERT_2_C | Check High                                       | Ueq as Compared to Neighbors for | 03                     |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | Si1                    |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | Si3                    |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | C1                     |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | C5                     |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | C25                    |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | C29                    |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | C41                    |
| PLAT242_ALERT_2_C | Check Low                                        | Ueq as Compared to Neighbors for | C45                    |

|                   |                       |                                  |             |
|-------------------|-----------------------|----------------------------------|-------------|
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C49         |
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C61         |
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C69         |
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C85         |
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C105        |
| PLAT342_ALERT_3_C | Low Bond Precision on | C-C Bonds .....                  | 0.0118 Ang. |

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### ● Alert level G

|                   |                                                  |                   |              |
|-------------------|--------------------------------------------------|-------------------|--------------|
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details             | in the CIF        | ? Do !       |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT                  | Unusually Large.  | 14.53        |
| PLAT154_ALERT_1_G | The su's on the Cell Angles are Equal .....      |                   | 0.00300 Deg. |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF:                         | U1 -- CS1 ..      | 3.86 Ang.    |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF:                         | U2 -- CS1 ..      | 4.22 Ang.    |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF:                         | CS1 -- O41 ..     | 3.63 Ang.    |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF:                         | CS1 -- SI2 ..     | 3.89 Ang.    |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF:                         | CS1 -- SI6 ..     | 3.94 Ang.    |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF:                         | CS1 -- SI3 ..     | 4.03 Ang.    |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # |                   | 451          |
|                   | 081 -SI5 -U2                                     | 1.555 1.555 1.555 | 40.18 Deg.   |

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 10 **ALERT level G** = General information/check it is not something unexpected

7 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
 23 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  
 2 ALERT type 4 Improvement, methodology, query or suggestion  
 1 ALERT type 5 Informative message, check

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## Datablock: 10

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Bond precision: C-C = 0.0181 A

Wavelength=0.71073

|              |                 |                 |                  |
|--------------|-----------------|-----------------|------------------|
| Cell:        | a=13.3139(4)    | b=13.6374(4)    | c=18.3661(7)     |
|              | alpha=90.824(3) | beta=106.789(3) | gamma=115.962(3) |
| Temperature: | 293 K           |                 |                  |

|                        | Calculated                          | Reported                  |
|------------------------|-------------------------------------|---------------------------|
| Volume                 | 2831.68(19)                         | 2831.69(17)               |
| Space group            | P -1                                | P -1                      |
| Hall group             | -P 1                                | ?                         |
| Moiety formula         | C72 H162 K2 N2 O24 Si6 U2, 2(C7 H8) | ?                         |
| Sum formula            | C86 H178 K2 N2 O24 Si6 U2           | C86 H178 K2 N2 O24 Si6 U2 |
| Mr                     | 2347.11                             | 2347.10                   |
| Dx, g cm <sup>-3</sup> | 1.376                               | 1.376                     |
| Z                      | 1                                   | 1                         |
| Mu (mm <sup>-1</sup> ) | 3.054                               | 3.054                     |
| F000                   | 1206.0                              | 1206.0                    |
| F000'                  | 1188.09                             |                           |
| h, k, l <sub>max</sub> | 19, 19, 26                          | 19, 19, 26                |
| Nref                   | 17299                               | 17272                     |
| Tmin, Tmax             | 0.243, 0.760                        | 0.260, 0.766              |
| Tmin'                  | 0.147                               |                           |

Correction method= ANALYTICAL

Data completeness= 0.998

Theta(max)= 30.510

R(reflections)= 0.0739( 13943)

wR2(reflections)= 0.1679( 17272)

S = 1.137

Npar= 601

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

DIFMX01\_ALERT\_2\_B The maximum difference density is > 0.1\*ZMAX\*1.00

\_refine\_diff\_density\_max given = 11.179

Test value = 9.200

|                   |                                                  |            |
|-------------------|--------------------------------------------------|------------|
| PLAT097_ALERT_2_B | Large Reported Max. (Positive) Residual Density  | 11.18 eA-3 |
| PLAT220_ALERT_2_B | Large Non-Solvent C Ueq(max)/Ueq(min) ...        | 4.7 Ratio  |
| PLAT242_ALERT_2_B | Check Low Ueq as Compared to Neighbors for       | C41        |
| PLAT250_ALERT_2_B | Large U3/U1 Ratio for Average U(i,j) Tensor .... | 6.9        |
| PLAT331_ALERT_2_B | Small Average Phenyl C-C Dist. C71 -C73_b        | 1.35 Ang.  |

### Alert level C

DIFMX02\_ALERT\_1\_C The maximum difference density is > 0.1\*ZMAX\*0.75

The relevant atom site should be identified.

|                   |                                                  |           |
|-------------------|--------------------------------------------------|-----------|
| PLAT094_ALERT_2_C | Ratio of Maximum / Minimum Residual Density .... | 2.84      |
| PLAT165_ALERT_3_C | Nr. of Status R Flagged Non-Hydrogen Atoms ..... | 6         |
| PLAT213_ALERT_2_C | Atom C23 has ADP max/min Ratio .....             | 3.4 prola |
| PLAT213_ALERT_2_C | Atom C24 has ADP max/min Ratio .....             | 3.1 prola |
| PLAT213_ALERT_2_C | Atom C42 has ADP max/min Ratio .....             | 3.2 prola |
| PLAT213_ALERT_2_C | Atom C43 has ADP max/min Ratio .....             | 3.1 prola |
| PLAT213_ALERT_2_C | Atom C44 has ADP max/min Ratio .....             | 3.2 prola |
| PLAT213_ALERT_2_C | Atom C50 has ADP max/min Ratio .....             | 3.2 prola |



|                   |                       |                                  |             |
|-------------------|-----------------------|----------------------------------|-------------|
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C21         |
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C29         |
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C45         |
| PLAT242_ALERT_2_C | Check Low             | Ueq as Compared to Neighbors for | C49         |
| PLAT244_ALERT_4_C | Low 'Solvent'         | Ueq as Compared to Neighbors of  | C71         |
| PLAT342_ALERT_3_C | Low Bond Precision on | C-C Bonds .....                  | 0.0181 Ang. |

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### ● Alert level G

|                   |                                                  |              |
|-------------------|--------------------------------------------------|--------------|
| PLAT002_ALERT_2_G | Number of Distance or Angle Restraints on AtSite | 3            |
| PLAT003_ALERT_2_G | Number of Uiso or Uij Restrained non-H Atoms ... | 7            |
| PLAT005_ALERT_5_G | No _iucr_refine_instructions_details in the CIF  | ? Do !       |
| PLAT083_ALERT_2_G | SHELXL Second Parameter in WGHT Unusually Large. | 37.26        |
| PLAT152_ALERT_1_G | The Supplied and Calc. Volume s.u. Differ by ... | 2 Units      |
| PLAT154_ALERT_1_G | The su's on the Cell Angles are Equal .....      | 0.00300 Deg. |
| PLAT199_ALERT_1_G | Check the Reported _cell_measurement_temperature | 293 K        |
| PLAT200_ALERT_1_G | Check the Reported _diffrn_ambient_temperature   | 293 K        |
| PLAT244_ALERT_4_G | Low 'Solvent' Ueq as Compared to Neighbors of    | C66          |
| PLAT302_ALERT_4_G | Note: Anion/Solvent Disorder .....               | 43 %         |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF: U1 -- K1 ..             | 3.62 Ang.    |
| PLAT774_ALERT_1_G | Suspect X-Y Bond in CIF: K1 -- SI2 ..            | 3.50 Ang.    |
| PLAT779_ALERT_4_G | Suspect or Irrelevant (Bond) Angle in CIF .... # | 360          |
|                   | C74 -C71 -H71 1.555 1.555 1.555                  | 5.80 Deg.    |
| PLAT860_ALERT_3_G | Note: Number of Least-Squares Restraints .....   | 44           |

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

7 **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  
 3 **ALERT type 3** Indicator that the structure quality may be low  
 4 **ALERT type 4** Improvement, methodology, query or suggestion  
 1 **ALERT type 5** Informative message, check

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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.























