Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

The monohydrates of the four polar dipeptides L-seryl-L-asparagine, L-seryl-L-tyrosine, L-tryptophanyl-L-serine and L-tyrosyl-L-tryptophan

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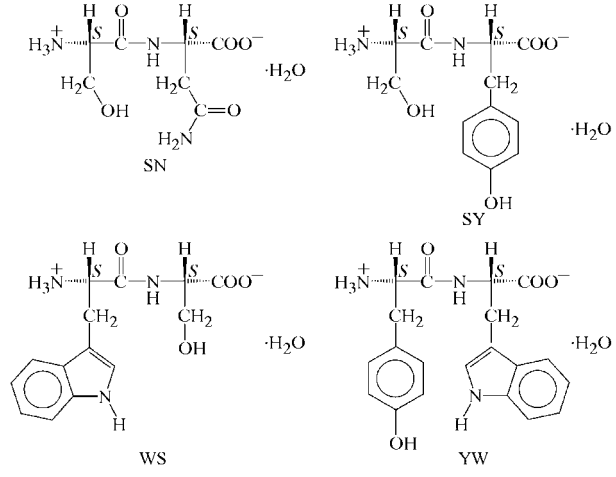
Received 3 December 2007
Accepted 11 February 2008
Online 23 February 2008

The crystal structures of the four dipeptides L-seryl-L-asparagine monohydrate, $C_7H_{13}N_3O_5\cdot H_2O$, L-seryl-L-tyrosine monohydrate, $C_{12}H_{16}N_2O_5\cdot H_2O$, L-tryptophanyl-L-serine monohydrate, $C_{14}H_{17}N_3O_4\cdot H_2O$, and L-tyrosyl-L-tryptophan monohydrate, $C_{20}H_{21}N_3O_4\cdot H_2O$, are dominated by extensive hydrogen-bonding networks that include cocrystallized solvent water molecules. Side-chain conformations are discussed on the basis of previous observations in dipeptides. These four dipeptide structures greatly expand our knowledge on dipeptides incorporating polar residues such as serine, asparagine, threonine, tyrosine and tryptophan.

Comment

A total of 36 dipeptides can be constructed from the six polar residues asparagine (Asn), glutamine (Gln), serine (Ser), threonine (Thr), tyrosine (Tyr) and tryptophan (Trp), but the structure of only one, Tyr–Tyr hydrate (Cotrait *et al.*, 1984), has been investigated previously by single-crystal X-ray diffraction. The title compounds, *viz*. Ser–Asn monohydrate (SN), Ser–Tyr monohydrate (SY), Trp–Ser monohydrate (WS) and Tyr–Trp monohydrate (YW), were studied as part of an effort to increase our knowledge of such dipeptides. The asymmetric units of the four dipeptides are shown in Fig. 1, while essential torsion angles are listed in Tables 1, 3, 5 and 7.



The molecules occur in unconstrained, extended conformations with close to planar peptide bonds and deviations from a perfectly staggered orientation of the amine group reaching a maximum value of 25° for YW.

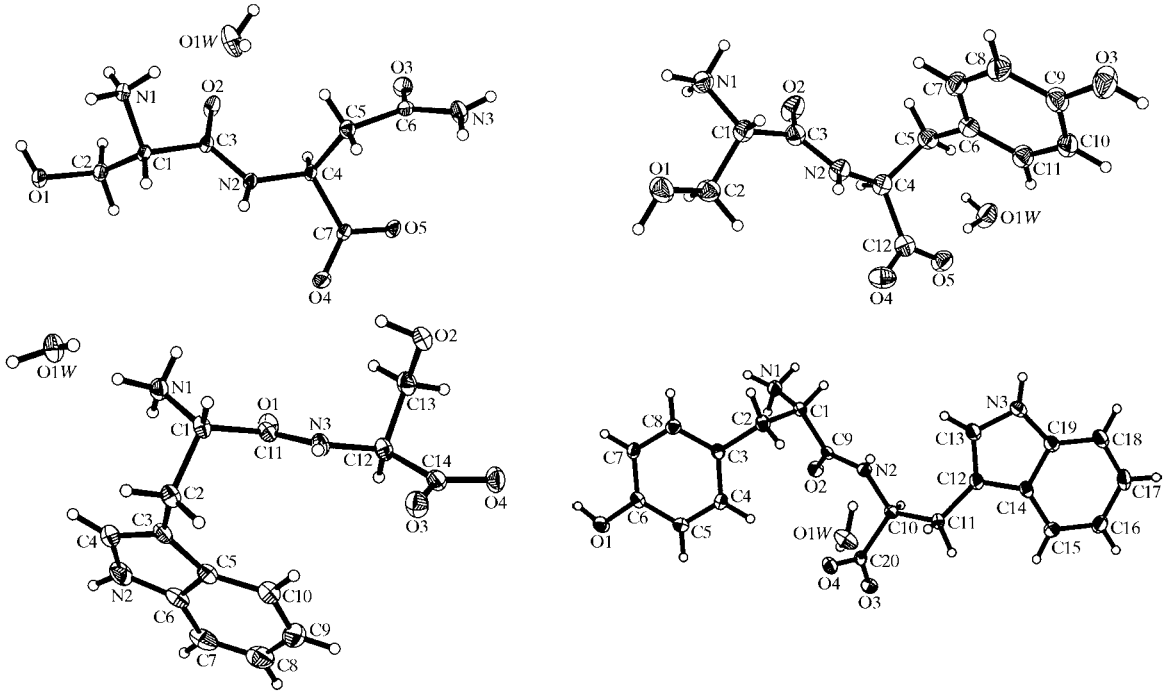


Figure 1
The molecular structures of SN (top left), SY (top right), WS (bottom left) and YW (bottom right). Displacement ellipsoids are shown at the 50% probability level and H atoms are shown as spheres of arbitrary size.

 DOI: 10.1107/S0108270108004228

The side-chain conformations for the title compounds were compared with those of related dipeptides in the Cambridge Structural Database (CSD; Version 5.29 of November 2007; Allen 2002). It is noted that the side chains of N-terminal Ser residues in the CSD are always in a *gauche*− orientation (the *gauche*+/*trans*/*gauche*− distribution is 0:0:5), while C-terminal Ser on the other hand displays a 7:5:1 distribution. An opposite trend is found for Trp, with distributions of 3:0:0 and 1:0:5 for N- and C-terminal residues, respectively. Tyr has the same preference as Trp for *gauche*+ at the N-terminus (5:2:1), but uniquely has *trans* as the most favoured C-terminal orientation (1:3:1). There are only two other dipeptides with a C-terminal Asn residue in the CSD, one each in a *gauche*+ and a *gauche*− orientation. The side-chain conformations found for the four title dipeptides (Tables 1, 3, 5 and 7) agree with the CSD statistics; only for the Tyr residue of SY do we find a conformation (*gauche*+) that is not also the most frequently observed among dipeptides in the CSD (*trans*).

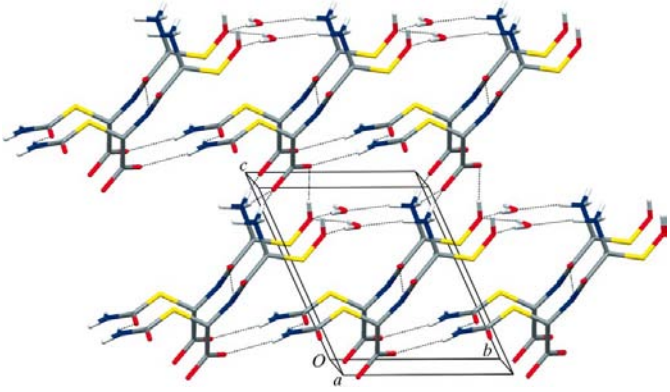


Figure 2
The crystal packing arrangement of SN viewed approximately along the *a* axis, showing the hydrophobic parts of the Ser and Asn side chains (in yellow in the electronic version of the paper). In Figs. 2, 3, 4 and 6, H atoms not involved in the motifs shown have been omitted for clarity, while short hydrogen bonds are indicated by dashed lines.

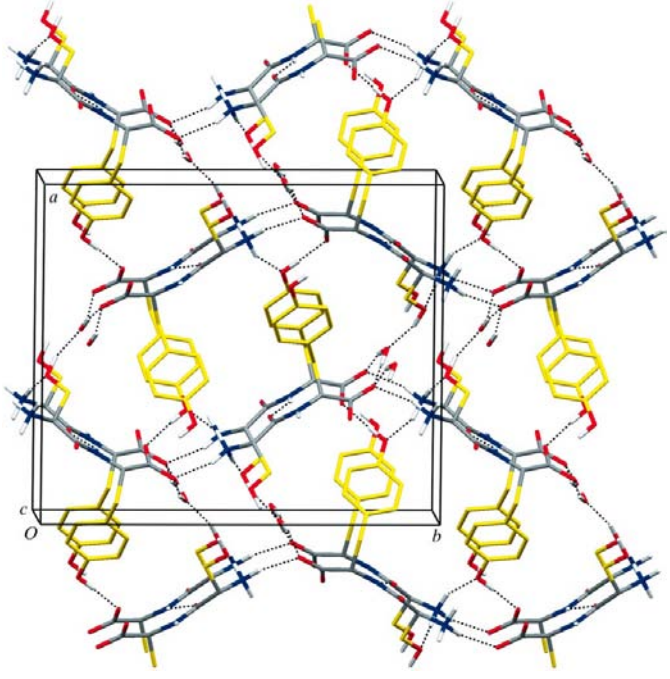


Figure 3
The crystal packing arrangement of SY viewed approximately along the *c* axis, with hydrophobic parts of the Ser and Tyr side chains shown lighter (in yellow in the electronic version of the paper).

It is noteworthy that all four polar dipeptides have been obtained as hydrates. This observation is of particular interest for WS and YW, as all seven dipeptides with a Trp residue in the CSD are also hydrates, indicating a very high propensity for cocrystallization with water molecules for this particular residue. In contrast, SN is the first Ser–Xaa (Xaa is any amino acid) dipeptide to crystallize as a hydrate.

Among the four dipeptides studied, SN has the smallest hydrophobic units in the side chains, which generate inconspicuous hydrophobic columns along the short (4.75 Å) *a* axis (Fig. 2). Accordingly, the hydrogen-bonding network is three-dimensional, and as in all N-terminal Ser-residue dipeptide crystal structures, the hydroxy H atom hydrogen bonds to a carboxylate acceptor (Table 2). This group also accepts two of the amine H atoms, but the third amino H atom, which is usually donated to the Ser hydroxy group, is instead accepted by the cocrystallized water molecule that acts as a bridge between the two groups.

Unlike SN, the crystal packing of SY (Fig. 3) is clearly divided into layers. There is, however, only one head-to-tail chain involving the charged N- and C-terminal groups (Table 4). The remaining two amine H atoms are accepted by the hydroxy groups of the Ser and Tyr side chains. Adding to the three-dimensional hydrogen-bonding pattern, the hydroxy groups also act as donors and span the main-chain layers by interacting with the carboxylate groups in a direct fashion for the Tyr OH group and in an indirect fashion, using the cocrystallized water as a bridging molecule, for the Ser OH group sitting on a shorter side chain. The extra OH group of Tyr compared with Phe means that SY has a completely

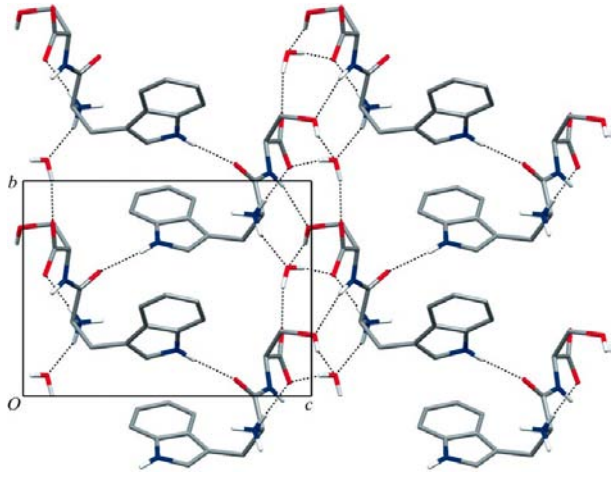


Figure 4
The crystal packing arrangement of WS viewed along the *a* axis.

different structure from Ser–Phe (Helle *et al.*, 2004). Glu–Glu (Eggleston & Hodgson, 1982), on the other hand, shows some of the same traits, with the N-terminal Glu replacing the Ser residue as well as the cocrystallized water molecule in SY.

The structure of WS adds to a series of structures of dipeptides with a C-terminal Ser residue studied previously, including Gly–Ser (Görbitz, 1999), Leu–Ser (Görbitz *et al.*, 2005), Val–Ser trihydrate (Johansen *et al.*, 2005), Val–Ser trifluoroethanol solvate (Görbitz, 2005), Ile–Ser hydrate, Met–Ser hydrate and Phe–Ser (Görbitz *et al.*, 2006), Ala–Ser hydrate (Jones *et al.*, 1978), Arg–Ser acetate hydrate (Verdaguer *et al.*, 1991), and His–Ser in complex with Gly–Glu (Suresh & Vijayan, 1985). In this group, Ile–Ser and Met–Ser have rather similar structures, while all other compounds have individually unique crystal packing arrangements. This is also true for WS, shown in Fig. 4, which, as expected from a dipeptide with large hydrophobic entities, is clearly divided into layers. The hydrogen-bonding pattern (Table 6) is nevertheless completely different even from that of its presumably closest relative Phe–Ser (Görbitz *et al.*, 2006). The most unusual feature is the amine H atom that is not involved in a strong hydrogen bond to an O-atom acceptor, but instead is squeezed in between two Trp side chains where it acts as a donor in weak inter- and intramolecular interactions with C-atom acceptors (Desiraju & Steiner, 1999; Fig. 5).

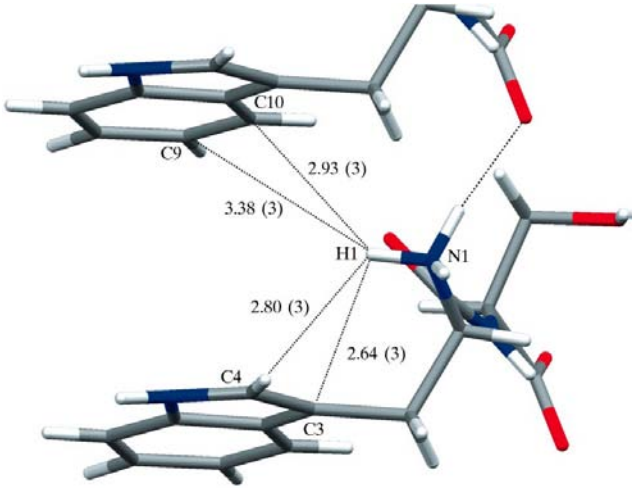


Figure 5
A structural detail showing amino–π N—H···C interactions in WS, with H···C distances in Å.

The structure of YW (Fig. 6) has a 'Big Mac' construction, with two different types of hydrophobic layers, one generated from Tyr side chains and one from Trp side chains, separated by the same type of hydrophilic layers constituted by the peptide main chains. The same pattern was found for the related compounds Tyr–Val (Ramakrishnan *et al.*, 1984), Tyr–Leu (Ramakrishnan & Viswamitra, 1988) and Tyr–Phe (Murali & Subramanian, 1987). It follows that the $N^{\varepsilon}H$ donor of the Trp side chain is involved only in a comparatively weak interaction, with the C atom (C14) of a neighbouring Trp side chain as the acceptor (Table 8). The hydrogen-bonding pattern of this group of dipeptides is furthermore interesting in that, as for WS, one of the amine H atoms does not participate in a strong N—H···O interaction. Instead, it is sandwiched between two aromatic rings, where it is involved in weaker inter- and intramolecular N—H···C contacts (Fig. 7). The complete absence of direct head-to-tail interactions between

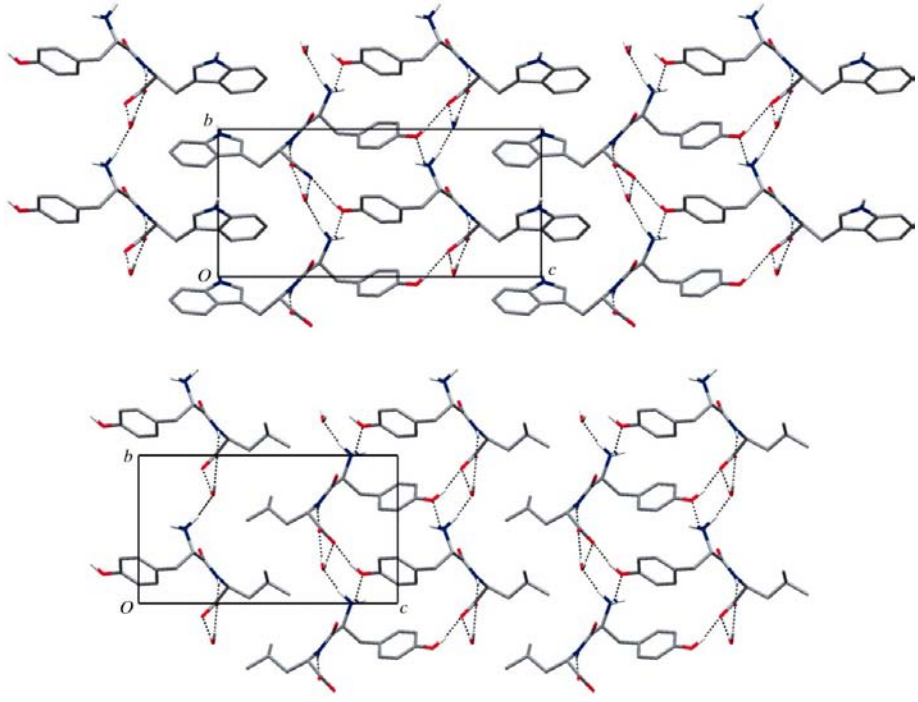


Figure 6
The crystal packing arrangement viewed along the *a* axis for YW (top) and Tyr–Leu (Ramakrishnan & Viswamitra, 1988) (bottom).

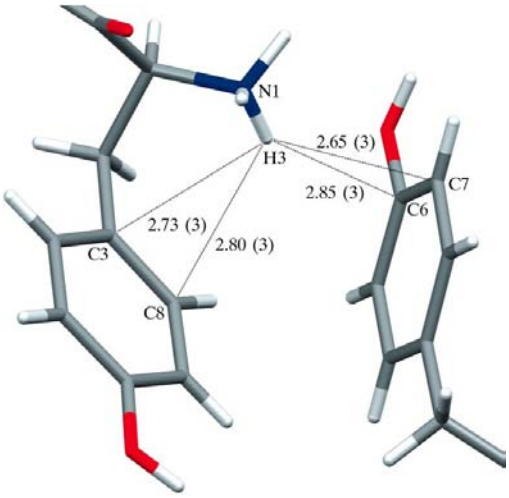


Figure 7
A structural detail showing amino–π N—H···C interactions in YW, with H···C distances in Å.

the charged N- and C-terminal groups in YW is a very rare phenomenon for dipeptide structures.

In summary, all four dipeptides display extensive hydrogen-bonding networks, but the gradual increase in the size of hydrophobic units in the side chains from SN through SY and WS to YW shifts the hydrophobic aggregation pattern from columns to layers and the dimensionality of the hydrogen-bonding pattern from three- to two-dimensional when only strong N—H···O and O—H···O interactions are considered. The presence of a large number of hydrogen-bonding donors and acceptors, including those present in cocrystallized water molecules, makes it possible for polar dipeptides to fulfil their hydrogen-bonding requirements while retaining peptide main chains and side chains in unconstrained conformations, but in both dipeptides with a Trp residue, WS and YW, unusual amino–π N—H···C interactions are observed.

Experimental

The title compounds were obtained from Bachem. Crystals were obtained by slow diffusion of acetonitrile into 30 µl of an aqueous solution containing about 0.2–2.0 mg of the peptide depending on the solubility.

Dipeptide SN

Crystal data

$C_7H_{13}N_3O_5\cdot H_2O$
M_r = 237.22
Triclinic, $P\overline{1}$
a = 4.7547 (1) Å
b = 7.5121 (2) Å
c = 8.5626 (2) Å
α = 115.691 (1)°
β = 90.266 (1)°
γ = 104.957 (1)°
V = 263.87 (1) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 105 (2) K
0.30 × 0.25 × 0.20 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.838, T_{max} = 0.974
2522 measured reflections
1289 independent reflections
1281 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.067
S = 1.09
1289 reflections
190 parameters
3 restraints
Only H-atom coordinates refined
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

Table 1
Selected torsion angles (°) for SN.

N1—C1—C3—N2	124.40 (13)	N1—C1—C2—O1	−57.08 (15)
C1—C3—N2—C4	−172.27 (12)	N2—C4—C5—C6	−169.42 (11)
C3—N2—C4—C7	−153.03 (13)	C4—C5—C6—O3	54.70 (19)
N2—C4—C7—O4	−7.36 (19)	C4—C5—C6—N3	−129.80 (14)

Table 2
Hydrogen-bond geometry (Å, °) for SN.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1W	0.88 (3)	1.88 (3)	2.7446 (18)	171 (2)
N1—H2···O5^{i}	0.91 (3)	1.92 (3)	2.7712 (16)	156 (2)
N1—H3···O5^{ii}	0.81 (3)	2.03 (3)	2.8037 (17)	169 (2)
N2—H4···O2^{iii}	0.86 (2)	2.12 (2)	2.9349 (16)	156 (2)
O1—H5···O4^{ii}	0.81 (3)	1.82 (3)	2.6418 (16)	174 (3)
C1—H11···O2^{iii}	0.98 (2)	2.45 (2)	3.2908 (18)	144.5 (18)
N3—H6···O4^{iv}	0.82 (3)	2.17 (3)	2.9784 (18)	165 (3)
N3—H7···O3^{iii}	0.86 (2)	2.08 (3)	2.9014 (19)	160 (3)
C5—H52···O3^{iii}	0.98 (2)	2.44 (2)	3.2899 (19)	144.2 (19)
O1W—H1W···O1^{iv}	0.88 (4)	1.90 (4)	2.7750 (21)	173 (3)
O1W—H2W···O1^{v}	0.78 (4)	2.31 (4)	3.0814 (20)	165 (3)

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

Dipeptide SY

Crystal data

$C_{12}H_{16}N_2O_5\cdot H_2O$
M_r = 286.28
Orthorhombic, $P2_12_12$
a = 15.3480 (9) Å
b = 17.8805 (11) Å
c = 4.7728 (3) Å
V = 1309.80 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 105 (2) K
0.80 × 0.50 × 0.20 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.814, T_{max} = 0.976
14151 measured reflections
1932 independent reflections
1655 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.102
S = 1.14
1932 reflections
206 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

Table 3
Selected torsion angles (°) for SY.

N1—C1—C3—N2	171.4 (2)	N1—C1—C2—O1	−68.9 (3)
C1—C3—N2—C4	169.2 (2)	N2—C4—C5—C6	62.4 (3)
C3—N2—C4—C12	−148.6 (2)	C4—C5—C6—C7	−88.7 (3)
N2—C4—C12—O4	6.1 (3)		

Table 4
Hydrogen-bond geometry (Å, °) for SY.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.99 (3)	1.96 (3)	2.936 (3)	171 (3)
N1—H2···O5^{ii}	0.99 (3)	1.96 (3)	2.903 (3)	158 (3)
N1—H3···O3^{iii}	0.95 (3)	1.83 (3)	2.721 (3)	155 (3)
O1—H4···O1W^{iv}	0.95 (3)	1.76 (3)	2.679 (3)	163 (3)
N2—H5···O2^{v}	0.82 (3)	2.34 (3)	3.092 (3)	153 (3)
O3—H6···O4^{vi}	0.87 (4)	1.74 (4)	2.612 (3)	173 (4)
C1—H11···O2^{v}	1.00	2.37	3.004 (3)	121
O1W—H1W···O5^{i}	0.846 (17)	2.07 (2)	2.904 (3)	167 (4)
O1W—H2W···O5	0.846 (17)	1.940 (18)	2.782 (3)	164 (3)

Symmetry codes: (i) $x, y, z+1$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+1$; (iii) $-x+1, -y+1, z+1$; (iv) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+1$; (v) $x, y, z-1$; (vi) $x+\frac{1}{2}, -y+\frac{3}{2}, -z$.

Dipeptide WS

Crystal data

$C_{14}H_{17}N_3O_4\cdot H_2O$
M_r = 309.32
Monoclinic, $P2_1$
a = 6.5613 (5) Å
b = 9.1474 (7) Å
c = 12.5052 (9) Å
β = 101.973 (1)°
V = 734.22 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 105 (2) K
0.40 × 0.25 × 0.08 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.893, T_{max} = 0.991
4829 measured reflections
1827 independent reflections
1623 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.091
S = 1.04
1827 reflections
225 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 5
Selected torsion angles (°) for WS.

N1—C1—C11—N3	157.96 (19)	N1—C1—C2—C3	61.6 (3)
C1—C11—N3—C12	−178.97 (19)	C1—C2—C3—C4	−95.8 (3)
C11—N3—C12—C14	−167.49 (19)	N3—C12—C13—O2	66.3 (2)
N3—C12—C14—O3	7.1 (3)		

Table 6
Hydrogen-bond geometry (Å, °) for WS.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···C3	0.90 (3)	2.64 (3)	3.012 (3)	106 (2)
N1—H2···O3^{i}	0.87 (3)	1.86 (3)	2.726 (3)	170 (3)
N1—H3···O1W	0.94 (4)	1.88 (3)	2.762 (3)	156 (3)
N2—H4···O1^{ii}	0.87 (3)	2.01 (3)	2.802 (3)	151 (3)
N3—H5···O2^{iii}	0.84 (3)	2.16 (3)	2.956 (2)	159 (3)
O2—H6···O1W^{iv}	0.91 (3)	1.87 (3)	2.756 (3)	164 (3)
C1—H11···O2^{iii}	1.00	2.47	3.114 (3)	122
C1—H11···O4^{iii}	1.00	2.46	3.403 (3)	158
C9—H91···C6^{v}	0.95	2.71	3.537 (4)	146
O1W—H1W···O4^{vi}	0.84 (4)	1.87 (4)	2.683 (2)	164 (4)
O1W—H2W···O3^{iii}	0.87 (4)	1.83 (4)	2.694 (2)	171 (4)

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

Dipeptide YW

Crystal data

$C_{20}H_{21}N_3O_4\cdot H_2O$
M_r = 385.41
Monoclinic, $P2_1$
a = 5.7309 (3) Å
b = 8.1960 (4) Å
c = 19.0952 (9) Å
β = 91.694 (1)°
V = 896.52 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 105 (2) K
0.36 × 0.20 × 0.14 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.882, T_{max} = 0.986
5858 measured reflections
2245 independent reflections
2089 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.080
S = 1.02
2245 reflections
284 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 7
Selected torsion angles (°) for YW.

N1—C1—C9—N2	161.60 (15)	N1—C1—C2—C3	47.2 (2)
C1—C9—N2—C10	177.26 (15)	C1—C2—C3—C4	78.8 (2)
C9—N2—C10—C20	−67.6 (2)	N2—C10—C11—C12	−64.5 (2)
N2—C10—C20—O3	147.54 (16)	C10—C11—C12—C13	58.1 (3)

Table 8
Hydrogen-bond geometry (Å, °) for YW.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.95 (3)	2.16 (3)	2.915 (2)	137 (2)
N1—H2···O1W^{ii}	0.99 (3)	1.63 (3)	2.611 (2)	170 (2)
N1—H3···C7^{iii}	0.87 (3)	2.66 (3)	3.298 (3)	131 (2)
O1—H4···O4^{i}	0.86 (3)	1.86 (3)	2.653 (2)	153 (3)
N2—H5···O3^{iv}	0.87 (3)	1.96 (3)	2.825 (2)	170 (2)
N3—H6···C14^{v}	0.88 (3)	2.65 (3)	3.419 (3)	147 (2)
O1W—H1W···O4	0.850 (18)	1.877 (17)	2.725 (2)	177 (3)
O1W—H2W···O3^{iv}	0.857 (18)	1.805 (19)	2.653 (2)	170 (3)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+1$; (ii) $x, y+1, z$; (iii) $-x, y+\frac{1}{2}, -z+1$; (iv) $x-1, y, z$; (v) $-x, y+\frac{1}{2}, -z+2$.

Positional parameters were refined for all H atoms of SN. For the three other structures, positional parameters were refined only for H atoms involved in short hydrogen bonds. Other H atoms were positioned with idealized geometry and fixed C—H distances in the range 0.95–1.00 Å. U_{iso}(H) values were refined for the water molecule in WS; for all other H atoms, U_{iso}(H) values were set at 1.2U_{eq} of the carrier atom, or 1.5U_{eq} for the amine and hydroxy groups, and for the cocrystallized water molecules. In the absence of significant anomalous scattering effects, Friedel pairs were merged.

For all compounds, data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The purchase of the Siemens SMART CCD diffractometer was made possible through support from the Research Council of Norway (NFR).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GG3137). Services for accessing these data are described at the back of the journal.

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