

SUPPLEMENTARY MATERIAL

Electron Density and electrostatic properties of two Peptide Molecules: Tyrosyl-Glycyl-Glycine Monohydrate and Glycyl-Aspartic Acid Dihydrate

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Abstract

The electron density and the electrostatic properties of Tyr-Gly-Gly and Gly-Asp molecules have been determined from high-resolution X-Ray diffraction data at 123K. Topological properties of the charge distribution are discussed and compared to those derived from other experimental studies on peptide molecules and the characteristics of the (3,-1) critical points of the C=O, C-N, C-C bonds are analysed.

crystal data for Tyr-Gly-Gly: C₁₃O₅N₃H₁₇; H₂O, Mr = 313, orthorhombic, P₂₁2₁2₁, Z = 4, T = 123 ± 2K, lattice parameters: a = 7.984(2) Å, b = 9.535(3) Å, c = 18.352(5) Å, V = 1397.1(6)Å³, D_x = 1.49 g cm⁻³, μ = 1.2 cm⁻¹ for λ_{M0} = 0.7107 Å.

crystal data for Gly-Asp: C₆O₅N₂H₁₀; 2H₂O, Mr = 212, orthorhombic, P₂₁2₁2₁, Z = 4, T = 123 ± 2K, lattice parameters: a = 9.659(1) Å, b = 9.672(1) Å, c = 10.739(1) Å, V = 1003.3(4)Å³, D_x = 1.40 g cm⁻³, μ = 1.3 cm⁻¹ for λ_{M0} = 0.7107 Å.

FIGURES CAPTION FOR SUPPLEMENTARY MATERIAL

Figures : Residual electron density in peptide, carboxyl and tyrosine planes of YGG and GD. Contour interval 0.05 eÅ⁻³; positive solid line, negative dashed line, zero contour omitted.

Figures : Experimental deformation density in peptide, carboxyl and tyrosine planes of YGG and GD. Contour interval 0.05 eÅ⁻³; positive solid line, negative dashed line, zero contour omitted.

Table: Thermal displacement parameters of YGG (\AA^2).

The standard deviation is between parentheses.

The form of the temperature factor for non-hydrogen atoms is

$$T = \exp(-2p^2 \sum_i \sum_j h_i h_j a_i^* a_j^* U_{ij})$$

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
O1	0.0121(2)	0.0216(3)	0.0108(2)	0.0029(2)	0.0021(2)	0.0001(2)
O2	0.0175(2)	0.0135(2)	0.0099(2)	-0.0020(2)	-0.0009(2)	-0.0012(2)
O31	0.0145(2)	0.0098(2)	0.0184(2)	-0.0029(2)	0.0020(2)	-0.0029(2)
O32	0.0125(2)	0.0126(2)	0.0209(2)	-0.0021(2)	0.0050(2)	-0.0031(2)
OH1	0.0181(3)	0.0151(2)	0.0242(3)	0.0050(2)	0.0068(2)	0.0053(2)
O6	0.0182(2)	0.0129(2)	0.0160(2)	0.0010(2)	0.0007(2)	0.0016(2)
N1	0.0133(2)	0.0129(2)	0.0104(2)	-0.0009(2)	0.0003(2)	0.0001(2)
N2	0.0112(2)	0.0120(2)	0.0099(2)	0.0020(2)	-0.0007(2)	-0.0011(2)
N3	0.0168(3)	0.0092(2)	0.0120(2)	-0.0023(2)	0.0007(2)	-0.0011(2)
C1	0.0109(3)	0.0114(3)	0.0087(2)	0.0010(2)	-0.0010(2)	-0.0006(2)
C1A	0.0119(3)	0.0118(3)	0.0087(2)	0.0013(2)	-0.0011(2)	0.0000(2)
C1B	0.0117(3)	0.0140(3)	0.0100(3)	0.0005(2)	-0.0027(2)	-0.0011(2)
C2	0.0122(3)	0.0096(3)	0.0099(2)	-0.0002(2)	0.0011(2)	-0.0009(2)
C2A	0.0154(3)	0.0110(3)	0.0095(2)	-0.0023(3)	0.0009(2)	-0.0018(2)
C3A	0.0123(3)	0.0100(3)	0.0186(3)	-0.0012(2)	0.0016(3)	-0.0040(2)
C3	0.0114(3)	0.0095(3)	0.0106(2)	-0.0010(2)	0.0004(2)	-0.0007(2)
C1G	0.0109(3)	0.0113(3)	0.0104(2)	0.0001(2)	-0.0000(2)	-0.0010(2)
C1E1	0.0130(3)	0.0135(3)	0.0120(3)	0.0015(3)	0.0019(2)	-0.0019(2)
C1D1	0.0141(3)	0.0140(2)	0.0096(2)	0.0001(3)	0.0024(2)	-0.0012(2)
C1Z	0.0119(3)	0.0118(3)	0.0139(3)	-0.0005(2)	0.0012(2)	-0.0002(2)
C1D2	0.0115(3)	0.0127(3)	0.0135(3)	-0.0004(2)	0.0035(2)	-0.0013(2)
C1E2	0.0132(3)	0.0132(3)	0.0136(3)	-0.0003(3)	0.0041(2)	0.0013(2)
H1A	0.0143					
H1B1	0.0156					
H1B2	0.0156					
H2A1	0.0156					
H2A2	0.0156					
H3A1	0.0182					
H3A2	0.0182					
HN11	0.0156					
HN12	0.0156					
HN13	0.0156					
HN2	0.0156					
HN3	0.0156					
H1D1	0.0169					
H1E1	0.0169					
H1D2	0.0169					
H1E2	0.0169					
HO5	0.0150					
Hw1	0.0208					
Hw2	0.0208					

Table: Thermal displacement parameters of GD (Å²).

The standard deviation is between parentheses.

The form of the temperature factor for non-hydrogen atoms is

$$T = \exp(-2p^2 \sum_i \sum_j h_i h_j a_i^* a_j^* U_{ij})$$

	U ₁₁	U ₂₂	U ₃₃	U ₁₂	U ₁₃	U ₂₃
O21	0.0157(1)	0.0136(1)	0.0161(1)	0.0003(1)	0.0004(1)	0.0034(1)
O22	0.0135(1)	0.0138(1)	0.0243(2)	0.0006(1)	0.0039(1)	0.0003(1)
C2	0.0133(2)	0.0109(1)	0.0128(2)	0.0002(1)	0.0009(1)	-0.0011(1)
C2A	0.0137(2)	0.0097(1)	0.0153(2)	0.0000(1)	0.0000(2)	-0.0012(1)
N2	0.0131(1)	0.0101(1)	0.0191(2)	-0.0000(1)	0.0019(1)	-0.0020(1)
C1	0.0135(2)	0.0094(1)	0.0137(2)	0.0006(1)	0.0003(1)	-0.0006(1)
O1	0.0170(2)	0.0098(1)	0.0255(2)	-0.0001(1)	0.0037(2)	-0.0032(1)
C1A	0.0149(2)	0.0125(2)	0.0184(2)	-0.0015(1)	0.0021(2)	-0.0037(2)
N1	0.0164(2)	0.0127(2)	0.0165(2)	-0.0011(1)	0.0034(1)	-0.0018(1)
C2B	0.0194(2)	0.0117(2)	0.0159(2)	-0.0030(2)	-0.0024(2)	0.0025(1)
C2G	0.0164(2)	0.0117(2)	0.0130(2)	-0.0019(2)	-0.0011(1)	0.0019(1)
O2D1	0.0267(2)	0.0125(1)	0.0170(2)	0.0017(1)	-0.0051(2)	-0.0001(1)
O2D2	0.0263(2)	0.0163(2)	0.0245(2)	-0.0039(2)	-0.0123(2)	0.0038(2)
Ow1	0.0191(2)	0.0159(2)	0.0180(2)	0.0033(1)	-0.0023(1)	0.0000(1)
Ow2	0.0275(2)	0.0215(2)	0.0213(2)	-0.0087(2)	0.0050(2)	-0.0060(2)
H2A	0.0164					
HN2	0.0199					
H1A1	0.0204					
H1A2	0.0241					
HN11	0.0224					
HN12	0.0154					
HN13	0.0193					
H2B1	0.0213					
H2B2	0.0195					
HD22	0.0304					
Hw11	0.0202					
Hw12	0.0235					
Hw21	0.0327					
Hw22	0.0308					

