# 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 {{abstype}} absorption correction using {{abs\_details}} was applied.[1,2] The structure were solved by {{solution\_method}} methods with {{solution\_program}} and refined by full-matrix least-squares methods against *F*2 using {{refinement\_prog}}.[3,4] All non-hydrogen atoms were refined with anisotropic displacement parameters. {%if cif.hydrogen\_atoms\_present%}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. {%endif%}Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre.[5] CCDC {%if cif.\_database\_code\_depnum\_ccdc\_archive%}{{cif.\_database\_code\_depnum\_ccdc\_archive}}{%else%}??????{%endif%} 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 %} *U*eq is defined as 1/3 of the trace of the orthogonalized *Uij* tensor.

## Table 3. Bond lengths and angles for {{ cif.block.name }}

|  |  |
| --- | --- |
| **Atom–Atom** | **Length [Å]** |
| {%tr for b in bonds %} |  |
| {{b.atoms}} | {{b.dist}} |
| {%tr endfor %} |  |
|  |  |
| **Atom–Atom–Atom** | **Angle [°]** |
| {%tr for a in angles %} |  |
| {{a.atoms}} | {{a.angle}} |
| {%tr endfor %} |  |

{% if options.without\_h %}Bonds and angles to hydrogen atoms were omitted.{% endif %}{%if ba\_symminfo%}{{ ba\_symminfo}}{%endif%}

## Table 4. Torsion angles for {{ cif.block.name }}

|  |  |
| --- | --- |
| **Atom–Atom–Atom–Atom** | **Torsion Angle [°]** |
| {%tr for t in torsions %} |  |
| {{t.atoms}} | {{t.angle}} |
| {%tr endfor %} |  |

{%if torsion\_symminfo%}{{ torsion\_symminfo}}{%endif%}

## Table 5. Hydrogen bonds for {{ cif.block.name }}

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **D–H⋯A [Å]** | **d(D–H) [Å]** | **d(H⋯A) [Å]** | **d(D⋯A) [Å]** | **<(DHA) [°]** |
| {%tr for h in hydrogen\_bonds %} |  |  |  |  |
| {{h.atoms}} | {{h.dist\_dh}} | {{h.dist\_ha}} | {{h.dist\_da}} | {{h.angle\_dha}} |
| {%tr endfor %} |  |  |  |  |

{%if hydrogen\_symminfo%}{{hydrogen\_symminfo}}{%endif%}