Electronic supplementary information for:

Amino acid hydrogen oxalate quasiracemates – hydrocarbon side chains

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Electronic Supplementary Information

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S1. Crystal Growth Experiments

General Considerations. All chemicals and solvents were purchased from the MilliporeSigma, TCI America, or Acros Chemicals and used as received without further purification unless stated otherwise.

Crystal Growth of Racemates DL-Ile·HOx, DL-Leu·HOx, DL-Nle·HOx, DL-Nva·HOx. To a 2-dram vial was added a 1:1:2 molar ratio of the enantiomers (40 – 60 mg total) and oxalic acid dihydrate. The contents of the vial were dissolved in 2 mL of distilled water with the aid of agitation and heat (*ca.* 60 °C) and allowed to crystallize via slow evaporation to give needle-like crystals after several days.

Crystal Growth of Quasiracemates L-Ile·D-Leu·2HOx, L-Ile·D-Nva·2HOx, L-Nva·D-Leu·2HOx, L-Nle·D-Leu·2HOx. To a 2-dram vial was added a 1:1:2 molar ratio of the quasienantiomers (40 – 60 mg total) and oxalic acid dihydrate. The contents of the vial were dissolved in 2 mL of distilled water with the aid of agitation and heat (*ca.* 60 °C) and allowed to crystallize via slow evaporation at room temperature to give needle-like crystals after several days.

S2. X-ray Crystallography

Crystallographic details for each amino acid racemic and quasiracemic compound are summarized in Table S1. X-ray data were collected on a Bruker Venture D8 diffractometer diffractometer using phi and omega scans with graphite monochromatic Cu $K\alpha$ (λ = 1.54178 Å) radiation. Data sets were corrected for Lorentz and polarization effects as well as absorption. The criterion for observed reflections is $I > 2\sigma(I)$. Lattice parameters were determined from least-squares analysis and reflection data. Empirical absorption corrections were applied using SADABS.[1] Structures were solved by direct methods and refined by full-matrix least-squares analysis on F^2 using X-SEED[2] equipped with SHELXT[3]. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares on F^2 using the SHELXL[44] program. H atoms attached to nitrogen or oxygen were located in difference Fourier synthesis and refined isotropically with independent O/N-H distances or restrained to 0.85(2) Å. The remaining H atoms were included in idealized geometric positions with U_{iso}=1.2U_{eq} of the atom to which they were attached (U_{iso}=1.5U_{eq} for methyl groups). Molecular configurations were compared to both the known chirality of the amino acid and estimated Flack parameters[5] and where applicable, atomic coordinates were inverted to achieve correct structural configurations. Hydrogen bond parameters are given in Table S2.

1. SADABS-2016/2 (Bruker AXS). L. Krause, R. Herbst-Irmer, G. M. Sheldrick and D. Stalke, *J. Appl. Cryst.,* 2015, **48**, 3-10.
2. L. J. Barbour, *J. Appl. Cryst*., 2020, **53***,* 1141.
3. G. M. Sheldrick, *Acta Cryst*., 2015, **A71**, 3-8.
4. G. M. Sheldrick, *Acta Cryst*., 2015, **C71**, 3-8.
5 . H. D. Flack, *Acta Crystallogr.,* 1983, **39**¸ 876-881.

Table S1. Crystallographic Data for Hydrogen Oxalate Amino Acids.

	DL-Ile·HOx	DL-Leu·HOx	DL-Nle·HOx	DL-Nva·HOx
Crystal data				
CCDC deposit no.	2017245	2017256	2105696	2017249
Empirical formula	$C_8H_{15}NO_6$	$C_8H_{15}NO_6$	$C_8H_{15}NO_6$	$C_7H_{13}NO_6$
Crystal System, space group	Monoclinic *P*21/n	Triclinic *P*-1	Triclinic *P*-1	Triclinic *P*-1
M_r	221.21	221.21	221.21	207.18
a, Å	9.7133(5)	5.6792(4)	5.6270(5)	5.7278(2)
b, Å	5.7496(3)	9.5687(7)	9.4327(9)	9.4026(3)
c, Å	19.3839(12)	9.9416(8)	10.4431(10)	9.8028(2)
α, deg	90	84.722(3)	88.922(4)	77.211(2)
ϐ, deg	104.238(2)	74.876(3)	75.976(4)	78.253(2)
γ, deg	90	82.793(3)	83.757(4)	78.876(2)
V, (Å^3)	1049.29(10)	516.43(7)	534.57(9)	497.98(3)
Z, *Z'*	4, 1	2, 1	2, 1	2, 1
D_{calc} (g cm^{-3})	1.400	1.423	1.374	1.382
μ (mm^{-1}), rad. type	1.039	1.056	1.020	1.058
F_{000}	472	236	236	220
temp (K)	100(2)	100(2)	100(2)	100(2)
Crystal form, color	needle, colorless	needle, colorless	needle, colorless	needle, colorless
Crystal size, mm	0.095x0.112x0.219	0.063x0.109x0.228	0.028x0.122x0.401	0.052x0.131x0.197
Data collection				
Diffractometer	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD
T_{min}/ T_{max}	0.6928,0.7536	0.6190/0.7531	0.5918/0.7530	0.6102/0.7530
No. of refls. (meas., uniq., and obs.)	15413/2043/2008	10477/1874/1778	9427/1944/1788	5325/1802/1545
R_{int}	0.0258	0.0393	0.0572	0.0288
ϑ_{max} (°)	72.284	68.359	68.281	68.282
Refinement				
R/R^2_ω (obs data)	0.0295/0.0765	0.0366/0.0958	0.0476/0.1258	0.0340/0.0825
R/R^2_ω (all data)	0.0298/0.0.768	0.0381/0.0978	0.0506/0.1297	0.0416/0.0870
S	1.077	1.071	1.075	1.058
No. of refls.	2043	1874	1944	1802
No. of parameters	153	153	194	143
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.310/-0.205	0.305/-0.234	0.764/-0.227	0.226/-0.206
flack	-	-	-	-

Table S1. Crystallographic Data for Hydrogen Oxalate Amino Acids. (Continued)

	L-Ile·D-Leu·2HOx	L-Ile·D-Nva·2HOx	L-Nva·D-Leu·2HOx	L-Nle·D-Leu·2HOx
Crystal data				
CCDC deposit no.	2017253	2017247	2017254	2017255
Empirical formula	$C_{16}H_{30}N_2O_{12}$	$C_{15}H_{28}N_2O_{12}$	$C_{15}H_{28}N_2O_{12}$	$C_{16}H_{30}N_2O_{12}$
Crystal System, space group	Triclinic *P*1	Triclinic *P*1	Triclinic *P*1	Triclinic *P*1
M_r	442.42	428.39	428.39	442.42
a, Å	5.6883(2)	5.7100(4)	5.6561(5)	5.6629(5)
b, Å	9.7485(3)	9.5809(7)	9.5934(8)	9.5020(9)
c, Å	9.8768(4)	9.8621(7)	9.7572(9)	10.2123(10)
α, deg	81.291(2)	74.666(3)	85.735(3)	95.275(6)
β, deg	74.807(2)	79.160(3)	75.315(3)	101.163(5)
γ, deg	81.290(2)	79.281(3)	82.514(3)	97.232(5)
V, (Å^3)	518.86(3)	505.72(6)	507.31(8)	530.99(9)
Z, *Z′*	1, 1	1, 1	1, 1	1, 1
D_{calc} (g cm^{-3})	1.416	1.407	1.402	1.384
μ (mm^{-1}), rad. type	1.051	1.060	1.057	1.027
F_{000}	236	228	228	236
temp (K)	100(2)	100(2)	100(2)	100(2)
Crystal form, color	needle, colorless	needle, colorless	needle, colorless	needle, colorless
Crystal size, mm	0.025x0.084x0.219	0.356x0.055x0.043	0.033x0.058x0.324	0.326x0.111x0.068
Data collection				
Diffractometer	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD	Bruker D8 Venture CCD
T_{min}/ T_{max}	0.6825/0.7531	0.6201/0.7535	0.467620/0.753579	0.5865/0.7531
No. of refls. (meas., uniq., and obs.)	11263/3656/3392	12329/3780/3501	1772/1772/1687	7892/3399/3072
R_{int}	0.0395	0.0407	0.01643	0.0547
ϑ_{max} (°)	68.242	72.193	68.184	68.591
Refinement				
R/R^2_ω (obs data)	0.0322/0.0734	0.0304/0.0783	0.0669/0.1715	0.0497/0.1265
R/R^2_ω (all data)	0.0366/0.0761	0.0333/0.0803	0.0700/0.1741	0.0560/0.1322
S	1.069	1.085	1.101	1.060
No. of refls.	3656	3780	1772	3399
No. of parameters	305	295	280	304
$\Delta\rho_{max/min}$ (e·Å^{-3})	0.232/ -0.184	0.253/-0.155	0.506/-0.344	0.392/-0.244
flack	0.12(12)	0.07(14)	0.5(10)	-0.23(19)

Table S2. Hydrogen Bond Parameters for Racemic and Quasiracemic Hydrogen Oxalate Amino Acids.

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
DL-Ile·HOx	O3–H3···O5^{i}	0.906(16)	1.689(16)	2.5920(10)	174.9(14)
	N1–H1A···O6^{ii}	0.916(15)	1.931(15)	2.8278(12)	165.6(13)
	N1–H1C···O5^{iv}	0.914(15)	1.996(15)	2.8509(11)	155.0(13)
	N1–H1B···O2^{ii}	0.899(15)	1.985(15)	2.8542(12)	162.3(13)
	O1–H1···O6^{iii}	0.865(16)	1.724(17)	2.5736(10)	166.7(15)

Symmetry codes: (i) *x, y*-1, *z;* (ii) 1-*x*, -*y*, 1-*z*; (iii) *x*-1/2, 1/2-*y, z*-1/2; (iv) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
DL-Leu·HOx	O1–H1···O6^{v}	0.93(2)	1.66(2)	2.5773(13)	165.6(17)
	O3–H3···O5^{i}	0.917(19)	1.699(19)	2.6132(13)	174.8(16)
	N1–H1A···O2^{ii}	0.912(18)	1.940(18)	2.8127(15)	159.6(15)
	N1–H1B···O5^{iii}	0.938(18)	1.897(18)	2.8164(15)	166.1(15)
	N1–H1C···O6^{iv}	0.911(18)	1.940(19)	2.8504(15)	176.8(15)

Symmetry codes: (i) *x*-1*, y*, *z;* (ii) -*x*, 1-*y,* 2-*z*; (iii) *x*-1, *y*+1*, z*; (iv) 1-*x,* 1-*y,* 2-*z*; (v) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
DL-Nle·HOx	O6–H6···O4^{i}	0.84(2)	1.74(2)	2.5820(15)	176(2)
	O1a–H1···O3^{ii}	0.79(2)	1.81(3)	2.5736(18)	164(2)
	O1A–H1···O3^{iii}	0.98(3)	1.81(3)	2.687(17)	147(2)
	N1a–H1A···O4^{iv}	0.91(3)	1.91(3)	2.809(2)	168(2)
	N1a–H1B···O2^{vii}	0.82(3)	2.01(3)	2.768(2)	152(2)
	N1a–H1C···O3^{vii}	0.94(3)	1.97(3)	2.907(2)	175(2)
	N1A–H1A1···O4^{ii}	0.91	1.90	2.64(2)	136.8
	N1A–H1A3···O5^{vi}	0.91	2.05	2.92(3)	159.4

Symmetry codes: (i) *x*-1*, y*, *z;* (ii) *x*-1, *y*+1*, z*; (iii) 1-*x*, 1-*y*, -*z*; (iv) 2-*x,* 1-*y*, -*z*; (v) *x*-1*, y*+1*, z*; (vi) *x, y*+1, *z*; (vii) *x, y*, *z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
DL-Nva·HOx	O1–H1···O6^{v}	0.88(2)	1.73(2)	2.5771(14)	161.6(19)
	O3–H3···O5^{i}	0.89(2)	1.75(2)	2.6348(14)	173.8(18)
	N1–H1A···O6^{ii}	0.92(2)	1.95(2)	2.8529(17)	166.4(16)
	N1–H1B···O2^{iii}	0.93(2)	1.94(2)	2.8408(16)	161.9(17)
	N1–H1C···O5^{iv}	0.92(2)	1.94(2)	2.8082(16)	157.7(17)

Symmetry codes: (i) *x*-1*, y*, *z;* (ii) 1-*x*, 2-*y,* 1-*z*; (iii) -*x*, 2-*y,* 1-*z*; (iv) *x*-1*, y, z*+1; (v) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Ile·D-Leu·2HOx	O1–H1···O8^{i}	0.76(4)	1.83(4)	2.571(3)	164(4)
	O3–H3···O12^{ii}	1.00(4)	1.58(5)	2.570(3)	172(4)
	O5–H5···O7^{iii}	0.82(5)	1.83(5)	2.639(3)	171(4)
	O9–H9···O11^{iv}	0.99(4)	1.61(4)	2.601(3)	172(4)
	N1–H1B···O4^{vii}	0.87(4)	1.99(4)	2.803(4)	155(4)
	N1–H1C···O12^{v}	0.91(5)	1.92(5)	2.828(4)	173(4)
	N1–H1A···O7^{vii}	0.85(5)	2.02(5)	2.849(4)	168(4)
	N2–H2A···O11^{vii}	0.93(5)	1.94(5)	2.827(4)	158(4)
	N2–H2C···O8^{vi}	0.92(5)	1.93(5)	2.833(4)	169(4)
	N2–H2B···O2^{vii}	0.88(5)	2.04(5)	2.833(4)	169(4)

Symmetry codes: (i) 1+*x, y*-1, *z;* (ii) *x*-1, 1+*y, z*; (iii) *x*-1, *y, z*; (iv) 1+*x, y, z*; (v) *x,* 1+*y, z*; (vi) *x, y*-1, *z;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Ile·D-Nva·2HOx	O1–H1···O8^{i}	0.84(2)	1.77(3)	2.550(4)	153(5)
	O3–H3···O12^{ii}	0.91(4)	1.69(4)	2.592(4)	169(4)
	O5–H5···O7^{iii}	0.88(2)	1.75(3)	2.619(4)	175(4)
	O9–H9···O11^{iv}	0.87(2)	1.77(3)	2.621(4)	168(4)
	N1–H1B···O4^{vii}	0.86(2)	2.06(3)	2.857(4)	156(4)
	N1–H1C···O12^{v}	0.88(3)	2.00(3)	2.862(4)	169(4)
	N1–H1A···O7^{vii}	0.86(2)	1.97(3)	2.807(4)	163(4)
	N2–H2A···O11^{vii}	0.87(2)	2.03(3)	2.830(4)	154(4)
	N2–H2C···O8^{vi}	0.88(2)	1.95(3)	2.815(5)	164(4)
	N2–H2B···O2^{vii}	0.88(2)	1.99(3)	2.841(4)	165(5)

Symmetry codes: (i) 1+*x, y, z*-1*;* (ii) *x*-1, *y,* 1+*z*; (iii) *x*-1, *y, z*; (iv) 1+*x, y, z*; (v) *x, y,* 1+*z*; (vi) *x, y, z*-1*;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Nva·D-Leu·2HOx	O1–H1···O8^{i}	0.92(3)	1.66(4)	2.572(5)	171(7)
	O3–H3···O12^{ii}	0.92(4)	1.67(4)	2.577(5)	170(9)
	O5–H5···O7^{iii}	0.92(4)	1.68(4)	2.599(5)	175(7)
	O9–H9···O11^{iv}	0.92(3)	1.67(4)	2.589(5)	174(7)
	N1–H1B···O4^{vii}	0.91	1.95	2.819(6)	158.5
	N1–H1C···O7^{vii}	0.91	1.94	2.814(5)	161.0
	N1–H1A···O12^{v}	0.91	1.92	2.833(6)	176.7
	N2–H2A···O8^{vi}	0.91	1.98	2.882(6)	172.7
	N2–H2C···O11^{vii}	0.91	1.94	2.822(6)	163.8
	N2–H2B···O2^{vii}	0.91	1.94	2.791(6)	154.3

Symmetry codes: (i) 1+*x, y*-1, *z;* (ii) *x*-1, 1+*y,* 1; (iii) *x*-1, *y, z*; (iv) 1+*x, y, z*; (v) *x,* 1+*y, z*; (vi) *x, y*-1, *z;* (vii) *x, y, z*

Compound	D–H···A	D–H (Å)	H···A (Å)	D···A (Å)	D–H···A (°)
L-Nle·D-Leu·2HOx	O1–H1···O8^{i}	0.86(3)	1.74(3)	2.581(4)	167(6)

O3–H3···O12^{ii}	0.85(3)	1.73(3)	2.575(4)	169(7)
O5–H5···O7^{iii}	0.85(3)	1.78(3)	2.603(4)	165(6)
O9–H9···O11^{iv}	0.85(3)	1.77(3)	2.605(4)	167(6)
N1–H1B···O7^{vii}	0.98(7)	1.85(6)	2.786(5)	159(5)
N1–H1C···O12^{v}	0.88(7)	1.98(7)	2.858(5)	174(6)
N1–H1A···O4^{vii}	0.90(7)	1.95(7)	2.800(4)	158(6)
N2–H2A···O8^{vi}	0.85(6)	2.00(7)	2.842(5)	166(5)
N2–H2C···O11^{vii}	0.88(7)	1.97(7)	2.808(5)	160(6)
N2–H2B···O2^{vii}	0.90(6)	2.01(6)	2.806(4)	147(6)

Symmetry codes: (i) *x*-1, *y*-1, *z;* (ii) 1+*x*, 1+*y,* 1; (iii) 1+*x*, *y, z*; (iv) *x*-1, *y, z*; (v) *x,* 1+*y, z*; (vi) *x, y*-1, *z;* (vii) *x, y, z*

S3. DL-Nle·HOx Crystal Photograph and View of Crystal Structure

A) B)

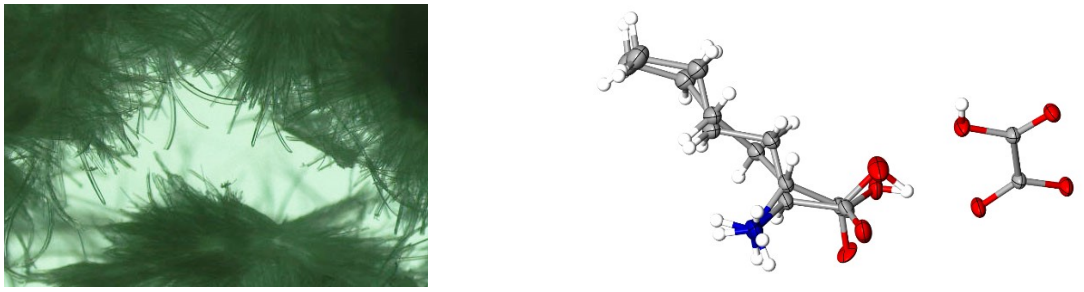

Fig. S1 DL-Nle·HOx A) crystal morphology and B) view of whole-molecule Nle disorder.

S4. Structure Indices (χ_{RMS} and C_i)

Conformational Assessments (χ_{RMS}). Each quasiracemic hydrogen oxalate amino acid structure was processed using X-SEED[2] where each amino acid component was isolated, configuration inverted to L if necessary, and saved as an individual file. These structure files were then loaded into CCDC-Mercury[6] and processed using the structure overlay feature. Hydrogen atoms were omitted from the assessments. The initial overlay process involved matching common atoms from the core N-C(C)-CO_2 fragments to determine the root-mean-squared best fit value (χ_{RMS}). Additional overlay calculations were performed on the two molecules by including the core fragments and the next atom associated with the side chain *R* group. These sequential assessments provided a range of χ_{RMS} values that shows the dependency of molecular conformations to chain length.

6. C. F. Macrae, I. Sovago, S. J. Cottrell, P. T. A. Galek, P. McCabe, E. Pidcock, M. Platings, G. P. Shields, J. S. Stevens, M. Towler and P. A. Wood, *J. Appl. Cryst.*, 2020, **53**, 226 – 235.

Inversion Symmetry Assessments (C_i). The quasiracemic crystal structures were initially processed using X-SEED[2]. The hydrogen oxalate fragments, hydrogen atoms, and non-hydrogen atoms lacking an equivalent partner were omitted. Each quasienantiomeric pair was organized with the same packing motifs – *i.e.,* $R_2^2(10)$ patterns – to provide consistent processing of the structures. A series of structure files were then generated that differed by the length of the *R* groups. These files containing near inversion related quasiracemate fragments and were assessed using Avnir's *Continuous Symmetry Measures* online tools.[7] The output from this process gave a quantitative measure (C_i values) of the degree of inversion symmetry for each structural fragment as a function of side chain length.

Table S3. Symmetry (C_i values) and Conformation (χ_{RMS} values) Data for Quasiracemates

Compound	Molecular section	χ_{RMS} L-Ile·D-Leu·2HOx	χ_{RMS} FITNIF	C_i L-Ile·D-Leu·2HOx	C_i FITNIF
L-Ile·D-Leu·2HOx	1	0.166	0.100	0.3864	0.0879
	2	0.559	0.169	1.0040	0.3256
	3	0.537	0.285	0.7870	0.8640

Compound	Molecular section	χ_{RMS} L-Ile·D-Nva·2HOx	χ_{RMS} FITJEX	C_i L-Ile·D-Nva·2HOx	C_i FITJEX
L-Ile·D-Nva·2HOx	1	0.016	0.060	0.0060	0.0651
	2	0.026	0.102	0.0065	0.1567
	3	0.035	0.124	0.0096	0.2743

Compound	Molecular section	χ_{RMS} L-Nva·D-Leu·2HOx	χ_{RMS} BERNER	C_i L-Nva·D-Leu·2HOx	C_i BERNER
L-Nva·D-Leu·2HOx	1	0.036	0.017	0.0109	0.0021
	2	0.063	0.018	0.0447	0.0034
	3	0.063	0.023	0.0490	0.0031

Compound	Molecular section	χ_{RMS} L-Nle·D-Leu·2HOx	χ_{RMS} GOLWEJ	C_i L-Nva·D-Leu·2HOx	C_i GOLWEJ
L-Nle·D-Leu·2HOx	1	0.020	0.102	0.0050	0.1389
	2	0.036	0.129	0.0178	0.3242
	3	0.118	0.215	0.1146	0.7480

7. P. Alemany, D. Casanova, S. Alvarez, C. Dryzun and David Avnir, "Continuous Symmetry Measures: A New Tool in Quantum Chemistry" Reviews in Computational Chemistry, Volume 30, Abby L. Parrill and Kenneth B. Lipkowitz, Editors, Chapter 7, p. 289 – 352, Wiley, 2017. M. Pinsky, C. Dryzun, D. Casanova, P. Alemany and D. Avnir, *J. Comput. Chem*., 2008, **29**, 2712 – 2721. H. Zabrodsky, S. Peleg and D. Avnir, *J. Am. Chem. Soc*., 1992, **114**, 7843 – 7851.

S5. Hydrogen Oxalate Cambridge Crystallographic Database (CSD) Search

The following data were generated *via* a search of the *CCDC-Cambridge Structural Database* (CSD, version 5.42, update 2) for O-H···O^- hydrogen oxalate-hydrogen oxalate interactions.

Table S4. CSD Search Data for Crystal Structures Containing Hydrogen Oxalate Anions.

REFCODE	Frag.	OH···O (°)	O···O^- (Å)	Space Group Number	Space Group Symbol	Z'	Z	HOx Hbond Strand Symm.	Primary Molecule Type	Oxalate stacking	HOx stacking distance	Stacking motif
Current Study												
DL-Ile·HOx	1	174.9	2.592	14	P21/n	1	4	translation	amino acid	Y	3.039	dimer
DL-Leu·HOx	1	174.8	2.613	2	P-1	1	2	translation	amino acid	Y	3.056	dimer
DL-Nle·HOx	1	176	2.582	2	P-1	1	2	translation	amino acid	Y	2.972	dimer
DL-Nva·HOx	1	161.6	2.577	2	P-1	1	2	translation	amino acid	Y	3.135	dimer
L-Leu·D-Ile·2HOx	1	171	2.639	1	P1	1	1	translation	amino acid	Y	3.003	dimer
	2	172	2.601									
L-Nva·D-Ile·2HOx	1	175	2.619	1	P1	1	1	translation	amino acid	Y	3.145	dimer
	2	168	2.621									
L-Leu·D-Nva·2HOx	1	175	2.599	1	P1	1	1	translation	amino acid	Y	3.035	dimer
	2	174	2.589									
L-Leu·D-Nle·2HOx	1	165	2.603	1	P1	1	1	translation	amino acid	Y	3.080	dimer
	2	167	2.605									
CSD Entries												
LOSHUZ	1	174.733	2.459	2	P-1	1	2	translation	quat amine	Y	4.238	dimer
ZOZMOT	1	174.75	2.545	2	P-1	1	2	translation	triazolium	Y	3.093	dimer
ACOQER	1	171.139	2.587	14	P21/n	1	4	translation	amino acid	Y	3.295	dimer
AFIVAO01	1	175.526	2.596	148	R-3	1	18	31 screw	triazolium	Y	3.109	dimer
AHOXLH02	1	160.958	2.553	14	P21/n	2	8	n glide	quat amine	Y	3.115	inf
AHOKLH02		172.38	2.557					n glide		Y	3.267	
AHOXLH03	1	176.92	2.563	62	Pnma	1	8	n glide	quat amine	Y	3.021	Inf

AJUMOH	1	178.034	2.558	15	C2/c	1	8	translation	quat amine	Y	3.135	dimer
AMTBUB	1	167.235	2.507	2	P-1	1	2	translation	amino acid	N		
ARAHEG	1	166.873	2.562	14	P21/n	1	4	21 screw	quat amine	N		
BASZUT	1	171.359	2.651	4	P21	1	2	21 screw	quat amine	N		
BEJLAG	1	178.772	2.468	14	P21/c	1	4	translation	quat. amine	N		
BEZCOY	1	151.766	2.461	14	P21/c	1	4	translation	quat. amine	N		
BOBQAK	1	179.797	2.483	43	Fdd2	1	16	translation	quat amine	N		
CABZAJ	1	168.706	2.522	14	P21/c	1	4	c glide	quat amine	N		
CIGQIV	1	174.377	2.502	14	P21/c	1	4	translation	quat amine	N		
CIKNUI01	1	173.183	2.587	14	P21/c	1	4	translation	quat amine	N		
CIRXEH	1	177.652	2.532	4	P21	1	2	translation	quat amine	Y	3.162	inf
CITSED10	1	171.81	2.471	7	Pc	2	4	translation	quat amine	Y	2.975	inf
CITSED10	2	173.46	2.514					translation		N		
CONGAP	1	171.182	2.573	2	P-1	1	2	translation	quat amine	N		
COSDUK	1	171.511	2.583	14	P21/c	1	4	translation	pyridinium	Y	2.983	inf
DAQXOJ	1	171.415	2.539	14	P21/c	0.5	2	c glide	quat amine	N		
DMAHOX	1	176.952	2.533	14	P21/c	1	4	translation	quat amine	Y	3.127	dimer
DUJKOK	1	169.43	2.537	1	P1	2	2	translation	quat amine	Y	3.030	dimer
DUJKOK	2	168.563	2.538	1	P1		2	translation		N		
DUJKOK	3	157.247	2.552	1	P1		2	translation		N		
DUJKOK	4	169.023	2.556	1	P1		2	translation		N		
EGOPAS	1	151.07	2.51	4	P21	2	4	21 screw	quat amine	N		
EMUDAS	1	171.633	2.554	2	P-1	2	4	translation	quat amine	Y	3.167	inf
EMUDAS	2	170.255	2.561	2	P-1		4	translation		N		
EVEPIF	1	171.866	2.579	2	P-1	1	2	translation	imidizolium	N		
FAHQUB	1	173.405	2.584	4	P21	2	4	translation	quat amine	Y	3.066	dimer
FAYFAN	1	175.772	2.699	15	C2/c	0.5	4	c glide	pyridinium	Y	3.204	inf
FIBCUR	1	172.978	2.469	61	Pbca	1	8	translation	quat amine	N		
FOMBIU	1	171.954	2.548	15	C2/c	1	8	translation	quat amine	Y	3.142	dimer
FOSJOP	1	173.959	2.582	2	P-1	1	2	translation	quat amine	Y	3.260	dimer

GALMIS	1	166.594	2.508	14	P21/c	1	4	c glide	pyridinium	N		
GENQOG01	1	175.741	2.584	15	C2/c	1	8	translation	quat amine	N		
GOLDES	1	179.095	2.556	15	C2/c	1	8	translation	quat amine	Y	3.115	dimer
GUSKAH	1	170.172	2.453	4	P21	2	4	translation	quat amine	N		
GUSKAH	2	176.12	2.487					translation		N		
GUWPOF	1	153.587	2.573	14	P21/n	1	4	n glide	quat amine	N		
HAGZUL	1	172.668	2.577	1	P1	2	2	translation	amino acid	Y	3.142	dimer
HAGZUL	2	177.061	2.617	1	P1		2	translation		N		
HIQXUD	1	176.388	2.546	14	P21/c	1	4	translation	imidazolium	N		
HOVFEF	1	170.519	2.567	4	P21	1	2	21 screw	imidazolium	N		
HUZQEA	1	173.858	2.503	4	P21	1	2	translation	quat amine	N		
IMEGIR18	1	175.448	2.566	14	P21/c	1	4	c glide	amino acid	Y	2.986	inf
JAZROU	1	173.532	2.508	29	Pca21	2	8	a glide	quat amine	N		
JAZROU	2	172.043	2.550	29	Pca21		8	a glide		N		
KAKYIH	1	170.295	2.472	4	P21	1	2	21 screw	quat amine	N		
KHOXAL11	1	173.818	2.523	14	P21/c	1	4	c glide	K+	Y	2.780	inf
KIGJUG	1	173.404	2.559	62	Pnma	1	8	n glide	H3O+	Y	3.025	inf
KUDWEN	1	174.027	2.564	2	P-1	1	2	translation	quat amine	Y	3.108	dimer
LARXAG	1	175.515	2.465	18	P21212	0.5	2	translation	quat amine	Y	3.306	dimer
LHOXAL01	1	171.016	2.490	1	P1	1	1	translation	Li+	Y	2.947	inf
LOCLOF	1	172.414	2.535	19	P212121	1	4	21 screw	amino acid	N		
MAMHOX	1	174.476	2.515	14	P21/n	1	4	n glide	quat amine	Y	3.520	inf
MEQPAZ02	1	174.792	2.590	14	P21/n	1	4	translation	imidazolium	Y	3.207	inf
MIFRAU	1	172.156	2.610	15	C2/c	1	8	translation	amino acid,	Y	3.303	dimer
MIKXEK	1	175.12	2.589	19	P212121	1	4	21 screw	quat amine	N		
MOHDIX	1	169.427	2.608	19	P212121	1	4	translation	amino acid	Y	2.970	dimer
MOSNAK01	1	173.504	2.627	15	C2/c	1	8	translation	pyridinium	Y	3.099	dimer
NELPUP	1	173.955	2.587	14	P21/n	1	4	translation	amino acid	Y	3.063	inf
NHOXAL06	1	175.475	2.567	2	P-1	1	2	translation	Na+	Y	3.068	inf
NORGEH	1	171.146	2.632	33	Pna21	1	4	21 screw	pyridinium	N		

NOSXAU	1	164.511	2.578	14	P21/c	1	4	c glide	amino acid	N		
NUZQOO	1	166.594	2.585	33	Pbn21	1	4	translation	quat amine	Y	3.609	inf
OJITEH	1	173.134	2.516	2	P-1	1	2	translation	quat amine	Y	3.945	dimer
OKAVED	1	176.266	2.463	14	P21/n	2	8	translation	quat amine	N		
OKAVED	2	171.08	2.589	14	P21/n		8	translation		N		
PAVQEK	1	178.379	2.559	13	P2/c	1	4	translation	quat amine	Y	3.104	dimer
PEPMOM01	1	173.233	2.578	15	C2/c	0.5	4	translation	quat amine	N		
PEPQEG	1	175.509	2.573	56	Pccn	0.5	4	translation	quat amine	Y	3.454	inf
PEPQEG01	1	174.233	2.550	18	P21212	0.5	2	translation	quat amine	N		
PEXCIH	1	173.919	2.536	19	P212121	1	4	21 screw	quat amine	N		
PONSAO	1	175.296	2.562	15	C2/c	1	8	translation	quat amine	Y	3.156	dimer
QIGCEO02	1	174.076	2.544	15	C2/c	0.5	4	translation	quat amine	Y	3.026	dimer
QIQKEI	1	174.14	2.495	4	P21	2	4	translation	quat amine	Y	4.192	dimer
QIQKEI	1	171.91	2.503					translation		N		
QIQKOS	1	178.796	2.636	14	P21/n	1	4	translation	quat amine	Y	3.411	dimer
QOCCUI	1	169.97	2.449	2	P-1	1	2	translation	pyridinium	Y	2.860	dimer
RIDNUQ03	1	165.47	2.510	14	P21/n	1	4	translation	quat amine	N		
ROBXOY	1	168.997	2.607	15	C2/c	1	8	translation	quat amine	Y	3.061	dimer
SANQUU	1	167.376	2.526	14	P21/c	1	4	translation	quat amine	N		
SEBZAD	1	162.402	2.625	61	Pbca	1	8	c glide	quat amine	N		
TAMFIZ	1	160.083	2.473	1	P1	2	2	translation	quat amine	N		
TAMFIZ	2	168.206	2.478	1	P1		2	translation		N		
TERSEP	1	176.694	2.473	14	P21/n	1	4	translation	quat amine	Y	3.262	dimer
TMAHOX	1	175.167	2.489	11	P21/m	0.5	2	translation	quat amine	N		
TODDUN	1	166.9	2.524	15	C2/c	1	8	translation	quat amine	Y	2.844	dimer
TODDUN	2	169.368	2.547	15	C2/c	1	8	translation		Y	3.152	
TOQGUD	1	174.111	2.606	4	P21	1	2	21 screw	pyridinium	N		
VEHGEU	1	170.495	2.616	14	P21/c	1	4	c glide	quat amine	N		
VURYEN	1	162.55	2.462	9	Cc	4	16	translation	quat amine	N		
VURYEN	2	147.16	2.462					translation		N		

VURYEN	3	170.06	2.462					translation		N		
VURYEN	4	156.44	2.462					translation		N		
WACZEG	1	171.432	2.611	14	P21/n	1	4	21 screw	quat amine	N		
WIFHUR	1	175.82	2.642	9	Ia	1	4	a glide	quat amine	N		
WIFJON	1	174.52	2.549	14	P21/c	1	4	c glide	quat amine	N		
WIPQOE	1	176.162	2.632	2	P-1	1	2	translation	amino acid	Y	3.107	dimer
WIZBEN	1	177.601	2.468	15	C2/c	1	8	translation	quat amine	N		
WIZBOX	1	159.624	2.480	29	Pca21	2	8	c glide	quat amine	N		
WIZBOX	2	166.69	2.486					c glide		N		
WOVYOV	1	176.954	2.54	14	P21/c	1	4	translation	amino acid	Y	2.943	dimer
XANSOW	1	172.691	2.641	4	P21	1	2	translation	quat amine	N		
XIZPEE	1	169.603	2.549	2	P-1	2	4	translation	quat amine	Y	3.880	dimer
XIZPEE	2	171.474	2.565	2	P-1		4	translation		Y	3.634	
XOCGOO	1	169.902	2.517	14	P21/c	1	4	translation	imidazolium	N		
XUJNOH	1	175.692	2.587	19	P212121	1	4	translation	quat amine	Y	3.208	inf
YEJYIV	1	171.553	2.545	19	P212121	1	4	translation	amino acid	Y	3.894	inf
YEPBEB	1	166.39	2.661	4	P21	1	2	translation	quat amine	N		
YIRGUE	1	170.791	2.553	2	P-1	2	4	translation	pyridinium	N		
ZAQJEI	1	174.776	2.492	2	P-1	1	2	translation	pyridinium	Y	3.719	dimer
ZENZUN	1	172.725	2.520	2	P-1	1	2	translation	quat amine	N		