

```

C:\WINDOWS\system32\cmd.exe

wR2 = 0.0752 before cycle 0 for 17657 data and 0% / 8% parameters
GoF = 2 = 1.000; Restrained GoF = 1.000 for 0 restraints
Rms shift/eqd = 0.000 Rmsdev = 0.000 for x h25 at 21:17:27
Rms shift = 0.000 Å for O45 Rms. sh = 0.000 for O45
wR2 = 0.0752 before cycle 7 for 17657 data and 0% / 8% parameters
GoF = 2 = 1.000; Restrained GoF = 1.000 for 0 restraints
Rms shift/eqd = 0.000 Rmsdev = 0.000 for x h25 at 21:17:28
Rms shift = 0.000 Å for H122 Rms. sh = 0.000 for O45
wR2 = 0.0752 before cycle 10 for 17657 data and 0% / 8% parameters
GoF = 2 = 1.000; Restrained GoF = 1.000 for 0 restraints
Rms shift/eqd = 0.000 Rmsdev = 0.000 for x h25 at 21:17:29
Rms shift = 0.000 Å for O45 Rms. sh = 0.000 for O45
wR2 = 0.0752 before cycle 11 for 17657 data and 0 / 8% parameters
GoF = 2 = 1.000; Restrained GoF = 1.000 for 0 restraints
R1 = 0.0278 for 17657 Pa 2-4mgFe2 and 0.0379 for all 17657 data
wR2 = 0.0752, GoF = 2 = 1.000, Restrained GoF = 1.000 for all data
0 atoms may be split and 0 atoms H2S
R1 = 0.0306 for 17657 unique reflections after merging for Fourier
Highest peak 2.38 at 0.0167 0.3834 0.4271 1 0.86 Å from O45 1
Deepest hole -0.91 at 0.5106 0.8579 0.4629 1 0.95 Å from F10 1
=====
+ m_0616287 Finished at 21:17:29 Total elapsed time: 7.32 min +
=====
请检查数据质量。

```