**Supplumentary materials**

**Figures :**

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| H:\article 12-10-2021\article\direction (a) a and (b) b.tif |
| **Figure S1:** Projection of the structure: **(a**) along the axis and **(b)** along the axis. |

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| H:\article 12-10-2021\article\H-bond.tif |
| **Figure S2:** Hydrogen bond motif in PMDT compound. |

|  |  |
| --- | --- |
| **H:\Revised PMDT\Figure S3-.tif**  **(a)** | **C:\Users\lpq11\Desktop\Graph1.tif**  **(b)** |
| **Figure S3: (a)** experimental and **(b)** theoretical IR absorption spectrum of PMDT compound. | |

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| H:\article 12-10-2021\article\optimized structure.tif |
| **Figure S4:** Optimized geometrical structure of the title molecule PMDT. |

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| H:\article 12-10-2021\article\AIMmolecule.tif |
| **Figure S5:** AIM critical points of the studied molecule PMDT. |

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| H:\article 12-10-2021\article\HS.tif |
| **Figure S6:** Asymmetric unit: **(a)** Hirshfeld surfaces,**(b)** dnorm and **(c)**full 2D fingerprint of C9H26N3(NO3) 3. |

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| H:\article 12-10-2021\article\dnorm.tif |
| **Figure S7:** Different hydrogen bonds observed in C9H26N3 (NO3) 3by dnorm mapping. |

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| H:\article 12-10-2021\article\Potential electrostatic HS.tif |
| **Figure S8:** Electrostatic potential of C9H26N3 (NO3) 3mapped to the Hirshfeld surface. |

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| **Figure S9:** 2D fingerprints of the intermolecular contacts involved in the compound C9H26N3 (NO3) 3. |

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| H:\Revised PMDT\Figure S10.tif |
| **Figure S10:** Molecular electrostatic potential surfaces analysis of PMDT in gas, water and DMSO solvatation. |

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| H:\article PMDT\Figure 15.tif |
| **Figure S11:** The frontier molecular orbital FMO's of PMDT compound in gas, water and DMSO solvatation. |

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| H:\article PMDT\Figure 16.tif |
| **Figure S12:** Density of state (DOS) spectrum of our compound PMDT in various phases. |

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| E:\PMDT revised\Figure S8 .tif |
| **Figure S13:** DTA and TGA curves of C9H26N3 (NO3) 3. |

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| H:\article 12-10-2021\article\DSC.tif |
| **Figure S14:** Differential scanning calorimetric analysis thermogram of C9H26N3 (NO3) 3. |

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| **Figure S15:** Variation of Ln (σ.T) as a function of 103 / T of C9H26N3 (NO3) 3. |

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| **Figure S16:** Variation of dielectric constants ε’ (Fig. a) and ε’’ (Fig. b) as a function of frequency at different temperatures. |

**Table**

**Table S1:** Crystallographic data of PMDT.

|  |  |
| --- | --- |
| Temperature | 293 K |
| Cristal size (mm) | 0.4 × 0.35 × 0.3 |
| Empirical formula | C9H26N6O9 |
| Formula weight (g mol-1) | 362.36 |
| Crystal system | Triclinic |
| Space group | P |
| a (Å) | 5.964(2) |
| b (Å) | 7.018 (1) |
| c (Å) | 21.688 (2) |
| α (°) | 91.90 (2) |
| β (°) | 90.60 (2) |
|  (°) | 102.45(3) |
| Z (Å) | 2 |
| V (Å3) | 885.8(3) |
| F(000) | 388 |
| Radiation type | Ag Kα |
| λ (Å) | 0.56083 |
| Reflections collected | 3582 |
| Independent reflections | 3128 |
| Reflections with I > 2σ(I) | 2125 |
| Rint | 0.030 |
| μ (mm-1) | 0.072 |
| Refined parameters | 234 |
| R[F2> 2σ(F2)] | 0.063 |
| wR(F2) | 0.184 |
| Δρmax = 0.29 e Å3 | Δρmin = −0.24 eÅ3 |

**Table S2:** Experimental and theoretical parameters of 1,1,4,7,7-Pentamethyldiethylenetriammonium trinitrate.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **B3LYP/6-31++G(d.p)** | | | | |
| **Bond lengths (A°)** | | **Bond angles (°)** | | |
| **Atom position** | **Theo.** | **Exp.** | **Atom position** | **Theo.** | **Exp.** |
| N1-C4 | 1.495 | 1.484(4) | C4-N1-C16 | 111.4 | 109.8(2) |
| N1-C16 | 1.489 | 1.484(4) | C4-N1-C20 | 113.3 | 113.2(3) |
| N1-C20 | 1.489 | 1.476(5) | C4-N1-H36 | 105.3 | 103(2) |
| N1-H36 | 1.132 | 0.90(3) | C16-N1-C20 | 110.9 | 111.1(3) |
| N2-C7 | 1.504 | 1.495(4) | C16-N1-H36 | 107.4 | 108(2) |
| N2-C10 | 1.506 | 1.498(4) | C20-N1-H36 | 108.1 | 112(2) |
| N2-C24 | 1.499 | 1.499(4) | C7-N2-C10 | 112.3 | 111.8(2) |
| N2-H37 | 1.099 | 0.87(3) | C7-N2-C24 | 111.6 | 112.4(2) |
| N3-C13 | 1.502 | 1.480(4) | C7-N2-H37 | 109.3 | 110.1(2) |
| N3-C28 | 1.491 | 1.490(5) | C10-N2-C24 | 109.6 | 110.1(2) |
| N3-C32 | 1.493 | 1.489(4) | C10-N2-H37 | 107.2 | 104(2) |
| N3-H38 | 1.122 | 0.87(3) | C24-N2-H37 | 106.6 | 109(2) |
| C4-H5 | 1.092 | 0.970 | C13-N3-C28 | 110.9 | 110.9(2) |
| C4-H6 | 1.092 | 0.970 | C13-N3-C32 | 112.7 | 112.2(2) |
| C4-C7 | 1.542 | 1.509(4) | C13-N3-H38 | 107.9 | 109(2) |
| C7-H8 | 1.094 | 0.970 | C28-N3-C32 | 111.2 | 110.5(2) |
| C7-H9 | 1.089 | 0.970 | C28-N3-H38 | 106.2 | 111(2) |
| C10-H11 | 1.092 | 0.970 | C32-N3-H38 | 107.6 | 104(2) |
| C10-H12 | 1.092 | 0.971 | N1-C4-H5 | 106.5 | 109.3 |
| C10-C13 | 1.541 | 1.515(4) | N1-C4-H6 | 110.2 | 109.4 |
| C13-H14 | 1.089 | 0.970 | N1-C4-C7 | 111.6 | 111.5(2) |
| C13-H15 | 1.095 | 0.970 | H5-C4-H6 | 107.4 | 108.0 |
| C16-H17 | 1.091 | 0.960 | H5-C4-C7 | 110.5 | 109.4 |
| C16-H18 | 1.09 | 0.959 | H6-C4-C7 | 110.7 | 109.3 |
| C16-H19 | 1.094 | 0.960 | N2-C7-C4 | 111.5 | 110.7(2) |
| C20-H21 | 1.094 | 0.960 | N2-C7-H8 | 107.0 | 109.5 |
| C20-H22 | 1.090 | 0.960 | N2-C7-H9 | 107.6 | 109.5 |
| C20-H23 | 1.091 | 0.959 | C4-C7-H8 | 111.4 | 109.6 |
| H21-O50 | 4.268 | - | C4-C7-H9 | 110.1 | 109.5 |
| H22-O50 | 2.687 | - | H8-C7-H9 | 109.1 | 108.1 |
| C24-H25 | 1.091 | 0.959 | N2-C10-H11 | 108.6 | 109.2 |
| C24-H26 | 1.089 | 0.959 | N2-C10-H12 | 106.2 | 109.3 |
| C24-H27 | 1.091 | 0.959 | N2-C10-C13 | 113.2 | 111.7(2) |
| C28-H29 | 1.093 | 0.960 | H11-C10-H12 | 107.1 | 108.0 |
| C28-H30 | 1.091 | 0.959 | H11-C10-C13 | 110.6 | 109.3 |
| C28-H31 | 1.091 | 0.959 | H12-C10-C13 | 110.9 | 109.3 |
| H29-O42 | 4.229 | - | N3-C13-C10 | 111.3 | 110.5(2) |
| C32-H33 | 1.093 | 0.960 | N3-C13-H14 | 106.4 | 109.5 |
| C32-H34 | 1.091 | 0.960 | N3-C13-H15 | 108.1 | 109.6 |
| C32-H35 | 1.09 | 0.959 | C10-C13-H14 | 109.5 | 109.6 |
| H37-O45 | 1.513 | - | C10-C13-H15 | 111.7 | 109.5 |
| N39-O40 | 1.224 | 1.250(4) | H14-C13-H15 | 109.7 | 108.1 |
| N39-O41 | 1.309 | 1.215(4) | N1-C16-H17 | 108.9 | 109.5 |
| N39-O42 | 1.262 | 1.223(4) | N1-C16-H18 | 108.0 | 109.5 |
| N43-O44 | 1.266 | 1.203(4) | N1-C16-H19 | 110.1 | 109.5 |
| N43-O45 | 1.301 | 1.248(4) | H17-C16-H18 | 109.1 | 109.5 |
| N43-O46 | 1.226 | 1.230(4) | H17-C16-H19 | 109.9 | 109.5 |
| N47-O48 | 1.223 | 1.221(5) | H18-C16-H19 | 110.9 | 109.5 |
| N47-O49 | 1.319 | 1.205(4) | N1-C20-H21 | 109.9 | 109.4 |
| N47-O50 | 1.253 | 1.237(4) | N1-C20-H22 | 107.9 | 109.4 |
|  |  |  | N1-C20-H23 | 109.7 | 109.5 |
|  |  |  | H21-C20-H22 | 110.8 | 109.5 |
|  |  |  | H21-C20-H23 | 109.9 | 109.5 |
|  |  |  | H22-C20-H23 | 108.5 | 109.5 |
|  |  |  | C20-H22-O50 | 114.8 | - |
|  |  |  | N2-C24-H25 | 109.6 | 109.4 |
|  |  |  | N2-C24-H26 | 109.8 | 109.5 |
|  |  |  | N2-C24-H27 | 108.4 | 109.5 |
|  |  |  | H25-C24-H26 | 108.8 | 109.6 |
|  |  |  | H25-C24-H27 | 110.7 | 109.4 |
|  |  |  | H26-C24-H27 | 109.5 | 109.5 |
|  |  |  | N3-C28-H29 | 109.9 | 109.5 |
|  |  |  | N3-C28-H30 | 108.2 | 109.5 |
|  |  |  | N3-C28-H31 | 108.5 | 109.5 |
|  |  |  | H29-C28-H30 | 110.9 | 109.5 |
|  |  |  | H29-C28-H31 | 109.8 | 109.4 |
|  |  |  | H30-C28-H31 | 109.4 | 109.4 |
|  |  |  | C28-H29-O42 | 31.7 | - |
|  |  |  | N3-C32-H33 | 109.9 | 109.4 |
|  |  |  | N3-C32-H34 | 108.4 | 109.4 |
|  |  |  | N3-C32-H35 | 110.1 | 109.4 |
|  |  |  | H33-C32-H34 | 110.2 | 109.5 |
|  |  |  | H33-C32-H35 | 109.1 | 109.5 |
|  |  |  | H34-C32-H35 | 109.2 | 109.5 |
|  |  |  | N2-H37-O45 | 171.6 | - |
|  |  |  | O40-N39-O41 | 119.4 | 120.7(3) |
|  |  |  | O40-N39-O42 | 123.4 | 117.7(3) |
|  |  |  | O41-N39-O42 | 117.2 | 121.7(3) |
|  |  |  | H29-O42-N39 | 107.9 | 121.3(3) |
|  |  |  | O44-N43-O45 | 117.4 | 116.2(3) |
|  |  |  | O44-N43-O46 | 122.9 | 122.3(3) |
|  |  |  | O45-N43-O46 | 119.7 | 121.5(3) |
|  |  |  | H37-O45-N43 | 110.4 | 125.2(3) |
|  |  |  | O48-N47-O50 | 118.8 | 114.9(3) |
|  |  |  | O48-N47-O50 | 124.3 | 119.9(3) |
|  |  |  | O49-N47-O50 | 116.9 | - |
|  |  |  | H21-O50-H22 | 14.5 | - |
|  |  |  | H21-O50-N47 | 109.3 | - |
|  |  |  | H22-O50-N47 | 118.6 | - |
| **RMSD** | 0.338 | | **RMSD** | 0.912 | |

**Table S3:** Enrichment ratios (RE) of the various contacts in C9H26N3(NO3)3.

|  |  |  |  |
| --- | --- | --- | --- |
| RE | H | N | O |
| H | 0.65 | 1.24 | 1.55 |
| N |  |  | 0.67 |
| O |  |  | 0.13 |
| % Surface | 60.4 | 2 | 37.6 |

**Table S4:** Natural bond orbital (NBO) analyses for weak interactions in our molecule PMDT.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Donor** | **Acceptor** | **E(2) kcal/mol** | **E(j)-E(i) (a.u)** | **F(i. j) (a.u)** |
| LP1 (O41) | σ\*(N3-H38) | 9.35 | 0.95 | 0.087 |
| LP2 (O41) | σ\*(N3-H38) | 81.76 | 0.73 | 0.219 |
| LP3 (O41) | σ\*(N3-H38) | 1.23 | 0.57 | 0.024 |
| LP3 (O41) | σ\*(C10-H12) | 0.29 | 0.69 | 0.014 |
| LP3 (O41) | σ\*(C28-H29) | 0.06 | 0.69 | 0.006 |
| LP1 (O42) | σ\*(N3-H38) | 0.53 | 1.09 | 0.022 |
| LP1 (O42) | σ\*(C10-H11) | 0.06 | 1.22 | 0.008 |
| LP1 (O42) | σ\*(C13-H15) | 0.11 | 1.22 | 0.010 |
| LP2 (O42) | σ\*(N3-H38) | 1.44 | 0.56 | 0.026 |
| LP2 (O42) | σ\*(C13-H14) | 0.10 | 0.69 | 0.008 |
| LP2 (O42) | σ\*(C13-H15) | 0.38 | 0.69 | 0.015 |
| LP2 (O42) | σ\*(C28-H30) | 0.20 | 0.71 | 0.011 |
| LP3 (O42) | σ\*(C10-H11) | 0.48 | 0.68 | 0.018 |
| LP3 (O42) | σ\*(C28-H30) | 0.22 | 0.70 | 0.012 |
| LP1 (O44) | σ\*(N2-H37) | 0.35 | 1.11 | 0.018 |
| LP1 (O44) | σ\*(C4-H6) | 0.40 | 1.23 | 0.020 |
| LP1 (O44) | σ\*(C13-H15) | 1.68 | 1.24 | 0.041 |
| LP2 (O44) | σ\*(N2-H37) | 1.22 | 0.58 | 0.024 |
| LP2 (O44) | σ\*(C4-H6) | 0.27 | 0.71 | 0.013 |
| LP2 (O44) | σ\*(C7-H8) | 0.20 | 0.69 | 0.011 |
| LP2 (O44) | σ\*(C13-H15) | 1.63 | 0.71 | 0.031 |
| LP3 (O44) | σ\*(C4-H6) | 0.85 | 0.70 | 0.024 |
| LP3 (O44) | σ\*(C13-H15) | 3.02 | 0.70 | 0.046 |
| LP1 (O45) | σ\*(N2-H37) | 8.60 | 0.97 | 0.084 |
| LP2 (O45) | σ\*(N2-H37) | 66.58 | 0.73 | 0.198 |
| LP3 (O45) | σ\*(N2-H37) | 0.76 | 0.59 | 0.020 |
| LP3 (O45) | σ\*(C4-H5) | 0.08 | 0.69 | 0.070 |
| LP3 (O45) | σ\*(C32-H35) | 0.37 | 0.72 | 0.016 |
| LP1 (O49) | σ\*(N1-H36) | 8.96 | 0.94 | 0.085 |
| LP1 (O49) | σ\*(C7-H8) | 0.26 | 1.06 | 0.015 |
| LP2 (O49) | σ\*(N1-H36) | 89.58 | 0.73 | 0.229 |
| LP2 (O49) | σ\*(C7-H8) | 0.07 | 0.85 | 0.007 |
| LP3 (O49) | σ\*(N1-H36) | 0.08 | 0.57 | 0.006 |
| LP3 (O49) | σ\*(C7-H8) | 0.83 | 0.69 | 0.023 |
| LP3 (O49) | σ\*(C24-H26) | 0.08 | 0.71 | 0.007 |
| LP1 (O50) | σ\*(N1-H36) | 0.70 | 1.08 | 0.026 |
| LP2 (O50) | σ\*(N1-H36) | 1.93 | 0.55 | 0.030 |
| LP2 (O50) | σ\*(C16-H18) | 0.23 | 0.71 | 0.012 |
| LP2 (O50) | σ\*(C16-H19) | 0.08 | 0.68 | 0.007 |
| LP2 (O50) | σ\*(C20-H21) | 0.08 | 0.67 | 0.007 |
| LP2 (O50) | σ\*(C20-H22) | 0.24 | 0.70 | 0.012 |
| LP3 (O50) | σ\*(C16-H18) | 0.10 | 0.69 | 0.008 |
| LP3 (O50) | σ\*(C20-H22) | 0.11 | 0.69 | 0.009 |

**Table S5:** CHELPG and Mulliken atomic charges calculation.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Atoms** | **Mulliken (e)** | **CHELPG (e)** | **Atoms** | **Mulliken (e)** | **CHELPG (e)** |
| **N1** | -0.625 | 0.187 | **H26** | 0.170 | 0.141 |
| **N2** | -0.654 | -0.077 | **H27** | 0.180 | 0.135 |
| **N3** | -0.499 | 0.138 | **C28** | -0.180 | -0.321 |
| **C4** | -0.236 | -0.006 | **H29** | 0.176 | 0.124 |
| **H5** | 0.178 | 0.025 | **H30** | 0.204 | 0.157 |
| **H6** | 0.254 | 0.106 | **H31** | 0.183 | 0.131 |
| **C7** | -0.375 | 0.097 | **C32** | -0.160 | -0.181 |
| **H8** | 0.211 | 0.058 | **H33** | 0.188 | 0.111 |
| **H9** | 0.166 | 0.028 | **H34** | 0.186 | 0.101 |
| **C10** | -0.232 | 0.021 | **H35** | 0.154 | 0.113 |
| **H11** | 0.241 | 0.118 | **H36** | 0.771 | 0.276 |
| **H12** | 0.172 | 0.067 | **H37** | 0.591 | 0.467 |
| **C13** | -0.626 | -0.400 | **H38** | 0.579 | 0.394 |
| **H14** | 0.201 | 0.189 | **N39** | -0.431 | 0.945 |
| **H15** | 0.251 | 0.210 | **O40** | -0.073 | -0.468 |
| **C16** | -0.228 | -0.307 | **O41** | -0.071 | -0.680 |
| **H17** | 0.161 | 0.129 | **O42** | -0.101 | -0.614 |
| **H18** | 0.211 | 0.165 | **N43** | -0.798 | 0.962 |
| **H19** | 0.171 | 0.104 | **O44** | 0.066 | -0.653 |
| **C20** | -0.240 | -0.250 | **O45** | 0.050 | -0.706 |
| **H21** | 0.164 | 0.096 | **O46** | -0.023 | -0.471 |
| **H22** | 0.210 | 0.153 | **N47** | -0.574 | 0.959 |
| **H23** | 0.155 | 0.091 | **O48** | -0.064 | -0.472 |
| **C24** | -0.137 | -0.265 | **O49** | -0.044 | -0.676 |
| **H25** | 0.199 | 0.135 | **O50** | -0.074 | -0.589 |

**Table S6:** Calculated quantum chemical parameters of PMDT compound.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Quantum**  **Parameters** | **EHOMO**  **(eV)** | **ELUMO**  **(eV)** | **│ΔE│**  **(eV)** | **I** | **A** | **χ** | **η** | **µ** | **ω** | **S** | **Qmax** |
| **DFT/**  **B3LYP/**  **6-31++G(d, p)** | **Gas** | | | | | | | | | | |
| -7.03 | -1.63 | 5.4 | 7.03 | 1.63 | 4.33 | 2.7 | -4.33 | 3.47 | 0.19 | 1.60 |
| **DMSO** | | | | | | | | | | |
| -7.49 | -1.70 | 5.79 | 7.49 | 1.70 | 4.60 | 2.90 | -4.60 | 3.65 | 0.17 | 1.59 |
| **Water** | | | | | | | | | | |
| -7.45 | -1.63 | 5.82 | 7.45 | 1.63 | 4.54 | 2.91 | -4.54 | 3.54 | 0.17 | 1.56 |

ΔE = │EHOMO - ELUMO│(eV), I = - EHOMO (eV), A = - ELUMO, χ = (I+A)/2, η = (I-A)/2, µ = - (I+A)/2, ω = µ2/2 η, S = 1/2 η, Qmax=- µ/ η.

**Table S7:** Evolution of the conductivity as a function of the temperature of C9H26N3(NO3) 3.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| T(K) | R (Ω) | σ (Ω- 1cm- 1) | Ln (σ.T) | 1000/T (K-1) |
| 313 | 183380 | 4.92.10-7 | -8.78 | 3.19 |
| 323 | 182610 | 4.94.10-7 | -8.74 | 3.09 |
| 333 | 126200 | 7.14.10-7 | -8.34 | 3 |
| 343 | 84147 | 1.072.10-6 | -7.90 | 2.91 |
| 353 | 73254 | 1.23.10-6 | -7.74 | 2.83 |
| 363 | 37588 | 2.40.10-6 | -7.04 | 2.75 |
| 373 | 29407 | 3.07.10-6 | -6.78 | 2.68 |

**Table S8:** The binding residue, bond length and interactions of PMDT to antibacterial targets.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Ligand** | **Target protein** | **Binding residue** | **Atoms** | **Bond length** | **Interactions** |
| **PMDT** | 4GXO | A:LYS21  A:LYS32  A:THR28  A:ASN29  Z:PRE999 | NZ  NZ  OG1  ND2  C7 | 5.37  4.17  2.87  2.68  3.28 | Attractive Charge  Attractive Charge  Conventional H-Bond  Conventional H-Bond  Carbon H-Bond |
| 6QXS | D:LYS19  D:ARG22  D:ARG217  Z:PRE999  D:ARG22  D:SER218  D:TYR260  Z:PRE999  Z:PRE999 | NZ  NH2  NH1  N6  NE  OG  OH  O2  N4 | 4.42  4.18  3.33  5.45  2.79  2.60  2.59  4.42  4.98 | Attractive Charge  Attractive Charge  Attractive Charge  Attractive Charge  Conventional H-Bond  Conventional H-Bond  Conventional H-Bond  Pi-Cation  Pi-Anion |
| 1AJ0 | A:MET1  Z:PRE999  A:HIS14  Z:PRE999 | N  N4  CD2  C8 | 3.07  5.01  3.50  3.36 | Attractive Charge  Attractive Charge  Carbon H-Bond  Carbon H-Bond |
| 1U1Z | A:ARG96  A:LYS94  A:ARG96  A:ARG98  Z:PRE999  A:LYS94  A:ARG96  A:ARG98  A:LYS94  Z:PRE999 | NH1  NZ  NH1  NH2  N6  NZ  N  NH2  CE  C4 | 2.75  5.22  5.52  4.33  3.44  2.62  3.18  2.60  3.77  3.26 | H-Bond  Electrostatic  Electrostatic  Electrostatic  Electrostatic  H-Bond  H-Bond  H-Bond  H-Bond  H-Bond |
| 7BYE | B:ARG28  B:LYS55  A:HIS63  A:HIS64  B:THR51  B:ASN52  B:GLN53  Z:PRE999 | NH2  NZ  ND1  N  OG1  N  N  C3 | 2.80  2.82  3.08  3.18  2.60  2.84  3.02  3.30 | Electrostatic  Electrostatic  H-Bond  H-Bond  H-Bond  H-Bond  H-Bond  H-Bond |