checkCIF/PLATON report (publication check)

No syntax errors found.
Please wait while processing ....

Datablock: Mn26

Bond precision: C-C = 0.0097 A   Wavelength=0.71073

Cell: a=34.6879(10) b=34.6879(10) c=34.6879(10)
             alpha=90   beta=90   gamma=90

Temperature: 100 K

	Calculated	Reported
Volume	41738(2)	41738(2)
Space group	F d -3	F d -3
Hall group	-F 2uv 2vw	-F 2uv 2vw
Moiety formula	C150 H150 Mn26 N24 O58, 3(O)	C150 H150 Mn26 N24 O58, 3(O)
Sum formula	C150 H150 Mn26 N24 O61	C150 H150 Mn26 N24 O61
Mr	4693.38	4693.38
Dx,g cm-3	1.494	1.494
Z	8	8
Mu (mm-1)	1.587	1.587
F000	18848.0	18848.0
F000'	18925.04	
h,k,lmax	42,42,42	42,42,42
Nref	3267	3201
Tmin,Tmax	0.690,0.867	0.678,0.863
Tmin'	0.635	

Correction method= AbsCorr=MULTI-SCAN

Data completeness= Ratio = 0.980   Theta(max)= 25.490

R(reflections)= 0.0580(1657)   wR2(reflections)= 0.1532(3201)

S = 0.994   Npar= 216

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
PLAT601_ALERT_2_A Structure Contains Solvent Accessible VOIDS of .   6344.00 A**3

Author Response: This is due to the space between the large 'spherical' molecules in the crystal structure,

and it likely contains very disordered solvent of crystallization.

Alert level B
PLAT230_ALERT_2_B Hirshfeld Test Diff for   O7   -- C13   ..   8.04 su

Author Response: O7 and C13 atoms constitute a disordered methanol molecule which exhibits orientational disorder about a 2-fold rotation axis.

Alert level C

PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Mn4   -- O6   ..   5.38 su
PLAT301_ALERT_3_C Main Residue Disorder ....   4.00 Perc.
PLAT311_ALERT_2_C Isolated Disordered Oxygen Atom (No H's ?) .....   <O8
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ...   10
PLAT731_ALERT_1_C Bond   Calc   1.910(4), Rep 1.9093(15) ......   2.67 su-Ra
                MN3 -O3   1.555   1.555
PLAT731_ALERT_1_C Bond   Calc   1.910(4), Rep 1.9092(15) ......   2.67 su-Ra
                O3   -MN3   1.555 48.555
PLAT731_ALERT_1_C Bond   Calc   1.910(4), Rep 1.9094(15) ......   2.67 su-Ra
                O3   -MN3   1.555 18.555
PLAT764_ALERT_4_C Overcomplete CIF Bond List Detected (Rep/Expd) .   1.43 Ratio

Alert level G

PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints   19
PLAT302_ALERT_4_G Anion/Solvent Disorder ....   25.00 Perc.

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

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

checkCIF publication errors

Alert level A

PUBL012_ALERT_1_A _publ_section_abstract is missing.
          Abstract of paper in English.
PUBL024_ALERT_1_A The number of authors is greater than 5.
            Please specify the role of each of the co-authors
            for your paper.

Alert level G

PUBL013_ALERT_1_G The _publ_section_comment (discussion of study) is
          missing. This is required for a full paper submission (but is
          optional for an electronic paper).
PUBL017_ALERT_1_G The _publ_section_references section is missing or
          empty.

```
   2 ALERT level A = Data missing that is essential or data in wrong format
   2 ALERT level G = General alerts. Data that may be required is missing
```

Publication of your CIF

You should always 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 nature of your study may justify the reported deviations from the submission requirements of the journal and these should be commented upon in the discussion or experimental section of a paper - after all, they might represent an interesting feature.

If level A alerts remain, which you believe to be justified deviations, and you intend to submit this CIF for publication in Acta Crystallographica Section C or Section E, you should additionally insert an explanation in your CIF using the Validation Reply Form (VRF) below. Your explanation will be considered as part of the review process.
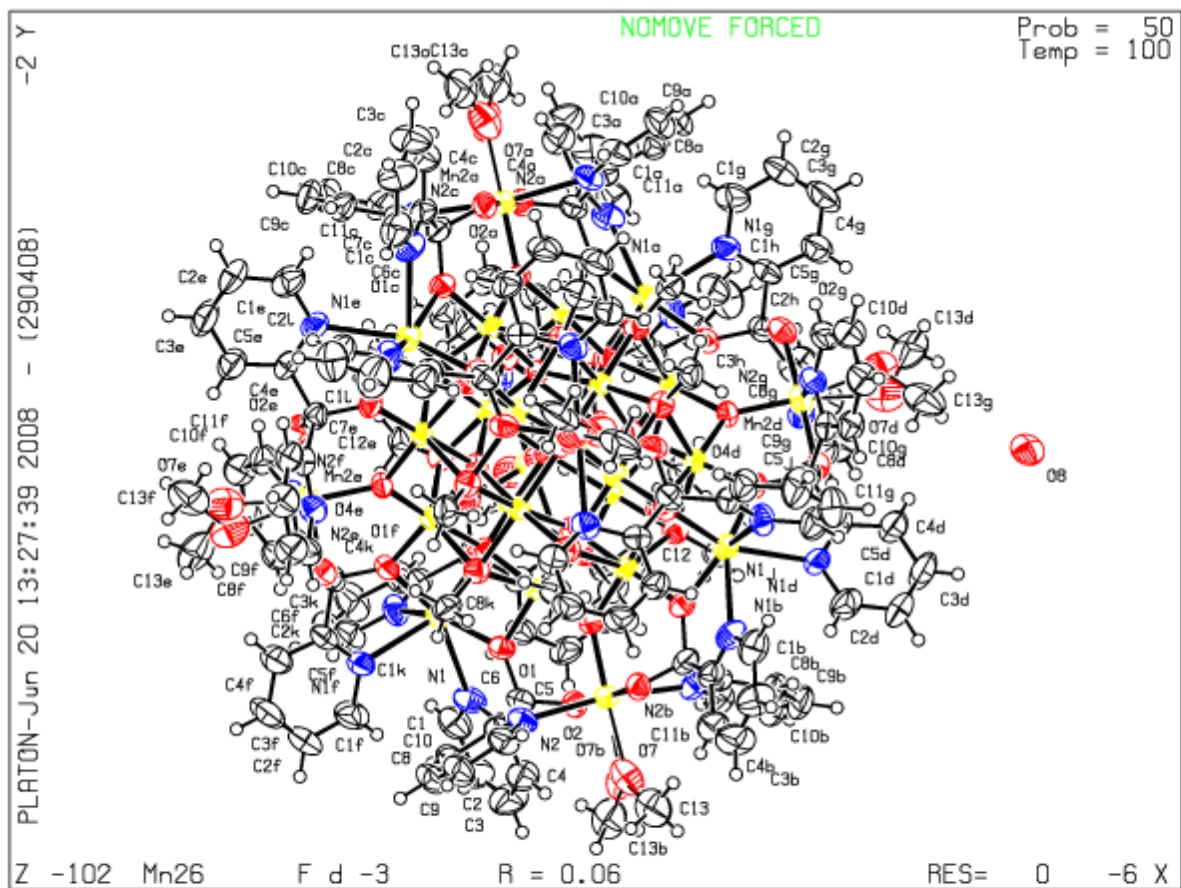
If you intend to submit to another section of Acta Crystallographica or Journal of Applied Crystallography or Journal of Synchrotron Radiation, you should make sure that at least a basic structural check is run on the final version of your CIF prior to submission.

```
# start Validation Reply Form
_vrf_PUBL012_GLOBAL
;
PROBLEM: _publ_section_abstract is missing.
RESPONSE: ...
;
_vrf_PUBL024_GLOBAL
;
PROBLEM: The number of authors is greater than 5.
RESPONSE: ...
;
# end Validation Reply Form
```

If you wish to submit your CIF for publication in Acta Crystallographica Section C or E, you should upload your CIF via the web. If your CIF is to form part of a submission to another IUCr journal, you will be asked, either during electronic submission or by the Co-editor handling your paper, to upload your CIF via our web site.

PLATON version of 29/04/2008; check.def file version of 22/04/2008

Datablock Mn26 - ellipsoid plot