# Structure Tables

{% if structure\_figure%}{{structure\_figure}}{%endif%}

**The following text is only a suggestion:** {{ crystallization\_method}} The data for {{cif.block.name}} were collected from a shock-cooled single crystal at {{cif.\_diffrn\_ambient\_temperature}} K on {{diffr\_type|inv\_article}} {{diffr\_type}} {{diffr\_device}} with {{diffr\_source|inv\_article}} {{diffr\_source}} using {{monochromator}} as monochromator and {{detector|inv\_article}} {{detector}} detector. The diffractometer {% if lowtemp\_dev %}was equipped with {{lowtemp\_dev|inv\_article}} {{lowtemp\_dev}} low temperature device and {%endif%}used {{radiation}} radiation {%if wavelength%}(λ={{wavelength}} Å){%endif%}. All data were integrated with {{integration\_progr}} and a multi-scan absorption correction using SADABS was applied.[1,2] The structure were solved by direct methods using SHELXT and refined by full-matrix least-squares methods against *F*2 by SHELXL-2018/3.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. The hydrogen atoms were refined isotropically on calculated positions using a riding model with their *U*iso values constrained to 1.5 times the *U*eq of their pivot atoms for terminal sp3 carbon atoms and 1.2 times for all other carbon atoms. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC ?????? contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/​structures. This report and the CIF file were generated using FinalCif.[6]

## Crystal data and structure refinement for {{ cif.block.name }}

|  |  |
| --- | --- |
| CCDC number | {{ cif.\_database\_code\_depnum\_ccdc\_archive }} |
| Empirical formula | {{ sum\_formula }} |
| Formula weight | {{ cif.\_chemical\_formula\_weight }} |
| Temperature [K] | {{cif.\_diffrn\_ambient\_temperature}} |
| Crystal system | {{ cif.\_space\_group\_crystal\_system }} |
| Space group (number) | {{p space\_group}} {{ itnum }} |
| *a* [Å] | {{cif.\_cell\_length\_a }} |
| *b* [Å] | {{cif.\_cell\_length\_b }} |
| *c* [Å] | {{cif.\_cell\_length\_c }} |
| α [Å] | {{cif.\_cell\_angle\_alpha }} |
| β [Å] | {{cif.\_cell\_angle\_beta }} |
| γ [Å] | {{cif.\_cell\_angle\_gamma }} |
| Volume [Å3] | {{cif.\_cell\_volume}} |
| *Z* | {{cif.\_cell\_formula\_units\_Z}} |
| *ρ*calc [g/cm3] | {{cif.\_exptl\_crystal\_density\_diffrn}} |
| *μ* [mm-1] | {{cif.\_exptl\_absorpt\_coefficient\_mu}} |
| *F*(000) | {{cif.\_exptl\_crystal\_F\_000}} |
| Crystal size [mm3] | {{crystal\_size}} |
| Crystal colour | {{cif.\_exptl\_crystal\_colour}} |
| Crystal shape | {{cif.\_exptl\_crystal\_description}} |
| Radiation | {{radiation}}{%if wavelength%} (λ={{wavelength}} Å){%endif%} |
| 2ϴ range [°] | {{theta\_range}} |
| Index ranges | {{index\_ranges}} |
| Reflections collected | {{cif.\_diffrn\_reflns\_number}} |
| Independent reflections | {{indepentent\_refl}}  *R*int = {{r\_int}} *R*sigma = {{r\_sigma}} |
| Completeness{%if theta\_full%} to  θ = {{theta\_full}}°{%endif%} | {{completeness}} |
| Data / Restraints / Parameters | {{data}} / {{restraints}} / {{parameters}} |
| Goodness-of-fit on *F*2 | {{ goof }} |
| Final *R* indexes  [*I*≥2σ(*I*)] | *R*1 = {{ls\_R\_factor\_gt}} w*R*2 = {{ls\_wR\_factor\_gt}} |
| Final *R* indexes  [all data] | *R*1 = {{ls\_R\_factor\_all}} w*R*2 = {{ls\_wR\_factor\_all}} |
| Largest peak/hole [eÅ3] | {{diff\_dens\_min}}/{{diff\_dens\_max}} |
| **{%tr if exti %}** |  |
| Extinction coefficient | {{exti}} |
| **{%tr endif %}** |  |
| **{%tr if flack\_x %}** |  |
| Flack X parameter | {{flack\_x}} |
| **{%tr endif %}** |  |

## {% if options.atoms\_table %}Table 2. Atomic coordinates and *U*eq [Å2] for {{ cif.block.name }}

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Atom** | ***x*** | ***y*** | ***z*** | ***U*eq** |
| {%tr for atom in atomic\_coordinates %} |  |  |  |  |
| {{ atom.label }} | {{ atom.x }} | {{ atom.y }} | {{ atom.z }} | {{ atom.u\_eq }} |
| {%tr endfor %} |  |  |  |  |

{% endif %}