Supporting information

Crystal structure and Hirshfeld surface analysis of pinaverium bromide dihydrate

Dezhen Chen1, Wangting Zhou1, Yujing Wei1, Chenghan Zhuang2, Yazheng He2, Xiaoli Li2, Kaibo Li2, Zhaoxia Zhang1\*, Guoqing Zhang1\*

*1 School of Materials Science and Engineering, Zhejiang Sci-Tech University, Hangzhou 310018, People’s Republic of China*

*2 Zhejiang Apeloa Jiayuan Pharmaceutical Co., Ltd., Dongyang, 322118, People’s Republic of China*

\*Corresponding author: Zhaoxia Zhang, E-mail: zhangzx@zstu.edu.cn; Guoqing Zhang, E-mail: [zgq@zstu.edu.cn](mailto:zgq@zstu.edu.cn).

Computing details

Data collection: *APEX2* (Bruker, 2016); Cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2013); Program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov et al., 2009); software used to prepare material for publication: *OLEX2*(Dolomanov et al., 2009).

Table Ⅰ. 4-[(2-bromo-4,5-dimethoxyphenyl)methyl]-4-[2-[2-(6,6-dimethylbicyclo[3,1,1]-hept-2-yl)ethoxy]ethyl]morpholinium bromide dihydrate.

|  |  |
| --- | --- |
| **Crystal data** |  |
| C26H41Br2NO4·2H2O | Z = 2 |
| *M*r = 627.45 | F(000) = 652 |
| Triclinic, *P* | *D*x = 1.391 g/m-3 |
| *a* = 7.3128(4) Å | Mo *Kα* radiation, *λ* = 0.71073 Å |
| *b* = 13.5547(7) Å | Cell parameters from 9545 reflections |
| *c* = 15.4049(8) Å | *θ* = 4.334­º―54.282º |
| *α* = 81.568(2) º | *µ* =2.75 mm−1 |
| *β* = 82.425(2) º | *T* = 296.15 K |
| *γ* = 85.881(2) º | Block, colourless |
| *V* = 1495.14(14) | 0.15 × 0.05 × 0.03 mm3 |
|  |  |
| **Data collection** |  |
| Bruker APEXⅡ CCD | 6610 independent reflections |
| diffractometer | 5072 reflections with *I* > 2*σ(I)* |
| φ and ω scans | *R*int = 0.0408 |
| Absorption correction: multi-scan | *θ*max = 25.12º, *θ*min = 2.69º |
| (SADABS; Bruker, 2016) | *h* = - 9 → 9 |
| *T*min = 0.607, *T*max = 0.746 | *k* = - 17 → 17 |
| 65718 measured reflections | *l* = - 19 → 19 |
|  |  |
| **Refinement** |  |
| Refinement on *F2* | Hydrogen site location: mixed |
| Least-squares matrix: full | H atoms treated by a mixture of independent |
| *R*[*F2* > 2*σ*(*F2*)] = 0.0596 | and constrained refinement |
| *wR*(*F2*) = 0.1997 | *w* = 1/[*σ2*(*Fo2*) + (0.1092*P*)2 + 1.3109*P*] |
| *S* = 1.054 | where *P* = (*Fo*2 + 2*Fc*2)/3 |
| 6610 reflections | (Δ/*σ*)max = 0.001 |
| 340 parameters | Δ*ρ*max = 0.64 e Å-3 |
| 125 restraints | Δ*ρ*min = - 0.62 e Å-3 |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | *x* | *y* | *z* | *U*iso\*/*U*eq |
| Br1 | 1.1201 (9) | 0.5513 (4) | 0.8423 (3) | 0.0895 (2) |
| O1 | 1.2723 (5) | 0.3303 (2) | 0.5876 (2) | 0.0744 (8) |
| O2 | 1.2761 (4) | 0.4790 (2) | 0.4636 (2) | 0.0663 (7) |
| O3 | 0.5037 (4) | 0.7053 (3) | 0.6766 (3) | 0.0851 (10) |
| N1 | 0.8821 (4) | 0.7578 (2) | 0.6755 (2) | 0.0484 (6) |
| C1 | 1.1444 (6) | 0.5342 (3) | 0.7207 (3) | 0.0593 (9) |
| C2 | 1.1888 (6) | 0.4374 (3) | 0.7020 (3) | 0.0616 (10) |
| H2 | 1.1925 | 0.3844 | 0.7475 | 0.074\* |
| C3 | 1.2274 (5) | 0.4209 (3) | 0.6147 (3) | 0.0590 (9) |
| C4 | 1.2253 (5) | 0.5018 (3) | 0.5465 (3) | 0.0540 (8) |
| C5 | 1.1727 (5) | 0.5955 (3) | 0.5672 (3) | 0.0522 (8) |
| H5 | 1.1657 | 0.6483 | 0.5216 | 0.063\* |
| C6 | 1.1290 (5) | 0.6145 (3) | 0.6550 (3) | 0.0511 (8) |
| C7 | 1.2781 (9) | 0.2444 (3) | 0.6523 (4) | 0.0900 (16) |
| H7A | 1.3130 | 0.1864 | 0.6236 | 0.135\* |
| H7B | 1.1583 | 0.2368 | 0.6857 | 0.135\* |
| H7C | 1.3668 | 0.2518 | 0.6912 | 0.135\* |
| C8 | 1.2877 (7) | 0.5586 (4) | 0.3921 (3) | 0.0759 (12) |
| H8A | 1.3284 | 0.5324 | 0.3378 | 0.114\* |
| H8B | 1.3741 | 0.6049 | 0.4015 | 0.114\* |
| H8C | 1.1683 | 0.5924 | 0.3887 | 0.114\* |
| C9 | 1.0861 (5) | 0.7205 (3) | 0.6716 (3) | 0.0520 (8) |
| H9A | 1.1567 | 0.7636 | 0.6252 | 0.062\* |
| H9B | 1.1290 | 0.7280 | 0.7271 | 0.062\* |
| C10 | 0.8020 (5) | 0.7388 (3) | 0.5941 (3) | 0.0541 (8) |
| H10A | 0.8605 | 0.7802 | 0.5426 | 0.065\* |
| H10B | 0.8287 | 0.6695 | 0.5856 | 0.065\* |
| C11 | 0.5955 (6) | 0.7612 (4) | 0.6019 (3) | 0.0720 (12) |
| H11A | 0.5693 | 0.8318 | 0.6054 | 0.086\* |
| H11B | 0.5492 | 0.7463 | 0.5493 | 0.086\* |
| C12 | 0.5652 (6) | 0.7292 (5) | 0.7541 (4) | 0.0840 (14) |
| H12A | 0.4974 | 0.6925 | 0.8057 | 0.101\* |
| H12B | 0.5400 | 0.8000 | 0.7572 | 0.101\* |
| C13 | 0.7693 (6) | 0.7041 (3) | 0.7550 (3) | 0.0648 (10) |
| H13A | 0.8071 | 0.7222 | 0.8083 | 0.078\* |
| H13B | 0.7930 | 0.6326 | 0.7560 | 0.078\* |
| C14 | 0.8753 (6) | 0.8705 (3) | 0.6771 (3) | 0.0582 (9) |
| H14A | 0.7487 | 0.8923 | 0.6957 | 0.070\* |
| H14B | 0.9079 | 0.9029 | 0.6172 | 0.070\* |
| H14C | 0.9780 | 0.8977 | 0.6365 | 0.070\* |
| H14D | 0.7627 | 0.8993 | 0.6545 | 0.070\* |
| C16 | 1.0788 (14) | 0.8968 (7) | 0.8784 (5) | 0.137 (3) |
| H16A | 1.1970 | 0.9146 | 0.8455 | 0.165\* |
| H16B | 1.0172 | 0.9570 | 0.8976 | 0.165\* |
| H16C | 1.1861 | 0.9370 | 0.8651 | 0.165\* |
| H16D | 0.9759 | 0.9410 | 0.8974 | 0.165\* |
| C17 | 1.1090 (20) | 0.8311 (11) | 0.9501 (10) | 0.238 (5) |
| H17A | 1.1757 | 0.7742 | 0.9270 | 0.285\* |
| H17B | 0.9877 | 0.8085 | 0.9752 | 0.285\* |
| C18 | 1.1975 (18) | 0.8454 (10) | 1.0240 (7) | 0.195 (4) |
| H18 | 1.1925 | 0.9170 | 1.0281 | 0.234\* |
| C19 | 1.4011 (19) | 0.8071 (10) | 1.0124 (9) | 0.224 (4) |
| H19 | 1.4758 | 0.8279 | 0.9559 | 0.269\* |
| C20 | 1.4279 (17) | 0.6963 (10) | 1.0570 (9) | 0.207 (3) |
| C21 | 1.4130 (20) | 0.7290 (12) | 1.1436 (9) | 0.233 (4) |
| H21 | 1.4943 | 0.6925 | 1.1845 | 0.279\* |
| C22 | 1.2140 (20) | 0.7418 (15) | 1.1803 (9) | 0.260 (5) |
| H22A | 1.1651 | 0.6771 | 1.2028 | 0.312\* |
| H22B | 1.2025 | 0.7812 | 1.2287 | 0.312\* |
| C23 | 1.1140 (20) | 0.7904 (13) | 1.1127 (9) | 0.259 (5) |
| H23A | 1.0288 | 0.8387 | 1.1397 | 0.310\* |
| H23B | 1.0385 | 0.7404 | 1.0984 | 0.310\* |
| C24 | 1.4690 (20) | 0.8348 (12) | 1.1024 (10) | 0.239 (4) |
| H24A | 1.6004 | 0.8446 | 1.0980 | 0.286\* |
| H24B | 1.3959 | 0.8884 | 1.1279 | 0.286\* |
| C25 | 1.3250 (30) | 0.6118 (11) | 1.0437 (14) | 0.308 (7) |
| H25A | 1.3504 | 0.6005 | 0.9831 | 0.462\* |
| H25B | 1.3618 | 0.5531 | 1.0815 | 0.462\* |
| H25C | 1.1949 | 0.6267 | 1.0576 | 0.462\* |
| C26 | 1.6190 (20) | 0.6779 (14) | 1.0134 (14) | 0.307 (8) |
| H26A | 1.6135 | 0.6568 | 0.9570 | 0.461\* |
| H26B | 1.6837 | 0.7383 | 1.0052 | 0.461\* |
| H26C | 1.6823 | 0.6268 | 1.0499 | 0.461\* |
| O4 | 0.9730 (20) | 0.8609 (11) | 0.8224 (6) | 0.091 (4) |
| O4A | 1.0430 (30) | 0.8720 (20) | 0.7983 (15) | 0.107 (10) |
| C15 | 0.9994 (15) | 0.9078 (5) | 0.7365 (6) | 0.069 (3) |
| C15A | 0.8820 (30) | 0.9049 (10) | 0.7648 (10) | 0.068 (5) |
| H15A | 1.1276 | 0.8967 | 0.7127 | 0.083\* |
| H15B | 0.9750 | 0.9792 | 0.7361 | 0.083\* |
| H15C | 0.8710 | 0.9773 | 0.7579 | 0.082\* |
| H15D | 0.7782 | 0.8799 | 0.8061 | 0.082\* |
| Br2 | 1.1866 (7) | 0.8574 (3) | 0.4227 (4) | 0.0788 (2) |
| O5 | 1.4655 (6) | 1.0023 (3) | 0.6971 (4) | 0.1032 (13) |
| H5A | 1.5311 | 1.0448 | 0.7105 | 0.161\* |
| H5B | 1.3978 | 0.9965 | 0.6564 | 0.161\* |
| O6 | 1.2372 (6) | 1.0247 (3) | 0.5568 (3) | 0.1075 (13) |
| H6A | 1.1285 | 1.0515 | 0.5634 | 0.161\* |
| H6B | 1.2609 | 1.0084 | 0.5051 | 0.161\* |

Table Ⅲ. Atomic displacement parameters (Å2).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | U11 | U22 | U33 | U12 | U13 | U23 |
| Br1 | 0.1297 (5) | 0.0719 (3) | 0.0711 (3) | 0.0155 (3) | -0.0348 (3) | -0.0136 (2) |
| O1 | 0.089 (2) | 0.0437 (14) | 0.095 (2) | 0.0120 (13) | -0.0239 (17) | -0.0217 (14) |
| O2 | 0.0656 (17) | 0.0583 (16) | 0.0759 (18) | 0.0010 (13) | -0.0020 (14) | -0.0207 (14) |
| O3 | 0.0451 (15) | 0.107 (3) | 0.106 (3) | -0.0133 (16) | -0.0020 (16) | -0.024 (2) |
| N1 | 0.0417(14) | 0.0449 (14) | 0.0582 (16) | 0.0010 (11) | -0.0054 (12) | -0.085 (12) |
| C1 | 0.060(2) | 0.052 (2) | 0.070 (2) | 0.0050 (16) | -0.0231 (18) | -0.0103 (17) |
| C2 | 0.067(2) | 0.0469 (19) | 0.075 (3) | 0.0065 (17) | -0.026 (2) | -0.0081 (17) |
| C3 | 0.0510 (19) | 0.0438 (18) | 0.086 (3) | 0.0065 (14) | -0.0209 (18) | -0.0144 (18) |
| C4 | 0.0444 (17) | 0.0509 (19) | 0.070 (2) | 0.0014 (14) | -0.011.8 (16) | -0.0181 (17) |
| C5 | 0.0414 (16) | 0.0432 (17) | 0.072 (2) | 0.0024 (13) | -0.0099 (15) | -0.0070 (15) |
| C6 | 0.0430 (17) | 0.0426 (17) | 0.070 (2) | 0.0010 (13) | -0.0138 (15) | -0.0113 (15) |
| C7 | 0.122 (4) | 0.046 (2) | 0.108 (4) | 0.014 (2) | -0.038 (3) | -0.016 (2) |
| C8 | 0.069 (3) | 0.079 (3) | 0.079 (3) | -0.006 (2) | 0.002 (2) | -0.019 (2) |
| C9 | 0.0412 (16) | 0.0430 (17) | 0.075 (2) | 0.0033 (13) | -0.0142 (16) | -0.0139 (16) |
| C10 | 0.0414 (17) | 0.060 (2) | 0.065 (2) | 0.0017 (15) | -0.0109 (15) | -0.0196 (17) |
| C11 | 0.048 (2) | 0.088 (3) | 0.084 (3) | 0.009 (2) | -0.016 (2) | -0.024 (2) |
| C12 | 0.055 (2) | 0.098 (4) | 0.094 (4) | -0.004 (2) | 0.010 (2) | -0.013 (3) |
| C13 | 0.062 (2) | 0.063 (2) | 0.065 (2) | -0.0008 (18) | 0.0024 (19) | -0.0059 (18) |
| C14 | 0.060 (2) | 0.0410 (17) | 0.076 (2) | 0.0070 (15) | -0.0177 (18) | -0.0123 (16) |
| C16 | 0.177 (8) | 0.148 (7) | 0.107 (5) | -0.007 (6) | -0.057 (5) | -0.052 (4) |
| C17 | 0.318 (10) | 0.196 (10) | 0.232 (7) | 0.032 (9) | -0.201 (8) | -0.010 (6) |
| C18 | 0.253 (7) | 0.198 (8) | 0.152 (5) | 0.047 (6) | -0.111 (5) | -0.034 (5) |
| C19 | 0.223 (6) | 0.248 (7) | 0.200 (6) | 0.006 (7) | -0.106 (5) | 0.035 (6) |
| C20 | 0.160 (6) | 0.241 (7) | 0.222 (7) | 0.018 (6) | -0.110 (6) | 0.024 (6) |
| C21 | 0.217 (7) | 0.280 (9) | 0.189 (6) | -0.023 (9) | -0.066 (7) | 0.048 (6) |
| C22 | 0.222 (8) | 0.348 (13) | 0.188 (7) | -0.015 (9) | -0.059 (6) | 0.062 (7) |
| C23 | 0.247 (7) | 0.313 (13) | 0.208 (6) | 0.027 (10) | -0.082 (6) | 0.020 (9) |
| C24 | 0.225 (8) | 0.270 (8) | 0.230 (9) | -0.048 (9) | -0.111 (7) | 0.023 (7) |
| C25 | 0.291 (15) | 0.258 (10) | 0.390 (20) | -0.024 (11) | -0.142 (16) | -0.016 (12) |
| C26 | 0.264 (10) | 0.246 (15) | 0.368 (18) | 0.020 (8) | 0.042 (14) | 0.012 (15) |
| O4 | 0.124 (9) | 0.080 (5) | 0.077 (4) | -0.011 (6) | -0.039 (5) | -0.010 (4) |
| C15 | 0.082 (7) | 0.051 (3) | 0.079 (5) | 0.002 (3) | -0.019 (5) | -0.018 (3) |
| O4A | 0.129 (19) | 0.085 (15) | 0.122 (19) | 0.031 (14) | -0.057 (15) | -0.041 (15) |
| C15A | 0.063 (10) | 0.052 (7) | 0.093 (12) | 0.012 (6) | -0.013 (8) | -0.024 (7) |
| Br2 | 0.0777 (3) | 0.0618 (3) | 0.0940 (4) | -0.0037 (2) | -0.0062 (2) | -0.0051 (2) |
| O5 | 0.085 (3) | 0.078 (2) | 0.142 (4) | 0.0062 (19) | -0.024 (2) | 0.001 (2) |
| O6 | 0.104 (3) | 0.105 (3) | 0.124 (4) | -0.003 (2) | -0.034 (3) | -0.034 (3) |

Table Ⅳ. Geometric parameters (Å, º).

|  |  |  |  |
| --- | --- | --- | --- |
| Br1—C1 | 1.904 (4) | C15—H15C | 0.9700 |
| O1—C3 | 1.358 (4) | C15—H15D | 0.9700 |
| O1—C7 | 1.420 (6) | C16—H16C | 0.9700 |
| O2—C4 | 1.356 (5) | C16—O4A | 1.387 (15) |
| O2—C8 | 1.423 (6) | C16—H16D | 0.9700 |
| O3—C11 | 1.401 (6) | C16—H16A | 0.9700 |
| O3—C12 | 1.417 (7) | C16—H16B | 0.9700 |
| O4A—C15A | 1.369 (17) | C16—C17 | 1.344 (14) |
| N1—C9 | 1.537 (4) | C16—O4 | 1.392 (10) |
| N1—C10 | 1.514 (5) | C17—H17A | 0.9700 |
| N1—C13 | 1.506 (5) | C17—H17B | 0.9700 |
| N1—C14 | 1.528 (4) | C17—C18 | 1.425 (14) |
| C1—C2 | 1.392 (5) | C18—H18 | 0.9800 |
| C1—C6 | 1.382 (5) | C18—C19 | 1.537 (14) |
| C2—H2 | 0.9300 | C18—C23 | 1.531 (14) |
| C2—C3 | 1.384 (6) | C19—H19 | 0.9800 |
| C3—C4 | 1.403 (6) | C19—C20 | 1.568 (13) |
| C4—C5 | 1.372 (5) | C19—C24 | 1.636 (14) |
| C5—H5 | 0.9300 | C20—C21 | 1.455 (14) |
| C5—C6 | 1.405 (6) | C20—C25 | 1.468 (14) |
| C6—C9 | 1.500 (5) | C20—C26 | 1.488 (14) |
| C7—H7A | 0.9600 | C21—H21 | 0.9800 |
| C7—H7B | 0.9600 | C21—C22 | 1.498 (14) |
| C7—H7C | 0.9600 | C21—C24 | 1.542 (14) |
| C8—H8A | 0.9600 | C22—H22A | 0.9700 |
| C8—H8B | 0.9600 | C22—H22B | 0.9700 |
| C8—H8C | 0.9600 | C22—C23 | 1.409 (13) |
| C9—H9A | 0.9700 | C23—H23A | 0.9700 |
| C9—H9B | 0.9700 | C23—H23B | 0.9700 |
| C10—H10A | 0.9700 | C24—H24A | 0.9700 |
| C10—H10B | 0.9700 | C24—H24B | 0.9700 |
| C10—C11 | 1.511 (5) | C25—H25A | 0.9600 |
| C11—H11A | 0.9700 | C25—H25B | 0.9600 |
| C11—H11B | 0.9700 | C25—H25C | 0.9600 |
| C12—H12A | 0.9700 | C26—H26A | 0.9600 |
| C12—H12B | 0.9700 | C26—H26B | 0.9600 |
| C12—C13 | 1.509 (7) | C26—H26C | 0.9600 |
| C13—H12A | 0.9700 | O4—C15 | 1.376 (12) |
| C13—H12B | 0.9700 | C15—H15A | 0.9700 |
| C14—H14C | 0.9700 | C15—H15B | 0.9700 |
| C14—H14D | 0.9700 | O5—H5A | 0.8403 |
| C14—C15A | 1.499 (13) | O5—H5B | 0.8630 |
| C14—H14A | 0.9700 | O6—H6A | 0.8499 |
| C14—H14B | 0.9700 | C6—H6B | 0.8501 |
| C14—C15 | 1.529 (8) |  |  |
|  |  |  |  |
| C3—O1—C7 | 118.8 (4) | N1—C14—C15 | 116.7 (4) |
| O4A—C15A—H15D | 109.4 | C14—C15A—H15C | 109.4 |
| O4A—C15A—H15C | 109.4 | H14A—C14—H14B | 107.3 |
| C4—O2—C8 | 118.2 (3) | C15—C14—H14A | 108.1 |
| H15C—C15A—H15D | 108.0 | C14—C15A—H15D | 109.4 |
| C11—O3—C12 | 109.7 (4) | C15—C14—H14B | 108.1 |
| C10—N1—C9 | 110.6 (3) | H16A—C16—H16B | 107.7 |
| C10—N1—C14 | 108.5 (3) | C17—C16—H16C | 106.0 |
| O4A—C15A—C14 | 111.3 (13) | C17—C16—O4A | 125.3 (17) |
| C15A—O4A—C16 | 120.7 (17) | C17—C16—H16A | 108.8 |
| H14—C14—H14D | 107.3 | C17—C16—H16D | 106.0 |
| C13—N1—C9 | 110.8 (3) | C17—C16—H16B | 108.8 |
| C15A—C14—H14D | 108.0 | C17—C16—O4 | 113.7 (10) |
| C13—N1—C10 | 107.6 (3) | O4—C16—H16A | 108.8 |
| C13—N1—C14 | 112.2 (3) | O4—C16—H16B | 108.8 |
| C14—N1—C9 | 107.2 (3) | C16—C17—H17A | 105.1 |
| C2—C1—Br1 | 116.1 (3) | C16—C17—H17B | 105.1 |
| C15A—C14—H14C | 108.0 | C16—C17—C18 | 128.7 (13) |
| C15A—C14—N1 | 117.0 (6) | H17A—C17—H17B | 105.9 |
| O4A—C16—H16C | 106.0 | C18—C17—H17A | 105.1 |
| O4A—C16—H16D | 106.0 | C18—C17—H17B | 105.1 |
| C6—C1—Br1 | 121.6 (3) | C17—C18—H18 | 108.6 |
| H16C—C16—H16D | 106.3 | C17—C18—C19 | 110.8 (12) |
| C6—C1—C2 | 122.3 (4) | C17—C18—C23 | 114.7 (14) |
| C1—C2—H2 | 120.4 | C19—C18—H18 | 108.6 |
| C3—C2—C1 | 119.3 (4) | C23—C18—H18 | 108.6 |
| C3—C2—H2 | 120.4 | C23—C18—C19 | 105.5 (10) |
| O1—C3—C2 | 125.1 (4) | C18—C19—H19 | 118.0 |
| O1—C3—C4 | 115.1 (4) | C18—C19—C20 | 111.8 (11) |
| N1—C14—H14C | 108.0 | C18—C19—C24 | 100.7 (11) |
| N1—C14—H14D | 108.0 | C20—C19—H19 | 118.0 |
| C2—C3—C4 | 119.8 (3) | C20—C19—C24 | 84.3 (8) |
| O2—C4—C3 | 115.5 (3) | C24—C19—H19 | 118.0 |
| O2—C4—C5 | 125.2 (4) | C21—C20—C19 | 90.6 (10) |
| C5—C4—C3 | 119.3 (4) | C21—C20—C25 | 120.5 (14) |
| C4—C5—H5 | 118.9 | C21—C20—C26 | 116.0 (13) |
| C4—C5—C6 | 122.2 (4) | C25—C20—C19 | 126.0 (11) |
| C6—C5—H5 | 118.9 | C25—C20—C26 | 105.4 (15) |
| C1—C6—C5 | 116.9 (3) | C26—C20—C19 | 96.5 (12) |
| C1—C6—C9 | 124.4 (4) | C20—C21—H21 | 115.7 |
| C5—C6—C9 | 118.4 (3) | C20—C21—C22 | 110.1 (13) |
| O1—C7—H7A | 109.5 | C20—C21—C24 | 91.7 (10) |
| O1—C7—H7B | 109.5 | C22—C21—H21 | 115.7 |
| O1—C7—H7C | 109.5 | C22—C21—C24 | 105.0 (15) |
| H7A—C7—H7B | 109.5 | C24—C21—H21 | 115.7 |
| H7A—C7—H7C | 109.5 | C21—C22—H22A | 109.9 |
| H7B—C7—H7C | 109.5 | C21—C22—H22B | 109.9 |
| O2—C8—H8A | 109.5 | H22A—C22—H22B | 108.3 |
| O2—C8—H8B | 109.5 | C23—C22—C21 | 109.0 (12) |
| O2—C8—H8C | 109.5 | C23—C22—H22A | 109.9 |
| H8A—C8—H8B | 109.5 | C23—C22—H22B | 109.9 |
| H8A—C8—H8C | 109.5 | C18—C23—H23A | 105.9 |
| H8B—C8—H8C | 109.5 | C18—C23—H23B | 105.9 |
| N1—C9—H9A | 108.2 | C22—C23—C18 | 125.6 (13) |
| N1—C9—H9B | 108.2 | C22—C23—H23A | 105.9 |
| C6—C9—N1 | 116.4 (3) | C22—C23—H23B | 105.9 |
| C6—C9—H9A | 108.2 | H23A—C23—H23B | 106.2 |
| C6—C9—H9B | 108.2 | C19—C24—H24A | 114.5 |
| H9A—C9—H9B | 107.3 | C19—C24—H24B | 114.5 |
| N1—C10—H10A | 109.2 | C21—C24—C19 | 85.1 (9) |
| N1—C10—H10B | 109.2 | C21—C24—H24A | 114.5 |
| H10A—C10—H10B | 107.9 | C21—C24—H24B | 114.5 |
| C11—C10—N1 | 111.8 (3) | H24A—C24—H24B | 111.6 |
| C11—C10—H10A | 109.2 | C20—C25—H25A | 109.5 |
| C11—C10—H10B | 109.2 | C20—C25—H25B | 109.5 |
| O3—C11—C10 | 111.8 (4) | C20—C25—H25C | 109.5 |
| O3—C11—H11A | 109.3 | H25A—C25—H25B | 109.5 |
| O3—C11—H11B | 109.3 | H25A—C25—H25C | 109.5 |
| C10—C11—H11A | 109.3 | H25B—C25—H25C | 109.5 |
| C10—C11—H11B | 109.3 | C20—C26—H26A | 109.5 |
| H11A—C11—C11B | 107.9 | C20—C26—H26B | 109.5 |
| O3—C12—H12A | 109.4 | C20—C26—H26C | 109.5 |
| O3—C12—H12B | 109.4 | H26A—C26—H26B | 109.5 |
| O3—C12—C13 | 111.3 (4) | H26A—C26—H26C | 109.5 |
| H12A—C12—H12B | 108.0 | H26B—C26—H26C | 109.5 |
| C13—C12—H12A | 109.4 | C15—O4—C16 | 113.6 (9) |
| C13—C12—H12B | 109.4 | C14—C15—H15A | 109.1 |
| N1—C13—C12 | 111.9 (4) | C14—C15—H15B | 109.1 |
| N1—C13—H13A | 109.2 | O4—C15—C14 | 112.7 (7) |
| N1—C13—H13B | 109.2 | O4—C15—H15A | 109.1 |
| C12—C13—H13A | 109.2 | O4—C15—H15B | 109.1 |
| C12—C13—H13B | 109.2 | H15A—C15—H15B | 107.8 |
| H13A—C13—H13B | 107.9 | H5A—O5—H5B | 138.7 |
| N1—C14—H14A | 108.1 | H6A—O6—H6B | 109.5 |
| N1—C14—H14B | 108.1 |  |  |
|  |  |  |  |
| Br1—C1—C2—C3 | -173.4 (3) | C13—N1—C14—C15 | 79.2 (6) |
| Br1—C1—C6—C5 | 172.0 (3) | C13—N1—C14—C15A | 39.8 (9) |
| Br1—C1—C6—C9 | -2.2 (5) | C14—N1—C9—C6 | -170.7 (3) |
| O1—C3—C4—O2 | -2.8 (5) | C14—N1—C10—C11 | -70.7 (4) |
| O1—C3—C4—C5 | 176.8 (3) | C14—N1—C13—C12 | 67.8 (5) |
| O2—C4—C5—C6 | -177.3 (3) | C16—C17—C18—C19 | -97.0 (2) |
| O3—C12—C13—N1 | 58.2 (6) | C16—C17—C18—C23 | 143.9 (17) |
| N1—C10—C11—O3 | -57.4 (5) | C16—O4—C15—C14 | -177.4 (9) |
| N1—C14—C15—O4 | -53.7 (14) | C16—O4A—C15A—C14 | 179.0 (2) |
| N1—C14—C15A—O4A | 62.0 (3) | C17—C16—O4—C15 | -156.4 (15) |
| C1—C2—C3—O1 | -179.9 (4) | C17—C16—O4A—C15A | 120.0 (3) |
| C1—C2—C3—C4 | 1.4 (6) | C17—C18—C19—C20 | -93.4 (13) |
| C1—C6—C9—N1 | -95.0 (4) | C17—C18—C19—C24 | 178.5 (12) |
| C2—C1—C6—C5 | -4.2 (6) | C17—C18—C23—C22 | 140.4 (17) |
| C2—C1—C6—C9 | -178.4 (4) | C18—C19—C20—C21 | -77.9 (12) |
| C2—C3—C4—O2 | 176.0 (3) | C18—C19—C20—C25 | 51.5 (19) |
| C2—C3—C4—C5 | -4.3 (6) | C18—C19—C20—C26 | 165.8 (13) |
| C3—C4—C5—C6 | 3.1 (5) | C18—C19—C24—C21 | 91.0 (12) |
| C4—C5—C6—C1 | 1.1 (5) | C19—C18—C23—C22 | 18.0 (2) |
| C4—C5—C6—C9 | 175.7 (3) | C19—C20—C21—C22 | 84.0 (14) |
| C5—C6—C9—N1 | 90.9 (4) | C19—C20—C21—C24 | -22.7 (11) |
| C6—C1—C2—C3 | 3.1 (6) | C20—C19—C24—C21 | -20.2 (10) |
| C7—O1—C3—C2 | 1.2 (6) | C20—C21—C22—C23 | -43 (2) |
| C7—O1—C3—C4 | 179.9 (4) | C20—C21—C24—C19 | 21.7 (10) |
| C8—O2—C4—C3 | -176.2 (4) | C21—C22—C23—C18 | -15.0 (3) |
| C8—O2—C4—C5 | 4.2 (6) | C22—C21—C24—C19 | -89.6 (12) |
| C9—N1—C10—C11 | 172.0 (3) | C23—C18—C19—C20 | 31.2 (15) |
| C9—N1—C13—C12 | -172.5 (4) | C23—C18—C19—C24 | -56.9 (13) |
| C9—N1—C14—C15 | -42.6 (6) | C24—C19—C20—C21 | 21.4 (11) |
| C9—N1—C14—C15A | -82.0 (9) | C24—C19—C20—C25 | 150.7 (16) |
| C10—N1—C9—C6 | -52.6 (4) | C24—C19—C20—C26 | -94.9 (13) |
| C10—N1—C13—C12 | -51.4 (4) | C24—C21—C22—C23 | 54.4 (19) |
| C10—N1—C14—C15 | -162.1 (5) | C25—C20—C21—C22 | -49.5 (18) |
| C10—N1—C14—C15A | 158.5 (9) | C25—C20—C21—C24 | -156.1 (12) |
| C11—O3—C12—C13 | -61.5 (5) | C26—C20—C21—C22 | -178.5 (14) |
| C12—O3—C11—C10 | 61.2 (5) | C26—C20—C21—C24 | 74.9 (15) |
| C13—N1—C9—C6 | 66.7 (4) | O4—C16—C17—C18 | -174.4 (16) |
| C13—N1—C10—C11 | 50.8 (4) | O4A—C16—C17—C18 | 159.5 (19) |

Table Ⅴ. Hydrogen-bond geometry (Å, º).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| D—H⋯A | D—H | H⋯A | D⋯A | D—H⋯A |
| C9—H9B⋯O4 | 0.97 | 2.6 | 3.205 (14) | 120.9 |
| C9—H9B⋯O4A | 0.97 | 2.38 | 3.01 (2) | 121.7 |
| C10—H10B⋯O2ⅰ | 0.97 | 2.46 | 3.313 (5) | 147.1 |
| C11—H11B⋯O1ⅰ | 0.97 | 2.64 | 3.337 (6) | 129.4 |
| C13—H13A⋯O4 | 0.97 | 2.36 | 3.053 (11) | 127.9 |
| C13—H13A⋯O4A | 0.97 | 2.73 | 3.33 (3) | 120.4 |
| C14—H14A⋯O5ⅱ | 0.97 | 2.46 | 3.379 (6) | 157.2 |
| O5—H5B⋯O6 | 0.86 | 2.03 | 2.869 (6) | 164.1 |
| O6—H6A⋯Br2ⅲ | 0.85 | 2.53 | 3.382 (5) | 176 |
| O6—H6B⋯Br2 | 0.85 | 2.68 | 3.353 (4) | 136.7 |

Symmetry codes: (ⅰ) - *x* + 2, - *y* + 1, - *z* + 1; (ⅱ) *x* - 1, *y*, *z*; (ⅲ) - *x* + 2 , - *y* + 2 , - *z* + 1.



Figure 8. The single crystal cell of pinaverium bromide dihydrate viewed along the b-axis direction. The blue line represents the hydrogen bonding.



Figure 9. The single crystal cell of pinaverium bromide dihydrate viewed along the c-axis direction. The blue line represents the hydrogen bonding.



Figure 10. The maximum and minimum features in the difference Fourier map, the maximum feature is represented by the dark blue area, and the minimum feature is indicated by the light red area.