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Crystal structure of sunvozertinib, $C_{29}H_{35}ClFN_7O_3$, from synchrotron X-ray powder data and DFT optimization

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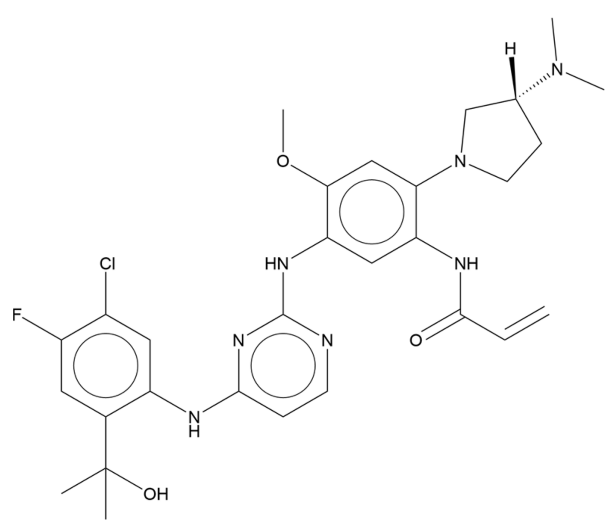
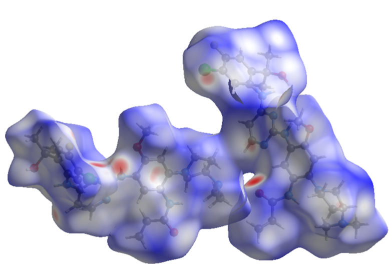
The crystal structure of sunvozertinib (systematic name: *N*-[5-({4-[5-chloro-4-fluoro-2-(2-hydroxypropan-2-yl)anilino]pyrimidin-2-yl}amino)-2-[(3*R*)-3-(dimethylamino)pyrrolidin-1-yl]-4-methoxyphenyl]prop-2-enamide), $C_{29}H_{35}ClFN_7O_3$, has been solved and refined using synchrotron X-ray powder diffraction data, and optimized using density functional theory techniques. The asymmetric unit in space group *C*2 contains two molecules, *A* and *B*, and the crystal structure consists of alternating layers of molecules *A* and *B* lying parallel to ($\overline{2}01$). O—H⋯O hydrogen bonds link the *B* molecules into chains propagating along the *b*-axis direction while pairwise N—H⋯N hydrogen bonds link the *A* molecules into dimers.

1. Chemical context

Sunvozertinib ($C_{29}H_{35}ClFN_7O_3$; marketed as Zegfrovy) is used to treat non-small-cell lung cancer (Wang *et al.*, 2022). It is administered to adult patients with locally advanced or metastatic non-small-cell lung cancer (NSCLC) when the disease has progressed on or after platinum-based chemotherapy. Its systematic name (CAS Registry Number 2370013-12-8) is *N*-[5-[[4-[5-chloro-4-fluoro-2-(2-hydroxypropan-2-yl)-anilino]pyrimidin-2-yl]amino]-2-[(3*R*)-3-(dimethylamino)pyrrolidin-1-yl]-4-methoxyphenyl]prop-2-enamide.





This work was carried out as part of a project (Kaduk *et al.*, 2014) to determine the crystal structures of large-volume commercial pharmaceuticals, and include high-quality powder diffraction data for them in the Powder Diffraction File (Kabekkodu *et al.*, 2024).

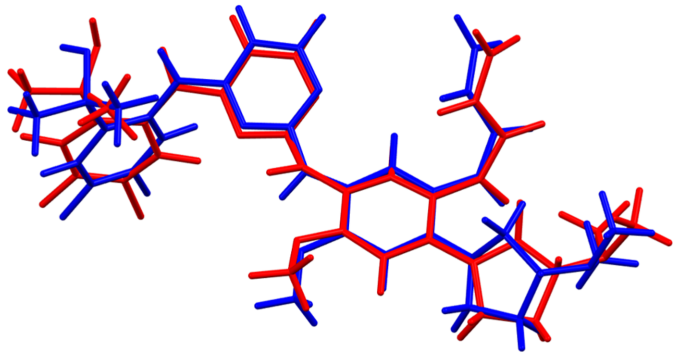


Figure 1
Comparison of the refined structure of sunvozertinib molecule *A* (red) to the *VASP*-optimized structure (blue). The comparison was generated using the *Mercury* Calculate/Molecule overlay tool; the r.m.s. difference is 0.838 Å.

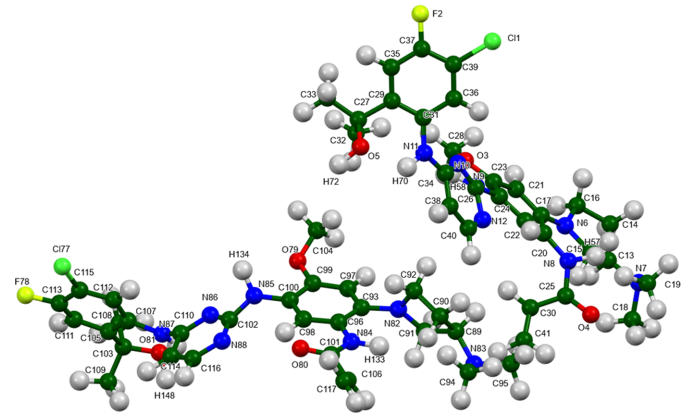


Figure 3
The asymmetric unit of sunvozertinib, with the atom numbering. The atoms are represented by 50% probability spheroids.

2. Structural commentary

Sunvozertinib crystallises in the monoclinic space group *C*2 with two molecules, *A* and *B*, in the asymmetric unit. The root-mean-square Cartesian displacements of the non-H atoms in the Rietveld-refined and DFT-optimized structures of molecules *A* and *B*, calculated using the *Mercury* Calculate/Molecule overlay tool (Macrae *et al.*, 2020), are 0.838 and 0.636 Å, respectively (Figs. 1 and 2). The differences are spread throughout the molecules. The agreements are outside of the normal range for correct structures (van de Streek & Neumann, 2014); however, this very complex structure, refined using limited data, might be expected to be less accurate than usual. In the refined structure, there is a close contact (overlap) between the vinyl group C95 of molecule *A* and one of the methylamine groups associated with atom N83 of molecule *B*. This contact is relieved on DFT optimization. The asymmetric unit is illustrated in Fig. 3. The remaining discussion will emphasize the *VASP*-optimized structure.

All of the bond distances, and most of the bond angles and torsion angles fall within the normal ranges indicated by a *Mercury* Mogul Geometry check (Macrae *et al.*, 2020). The angles C3—C25—N8 [116.2°; average = 113.8 (7)°; *Z*-score = 3.4], C104—O79—C99 [112.2°; average = 117.5 (15)°; *Z*-score = 3.5], and O79—C99—C100 [119.3°; average = 114.8 (12)°; *Z*-score = 3.7] are flagged as unusual. For all three, the uncertainty on average is exceptionally small, inflating the *Z*-scores, so these are not of concern. Torsion angles involving rotation about the C13—N7 and C89—N83 bonds (which reflect the orientations of the dimethylamino groups in the two molecules) lie in minor *trans* populations of a mainly *gauche* distribution. The torsion angles about C93—N82 lie in the middle of broad ranges. Torsion angles involving C110—N87 lie on the tails of distributions, so they are slightly unusual. Torsions about C25—N8 (amide) and O79—C99 (methoxy) are flagged as unusual.

The root-mean-square difference between molecules *A* and *B* is 1.706 Å (Fig. 4). As noted above, the differences are spread throughout the molecules. The interplanar angles between the aromatic rings in molecule *A* are 64.8 and 27.2°, and those in molecule *B* are 66.7 and 31.3°. Quantum chemical geometry optimization of the isolated sunvozertinib molecules (DFT/B3LYP/6-31G*/water) using *Spartan '24* (Wavefunction, 2025) indicated that molecule *B* is 1.8 kcal mol^{-1} lower in energy than molecule *A*. Since the expected uncertainty of

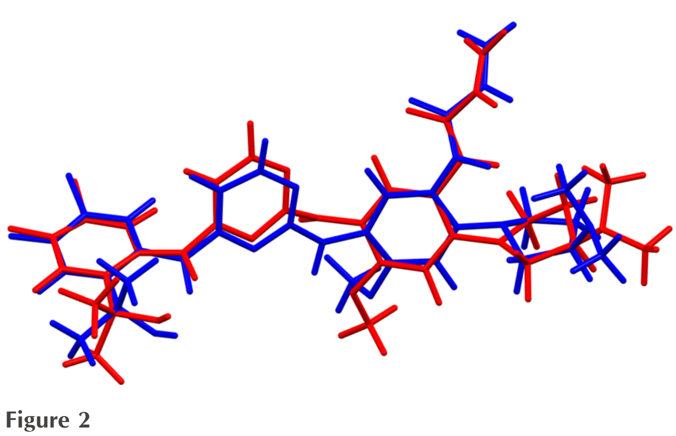


Figure 2
Comparison of the refined structure of sunvozertinib molecule *B* (red) to the *VASP*-optimized structure (blue). The comparison was generated using the *Mercury* Calculate/Molecule overlay tool; the r.m.s. difference is 0.636 Å.

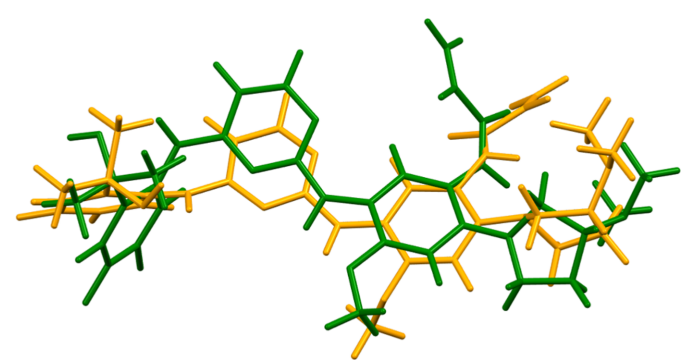


Figure 4
Comparison of the *VASP*-optimized structures of sunvozertinib molecule *A* (green) and molecule *B* (orange). The r.m.s. difference is 1.706 Å.

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N9—H58$\cdots$N10^{i}	1.03	2.10	3.022	148
N11—H70$\cdots$O5	1.02	2.18	2.872	124
N11—H70$\cdots$Cl77^{ii}	1.02	2.82	3.597	133
N85—H134$\cdots$Cl77^{iii}	1.02	2.47	3.424	155
N87—H146$\cdots$O81	1.03	1.96	2.705	127
O81—H148$\cdots$O80^{iv}	0.99	1.77	2.740	164
C38—H73$\cdots$O79^{v}	1.09	2.32	3.329	154
C90—H120$\cdots$N12^{vi}	1.10	2.51	3.358	133
C104—H136$\cdots$O5^{vii}	1.10	2.53	3.498	147
C108—H141$\cdots$N88^{iv}	1.10	2.33	3.400	165

Symmetry codes: (i) $-x+1, y, -z+2$; (ii) $-x+1, y-1, -z+2$; (iii) $-x+1, y, -z+1$; (iv) $x, y+1, z$; (v) $x, y-1, z+1$; (vi) $x, y, z-1$; (vii) $x, y+1, z-1$.

such calculations is of the order of 1 kcal mol^{-1}, the two molecules should be considered to be equivalent in energy. The molecule is apparently flexible: the global minimum-energy conformation is 233 kcal mol^{-1} lower in energy, but is much more compact, being folded on itself. Intermolecular interactions are thus important in determining the solid-state conformation.

3. Supramolecular features

The extended structure (Fig. 5) consists of alternating layers of molecules A and B lying parallel to the ($\bar{2}$01) plane. O—H$\cdots$O hydrogen bonds (Table 1) link the B molecules into chains propagating along the b-axis direction. N—H$\cdots$N hydrogen bonds link the A molecules into pairs. The *Mercury* Aromatics Analyser indicates two strong (d = 4.96 Å) interactions between the A molecules, and two moderate (d = 4.96 Å) parallel stacking interactions between the B molecules.

Analysis of the contributions to the total crystal energy of the structure using the Forcite module of *Materials Studio* (Dassault Systèmes, 2024) indicated that the intramolecular energy is dominated by torsion angle distortion terms, with a significant contribution from angle distortion terms. The intermolecular energy is dominated by van der Waals attractions, which in this force-field-based analysis include hydrogen bonds. The hydrogen bonds are better discussed using the results of the DFT calculation.

Hydrogen bonds are prominent in the structure. Strong O81—H148$\cdots$O80 hydrogen bonds link the B molecules into chains along the b-axis direction. The graph set descriptor (Etter, 1990; Bernstein *et al.*, 1995; Motherwell *et al.*, 2000) for this pattern is $C_1^1(16)$. The energy of the O—H$\cdots$O hydrogen bond (O81—H148$\cdots$O80 = 13.2 kcal mol^{-1}) was calculated using the correlation of Rammohan and Kaduk (2018). There are two intramolecular N—H$\cdots$O hydrogen bonds in molecule B. The energy of the N87—H146$\cdots$O81 hydrogen bond (5.4 kcal mol^{-1}) was calculated using the correlation of Wheatley and Kaduk (2019).

Pairwise N9—H58$\cdots$N10 bonds link the A molecules into dimers with crystallographic twofold symmetry, with a graph-set notation of $R_2^2(8)$. The O5—H72 group of molecule A does not form a hydrogen bond in the present model although an alternative orientation that would form an intermolecular O5—H72$\cdots$Cl77 link is possible.

Intramolecular N—H$\cdots$N bonds are present in both molecules. N—H$\cdots$Cl bonds also participate in the chains of molecules B. Several weak C—H$\cdots$N and C—H$\cdots$O hydrogen bonds also contribute to the cohesion of the structure.

The volume enclosed by the Hirshfeld surface of sunvozertinib (Fig. 6; Hirshfeld, 1977; Spackman *et al.*, 2021) is 1491.6 Å^3, some 98.7% of 1/4 of the unit-cell volume. The packing density is thus typical. The only significant close contacts (red in Fig. 6) involve the hydrogen bonds. The volume per non-hydrogen atom is normal, at 18.4 Å^3.

The Bravais–Friedel–Donnay–Harker (Bravais, 1866; Friedel, 1907; Donnay & Harker, 1937) algorithm suggests that we might expect elongated morphology for sunvozertinib, with [010] as the long axis. A 2nd order spherical harmonic model for preferred orientation was included. The texture index was 1.036 (3), indicating that the preferred orientation was small in this rotated capillary specimen.

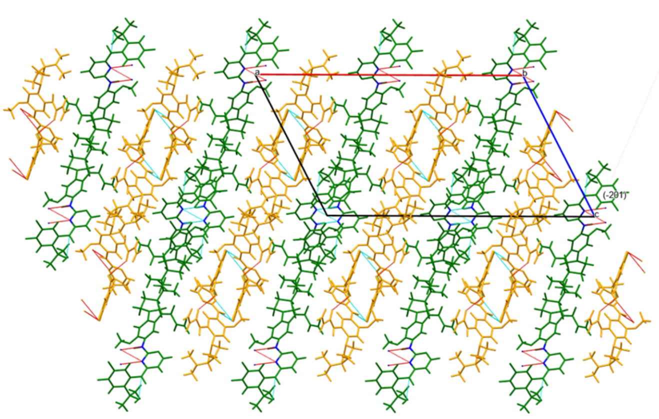


Figure 5
Crystal structure of sunvozertinib, viewed down the b-axis direction. Molecule A is green, and molecule B is orange.

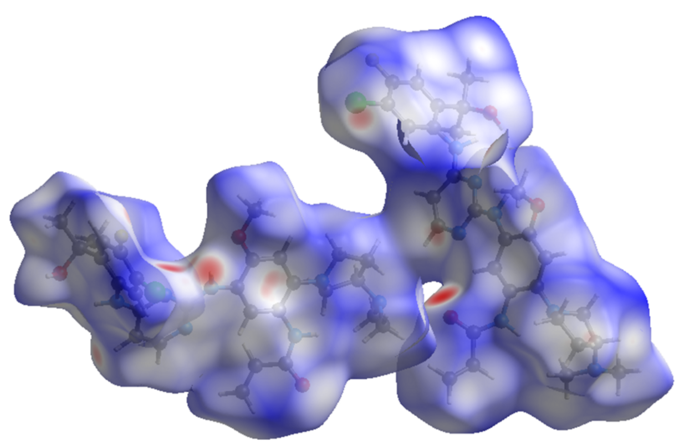


Figure 6
The Hirshfeld surface of sunvozertinib. Intermolecular contacts longer than the sums of the van der Waals radii are colored blue, and contacts shorter than the sums of the radii are colored red. Contacts equal to the sums of radii are white.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{29}H_{35}ClFN_7O_3$
M_r	584.09
Crystal system, space group	Monoclinic, *C*2
Temperature (K)	298
a, *b*, *c* (Å)	33.491 (9), 10.2237 (6), 19.857 (4)
β (°)	117.216 (9)
V (Å^3)	6046.4 (10)
Z	8
Radiation type	Synchrotron, λ = 0.81933 Å
μ (mm^{-1})	0.11
Specimen shape, size (mm)	Cylinder, 0.45 × 0.15
Data collection	
Diffractometer	Wiggler Low Energy Beamline, Brockhouse X-ray Diffraction and Scattering Sector, Canadian Light Source
Specimen mounting	Kapton capillary
Data collection mode	Transmission
Scan method	Step
2θ values (°)	$2\theta_{min}$ = 1.6, $2\theta_{max}$ = 75.0, $2\theta_{step}$ = 0.003
Refinement	
R factors and goodness of fit	R_p = 0.061, R_{wp} = 0.0993, R_{exp} = 0.002, $R(F^2)$ = 0.26899, χ^2 = 2361.571
No. of parameters	268
No. of restraints	222
$(\Delta/\sigma)_{max}$	4.249

Computer programs: *GSAS-II* (Toby & Von Dreele, 2013).

4. Database survey

A reduced cell search in the Cambridge Structural Database (CSD Conquest Build 2026.1.0; Groom *et al.*, 2016) yielded one hit for an unrelated structure, but no structures of sunvozertinib or its derivatives. We are unaware of any published X-ray powder diffraction data for sunvozertinib.

5. Synthesis and crystallization

Sunvozertinib is a commercial reagent, purchased from TargetMol (Batch #231941), and was used as-received.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The white powder was packed into a 0.5 mm diameter Kapton capillary, and rotated during the measurements at ∼2 Hz. The powder pattern was measured at 298 (1) K at the Wiggler Low Energy Beamline (Leontowich *et al.*, 2021) of the Brockhouse X-ray Diffraction and Scattering Sector of the Canadian Light Source using a wavelength of 0.819325 (2) Å (15.1 keV) from 1.6–75.0° 2θ with a step size of 0.0025° and a collection time per step of 3 minutes. The high-resolution powder diffraction data were collected using eight Dectris Mythen2 X series 1K linear strip detectors. NIST SRM 660b LaB_6 was used to calibrate the instrument and refine the monochromatic wavelength used in the experiment.

The pattern was indexed using *JADE Pro* (MDI, 2025) on a *C*-centered monoclinic cell with *a* = 33.43691, *b* = 10.20685, *c* = 19.80699 Å, β = 117.27°, *V* = 6008.62 Å^3, and *Z* = 8. The space group suggested by *EXPO2014* (Altomare *et al.*, 2013) was *C*2, which was confirmed by the successful solution and refinement of the structure.

The molecular structure of sunvozertinib was downloaded from PubChem (Kim *et al.*, 2023) as Conformer3D_COMPOUND_CID_139377809.sdf. It was converted to a *.mol2 file using *Mercury* (Macrae *et al.*, 2020). The crystal structure was solved by Monte Carlo simulated annealing techniques as implemented in *EXPO2014* (Altomare *et al.*, 2013) using the two sunvozertinib molecules as fragments, including a bump penalty on the non-H atoms.

Rietveld refinement was carried out with *GSAS-II* (Toby & Von Dreele, 2013). Only the 2.5–40.0° portion of the pattern was included in the refinements (d_{min} = 1.198 Å). All non-H bond distances and angles were subjected to restraints, based on a *Mercury* Mogul Geometry Check (Sykes *et al.*, 2011; Bruno *et al.*, 2004). The Mogul average and standard deviation for each quantity were used as the restraint parameters. The aromatic rings were restrained to be planar. The restraints contributed 13.6% to the overall χ^2. Decreasing the restraint weights led to disconnected molecular fragments. The hydrogen atoms were included in calculated positions, which were recalculated during the refinement using *Materials Studio* (Dassault Systèmes, 2024). Attempts to refine isotropic displacement coefficients (grouped by chemical similarity) led to unreasonably-large positive and negative values, so the U_{iso} were fixed at reasonable values. The peak profiles were described using a uniaxial microstrain model, with [010] as the unique axis. The background was modeled using a six-term shifted Chebyshev polynomial, with two peaks at 3.05 and 10.87° 2θ to model the scattering from the Kapton capillary and any amorphous component of the sample.

The final refinement of 268 variables using 15,001 observations and 222 restraints yielded the residual R_{wp} = 0.0993. The largest peak (1.42 Å from C15) and hole (2.15 Å from C93) in the difference-Fourier map are +0.53 (13) and

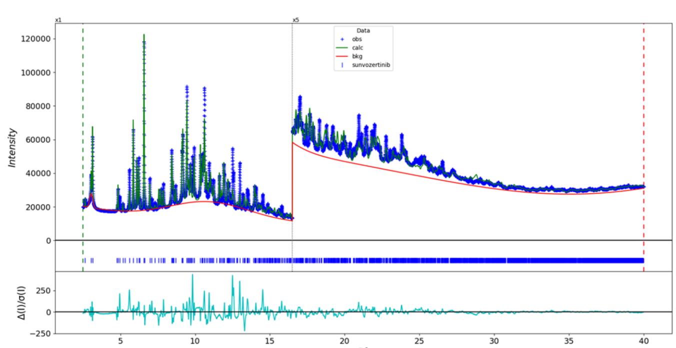


Figure 7
The Rietveld difference plot for sunvozertinib. The blue crosses represent the observed data points, and the green line is the calculated pattern. The cyan curve is the normalized error plot, and the red line is the background curve. The blue tick marks indicate the peak positions. The vertical scale has been multiplied by a factor of 5 for 2θ > 16.5°.

-0.47 (13) e Å^{-3}, respectively. The final Rietveld plot is shown in Fig. 7. The largest features in the normalized error plot are in the intensities and shapes of some of the strong low-angle peaks.

The crystal structure of sunvozertinib was optimized (fixed experimental unit cell) with density functional theory techniques using *VASP* (Kresse and Furthmüller, 1996) through the *MedeA* graphical interface (Materials Design, 2024). The calculation was carried out on 32 cores of a 144-core (768 Gb memory) HPE Superdome Flex 280 Linux server at North Central College. The calculation used the GGA-PBE functional, a plane wave cutoff energy of 400.0 eV, and a *k*-point spacing of 0.5 Å^{-1} leading to a $3 \times 3 \times 1$ mesh, and took ~2.9 days. Single-point density functional theory calculations (fixed experimental cell) and population analysis were carried out using *CRYSTAL23* (Erba *et al.*, 2023). The basis sets for the H, C, N and O atoms in the calculation were those of Gatti *et al.* (1994), and those for F and Cl were from Peintinger *et al.* (2013). The calculations were run on a 3.5 GHz PC using 8 *k*-points and the B3LYP functional, and took ~11.4 h.

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References

Altomare, A., Cuocci, C., Giacovazzo, C., Moliterni, A., Rizzi, R., Corriero, N. & Falcicchio, A. (2013). *J. Appl. Cryst.* **46**, 1231–1235.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N. L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bravais, A. (1866). *Etudes Cristallographiques.* Paris: Gauthier Villars.
Bruno, I. J., Cole, J. C., Kessler, M., Luo, J., Motherwell, W. D. S., Purkis, L. H., Smith, B. R., Taylor, R., Cooper, R. I., Harris, S. E. & Orpen, A. G. (2004). *J. Chem. Inf. Comput. Sci.* **44**, 2133–2144.
Dassault Systèmes. (2024). *BIOVIA Materials Studio 2025*. San Diego, CA. BIOVIA.
Donnay, J. D. H. & Harker, D. (1937). *Am. Mineral.* **22**, 446–467.
Erba, A., Desmarais, J. K., Casassa, S., Civalleri, B., Donà, L., Bush, I. J., Searle, B., Maschio, L., Edith-Daga, L., Cossard, A., Ribaldone, C., Ascrizzi, E., Marana, N. L., Flament, J.-P. & Kirtman, B. (2023). *J. Chem. Theory Comput.* **19**, 6891–6932.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Friedel, G. (1907). *Bull. Soc. Fr. Minéral.* **30**, 326–455.
Gatti, C., Saunders, V. R. & Roetti, C. (1994). *J. Chem. Phys.* **101**, 10686–10696.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hirshfeld, F. L. (1977). *Theor. Chim. Acta* **44**, 129–138.
Kabekkodu, S., Dosen, A. & Blanton, T. N. (2024). *Powder Diffr.* **39**, 47–59.
Kaduk, J. A., Crowder, C. E., Zhong, K., Fawcett, T. G. & Suchomel, M. R. (2014). *Powder Diffr.* **29**, 269–273.
Kim, S., Chen, J., Cheng, T., Gindulyte, A., He, J., He, S., Li, Q., Shoemaker, B. A., Thiessen, P. A., Yu, B., Zaslavsky, L., Zhang, J. & Bolton, E. E. (2023). *Nucleic Acids Res.* **51**, D1373–D1380.
Kresse, G. & Furthmüller, J. (1996). *Comput. Mater. Sci.* **6**, 15–50.
Leontowich, A. F. G., Gomez, A., Diaz Moreno, B., Muir, D., Spasyuk, D., King, G., Reid, J. W., Kim, C.-Y. & Kycia, S. (2021). *J. Synchrotron Rad.* **28**, 961–969.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Materials Design. (2024). *MedeA 3.7.2*. Materials Design Inc., San Diego, USA.
MDI. (2025). *JADE Pro version 9.3*. Materials Data, Livermore, USA.
Motherwell, W. D. S., Shields, G. P. & Allen, F. H. (2000). *Acta Cryst.* B**56**, 857–871.
Peintinger, M. F., Oliveira, D. V. & Bredow, T. (2013). *J. Comput. Chem.* **34**, 451–459.
Rammohan, A. & Kaduk, J. A. (2018). *Acta Cryst.* B**74**, 239–252.
Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.
Streek, J. van de & Neumann, M. A. (2014). *Acta Cryst.* B**70**, 1020–1032.
Sykes, R. A., McCabe, P., Allen, F. H., Battle, G. M., Bruno, I. J. & Wood, P. A. (2011). *J. Appl. Cryst.* **44**, 882–886.
Toby, B. H. & Von Dreele, R. B. (2013). *J. Appl. Cryst.* **46**, 544–549.
Wang, M., Yang, J. C., Mitchell, P. L., Fang, J., Camidge, D. R., Nian, W., Chiu, C.-H., Zhou, J., Zhao, Y., Su, W.-C., Yang, T.-Y., Zhu, V. W., Milward, M., Fan, Y., Huang, W.-T., Cheng, Y., Jiang, L., Brungs, D., Bazhenova, L., Lee, C. K., Gao, B., Xu, Y., Hsu, W.-H., Zheng, L. & Janne, P. A. (2022). *Cancer Discov.* **12**, 1676–1689.
Wavefunction, Inc. (2025). *Spartan '24. V. 1.3.1.* Wavefunction Inc., Irvine, USA.
Wheatley, A. M. & Kaduk, J. A. (2019). *Powder Diffr.* **34**, 35–43.

supporting information

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Computing details

N-[5-({4-[5-Chloro-4-fluoro-2-(2-hydroxypropan-2-yl)anilino]pyrimidin-2-yl}amino)-2-[(3*R*)-3-(dimethylamino)pyrrolidin-1-yl]-4-methoxyphenyl]prop-2-enamide (I)

Crystal data

$C_{29}H_{35}ClFN_7O_3$
M_r = 584.09
Monoclinic, *C*2
a = 33.491 (9) Å
b = 10.2237 (6) Å
c = 19.857 (4) Å
β = 117.216 (9)°
V = 6046.4 (10) Å^3
Z = 8
D_x = 1.283 Mg m^{-3}
Synchrotron radiation, λ = 0.81933 Å
μ = 0.11 mm^{-1}
T = 298 K
cylinder, 0.45 × 0.15 mm

Data collection

Wiggler Low Energy Beamline, Brockhouse X-ray Diffraction and Scattering Sector, Canadian Light Source diffractometer
Specimen mounting: Kapton capillary
Data collection mode: transmission
Scan method: step
$2\theta_{min}$ = −9.008°, $2\theta_{max}$ = 75.047°, $2\theta_{step}$ = 0.003°

Refinement

Least-squares matrix: full
R_p = 0.061
R_{wp} = 0.092
R_{exp} = 0.002
$R(F^2)$ = 0.26899
33623 data points
Profile function: Finger-Cox-Jephcoat function parameters U, V, W, X, Y, SH/L: peak variance(Gauss) = Utan(Th)^2+Vtan(Th)+W: peak HW(Lorentz) = X/cos(Th)+Ytan(Th); SH/L = S/L+H/L U, V, W in (centideg)^2, X & Y in centideg 6.157, -1.198, 1.258, 0.000, 0.667, 0.002,
268 parameters
222 restraints
0 constraints
Weighting scheme based on measured s.u.'s
$(\Delta/\sigma)_{max}$ = 4.249
Background function: Background function: "chebyschev-1" function with 6 terms: 1.038(5)e4, -6.46(6)e3, 2.14(4)e3, -3.6(8)e2, 6.9(7)e2, -1.9(3)e2, Background peak parameters: pos, int, sig, gam: 3.050(5), 2.13(10)e5, 103(9), 0.100, 10.894(31), 7.23(23)e6, 7.23(23)e4, 0.100,
Preferred orientation correction: Simple spherical harmonic correction Order = 2 Coefficients: 0:0:C(2,-2) = 0.126(18); 0:0:C(2,0) = -0.206(24); 0:0:C(2,2) = 0.270(18)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.6105 (9)	−0.58413	1.0397 (13)	0.0500*
F2	0.6809 (9)	−0.518 (6)	1.1997 (16)	0.0500*
O3	0.4737 (10)	0.158 (4)	0.9250 (19)	0.0500*
O4	0.2231 (10)	−0.037 (5)	0.6534 (18)	0.0500*
O5	0.5494 (17)	−0.365 (6)	1.294 (3)	0.0500*
N6	0.3421 (9)	0.219 (4)	0.6663 (15)	0.0500*
N7	0.2348 (11)	0.211 (5)	0.4865 (16)	0.0500*
N8	0.2994 (9)	0.021 (4)	0.7000 (14)	0.0500*
N9	0.4386 (15)	−0.065 (4)	0.9464 (16)	0.0500*
N10	0.4777 (8)	−0.241 (4)	1.0326 (19)	0.0500*
N11	0.5090 (9)	−0.377 (5)	1.1443 (15)	0.0500*
N12	0.3964 (8)	−0.225 (6)	0.964 (3)	0.0500*
C13	0.2774 (9)	0.263 (4)	0.5502 (16)	0.0500*
C14	0.3201 (12)	0.301 (7)	0.5406 (18)	0.0500*
C15	0.2969 (11)	0.164 (5)	0.6150 (18)	0.0500*
C16	0.3597 (11)	0.298 (5)	0.622 (2)	0.0500*
C17	0.3678 (11)	0.154 (5)	0.739 (2)	0.0500*
C18	0.1927 (12)	0.269 (7)	0.485 (4)	0.0500*
C19	0.2307 (19)	0.078 (5)	0.496 (4)	0.0500*
C20	0.3459 (8)	0.050 (4)	0.7550 (17)	0.0500*
C21	0.4122 (13)	0.191 (5)	0.794 (2)	0.0500*
C22	0.3712 (13)	−0.029 (4)	0.818 (2)	0.0500*
C23	0.4335 (17)	0.122 (5)	0.863 (2)	0.0500*
C24	0.4139 (14)	0.006 (5)	0.874 (2)	0.0500*
C25	0.2585 (8)	0.013 (4)	0.7043 (16)	0.0500*
C26	0.4381 (9)	−0.192 (4)	0.9756 (18)	0.0500*
C27	0.5832 (10)	−0.292 (3)	1.2855 (16)	0.0500*
C28	0.491 (2)	0.286 (5)	0.927 (3)	0.0500*
C29	0.5891 (8)	−0.370 (5)	1.2248 (17)	0.0500*
C30	0.2623 (15)	0.041 (9)	0.781 (3)	0.0500*
C31	0.5527 (8)	−0.391 (5)	1.1534 (15)	0.0500*
C32	0.567 (3)	−0.153 (4)	1.258 (3)	0.0500*
C33	0.6256 (12)	−0.289 (7)	1.361 (2)	0.0500*
C34	0.4728 (8)	−0.327 (7)	1.080 (3)	0.0500*
C35	0.6305 (9)	−0.427 (5)	1.2429 (13)	0.0500*
C36	0.5599 (9)	−0.445 (7)	1.0942 (15)	0.0500*
C37	0.6374 (9)	−0.484 (9)	1.1849 (18)	0.0500*
C38	0.4311 (10)	−0.361 (9)	1.074 (4)	0.0500*
C39	0.6023 (8)	−0.498 (5)	1.1111 (13)	0.0500*
C40	0.3940 (8)	−0.305 (9)	1.015 (4)	0.0500*
C41	0.227 (2)	0.016 (10)	0.798 (3)	0.0500*
H42	0.26773	0.35323	0.57321	0.0650*
H43	0.32498	0.22679	0.50215	0.0650*
H44	0.31608	0.40347	0.52569	0.0650*
H45	0.30100	0.06274	0.59493	0.0650*

H46	0.27521	0.15850	0.64551	0.0650*
H47	0.39018	0.24802	0.62253	0.0650*
H48	0.36898	0.40040	0.64795	0.0650*
H49	0.17173	0.31755	0.42782	0.0650*
H50	0.17226	0.18806	0.49413	0.0650*
H51	0.20247	0.34496	0.53193	0.0650*
H52	0.24345	0.02044	0.46055	0.0650*
H53	0.19392	0.05303	0.47699	0.0650*
H54	0.25135	0.05129	0.55827	0.0650*
H55	0.43002	0.27487	0.78049	0.0650*
H56	0.35699	−0.12617	0.82585	0.0650*
H57	0.29101	−0.00079	0.64024	0.0650*
H58	0.46590	−0.01532	0.99563	0.0650*
H59	0.46572	0.36177	0.92554	0.0650*
H60	0.49718	0.30010	0.87529	0.0650*
H61	0.52393	0.29850	0.98065	0.0650*
H62	0.29468	0.08373	0.82705	0.0650*
H63	0.56038	−0.14227	1.19667	0.0650*
H64	0.59364	−0.07973	1.29487	0.0650*
H65	0.53452	−0.13347	1.26195	0.0650*
H66	0.62020	−0.22161	1.40195	0.0650*
H67	0.63346	−0.39198	1.38574	0.0650*
H68	0.65485	−0.25122	1.35216	0.0650*
H69	0.65805	−0.42674	1.30400	0.0650*
H70	0.50097	−0.40691	1.19047	0.0650*
H71	0.53158	−0.44526	1.03372	0.0650*
H72	0.53887	−0.31169	1.33145	0.0650*
H73	0.42873	−0.43182	1.11637	0.0650*
H74	0.35995	−0.33061	1.01142	0.0650*
H75	0.19925	−0.05697	0.76289	0.0650*
H76	0.22510	0.06878	0.84758	0.0650*
Cl77	0.5504 (9)	0.766 (3)	0.7381 (12)	0.0500*
F78	0.5324 (12)	1.048 (3)	0.7594 (18)	0.0500*
O79	0.4365 (16)	0.507 (5)	0.236 (2)	0.0500*
O80	0.3326 (17)	0.085 (6)	0.3147 (16)	0.0500*
O81	0.3926 (16)	1.086 (4)	0.4255 (16)	0.0500*
N82	0.3283 (11)	0.178 (4)	0.0645 (13)	0.0500*
N83	0.2235 (11)	0.038 (4)	−0.090 (2)	0.0500*
N84	0.314 (2)	0.098 (6)	0.1912 (16)	0.0500*
N85	0.4176 (10)	0.443 (4)	0.3499 (17)	0.0500*
N86	0.415 (2)	0.649 (3)	0.406 (3)	0.0500*
N87	0.4160 (12)	0.842 (3)	0.4758 (15)	0.0500*
N88	0.3794 (19)	0.452 (4)	0.420 (3)	0.0500*
C89	0.2725 (11)	0.076 (4)	−0.0516 (16)	0.0500*
C90	0.2998 (14)	−0.026 (4)	0.011 (3)	0.0500*
C91	0.2877 (14)	0.211 (3)	−0.007 (2)	0.0500*
C92	0.3436 (10)	0.047 (4)	0.059 (3)	0.0500*
C93	0.3489 (14)	0.250 (5)	0.1366 (13)	0.0500*

C94	0.2177 (18)	−0.078 (7)	−0.051 (4)	0.0500*
C95	0.2047 (19)	0.005 (8)	−0.171 (2)	0.0500*
C96	0.343 (2)	0.206 (6)	0.1991 (19)	0.0500*
C97	0.3782 (19)	0.354 (6)	0.1475 (15)	0.0500*
C98	0.365 (3)	0.273 (7)	0.268 (2)	0.0500*
C99	0.4023 (12)	0.414 (5)	0.2184 (14)	0.0500*
C100	0.3942 (18)	0.377 (5)	0.2791 (19)	0.0500*
C101	0.3093 (13)	0.049 (5)	0.2491 (15)	0.0500*
C102	0.4009 (14)	0.521 (3)	0.389 (2)	0.0500*
C103	0.4180 (8)	1.143 (3)	0.4993 (16)	0.0500*
C104	0.464 (3)	0.506 (8)	0.194 (5)	0.0500*
C105	0.4454 (16)	1.039 (3)	0.5595 (16)	0.0500*
C106	0.2702 (13)	−0.038 (6)	0.226 (3)	0.0500*
C107	0.4492 (13)	0.906 (3)	0.5442 (18)	0.0500*
C108	0.4481 (17)	1.245 (5)	0.489 (4)	0.0500*
C109	0.3830 (16)	1.211 (6)	0.516 (3)	0.0500*
C110	0.4079 (15)	0.707 (4)	0.462 (2)	0.0500*
C111	0.4774 (13)	1.088 (3)	0.6320 (16)	0.0500*
C112	0.483 (2)	0.828 (4)	0.5983 (18)	0.0500*
C113	0.5053 (12)	1.002 (3)	0.6880 (15)	0.0500*
C114	0.386 (3)	0.641 (5)	0.497 (4)	0.0500*
C115	0.5117 (16)	0.876 (3)	0.6693 (15)	0.0500*
C116	0.373 (3)	0.514 (6)	0.474 (4)	0.0500*
C117	0.272 (2)	−0.144 (6)	0.259 (5)	0.0500*
H118	0.28524	0.07349	−0.09588	0.0650*
H119	0.30647	−0.11720	−0.01573	0.0650*
H120	0.28062	−0.05220	0.04362	0.0650*
H121	0.26006	0.25111	0.00512	0.0650*
H122	0.29572	0.28388	−0.04306	0.0650*
H123	0.36210	0.00034	0.11701	0.0650*
H124	0.36636	0.05290	0.03009	0.0650*
H125	0.21187	−0.16819	−0.08809	0.0650*
H126	0.18756	−0.06257	−0.03974	0.0650*
H127	0.24919	−0.09262	0.00504	0.0650*
H128	0.20973	−0.10374	−0.17712	0.0650*
H129	0.16729	0.02861	−0.20022	0.0650*
H130	0.22245	0.06447	−0.19771	0.0650*
H131	0.38313	0.39270	0.09798	0.0650*
H132	0.35886	0.24272	0.31814	0.0650*
H133	0.29429	0.05190	0.13494	0.0650*
H134	0.45471	0.43582	0.38196	0.0650*
H135	0.49728	0.55595	0.22973	0.0650*
H136	0.46976	0.40065	0.18220	0.0650*
H137	0.44497	0.56062	0.13813	0.0650*
H138	0.23668	−0.00967	0.17655	0.0650*
H139	0.56295	1.25964	0.57397	0.0650*
H140	0.51558	1.20985	0.48189	0.0650*
H141	0.55470	1.34162	0.48481	0.0650*

H142	0.63000	1.30174	0.52090	0.0650*
H143	0.64609	1.14119	0.49625	0.0650*
H144	0.60104	1.24086	0.42162	0.0650*
H145	0.47997	1.19761	0.64378	0.0650*
H146	0.39318	0.90156	0.42637	0.0650*
H147	0.48729	0.72246	0.58423	0.0650*
H148	0.35653	1.10057	0.40394	0.0650*
H149	0.37969	0.69231	0.54221	0.0650*
H150	0.35576	0.46125	0.50417	0.0650*
H151	0.30571	−0.17992	0.30551	0.0650*
H152	0.24050	−0.20457	0.24252	0.0650*

Geometric parameters (Å, º)

Cl1—C39	1.793 (11)	Cl77—C115	1.791 (11)
F2—C37	1.392 (17)	F78—C113	1.370 (18)
O3—C23	1.395 (8)	O79—C99	1.405 (8)
O3—C28	1.423 (14)	O79—C104	1.481 (14)
O4—C25	1.263 (10)	O80—C101	1.228 (10)
O5—C27	1.424 (7)	O81—C103	1.439 (8)
O5—H72	1.11 (5)	O81—H148	1.09 (5)
N6—C15	1.496 (9)	N82—C91	1.492 (9)
N6—C16	1.494 (8)	N82—C92	1.463 (8)
N6—C17	1.463 (11)	N82—C93	1.468 (11)
N7—C13	1.505 (10)	N83—H76^{iii}	1.30 (4)
N7—C18	1.52 (2)	N83—C89	1.512 (10)
N7—C19	1.38 (2)	N83—C94	1.479 (18)
N8—C20	1.467 (10)	N83—C95	1.465 (18)
N8—C25	1.413 (8)	N84—C96	1.430 (9)
N8—H57	1.11 (3)	N84—C101	1.331 (8)
N9—C24	1.482 (13)	N84—H133	1.11 (3)
N9—C26	1.425 (11)	N85—C100	1.426 (13)
N9—H58	1.11 (3)	N85—C102	1.401 (11)
N10—C26	1.384 (11)	N85—H134	1.11 (3)
N10—C34	1.354 (13)	N86—C102	1.380 (11)
N11—C31	1.397 (13)	N86—C110	1.369 (9)
N11—C34	1.390 (9)	N87—C107	1.458 (13)
N11—H70	1.11 (3)	N87—C110	1.415 (9)
N12—C26	1.347 (6)	N87—H146	1.11 (3)
N12—C40	1.334 (10)	N88—C102	1.346 (6)
C13—N7	1.505 (10)	N88—C116	1.348 (10)
C13—C14	1.578 (12)	C89—N83	1.512 (10)
C13—C15	1.527 (10)	C89—C90	1.559 (12)
C13—H42	1.14 (4)	C89—C91	1.583 (10)
C14—C13	1.578 (12)	C89—H118	1.14 (3)
C14—C16	1.555 (10)	C90—C89	1.559 (12)
C14—H43	1.14 (6)	C90—C92	1.530 (8)
C14—H44	1.08 (6)	C90—H119	1.14 (4)

C15—N6	1.496 (9)	C90—H120	1.14 (6)
C15—C13	1.527 (10)	C91—N82	1.492 (9)
C15—H45	1.14 (6)	C91—C89	1.583 (10)
C15—H46	1.14 (4)	C91—H121	1.14 (6)
C16—N6	1.494 (8)	C91—H122	1.14 (5)
C16—C14	1.555 (10)	C92—N82	1.463 (8)
C16—H47	1.14 (5)	C92—C90	1.530 (8)
C16—H48	1.15 (5)	C92—H123	1.14 (5)
C17—N6	1.463 (11)	C92—H124	1.14 (5)
C17—C20	1.407 (5)	C93—N82	1.468 (11)
C17—C21	1.428 (8)	C93—C96	1.410 (5)
C18—N7	1.52 (2)	C93—C97	1.397 (8)
C18—H49	1.14 (7)	C94—N83	1.479 (18)
C18—H50	1.14 (8)	C94—H125	1.14 (8)
C18—H51	1.14 (7)	C94—H126	1.14 (7)
C19—N7	1.38 (2)	C94—H127	1.14 (6)
C19—H52	1.14 (8)	C95—C41^{iii}	1.16 (7)
C19—H53	1.14 (6)	C95—H76^{iii}	0.89 (6)
C19—H54	1.14 (6)	C95—N83	1.465 (18)
C20—N8	1.467 (10)	C95—H128	1.14 (9)
C20—C17	1.407 (5)	C95—H129	1.14 (6)
C20—C22	1.407 (8)	C95—H130	1.14 (6)
C21—C17	1.428 (8)	C96—N84	1.430 (9)
C21—C23	1.420 (9)	C96—C93	1.410 (5)
C21—H55	1.14 (3)	C96—C98	1.408 (8)
C22—C20	1.407 (8)	C97—C93	1.397 (8)
C22—C24	1.398 (10)	C97—C99	1.402 (8)
C22—H56	1.14 (3)	C97—H131	1.14 (3)
C23—O3	1.395 (8)	C98—C96	1.408 (8)
C23—C21	1.420 (9)	C98—C100	1.397 (8)
C23—C24	1.413 (9)	C98—H132	1.14 (3)
C24—N9	1.482 (13)	C99—O79	1.405 (8)
C24—C22	1.398 (10)	C99—C97	1.402 (8)
C24—C23	1.413 (9)	C99—C100	1.401 (9)
C25—O4	1.263 (10)	C100—N85	1.426 (13)
C25—N8	1.413 (8)	C100—C98	1.397 (8)
C25—C30	1.491 (7)	C100—C99	1.401 (9)
C26—N9	1.425 (11)	C101—O80	1.228 (10)
C26—N10	1.384 (11)	C101—N84	1.331 (8)
C26—N12	1.347 (6)	C101—C106	1.473 (7)
C27—O5	1.424 (7)	C102—N85	1.401 (11)
C27—C29	1.529 (4)	C102—N86	1.380 (11)
C27—C32	1.524 (6)	C102—N88	1.346 (6)
C27—C33	1.524 (6)	C103—O81	1.439 (8)
C28—O3	1.423 (14)	C103—C105	1.548 (5)
C28—H59	1.14 (9)	C103—C108	1.528 (7)
C28—H60	1.14 (8)	C103—C109	1.525 (7)
C28—H61	1.14 (4)	C104—O79	1.481 (14)

C29—C27	1.529 (4)	C104—H135	1.14 (6)
C29—C31	1.402 (5)	C104—H136	1.14 (8)
C29—C35	1.395 (7)	C104—H137	1.14 (10)
C30—C25	1.491 (7)	C105—C103	1.548 (5)
C30—C41	1.41 (3)	C105—C107	1.411 (5)
C30—H62	1.14 (3)	C105—C111	1.436 (17)
C31—N11	1.397 (13)	C106—C101	1.473 (7)
C31—C29	1.402 (5)	C106—C117	1.26 (2)
C31—C36	1.416 (8)	C106—H138	1.14 (4)
C32—C27	1.524 (6)	C107—N87	1.458 (13)
C32—H63	1.14 (5)	C107—C105	1.411 (5)
C32—H64	1.14 (7)	C107—C112	1.401 (8)
C32—H65	1.14 (7)	C108—C103	1.528 (7)
C33—C27	1.524 (6)	C108—H139^{iv}	1.13 (6)
C33—H66	1.14 (3)	C108—H140^{iv}	1.14 (6)
C33—H67	1.14 (8)	C108—H141^{iv}	1.15 (7)
C33—H68	1.14 (6)	C109—C103	1.525 (7)
C34—N10	1.354 (13)	C109—H142^{iv}	1.14 (6)
C34—N11	1.390 (9)	C109—H143^{iv}	1.14 (6)
C34—C38	1.391 (10)	C109—H144^{iv}	1.14 (6)
C35—C29	1.395 (7)	C110—N86	1.369 (9)
C35—C37	1.399 (9)	C110—N87	1.415 (9)
C35—H69	1.14 (2)	C110—C114	1.400 (10)
C36—C31	1.416 (8)	C111—C105	1.436 (17)
C36—C39	1.408 (10)	C111—C113	1.391 (14)
C36—H71	1.14 (2)	C111—H145	1.14 (3)
C37—F2	1.392 (17)	C112—C107	1.401 (8)
C37—C35	1.399 (9)	C112—C115	1.384 (8)
C37—C39	1.406 (8)	C112—H147	1.14 (3)
C38—C34	1.391 (10)	C113—F78	1.370 (18)
C38—C40	1.387 (9)	C113—C111	1.391 (14)
C38—H73	1.14 (3)	C113—C115	1.387 (8)
C39—Cl1	1.793 (11)	C114—C110	1.400 (10)
C39—C36	1.408 (10)	C114—C116	1.391 (9)
C39—C37	1.406 (8)	C114—H149	1.13 (3)
C40—N12	1.334 (10)	C115—Cl77	1.791 (11)
C40—C38	1.387 (9)	C115—C112	1.384 (8)
C40—H74	1.14 (2)	C115—C113	1.387 (8)
C41—C30	1.41 (3)	C116—N88	1.348 (10)
C41—H75	1.14 (6)	C116—C114	1.391 (9)
C41—H76	1.14 (5)	C116—H150	1.13 (3)
C41—C95^{i}	1.16 (7)	C117—C106	1.26 (2)
C41—H130^{i}	0.53 (10)	C117—H151	1.14 (8)
H42—C13	1.14 (4)	C117—H152	1.14 (5)
H43—C14	1.14 (6)	H118—C89	1.14 (3)
H44—C14	1.08 (6)	H119—C90	1.14 (4)
H45—C15	1.14 (6)	H120—C90	1.14 (6)
H46—C15	1.14 (4)	H121—C91	1.14 (6)

H47—C16	1.14 (5)	H122—C91	1.14 (5)
H48—C16	1.15 (5)	H123—C92	1.14 (5)
H49—C18	1.14 (7)	H124—C92	1.14 (5)
H50—C18	1.14 (8)	H125—C94	1.14 (8)
H51—C18	1.14 (7)	H126—C94	1.14 (7)
H52—C19	1.14 (8)	H127—C94	1.14 (6)
H53—C19	1.14 (6)	H128—C95	1.14 (9)
H54—C19	1.14 (6)	H129—C95	1.14 (6)
H55—C21	1.14 (3)	H130—C41^{iii}	0.53 (10)
H56—C22	1.14 (3)	H130—C95	1.14 (6)
H57—N8	1.11 (3)	H131—C97	1.14 (3)
H58—N9	1.11 (3)	H132—C98	1.14 (3)
H59—C28	1.14 (9)	H133—N84	1.11 (3)
H60—C28	1.14 (8)	H134—N85	1.11 (3)
H61—C28	1.14 (4)	H135—C104	1.14 (6)
H62—C30	1.14 (3)	H136—C104	1.14 (8)
H63—C32	1.14 (5)	H137—H73^{v}	0.523
H64—C32	1.14 (7)	H137—C104	1.14 (10)
H65—C32	1.14 (7)	H138—C106	1.14 (4)
H66—C33	1.14 (3)	H139—C108^{iv}	1.13 (6)
H67—C33	1.14 (8)	H140—C108^{iv}	1.14 (6)
H68—C33	1.14 (6)	H141—C108^{iv}	1.15 (7)
H69—C35	1.14 (2)	H142—C109^{iv}	1.14 (6)
H70—N11	1.11 (3)	H143—C109^{iv}	1.14 (6)
H71—C36	1.14 (2)	H144—C109^{iv}	1.14 (6)
H72—O5	1.11 (5)	H145—C111	1.14 (3)
H73—C38	1.14 (3)	H146—N87	1.11 (3)
H73—H137^{ii}	0.523	H147—C112	1.14 (3)
H74—C40	1.14 (2)	H148—O81	1.09 (5)
H75—C41	1.14 (6)	H149—C114	1.13 (3)
H76—C41	1.14 (5)	H150—C116	1.13 (3)
H76—N83^{i}	1.30 (4)	H151—C117	1.14 (8)
H76—C95^{i}	0.89 (6)	H152—C117	1.14 (5)

C23—O3—C28	118.9 (7)	C91—N82—C92	109.1 (8)
C27—O5—H72	110 (3)	C91—N82—C93	129.7 (12)
C15—N6—C16	110.7 (8)	C92—N82—C93	120.7 (11)
C15—N6—C17	117.2 (11)	H76^{iii}—N83—C89	84.9 (19)
C16—N6—C17	127.7 (13)	H76^{iii}—N83—C94	140 (4)
C13—N7—C18	113.0 (10)	C89—N83—C94	108.4 (10)
C13—N7—C19	110.3 (10)	H76^{iii}—N83—C95	37 (2)
C18—N7—C19	103.9 (15)	C89—N83—C95	115.8 (10)
C20—N8—C25	134.2 (10)	C94—N83—C95	107.7 (15)
C20—N8—H57	120 (2)	C96—N84—C101	122.8 (9)
C25—N8—H57	105.9 (18)	C96—N84—H133	120 (2)
C24—N9—C26	137.8 (14)	C101—N84—H133	117 (2)
C24—N9—H58	120 (2)	C100—N85—C102	129.7 (14)
C26—N9—H58	103 (2)	C100—N85—H134	120 (3)

C26—N10—C34	115.4 (5)	C102—N85—H134	110 (3)
C31—N11—C34	125.5 (14)	C102—N86—C110	116.1 (4)
C31—N11—H70	120 (2)	C107—N87—C110	128.0 (15)
C34—N11—H70	115 (2)	C107—N87—H146	120 (2)
C26—N12—C40	116.0 (5)	C110—N87—H146	112 (3)
N7—C13—C15	110.5 (13)	C102—N88—C116	115.7 (4)
N7—C13—H42	107 (2)	N83—C89—C90	109.5 (11)
C15—C13—H42	107 (3)	N83—C89—H118	108 (2)
C16—C14—H43	112 (5)	C90—C89—H118	108 (4)
C16—C14—H44	104 (4)	C89—C90—C92	102.3 (9)
H43—C14—H44	120 (2)	C89—C90—H119	111 (4)
N6—C15—C13	103.5 (7)	C92—C90—H119	111 (3)
N6—C15—H45	109 (3)	C89—C90—H120	109 (3)
C13—C15—H45	112 (3)	C92—C90—H120	113 (3)
N6—C15—H46	111 (3)	H119—C90—H120	111 (3)
C13—C15—H46	110 (4)	N82—C91—H121	110 (4)
H45—C15—H46	110 (3)	N82—C91—H122	111 (3)
N6—C16—C14	104.1 (4)	H121—C91—H122	110 (3)
N6—C16—H47	111 (3)	N82—C92—C90	103.2 (4)
C14—C16—H47	110 (4)	N82—C92—H123	110 (3)
N6—C16—H48	109 (3)	C90—C92—H123	111 (3)
C14—C16—H48	112 (4)	N82—C92—H124	109 (4)
H47—C16—H48	110 (2)	C90—C92—H124	113 (3)
N6—C17—C20	115.6 (6)	H123—C92—H124	111 (2)
N6—C17—C21	124.6 (6)	N82—C93—C96	120.5 (7)
C20—C17—C21	119.8 (5)	N82—C93—C97	120.9 (7)
N7—C18—H49	109 (6)	C96—C93—C97	118.3 (5)
N7—C18—H50	109 (4)	N83—C94—H125	109 (5)
H49—C18—H50	109 (3)	N83—C94—H126	110 (5)
N7—C18—H51	110 (2)	H125—C94—H126	110 (4)
H49—C18—H51	110 (6)	N83—C94—H127	109 (3)
H50—C18—H51	110 (7)	H125—C94—H127	109 (6)
N7—C19—H52	110 (6)	H126—C94—H127	110 (5)
N7—C19—H53	110 (4)	C41^{iii}—C95—H76^{iii}	66 (5)
H52—C19—H53	109 (4)	C41^{iii}—C95—N83	120 (4)
N7—C19—H54	110 (3)	H76^{iii}—C95—N83	61 (3)
H52—C19—H54	109 (5)	C41^{iii}—C95—H128	83 (8)
H53—C19—H54	109 (6)	H76^{iii}—C95—H128	129 (8)
N8—C20—C17	118.1 (7)	N83—C95—H128	109 (4)
N8—C20—C22	123.4 (9)	C41^{iii}—C95—H129	122 (7)
C17—C20—C22	118.2 (5)	H76^{iii}—C95—H129	121 (9)
C17—C21—C23	119.5 (10)	N83—C95—H129	110 (5)
C17—C21—H55	119.8 (15)	H128—C95—H129	109 (4)
C23—C21—H55	120.8 (16)	C41^{iii}—C95—H130	27 (5)
C20—C22—C24	122.7 (7)	H76^{iii}—C95—H130	49 (3)
C20—C22—H56	120.0 (18)	N83—C95—H130	110 (3)
C24—C22—H56	117.3 (17)	H128—C95—H130	109 (6)
O3—C23—C21	125.4 (6)	H129—C95—H130	110 (6)

O3—C23—C24	114.4 (6)	N84—C96—C93	120.5 (8)
C21—C23—C24	120.2 (5)	N84—C96—C98	120.1 (9)
N9—C24—C22	123.7 (10)	C93—C96—C98	119.3 (5)
N9—C24—C23	118.1 (8)	C93—C97—C99	121.9 (6)
C22—C24—C23	118.1 (6)	C93—C97—H131	120.0 (18)
O4—C25—N8	123.8 (6)	C99—C97—H131	118.1 (18)
O4—C25—C30	120.4 (7)	C96—C98—C100	122.1 (6)
N8—C25—C30	114.5 (3)	C96—C98—H132	120.0 (18)
N9—C26—N10	118.4 (14)	C100—C98—H132	117.9 (18)
N9—C26—N12	111.0 (12)	O79—C99—C97	124.6 (6)
N10—C26—N12	125.6 (4)	O79—C99—C100	115.5 (5)
O5—C27—C29	102.2 (8)	C97—C99—C100	119.9 (4)
O5—C27—C32	110.5 (9)	N85—C100—C98	122.6 (9)
C29—C27—C32	110.9 (7)	N85—C100—C99	119.1 (8)
O5—C27—C33	109.2 (9)	C98—C100—C99	118.2 (5)
C29—C27—C33	112.9 (7)	O80—C101—N84	122.2 (6)
C32—C27—C33	110.7 (6)	O80—C101—C106	123.7 (7)
O3—C28—H59	109 (6)	N84—C101—C106	113.6 (4)
O3—C28—H60	110 (6)	N85—C102—N86	119.9 (12)
H59—C28—H60	109 (4)	N85—C102—N88	112.7 (12)
O3—C28—H61	110 (3)	N86—C102—N88	125.8 (4)
H59—C28—H61	109 (6)	O81—C103—C105	111.9 (8)
H60—C28—H61	110 (6)	O81—C103—C108	104.8 (9)
C27—C29—C31	120.9 (7)	C105—C103—C108	112.2 (7)
C27—C29—C35	119.2 (7)	O81—C103—C109	104.7 (9)
C31—C29—C35	119.7 (5)	C105—C103—C109	112.7 (7)
C25—C30—C41	121.7 (8)	C108—C103—C109	110.1 (6)
C25—C30—H62	120 (2)	O79—C104—H135	109 (5)
C41—C30—H62	118 (2)	O79—C104—H136	109 (4)
N11—C31—C29	119.3 (6)	H135—C104—H136	110 (7)
N11—C31—C36	120.0 (9)	O79—C104—H137	109 (7)
C29—C31—C36	120.1 (5)	H135—C104—H137	110 (5)
C27—C32—H63	110 (3)	H136—C104—H137	109 (5)
C27—C32—H64	110 (4)	C103—C105—C107	125.1 (7)
H63—C32—H64	109 (5)	C103—C105—C111	116.2 (10)
C27—C32—H65	110 (4)	C107—C105—C111	117.0 (8)
H63—C32—H65	109 (6)	C101—C106—C117	122.2 (6)
H64—C32—H65	109 (3)	C101—C106—H138	120 (4)
C27—C33—H66	109 (3)	C117—C106—H138	118 (4)
C27—C33—H67	109 (3)	N87—C107—C105	121.7 (6)
H66—C33—H67	110 (5)	N87—C107—C112	117.6 (8)
C27—C33—H68	109 (4)	C105—C107—C112	120.4 (5)
H66—C33—H68	109 (5)	C103—C108—H139^{iv}	110 (3)
H67—C33—H68	110 (3)	C103—C108—H140^{iv}	110 (3)
N10—C34—N11	122.9 (15)	H139^{iv}—C108—H140^{iv}	110 (5)
N10—C34—C38	122.6 (7)	C103—C108—H141^{iv}	109 (4)
N11—C34—C38	114.1 (11)	H139^{iv}—C108—H141^{iv}	109 (4)
C29—C35—C37	118.9 (8)	H140^{iv}—C108—H141^{iv}	109 (4)

C29—C35—H69	119.8 (16)	C103—C109—H142^{iv}	109 (3)
C37—C35—H69	121.3 (16)	C103—C109—H143^{iv}	110 (4)
C31—C36—C39	119.1 (9)	H142^{iv}—C109—H143^{iv}	109 (4)
C31—C36—H71	120.0 (15)	C103—C109—H144^{iv}	110 (3)
C39—C36—H71	120.9 (14)	H142^{iv}—C109—H144^{iv}	109 (5)
F2—C37—C35	118.8 (10)	H143^{iv}—C109—H144^{iv}	109 (4)
F2—C37—C39	119.3 (7)	N86—C110—N87	119.5 (12)
C35—C37—C39	121.7 (5)	N86—C110—C114	121.9 (5)
C34—C38—C40	116.4 (3)	N87—C110—C114	117.9 (14)
C34—C38—H73	120 (2)	C105—C111—C113	120.1 (11)
C40—C38—H73	123 (2)	C105—C111—H145	120.2 (16)
Cl1—C39—C36	120.1 (6)	C113—C111—H145	119.8 (17)
Cl1—C39—C37	121.1 (6)	C107—C112—C115	121.2 (5)
C36—C39—C37	118.8 (5)	C107—C112—H147	120.1 (13)
N12—C40—C38	123.8 (6)	C115—C112—H147	118.7 (13)
N12—C40—H74	120 (3)	F78—C113—C111	119.7 (9)
C38—C40—H74	116 (3)	F78—C113—C115	119.1 (6)
C30—C41—H75	120 (4)	C111—C113—C115	120.2 (8)
C30—C41—H76	120 (4)	C110—C114—C116	116.3 (3)
H75—C41—H76	120 (4)	C110—C114—H149	120 (3)
C30—C41—C95^{i}	164 (4)	C116—C114—H149	123 (3)
H75—C41—C95^{i}	75 (4)	Cl77—C115—C112	118.4 (8)
H76—C41—C95^{i}	45 (4)	Cl77—C115—C113	122.0 (6)
C30—C41—H130^{i}	100 (7)	C112—C115—C113	119.0 (6)
H75—C41—H130^{i}	121 (10)	N88—C116—C114	124.2 (4)
H76—C41—H130^{i}	46 (3)	N88—C116—H150	120 (3)
C95^{i}—C41—H130^{i}	74 (7)	C114—C116—H150	115 (3)
C38—H73—H137^{ii}	107.8 (17)	C106—C117—H151	120 (3)
C41—H76—N83^{i}	138 (5)	C106—C117—H152	120 (5)
C41—H76—C95^{i}	68 (5)	H151—C117—H152	120 (5)
N83^{i}—H76—C95^{i}	82 (3)	C41^{iii}—H130—C95	79 (5)
C99—O79—C104	120.3 (7)	H73^{v}—H137—C104	141 (2)
C103—O81—H148	112 (3)		

Symmetry codes: (i) *x*, *y*, *z*+1; (ii) *x*, *y*−1, *z*+1; (iii) *x*, *y*, *z*−1; (iv) −*x*+1, *y*, −*z*+1; (v) *x*, *y*+1, *z*−1.

(_I_VASP)

Crystal data

$C_{29}H_{35}ClFN_7O_3$
M_r = 584.09
Monoclinic, *C*2
a = 33.50300 Å
b = 10.22560 Å
c = 19.85680 Å
β = 117.25°
V = 6047.72 Å^3
Z = 8
T = 298 K

Data collection

h = →
k = →
l = →

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	B_{iso}*/B_{eq}
Cl1	0.59812	−0.58413	1.04564	
F2	0.67191	−0.45003	1.17408	
O3	0.48377	0.11957	0.91453	
O4	0.24456	−0.10020	0.64500	
O5	0.55683	−0.33363	1.30971	
N6	0.34915	0.24619	0.68556	
N7	0.25686	0.39103	0.53685	
N8	0.30706	0.02593	0.70343	
N9	0.44324	−0.08017	0.93775	
N10	0.47122	−0.21298	1.04107	
N11	0.50242	−0.34843	1.14852	
N12	0.39118	−0.17917	0.97070	
C13	0.29793	0.41198	0.60711	
C14	0.34032	0.40473	0.59514	
C15	0.30789	0.31617	0.67390	
C16	0.37561	0.33763	0.66573	
C17	0.37152	0.16903	0.75081	
C18	0.21686	0.43020	0.54248	
C19	0.25144	0.26033	0.50490	
C20	0.34924	0.06059	0.76289	
C21	0.41683	0.19026	0.80230	
C22	0.37171	−0.01886	0.82696	
C23	0.43926	0.10877	0.86452	
C24	0.41657	0.00336	0.87852	
C25	0.27296	−0.04877	0.70421	
C26	0.43381	−0.16071	0.98354	
C27	0.58156	−0.24716	1.28306	
C28	0.51074	0.20717	0.89716	
C29	0.58489	−0.31881	1.21824	
C30	0.27152	−0.05665	0.77750	
C31	0.54590	−0.36567	1.15499	
C32	0.55491	−0.12013	1.25828	
C33	0.62710	−0.21618	1.34960	
C34	0.46524	−0.29475	1.08812	
C35	0.62677	−0.34805	1.22221	
C36	0.55051	−0.44482	1.10127	
C37	0.63047	−0.42375	1.16747	
C38	0.42180	−0.32321	1.07900	
C39	0.59247	−0.47610	1.10733	
C40	0.38656	−0.26106	1.01980	
C41	0.24525	−0.14408	0.78792	
H42	0.29476	0.51106	0.62589	
H43	0.33326	0.34638	0.54452	
H44	0.35074	0.50212	0.58595	
H45	0.31333	0.36986	0.72572	

H46	0.27991	0.24813	0.66079
H47	0.40112	0.28441	0.65612
H48	0.39327	0.41025	0.71164
H49	0.20774	0.36284	0.57728
H50	0.18818	0.43304	0.48549
H51	0.22121	0.52838	0.56744
H52	0.24297	0.18481	0.53667
H53	0.28182	0.22898	0.50168
H54	0.22432	0.26225	0.44648
H55	0.43468	0.27194	0.79344
H56	0.35544	−0.10530	0.83494
H57	0.30306	0.04551	0.65014
H58	0.47590	−0.08894	0.94689
H59	0.54465	0.19813	0.94426
H60	0.49945	0.30937	0.89369
H61	0.51099	0.17942	0.84370
H62	0.29230	0.01186	0.82197
H63	0.55111	−0.07949	1.30615
H64	0.57357	−0.04974	1.24200
H65	0.52153	−0.13315	1.21031
H66	0.64678	−0.15019	1.33264
H67	0.64725	−0.30453	1.37436
H68	0.62151	−0.16672	1.39363
H69	0.65777	−0.31237	1.26876
H70	0.50014	−0.35770	1.19782
H71	0.52052	−0.48723	1.05572
H72	0.57605	−0.40921	1.33311
H73	0.41675	−0.39392	1.11529
H74	0.35208	−0.27899	1.00967
H75	0.22587	−0.21258	0.74259
H76	0.24209	−0.14828	0.84010
Cl77	0.55656	0.75824	0.74883
F78	0.55305	1.04286	0.75287
O79	0.44002	0.44922	0.20978
O80	0.33849	0.04332	0.32855
O81	0.42718	1.08565	0.42668
N82	0.32255	0.12378	0.08011
N83	0.22651	0.04533	−0.06503
N84	0.31064	0.10325	0.20321
N85	0.40961	0.48806	0.31334
N86	0.42039	0.65827	0.39359
N87	0.43505	0.83465	0.47409
N88	0.37256	0.47958	0.38964
C89	0.27285	0.07837	−0.04820
C90	0.30577	−0.03757	−0.01238
C91	0.29549	0.19141	0.00836
C92	0.34424	0.01576	0.06048
C93	0.34945	0.20495	0.14327

C94	0.21833	0.03461	0.00058
C95	0.19350	0.13005	−0.12233
C96	0.34142	0.19993	0.20704
C97	0.38290	0.28846	0.14539
C98	0.36108	0.29045	0.26621
C99	0.40504	0.37147	0.20649
C100	0.39139	0.38298	0.26411
C101	0.31233	0.02523	0.26036
C102	0.39973	0.54231	0.36764
C103	0.42947	1.11606	0.49959
C104	0.48330	0.40042	0.26343
C105	0.46308	1.02295	0.55845
C106	0.28043	−0.08639	0.23358
C107	0.46197	0.88571	0.54653
C108	0.44342	1.25966	0.51646
C109	0.38361	1.09639	0.49826
C110	0.41756	0.71057	0.45322
C111	0.49476	1.07227	0.62799
C112	0.49115	0.80379	0.60508
C113	0.52343	0.99041	0.68503
C114	0.39370	0.64537	0.48653
C115	0.52154	0.85585	0.67458
C116	0.36994	0.53492	0.44917
C117	0.28665	−0.19255	0.27662
H118	0.27110	0.10482	−0.10314
H119	0.28806	−0.11692	0.00022
H120	0.31819	−0.07668	−0.05072
H121	0.27180	0.25913	0.01425
H122	0.31669	0.24965	−0.01024
H123	0.35842	−0.05560	0.10698
H124	0.37214	0.05112	0.04970
H125	0.22127	0.12902	0.03036
H126	0.18415	−0.00282	−0.01754
H127	0.24198	−0.03487	0.04180
H128	0.15958	0.09392	−0.13702
H129	0.19531	0.23381	−0.10403
H130	0.19781	0.12847	−0.17396
H131	0.39247	0.28871	0.09974
H132	0.35212	0.29403	0.31223
H133	0.29431	0.06747	0.14871
H134	0.42803	0.55061	0.29840
H135	0.48711	0.40248	0.32163
H136	0.50846	0.46489	0.26003
H137	0.48795	0.29953	0.24894
H138	0.25225	−0.08029	0.17660
H139	0.47778	1.27479	0.52453
H140	0.44124	1.29561	0.56696
H141	0.42031	1.31793	0.46796

H142	0.35855	1.16325	0.45728
H143	0.37165	0.99595	0.48169
H144	0.38641	1.11568	0.55474
H145	0.49788	1.17687	0.63882
H146	0.43381	0.89455	0.43169
H147	0.49126	0.69904	0.59557
H148	0.39525	1.08678	0.38790
H149	0.39087	0.68730	0.53448
H150	0.34669	0.48739	0.46602
H151	0.26401	−0.27621	0.25675
H152	0.31520	−0.19854	0.33299

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N9—H58···N10^{i}	1.03	2.10	3.022	148
N11—H70···O5	1.02	2.18	2.872	124
N11—H70···Cl77^{ii}	1.02	2.82	3.597	133
N85—H134···Cl77^{iii}	1.02	2.47	3.424	155
N87—H146···O81	1.03	1.96	2.705	127
O81—H148···O80^{iv}	0.99	1.77	2.740	164
C38—H73···O79^{v}	1.09	2.32	3.329	154
C90—H120···N12^{vi}	1.10	2.51	3.358	133
C104—H136···O5^{vii}	1.10	2.53	3.498	147
C108—H141···N88^{iv}	1.10	2.33	3.400	165

Symmetry codes: (i) −*x*+1, *y*, −*z*+2; (ii) −*x*+1, *y*−1, −*z*+2; (iii) −*x*+1, *y*, −*z*+1; (iv) *x*, *y*+1, *z*; (v) *x*, *y*−1, *z*+1; (vi) *x*, *y*, *z*−1; (vii) *x*, *y*+1, *z*−1.