Hydrogen bond motifs in the crystals of hydrophobic amino acids – Supplementary Material

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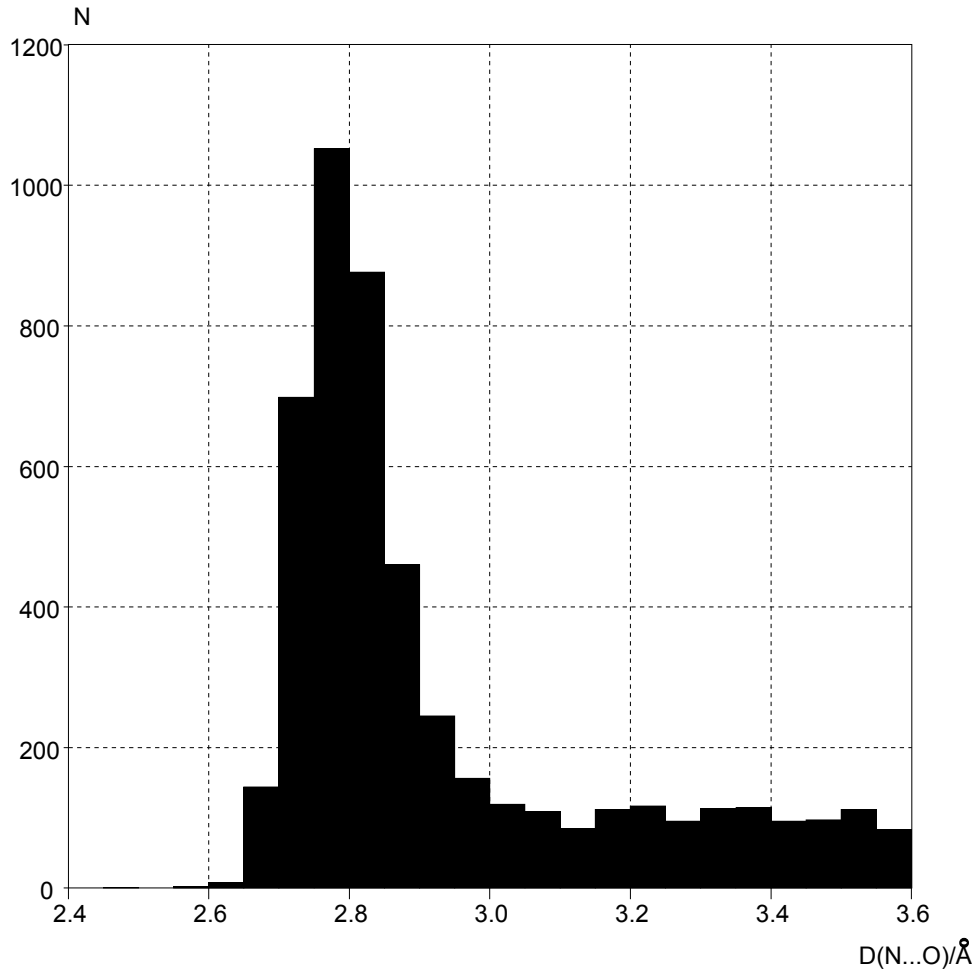

Fig. 1. Histogram of N···O distances in ammonium – carboxylate hydrogen bonds. 1206 error-free, ordered organic structures with an N···O distance of less than 3.6 Å and an N-H···O angle of at least 90° were included. N-H distances were normalised.

Table S1. Space group data and unit cell parameters for the structures discussed in the paper. Unit cell dimensions are given in Å and degrees.

REFCODE	Name	Space grp.	Z	a	b	c	α	β	γ
α-amino acids									
ACXTPY	4-Amino-thiapyran-4-carboxylic acid	$P2_1/c$	4	10.61	6.55	10.97	90.0	96.3	90.0
ACYHXA01	1-Amino-cyclohexane-1-carboxylic acid	$P2_1/a$	4	11.047	6.494	10.831	90.0	95.9	90.0
AHEJEC01	D-Valine	$P2_1$	4	9.661	5.2457	11.9408	90.0	90.5851	90.0
ALUCAL04	D-Alanine	$P2_12_12_1$	4	6.043	12.337	5.784	90.0	90.0	90.0
AMMPRA01	α-Ammonium-α-methylpropionoate	$C2/c$	8	10.6273	9.0102	11.337	90.0	93.749	90.0
BOQCUF	DL-Cysteine	$P2_1/a$	4	9.877	4.737	12.877	90.0	112.044	90.0
CEDFAS	*rac*-DL-Penicillamine	$P2_1/c$	4	11.624	5.919	11.482	90.0	114.48	90.0
CERGEL	DL-Selenomethionine	$P2_1/a$	4	9.893	4.713	17.082	90.0	101.63	90.0
CHEDGL10	*rac*-1,4-Cyclohexadiene-1-glycine	$P2_1/c$	4	15.864	4.81	10.022	90.0	98.03	90.0
DAILEU	D-Alloisoleucine	$P2_1$	4	9.76	5.33	14.26	90.0	98.6	90.0
DEYFOD	L-Selenomethionine	$P2_1$	4	9.5042	5.0999	15.6638	90.0	100.541	90.0
DLABUT03	DL-α-Amino-*n*-butyric acid (form D)	$I2/a$	8	9.88	4.79	24.21	90.0	102.3	90.0
DLABUT05	DL-α-Amino-*n*-butyric acid (form A)	$P2_1/a$	4	9.829	4.78	11.908	90.0	101.02	90.0
DLABUT11	DL-α-Amino-*n*-butyric acid (form B)	$P4_2/n$	8	13.4	13.4	5.82	90.0	90.0	90.0
DLALNI01	DL-Alanine	$Pna2_1$	4	12.0263	6.0321	5.829	90.0	90.0	90.0
DLILEU02	DL-Isoleucine	$P\bar{1}$	2	5.2289	5.4102	13.1095	96.332	90.622	109.493
DLLEUC	DL-Leucine	$P\bar{1}$	2	14.12	5.19	5.39	111.1	86.4	97.0
DLMETA02	DL-Methionine (α-form)	$P2_1/a$	4	9.89	4.7	16.74	90.0	102.3	90.0
DLMETA05	DL-Methionine (β-form)	$I2/a$	8	9.877	4.6915	32.603	90.0	106.25	90.0
DLNLUA01	DL-Norleucine (α-form)	$P2_1/a$	4	9.9069	4.737	16.382	90.0	104.681	90.0
DLNLUA02	DL-Norleucine (β-form)	$C2/c$	8	31.067	4.717	9.851	90.0	91.37	90.0
EXAXEG	4-Fluorophenyl-alanine	$P2_1$	4	8.8132	5.983	16.046	90.0	91.349	90.0
EXAXOQ	3,4,5-Trifluorophenyl-alanine	$P2_1$	4	12.2388	5.3956	14.684	90.0	98.179	90.0
FEGMAG	β-Chloro-L-alanine	$P2_12_12_1$	4	5.437	8.1423	12.21	90.0	90.0	90.0
FIVGEW	DL-2-Amino-2-phenylethanoic acid	$P2_1/c$	4	15.7794	4.8525	9.8771	90.0	97.952	90.0
GLYCIN16	Glycine (γ-form)	$P3_2$	3	6.975	6.975	5.473	90.0	90.0	120.0
GLYCIN19	Glycine (α-form)	$P2_1/n$	4	5.0993	11.9416	5.4608	90.0	111.784	90.0
GLYCIN27	Glycine (β-form)	$P2_1$	2	5.092	6.273	5.384	90.0	113.17	90.0
GLYCIN36	Glycine (δ-form)	Pn	2	4.973	5.939	5.483	90.0	115.76	90.0
GLYCIN68	Glycine (ϵ-form)	Pn	2	4.8887	5.7541	5.4419	90.0	116.682	90.0
ICAMOO	*S*-Benzyl-L-cysteine	$P2_1$	4	9.4224	5.0947	21.551	90.0	94.895	90.0
JOXBED	*S*-(2,2,2-Trifluoro-ethyl)-L-cysteine	$P2_1$	4	9.503	5.166	16.957	90.0	91.45	90.0
KEPJOE	(+/−)-2-*exo*-Amino-6-*endo*-(methylthio)-bicyclo[2.2.1]heptane-2-*endo*-carboxylic acid	$P2_1/c$	4	9.681	10.276	9.773	90.0	91.23	90.0
LALNIN12	L-Alanine	$P2_12_12_1$	4	6.025	12.324	5.783	90.0	90.0	90.0
LALXAX	*rac*-2-Amino-2-(2-fluorophenyl)acetic acid	$P2_1/c$	4	15.738	4.854	9.944	90.0	96.58	90.0
LARSUT	*rac*-2-Amino-4-fluoro-dodec-4-enecarboxylic acid	$P2_1/c$	4	28.081	4.874	9.694	90.0	93.21	90.0
LCYSTN04	L-Cysteine (form II)	$P2_1$	4	9.441	5.222	11.337	90.0	109.0	90.0
LCYSTN21	L-Cysteine (form I)	$P2_12_12_1$	4	8.1156	12.1849	5.4258	90.0	90.0	90.0
LCYSTN24	L-Cysteine (form III)	$P2_12_12_1$	4	8.0558	10.4883	5.3471	90.0	90.0	90.0
LCYSTN26	L-Cysteine (form IV)	$P2_1$	4	8.105	5.442	10.916	90.0	94.897	90.0
LEUCIN01	L-Leucine	$P2_1$	4	14.666	5.324	9.606	90.0	94.06	90.0
LEUCIN03	L-Leucine (high pressure form)	$C2$	4	8.807	5.975	14.193	90.0	96.17	90.0
LISLEU02	L-Isoleucine	$P2_1$	4	9.681	5.301	13.956	90.0	96.16	90.0
LMETON02	L-Methionine	$P2_1$	4	9.493	5.201	14.831	90.0	99.84	90.0
LNLEUC10	L-Norleucine	$C2$	4	9.55	5.26	15.377	90.0	95.6	90.0
LVALIN01	L-Valine	$P2_1$	4	9.682	5.247	11.93	90.0	90.57	90.0
SIMPEJ	(R)-Phenylalanine	$C2$	8	8.804	6.041	31.564	90.0	96.6	90.0
SIMRAH	*(R,S)*-Hexafluoro-valine	$P2_1/c$	4	11.726	6.607	10.1	90.0	109.35	90.0
VALIDL	DL-Valine (monoclinic)	$P2_1/c$	4	5.21	22.1	5.41	90.0	109.2	90.0
VALIDL02	DL-Valine (triclinic)	$P\bar{1}$	2	5.222	5.406	10.838	90.89	92.34	110.02
XADTUR	DL-2-Amino-4-pentenoic acid	$Pca2_1$	8	9.8588	4.8125	25.0546	90.0	90.0	90.0
YIJHOO	DL-Prop-2-ynyl-glycine	$P2_1/a$	4	9.881	4.734	13.017	90.0	108.04	90.0

Cocrystals									
BERNAN	L-Leucine D-2-aminobutanoic acid	$P2_1$	2	5.1673	23.9998	5.4029	90	112.026	90
BERNER	L-Leucine D-norvaline	$P1$	1	5.1639	5.4076	13.1241	91.779	98.138	111.823
BERNIV	L-Leucine D-methionine	$P2_1$	2	5.1451	28.0517	5.4068	90	111.423	90
BERPET	L-Leucine D-valine	$P2_1$	2	5.2002	25.1334	5.4157	90	110.796	90
BERQAQ	L-Valine D-2-aminobutanoic acid	$P2_1$	2	9.9562	4.7417	12.7833	90	106.843	90
BERQEU	L-Valine D-norvaline	$C2$	4	27.2288	4.7397	9.9535	90	96.091	90
BERQIY	L-Valine D-methionine	$P2_12_12_1$	4	28.9379	4.7032	10.0011	90	90	90
FITHIZ	L-Isoleucine D-alanine	$P2_1$	2	9.8944	4.7425	12.9045	90	93.374	90
FITJAT	L-Isoleucine D-2-aminobutanoic acid	$C2$	4	26.9873	4.7471	9.9652	90	94.546	90
FITJEX	L-Isoleucine D-norvaline	$C2$	4	29.0557	4.7551	9.9398	90	101.358	90
FITLEZ	L-Isoleucine D-norleucine	$P2_1$	4	10.012	4.7227	30.335	90	98.38	90
FITLID	L-Isoleucine D-methionine	$C2$	4	31.7681	4.717	10.0043	90	105.914	90
FITMEA	L-Isoleucine D-valine	$P2_1$	2	5.2528	23.9809	5.42	90	110.42	90
FITNIF	L-Isoleucine D-leucine	$P1$	1	5.1933	5.4064	13.6968	91.516	98.603	110.376
GOLVIM	L-Norvaline D-norleucine	$P2_1$	2	9.9166	4.7247	15.3292	90	102.349	90
GOLVOS	L-Methionine D-norleucine	$P2_1$	2	9.8756	4.7029	16.4192	90	107.3283	90
GOLVUY	L-Valine D-norleucine	$C2$	4	29.5751	4.7386	9.9402	90	102.7111	90
GOLWAF	L-*allo*-Isoleucine D-norleucine	$C2$	4	31.4433	4.7622	9.9363	90	100.8378	90
GOLWEJ	L-Leucine D-norleucine	$P2_1$	2	5.1778	27.8078	5.3995	90	112.303	90
XADVED	L-Isoleucine D-*allo*-isoleucine	$P1$	1	5.2438	5.3978	13.2562	93.042	92.811	109.897
XADVIH	DL-Isoleucine DL-*allo*-isoleucine	$P\bar{1}$	2	5.2493	5.4006	13.2778	92.9433	92.8659	109.8571
β-amino acids									
BALNIN01	β-Alanine	$Pbca$	8	9.882	13.807	6.086	90	90	90
GIKNOD	(2*S*,3*R*)-3-Amino-2-phenylthiobutanoic acid	$P2_12_12_1$	4	8.723	19.337	6.365	90	90	90
DASBAB	*cis*-2-Aminocyclopentanecarboxylic acid	$P\bar{1}$	2	5.123	6.374	10.931	97.9	99.08	110.49
DASBEF	*cis*-2-Aminocyclohexanecarboxylic acid	$P\bar{1}$	2	5.160	6.383	12.281	95.11	100.51	108.97
DASBIJ	*cis*-2-Aminocycloheptanecarboxylic acid	$P\bar{1}$	2	5.134	6.317	13.468	101.5	96.17	106.25
DASBOP	*cis*-2-Aminocyclooctanecarboxylic acid	$P\bar{1}$	2	5.397	6.338	13.743	94.49	98.66	105.94
DASBUV	*cis*-2-Aminocyclohex-4-enecarboxylic acid	$P2_1/c$	4	11.757	5.159	12.075	90	110.27	90
DASCAC	3-*exo*-Aminobicyclo-(2.2.1)heptane-2-exo-carboxylic acid	$Pbcn$	8	23.387	6.654	10.007	90	90	90
DATMAN	*trans*-2-Aminocyclohexanecarboxylic acid	$P2_1/c$	4	11.597	5.640	13.011	90	111.07	90
DATMER	*trans*-2-Amino-cyclohex-4-ene-carboxylic acid	$P2_1/c$	4	10.961	5.448	12.994	90	110.97	90
γ-amino acids									
ACIJEC	Vigabatrin	$Fdd2$	16	16.471	22.717	7.203	90	90	90
CIDDEZ	(*S*)-3-Aminomethyl-5-methylhexanoate	$P2_12_12_1$	4	6.464	7.822	18.612	90	90	90
GAMBUT02	γ-Aminobutyric acid (monoclinic form)	$P2_1/a$	4	8.214	10.000	7.208	90	110.59	90
GAMBUT04	γ-Aminobutyric acid (tetragonal form)	$I4_1cd$	16	11.963	11.963	15.282	90	90	90
HAXKEW	4-Amino-3-(2-thienyl)butyric acid	$P2_1/c$	4	13.288	5.231	12.388	90	92.3	90
POSFAE	4-Amino-3-(2-benzothiophen)butyric acid	$P2_1/c$	4	17.857	5.183	12.587	90	100.07	90
QIMKIG	Gabapentin	$P2_1/c$	4	5.8759	6.9198	22.262	90	90.08	90
VICGOE	3-Aminoadamantane-1-carboxylic acid	$P2_1/c$	4	9.357	6.652	15.807	90	102.03	90

Table S2. References for the CSD refcodes used in the paper.

CSD refcode	Reference
ACIJEC	Haramura, M.; Tanaka, A.; Akimoto T.; Hirayama, N. (2004). *Anal. Sci: X-Ray Struct. Anal. Online*, **20**, x9.
ACXTPY	Bhattacharjee, S.K.; Chacko, K.K.; Zand, R. (1975). *J. Cryst. Mol. Struct.*, **5**, 403.
ACYHXA01	Valle, G.; Crisma, M.; Toniolo, C.; Sen, N.; Sukumar, M.; Balaram, P. (1988). *J. Chem. Soc., Perkin Trans. 2* , 393.
AHEJEC01	Wang, W.; Gong, Y.; Li, C. (2002). *Chin. Sci. Bull.*, **47**, 603.
ALUCAL04	Wilson, C.C.; Myles, D.; Ghosh, M.; Johnson, L.N.; Wang, W. (2005). *New J.Chem.*, **29**, 1318.
AMMPRA01	Lynch, D.E.; McClenaghan, I. (2002). *Acta Cryst.*, E**58**, o706.
BALNIN01	Papavinasam, E.; Natarajan, S.; Shivaprakash, N.C. (1986). *Int. J. Pept. Protein Res.*, **28**, 525.
BERNAN	Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, C**55**, 1547.
BERNER	Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, C**55**, 1547.
BERNIV	Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, C**55**, 1547.
BERPET	Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, C**55**, 1547.
BERQAQ	Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, C**55**, 1547.
BERQEU	Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, C**55**, 1547.
BERQIY	Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, C**55**, 1547.
BOQCUF	Luger, P.; Weber, M. (1999). *Acta Cryst.*, C**55**, 1882.
CEDFAS	Howard-Lock, H.E.; Lock, C.J.L.; Smalley, P.S. (1983). *J. Crystallogr. Spectrosc. Res.*, **13**, 333.
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DASBEF	Fábián, L.; Kálmán, A.; Argay, Gy.; Bernáth, G.; Gyarmati, Zs.Cs. (2005). *Cryst. Growth Des.*, **5**, 773.
DASBIJ	Fábián, L.; Kálmán, A.; Argay, Gy.; Bernáth, G.; Gyarmati, Zs.Cs. (2005). *Cryst. Growth Des.*, **5**, 773.
DASBOP	Fábián, L.; Kálmán, A.; Argay, Gy.; Bernáth, G.; Gyarmati, Zs.Cs. (2005). *Cryst. Growth Des.*, **5**, 773.
DASBUV	Fábián, L.; Kálmán, A.; Argay, Gy.; Bernáth, G.; Gyarmati, Zs.Cs. (2005). *Cryst. Growth Des.*, **5**, 773.

DASCAC Fábián, L.; Kálmán, A.; Argay, Gy.; Bernáth, G.; Gyarmati, Zs.Cs. (2005). *Cryst. Growth Des.*, **5**, 773.

DATMAN Fábián, L.; Kálmán, A.; Argay, Gy.; Bernáth, G.; Gyarmati, Zs.Cs. (2005). *Cryst. Growth Des.*, **5**, 773.

DATMER Fábián, L.; Kálmán, A.; Argay, Gy.; Bernáth, G.; Gyarmati, Zs.Cs. (2005). *Cryst. Growth Des.*, **5**, 773.

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EXAXOQ In, Y.; Kishima, S.; Minoura, K.; Nose, T.; Shimohigashi, Y.; Ishida, T. (2003). *Chem. Pharm. Bull.*, **51**, 1258.

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FITMEA Dalhus, B.; Görbitz, C.H. (1999). *Acta Cryst.*, B**55**, 424.

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