# Structure Tables

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

## Table 1 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 [°] | {{ cif.\_cell\_angle\_alpha }} |
| β [°] | {{ cif.\_cell\_angle\_beta }} |
| γ [°] | {{ cif.\_cell\_angle\_gamma }} |
| Volume [Å3] | {{ cif.\_cell\_volume }} |
| *Z* | {{ cif.\_cell\_formula\_units\_Z }} |
| *ρ*calc [gcm−3] | {{ 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 | {{ crystal\_colour }} |
| Crystal shape | {{ crystal\_shape }} |
| 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\_ref }} |
| Largest peak/hole [eÅ−3] | {{ diff\_dens\_max }}/{{ diff\_dens\_min }} |
| {%tr if exti %} |  |
| Extinction coefficient | {{ exti }} |
| {%tr endif %} |  |
| {%tr if flack\_x %} |  |
| Flack X parameter | {{ flack\_x }} |
| {%tr endif %} |  |

## {%p if refinement\_details %}

## Refinement details for {{ cif.block.name }}

{{ refinement\_details }}

## {%p endif %}

## {%p if atomic\_coordinates %}

## Table 1 Atomic coordinates and Ueq [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 %} |  |  |  |  |

*U*eq is defined as 1/3 of the trace of the orthogonalized *Uij* tensor.

{%p endif %}

{%p if displacement\_parameters %}

## Table 1 Anisotropic displacement parameters (Å2) for {{ cif.block.name }}. The anisotropic displacement factor exponent takes the form: −2π2[*h*2*(a\*)*2*U*11*+ k*2*(b\*)*2*U*22 + … + *2hka\*b\*U*12 ]

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Atom** | ***U*11** | ***U*22** | ***U*33** | ***U*23** | ***U*13** | ***U*12** |
| {%tr for atom in displacement\_parameters %} |  |  |  |  |  |  |
| {{ atom.label }} | {{ atom.U11 }} | {{ atom.U22 }} | {{ atom.U33 }} | {{ atom.U23 }} | {{ atom.U13 }} | {{ atom.U12 }} |
| {%tr endfor %} |  |  |  |  |  |  |

{%p endif %}

{%p if bonds %}

## Table 1 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 %} |  |

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

{%r endif %}{% if ba\_symminfo %}{{ ba\_symminfo }}{% endif %}

{%p endif %}

{%p if torsions%}

## Table 1 Torsion angles for {{ cif.block.name }}

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

Bonds and angles to hydrogen atoms were omitted.

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

{%p endif %}

{%p if hydrogen\_bonds %}

## Table 1 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}}

{%r endif %}

{%p endif %}

{%p if options.hydrogen\_bonds and hydrogen\_bonds %}

## Table 1 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 %} |  |  |  |  |

{%r if hydrogen\_symminfo %}

{{hydrogen\_symminfo}}

{%r endif %}

{%p endif %}