Table 1. Hydrogen-bonds for compound 1 [A and deg.].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(1W)-H(11)...O(9W)#1 | 0.85 | 2.20 | 2.88(3) | 136.9 |
| O(1W)-H(12)...O(53A)#2 | 0.85 | 1.99 | 2.82(3) | 166.2 |
| O(2W)-H(21)...O(21A)#3 | 0.85 | 2.09 | 2.88(3) | 155.5 |
| O(2W)-H(22)...O(43A)#4 | 0.85 | 2.06 | 2.90(3) | 168.6 |
| O(3W)-H(31)...O(15W)#3 | 0.85 | 2.16 | 2.99(3) | 165.0 |
| O(3W)-H(32)...O(52A) | 0.85 | 2.08 | 2.86(3) | 151.4 |
| O(4W)-H(41)...O(3B)#5 | 0.85 | 1.84 | 2.69(3) | 175.6 |
| O(4W)-H(42)...O(23A)#6 | 0.85 | 2.19 | 2.98(3) | 154.2 |
| O(5W)-H(51)...O(21B)#7 | 0.85 | 2.30 | 3.14(3) | 169.4 |
| O(5W)-H(52)...O(51B)#8 | 0.85 | 2.07 | 2.91(3) | 168.2 |
| O(6W)-H(61)...O(52B) | 0.85 | 2.06 | 2.89(3) | 165.6 |
| O(6W)-H(62)...O(52B)#8 | 0.85 | 2.17 | 3.00(3) | 166.6 |
| O(7W)-H(71)...O(32B)#7 | 0.85 | 2.02 | 2.87(3) | 179.0 |
| O(7W)-H(72)...O(43B)#9 | 0.85 | 2.09 | 2.94(3) | 176.4 |
| O(8W)-H(81)...O(32B)#7 | 0.85 | 2.04 | 2.89(3) | 170.1 |
| O(8W)-H(82)...O(26W)#9 | 0.85 | 1.98 | 2.73(3) | 146.7 |
| O(9W)-H(91)...O(4W) | 0.85 | 1.94 | 2.79(3) | 173.5 |
| O(9W)-H(92)...O(13A)#3 | 0.85 | 2.14 | 2.98(3) | 175.0 |
| O(10W)-H(101)...O(2W) | 0.85 | 1.98 | 2.81(3) | 163.3 |
| O(10W)-H(102)...O(3W) | 0.85 | 1.89 | 2.72(3) | 163.3 |
| O(11W)-H(111)...O(23A)#3 | 0.85 | 2.18 | 3.00(3) | 163.2 |
| O(11W)-H(112)...O(52A)#1 | 0.85 | 1.92 | 2.77(3) | 175.6 |
| O(12W)-H(121)...O(32A) | 0.85 | 2.06 | 2.91(3) | 178.7 |
| O(12W)-H(122)...O(28W) | 0.85 | 1.82 | 2.66(3) | 179.0 |
| O(13W)-H(131)...O(19W) | 0.85 | 2.16 | 3.00(3) | 165.6 |
| O(13W)-H(132)...O(27W) | 0.85 | 1.82 | 2.67(3) | 176.3 |
| O(14W)-H(141)...O(10W) | 0.85 | 1.90 | 2.74(3) | 171.4 |
| O(14W)-H(142)...O(19W) | 0.85 | 1.91 | 2.75(3) | 172.4 |
| O(15W)-H(151)...O(13A) | 0.85 | 1.92 | 2.70(2) | 151.7 |
| O(15W)-H(152)...O(20W)#1 | 0.85 | 1.79 | 2.63(3) | 168.6 |
| O(16W)-H(161)...O(43A) | 0.85 | 1.87 | 2.69(3) | 161.4 |
| O(16W)-H(162)...O(12A)#6 | 0.85 | 1.91 | 2.74(3) | 166.0 |
| O(17W)-H(171)...O(4A) | 0.85 | 1.86 | 2.70(2) | 171.5 |
| O(17W)-H(172)...O(7W)#7 | 0.85 | 1.96 | 2.80(3) | 172.4 |
| O(18W)-H(181)...O(8W)#7 | 0.88 | 2.49 | 3.24(3) | 143.9 |
| O(18W)-H(182)...O(52B)#8 | 0.85 | 2.09 | 2.93(3) | 175.9 |
| O(19W)-H(191)...O(52A) | 0.85 | 2.30 | 3.15(3) | 178.8 |
| O(19W)-H(192)...O(31A)#3 | 0.85 | 2.08 | 2.93(3) | 178.8 |
| O(20W)-H(201)...O(51A) | 0.85 | 2.00 | 2.84(3) | 172.4 |
| O(20W)-H(202)...O(9W) | 0.85 | 1.94 | 2.79(3) | 173.0 |
| O(21W)-H(211)...O(43B) | 0.85 | 1.97 | 2.78(2) | 159.5 |
| O(21W)-H(212)...O(26W) | 0.85 | 1.99 | 2.82(3) | 165.2 |
| O(22W)-H(222)...O(23B)#5 | 0.85 | 1.84 | 2.69(2) | 175.5 |
| O(23W)-H(231)...O(17W) | 0.85 | 1.95 | 2.80(3) | 179.7 |
| O(23W)-H(232)...O(21B)#5 | 0.85 | 1.94 | 2.79(3) | 179.1 |
| O(24W)-H(241)...O(18W) | 0.85 | 2.08 | 2.73(3) | 132.4 |
| O(24W)-H(242)...O(12B)#6 | 0.85 | 1.94 | 2.72(3) | 151.8 |
| O(25W)-H(251)...O(33B)#5 | 0.85 | 1.87 | 2.69(3) | 162.4 |
| O(25W)-H(252)...O(53B)#8 | 0.85 | 1.83 | 2.68(3) | 177.4 |
| O(26W)-H(261)...O(22W) | 0.85 | 1.96 | 2.69(3) | 144.1 |
| O(26W)-H(262)...O(11B)#5 | 0.85 | 2.31 | 3.11(3) | 157.1 |
| O(27W)-H(271)...O(2A) | 0.85 | 2.32 | 3.15(3) | 166.6 |
| O(27W)-H(272)...O(5A) | 0.85 | 2.24 | 3.07(3) | 165.6 |
| O(28W)-H(281)...O(27W) | 0.85 | 2.06 | 2.75(4) | 138.3 |
| O(28W)-H(282)...O(10W)#1 | 0.85 | 2.00 | 2.71(4) | 139.6 |
| O(1A)-H(1A)...O(5A) | 0.84 | 1.91 | 2.71(2) | 158.6 |
| O(3A)-H(3A)...O(2A) | 0.84 | 1.93 | 2.75(3) | 164.8 |
| O(4A)-H(4A)...O(3A) | 0.84 | 1.90 | 2.74(2) | 173.8 |
| O(1B)-H(1B)...O(2B) | 0.84 | 2.12 | 2.91(2) | 156.2 |

| | | | | |
|---|---|---|---|---|
| O(2B)-H(2B)...O(4W)#10 | 0.84 | 2.60 | 3.31(3) | 143.1 |
| O(3B)-H(3B)...O(4B) | 0.84 | 1.92 | 2.75(2) | 168.8 |
| O(4B)-H(4B)...O(5B) | 0.84 | 2.06 | 2.86(2) | 159.1 |
| O(5B)-H(5B)...O(1B) | 0.84 | 2.50 | 3.31(2) | 162.8 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,y-1/2,-z+1/2 #2 -x,-y+2,-z+1 #3 -x,y+1/2,-z+1/2
#4 -x,-y+2,-z #5 -x+1,y+1/2,-z+1/2 #6 x,-y+3/2,z-1/2
#7 -x+1,-y+1,-z+1 #8 -x+1,-y+2,-z+1 #9 x,-y+3/2,z+1/2
#10 -x+1,y-1/2,-z+1/2

Table 2. Hydrogen-bonds for compound 2 [A and deg.].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(1)-H(1)...O(2) | 0.84 | 1.96 | 2.713(9) | 148.7 |
| O(2)-H(2)...O(3) | 0.84 | 1.85 | 2.661(9) | 161.1 |
| O(3)-H(3)...O(4) | 0.84 | 1.83 | 2.662(9) | 170.5 |
| O(4)-H(4)...O(1) | 0.84 | 1.88 | 2.718(9) | 177.6 |
| O(2W)-H(2WA)...O(1W) | 0.85 | 1.89 | 2.744(12) | 178.2 |
| O(2W)-H(2WB)...O(4W) | 0.85 | 1.97 | 2.819(11) | 178.3 |
| O(3W)-H(3WA)...O(11W) | 0.85 | 1.97 | 2.803(10) | 168.2 |
| O(3W)-H(3WB)...O(22)#2 | 0.85 | 2.02 | 2.853(10) | 168.2 |
| O(4W)-H(4WA)...O(21)#2 | 0.85 | 1.98 | 2.820(10) | 168.1 |
| O(4W)-H(4WB)...O(22) | 0.85 | 2.03 | 2.793(11) | 149.7 |
| O(5W)-H(5WA)...O(31)#1 | 0.85 | 2.00 | 2.840(11) | 171.9 |
| O(5W)-H(5WB)...O(2W)#1 | 0.85 | 2.12 | 2.963(13) | 172.1 |
| O(6W)-H(6WA)...O(43)#1 | 0.85 | 2.11 | 2.850(10) | 146.0 |
| O(6W)-H(6WB)...O(3W)#2 | 0.85 | 2.06 | 2.891(10) | 164.6 |
| O(7W)-H(7WA)...O(8W) | 0.85 | 1.94 | 2.776(12) | 168.1 |
| O(7W)-H(7WB)...O(18W)#3 | 0.85 | 2.14 | 2.774(12) | 131.2 |
| O(8W)-H(8WA)...O(32) | 0.85 | 2.02 | 2.866(10) | 171.1 |
| O(8W)-H(8WB)...O(9W)#4 | 0.85 | 2.10 | 2.939(11) | 171.2 |
| O(9W)-H(9WA)...O(10W) | 0.85 | 2.01 | 2.809(11) | 156.3 |
| O(9W)-H(9WB)...O(18W)#5 | 0.85 | 2.05 | 2.847(10) | 156.4 |
| O(10W)-H(101)...O(21) | 0.85 | 2.05 | 2.843(11) | 154.2 |
| O(10W)-H(102)...O(6W)#2 | 0.85 | 1.99 | 2.776(11) | 153.9 |
| O(11W)-H(111)...O(13)#6 | 0.85 | 1.91 | 2.755(8) | 174.8 |
| O(11W)-H(112)...O(23)#2 | 0.85 | 2.19 | 3.039(9) | 174.9 |
| O(12W)-H(121)...O(12)#6 | 0.85 | 2.02 | 2.857(9) | 168.5 |
| O(12W)-H(122)...O(43)#7 | 0.85 | 1.90 | 2.734(9) | 168.2 |
| O(13W)-H(131)...O(42) | 0.85 | 1.90 | 2.728(8) | 164.7 |
| O(13W)-H(132)...O(8W)#8 | 0.85 | 1.97 | 2.800(10) | 164.8 |
| O(14W)-H(141)...O(1W) | 0.85 | 1.88 | 2.726(11) | 173.7 |
| O(14W)-H(142)...O(3W) | 0.85 | 1.88 | 2.725(9) | 174.1 |
| O(15W)-H(151)...O(21)#2 | 0.85 | 2.76 | 3.580(10) | 163.4 |
| O(15W)-H(152)...O(31)#1 | 0.85 | 1.94 | 2.762(10) | 161.8 |
| O(16W)-H(161)...O(32)#1 | 0.85 | 1.93 | 2.784(9) | 179.5 |
| O(16W)-H(162)...O(42)#7 | 0.85 | 1.88 | 2.727(9) | 179.5 |
| O(17W)-H(171)...O(41) | 0.85 | 1.99 | 2.839(9) | 175.1 |
| O(17W)-H(172)...O(2W) | 0.85 | 1.85 | 2.696(11) | 175.0 |
| O(18W)-H(181)...O(13) | 0.85 | 1.88 | 2.726(10) | 179.6 |
| O(18W)-H(182)...O(23)#8 | 0.85 | 1.93 | 2.777(10) | 179.7 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y,-z #2 -x,-y+1,-z #3 x,y,z-1 #4 -x+1,-y+1,-z
#5 -x+1,-y+1,-z+1 #6 -x,-y+1,-z+1 #7 -x,-y,-z+1
#8 x,y,z+1

Table 3. Hydrogen-bonds for compound 3 [A and deg.].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(1)-H(1)...O(2) | 0.84 | 1.95 | 2.711(6) | 150.1 |
| O(2)-H(2)...O(3) | 0.84 | 1.92 | 2.703(5) | 154.2 |
| O(3)-H(3)...O(4) | 0.84 | 1.85 | 2.670(5) | 164.9 |
| O(4)-H(4)...O(1) | 0.84 | 1.93 | 2.710(5) | 154.8 |
| O(2W)-H(2WA)...O(1W) | 0.85 | 1.82 | 2.666(7) | 177.5 |
| O(2W)-H(2WB)...O(4W) | 0.85 | 1.97 | 2.817(6) | 177.6 |
| O(3W)-H(3WA)...O(11W) | 0.85 | 2.43 | 3.251(6) | 164.0 |
| O(3W)-H(3WB)...O(22)#1 | 0.85 | 2.34 | 3.169(5) | 163.8 |
| O(4W)-H(4WA)...O(21)#1 | 0.85 | 2.04 | 2.889(7) | 175.1 |
| O(4W)-H(4WB)...O(22) | 0.85 | 1.96 | 2.770(5) | 158.1 |
| O(5W)-H(5WA)...O(31)#2 | 0.85 | 1.96 | 2.797(6) | 169.3 |
| O(5W)-H(5WB)...O(2W)#2 | 0.85 | 2.21 | 3.046(7) | 169.6 |
| O(6W)-H(6WA)...O(43)#2 | 0.85 | 2.09 | 2.825(5) | 144.1 |
| O(6W)-H(6WB)...O(3W)#1 | 0.85 | 2.08 | 2.895(5) | 161.1 |
| O(7W)-H(7WA)...O(8W) | 0.85 | 2.21 | 3.016(8) | 158.0 |
| O(7W)-H(7WB)...O(18W)#3 | 0.85 | 2.35 | 2.754(11) | 109.7 |
| O(8W)-H(8WA)...O(32) | 0.85 | 1.99 | 2.828(6) | 169.3 |
| O(8W)-H(8WB)...O(9W)#4 | 0.85 | 2.03 | 2.867(10) | 169.3 |
| O(9W)-H(9WA)...O(10W) | 0.85 | 1.99 | 2.790(12) | 156.4 |
| O(9W)-H(9WB)...O(18W)#5 | 0.85 | 2.00 | 2.801(13) | 156.5 |
| O(10W)-H(101)...O(21) | 0.85 | 2.30 | 3.127(10) | 163.5 |
| O(10W)-H(102)...O(6W)#1 | 0.85 | 1.76 | 2.577(9) | 162.1 |
| O(11W)-H(111)...O(13)#6 | 0.85 | 1.92 | 2.759(5) | 171.0 |
| O(11W)-H(112)...O(23)#1 | 0.85 | 1.85 | 2.693(5) | 171.0 |
| O(12W)-H(121)...O(12)#6 | 0.85 | 2.14 | 2.969(6) | 165.2 |
| O(12W)-H(122)...O(43)#7 | 0.85 | 1.90 | 2.727(4) | 164.7 |
| O(13W)-H(131)...O(42) | 0.85 | 1.90 | 2.736(4) | 166.9 |
| O(13W)-H(132)...O(8W)#8 | 0.85 | 1.87 | 2.707(5) | 166.9 |
| O(14W)-H(141)...O(1W) | 0.85 | 1.87 | 2.722(6) | 178.6 |
| O(14W)-H(142)...O(3W) | 0.85 | 1.88 | 2.730(5) | 178.6 |
| O(15W)-H(151)...O(21)#1 | 0.85 | 2.09 | 2.934(7) | 169.6 |
| O(15W)-H(152)...O(31)#2 | 0.85 | 1.86 | 2.702(5) | 169.2 |
| O(16W)-H(161)...O(32)#2 | 0.85 | 1.90 | 2.746(5) | 176.9 |
| O(16W)-H(162)...O(42)#7 | 0.85 | 1.87 | 2.721(4) | 176.9 |
| O(17W)-H(171)...O(41) | 0.85 | 1.97 | 2.815(4) | 177.0 |
| O(17W)-H(172)...O(2W) | 0.85 | 1.84 | 2.686(5) | 176.9 |
| O(18W)-H(181)...O(13) | 0.85 | 1.67 | 2.516(11) | 177.4 |
| O(18W)-H(182)...O(23)#8 | 0.85 | 1.51 | 2.362(12) | 177.3 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z #2 -x,-y,-z #3 x,y,z-1 #4 -x+1,-y+1,-z
#5 -x+1,-y+1,-z+1 #6 -x,-y+1,-z+1 #7 -x,-y,-z+1
#8 x,y,z+1

Table 4. Hydrogen-bonds for compound 4 [A and deg.].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(1)-H(1)...O(2) | 0.84 | 1.98 | 2.723(9) | 147.4 |
| O(2)-H(2)...O(3) | 0.84 | 1.84 | 2.664(9) | 168.5 |
| O(3)-H(3)...O(4) | 0.84 | 1.84 | 2.671(9) | 167.6 |
| O(4)-H(4)...O(1) | 0.84 | 1.93 | 2.724(9) | 158.1 |
| O(2W)-H(2WA)...O(1W) | 0.85 | 1.90 | 2.747(14) | 178.7 |
| O(2W)-H(2WB)...O(4W) | 0.85 | 1.97 | 2.816(12) | 178.7 |
| O(3W)-H(3WA)...O(11W) | 0.85 | 1.97 | 2.806(11) | 169.1 |
| O(3W)-H(3WB)...O(22)#1 | 0.85 | 2.01 | 2.848(11) | 169.4 |
| O(4W)-H(4WA)...O(21)#1 | 0.85 | 1.97 | 2.803(11) | 167.4 |
| O(4W)-H(4WB)...O(22) | 0.85 | 2.05 | 2.815(12) | 148.9 |
| O(5W)-H(5WA)...O(31)#2 | 0.85 | 2.02 | 2.860(12) | 172.5 |

| | | | | |
|---|---|---|---|---|
| O(5W)-H(5WB)...O(2W)#2 | 0.85 | 2.07 | 2.919(14) | 172.5 |
| O(6W)-H(6WA)...O(43)#2 | 0.85 | 2.12 | 2.859(11) | 145.2 |
| O(6W)-H(6WB)...O(3W)#1 | 0.85 | 2.05 | 2.879(11) | 163.6 |
| O(7W)-H(7WA)...O(8W) | 0.85 | 1.93 | 2.765(14) | 167.5 |
| O(7W)-H(7WB)...O(18W)#3 | 0.85 | 2.13 | 2.769(13) | 131.2 |
| O(8W)-H(8WA)...O(32) | 0.85 | 1.99 | 2.839(12) | 172.0 |
| O(8W)-H(8WB)...O(9W)#4 | 0.85 | 2.08 | 2.920(13) | 171.7 |
| O(9W)-H(9WA)...O(10W) | 0.85 | 2.00 | 2.798(12) | 156.0 |
| O(9W)-H(9WB)...O(18W)#5 | 0.85 | 2.06 | 2.855(12) | 155.5 |
| O(10W)-H(101)...O(21) | 0.85 | 2.05 | 2.849(12) | 155.3 |
| O(10W)-H(102)...O(6W)#1 | 0.85 | 1.97 | 2.759(12) | 154.7 |
| O(11W)-H(111)...O(13)#6 | 0.85 | 1.88 | 2.729(9) | 176.6 |
| O(11W)-H(112)...O(23)#1 | 0.85 | 2.19 | 3.044(10) | 176.5 |
| O(12W)-H(121)...O(12)#6 | 0.85 | 2.02 | 2.856(9) | 167.9 |
| O(12W)-H(122)...O(43)#7 | 0.85 | 1.89 | 2.727(9) | 167.8 |
| O(13W)-H(131)...O(42) | 0.85 | 1.90 | 2.727(9) | 164.4 |
| O(13W)-H(132)...O(8W)#8 | 0.85 | 2.00 | 2.833(11) | 164.6 |
| O(14W)-H(141)...O(1W) | 0.85 | 1.86 | 2.701(11) | 173.2 |
| O(14W)-H(142)...O(3W) | 0.85 | 1.88 | 2.726(10) | 173.7 |
| O(15W)-H(151)...O(23)#1 | 0.85 | 1.95 | 2.802(10) | 174.4 |
| O(15W)-H(152)...O(31)#2 | 0.85 | 1.90 | 2.747(10) | 174.3 |
| O(16W)-H(161)...O(32)#2 | 0.85 | 1.93 | 2.783(10) | 178.7 |
| O(16W)-H(162)...O(42)#7 | 0.85 | 1.89 | 2.736(9) | 178.5 |
| O(17W)-H(171)...O(41) | 0.85 | 2.00 | 2.848(10) | 174.7 |
| O(17W)-H(172)...O(2W) | 0.85 | 1.85 | 2.701(11) | 174.6 |
| O(18W)-H(181)...O(13) | 0.85 | 1.88 | 2.730(10) | 178.5 |
| O(18W)-H(182)...O(23)#8 | 0.85 | 1.94 | 2.786(12) | 179.2 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z #2 -x,-y,-z #3 x,y,z-1 #4 -x+1,-y+1,-z
#5 -x+1,-y+1,-z+1 #6 -x,-y+1,-z+1 #7 -x,-y,-z+1
#8 x,y,z+1

Table 5. Hydrogen-bonds for compound 5 [A and deg.].

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| O(1)-H(1)...O(2) | 0.84 | 1.86 | 2.702(9) | 178.3 |
| O(2)-H(2)...O(3) | 0.84 | 1.95 | 2.703(7) | 149.5 |
| O(3)-H(3)...O(4) | 0.84 | 1.84 | 2.677(8) | 177.9 |
| O(4)-H(4)...O(1) | 0.84 | 1.95 | 2.723(7) | 153.2 |
| O(2W)-H(2WA)...O(1W) | 0.85 | 1.76 | 2.608(12) | 176.5 |
| O(2W)-H(2WB)...O(4W) | 0.85 | 1.94 | 2.790(13) | 177.4 |
| O(3W)-H(3WA)...O(11W) | 0.85 | 2.36 | 3.184(10) | 163.3 |
| O(3W)-H(3WB)...O(22)#1 | 0.85 | 2.17 | 2.984(11) | 160.5 |
| O(3W)-H(3WB)...O(22') | 0.85 | 2.29 | 2.761(12) | 115.3 |
| O(4W)-H(4WA)...O(21)#1 | 0.85 | 1.87 | 2.708(12) | 166.8 |
| O(4W)-H(4WB)...O(22) | 0.85 | 1.89 | 2.705(10) | 160.9 |
| O(4W)-H(4WA)...O(21')#1 | 0.85 | 2.27 | 3.114(13) | 173.5 |
| O(4W)-H(4WB)...O(22') | 0.85 | 2.13 | 2.900(12) | 150.0 |
| O(5W)-H(5WA)...O(31)#2 | 0.85 | 1.94 | 2.778(10) | 169.0 |
| O(5W)-H(5WB)...O(2W)#2 | 0.85 | 2.24 | 3.081(13) | 169.6 |
| O(6W)-H(6WA)...O(43)#2 | 0.85 | 2.10 | 2.820(8) | 141.5 |
| O(6W)-H(6WB)...O(3W)#1 | 0.85 | 2.05 | 2.868(10) | 161.4 |
| O(7W)-H(7WA)...O(8W) | 0.85 | 2.16 | 2.972(17) | 158.8 |
| O(7W)-H(7WB)...O(18W)#3 | 0.85 | 2.29 | 2.727(18) | 112.1 |
| O(7W)-H(7WB)...O(23') | 0.85 | 2.33 | 3.168(13) | 168.8 |
| O(8W)-H(8WA)...O(32) | 0.85 | 2.02 | 2.857(10) | 170.5 |
| O(8W)-H(8WB)...O(9W)#4 | 0.85 | 2.05 | 2.890(16) | 169.6 |
| O(9W)-H(9WA)...O(10W) | 0.85 | 1.99 | 2.786(19) | 156.2 |
| O(9W)-H(9WB)...O(18W)#5 | 0.85 | 1.95 | 2.73(2) | 153.5 |
| O(10W)-H(101)...O(21) | 0.85 | 2.20 | 2.979(16) | 151.6 |

| | | | | |
|---|---|---|---|---|
| O(10W)-H(102)...O(6W)#1 | 0.85 | 1.81 | 2.626(16) | 159.3 |
| O(10W)-H(101)...O(21') | 0.85 | 2.41 | 3.247(16) | 170.7 |
| O(11W)-H(111)...O(13)#6 | 0.85 | 1.88 | 2.722(8) | 172.0 |
| O(11W)-H(112)...O(23)#1 | 0.85 | 1.90 | 2.731(10) | 167.3 |
| O(11W)-H(112)...O(23')#1 | 0.85 | 1.95 | 2.759(10) | 159.8 |
| O(12W)-H(121)...O(12)#6 | 0.85 | 2.07 | 2.903(8) | 166.3 |
| O(12W)-H(122)...O(43)#7 | 0.85 | 1.90 | 2.730(7) | 165.9 |
| O(13W)-H(131)...O(42) | 0.85 | 1.91 | 2.739(6) | 165.7 |
| O(13W)-H(132)...O(8W)#8 | 0.85 | 1.89 | 2.721(9) | 165.7 |
| O(14W)-H(141)...O(1W) | 0.85 | 1.87 | 2.722(10) | 178.4 |
| O(14W)-H(142)...O(3W) | 0.85 | 1.85 | 2.705(8) | 179.6 |
| O(15W)-H(151)...O(23)#1 | 0.85 | 2.14 | 2.925(11) | 154.4 |
| O(15W)-H(152)...O(31)#2 | 0.85 | 1.87 | 2.718(9) | 177.8 |
| O(15W)-H(151)...O(21')#1 | 0.85 | 1.97 | 2.769(10) | 156.1 |
| O(16W)-H(161)...O(32)#2 | 0.85 | 1.89 | 2.742(7) | 175.7 |
| O(16W)-H(162)...O(42)#7 | 0.85 | 1.88 | 2.724(6) | 175.5 |
| O(17W)-H(171)...O(41) | 0.85 | 1.97 | 2.818(6) | 176.9 |
| O(17W)-H(172)...O(2W) | 0.85 | 1.82 | 2.668(9) | 176.5 |
| O(18W)-H(181)...O(13) | 0.85 | 1.73 | 2.580(17) | 177.5 |
| O(18W)-H(182)...O(23)#8 | 0.85 | 1.88 | 2.72(2) | 169.2 |
| O(18W)-H(182)...O(23')#8 | 0.85 | 1.38 | 2.194(18) | 159.8 |

Symmetry transformations used to generate equivalent atoms:
#1 -x,-y+1,-z #2 -x,-y,-z #3 x,y,z-1 #4 -x+1,-y+1,-z
#5 -x+1,-y+1,-z+1 #6 -x,-y+1,-z+1 #7 -x,-y,-z+1
#8 x,y,z+1