Supporting Information for

"Crystal packing predictions of the alpha-amino acids: methods assessment and structural observations"

Supporting Information contains:

1) unit cell parameters and calculated energies of the lowest energy predicted crystal structures, after the final (DMAflex) re-minimisations

2) A CIF structure file of the lowest energy predicted structures is provided for each molecule, with structures given in order of increasing energy.

Table S1. Unit cells and relative energies of the predicted crystal structures of DL-alanine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	*Pna*2$_1$	0.00	11.782	6.093	5.881	90.00	90.00	90.00	422.12	105.53
2	*Pna*2$_1$	3.41	10.044	7.595	5.838	90.00	90.00	90.00	445.35	111.34
3	*P*2$_1$/*c*	4.22	5.464	8.567	9.932	90.00	96.02	90.00	462.36	115.59
4	*Pbcn*	4.42	10.115	8.957	9.796	90.00	90.00	90.00	887.48	110.94
5	*Pna*2$_1$	4.69	5.725	12.668	5.970	90.00	90.00	90.00	433.01	108.25
6	*C*2/*c*	5.27	10.117	9.161	10.820	90.00	91.94	90.00	1002.15	125.27
7	*C*2/*c*	5.30	15.707	6.491	10.676	90.00	126.83	90.00	871.20	108.90
8	*P*2$_1$/*c*	5.38	7.100	7.893	10.342	90.00	132.30	90.00	428.63	107.16
9	*P*2$_1$/*c*	5.56	5.398	9.954	9.891	90.00	119.47	90.00	462.68	115.67
10	*P*2$_1$/*c*	5.67	9.747	5.963	8.033	90.00	97.95	90.00	462.43	115.61
11	*P*2$_1$/*c*	5.78	5.380	11.097	9.498	90.00	122.81	90.00	476.56	119.14
12	*C*2/*c*	5.87	20.033	5.969	8.026	90.00	105.32	90.00	925.60	115.70
13	*C*2/*c*	7.01	18.426	5.975	8.888	90.00	101.69	90.00	958.28	119.79
14	*P*2$_1$/*c*	7.13	5.367	7.969	11.362	90.00	95.47	90.00	483.73	120.93
15	*P*-1	7.39	5.049	5.358	9.245	82.21	77.28	69.09	227.47	113.74
16	*P*2$_1$/*c*	7.84	10.385	4.737	9.727	90.00	95.68	90.00	476.20	119.05
17	*Pbcn*	7.86	10.281	9.122	9.466	90.00	90.00	90.00	887.66	110.96
18	*Pbca*	8.11	7.731	5.967	21.186	90.00	90.00	90.00	977.19	122.15
19	*P*2$_1$/*c*	8.61	4.961	18.142	5.730	90.00	119.93	90.00	446.93	111.73
20	*P*-1	9.62	4.563	4.889	10.041	100.35	93.56	98.78	216.80	108.40
21	*P*2$_1$/*c*	9.92	4.884	20.294	4.597	90.00	99.45	90.00	449.46	112.37
22	*P*-1	11.32	4.657	4.750	10.547	79.42	77.87	83.54	223.57	111.79
23	*P*-1	11.33	4.664	4.749	9.981	78.77	85.04	83.51	214.94	107.47

[a] All energies are relative to the lowest energy predicted crystal structure.

Table S2. Unit cells and relative energies of the predicted crystal structures of L-alanine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	*P*2$_1$2$_1$2$_1$	3.32	5.772	6.109	12.225	90.00	90.00	90.00	431.06	107.77
2	*P*2$_1$2$_1$2$_1$	4.70	5.577	8.410	9.629	90.00	90.00	90.00	451.63	112.91
3	*P*2$_1$2$_1$2$_1$	6.55	4.787	9.189	9.712	90.00	90.00	90.00	427.17	106.79
4	*C*2	7.34	10.509	8.750	5.369	90.00	93.40	90.00	492.84	123.21
5	*P*2$_1$	9.97	5.946	5.882	6.316	90.00	95.83	90.00	219.76	109.88
6	*C*2	10.00	9.486	5.198	9.965	90.00	92.09	90.00	491.02	122.76
7	*C*2	10.79	9.468	5.208	11.026	90.00	112.45	90.00	502.52	125.63
8	*P*2$_1$2$_1$2$_1$	11.05	5.316	8.984	9.453	90.00	90.00	90.00	451.45	112.86

9	*C*2	11.68	7.606	5.950	10.420	90.00	92.08	90.00	471.19	117.80
10	$P2_12_12_1$	12.07	5.273	8.223	9.781	90.00	90.00	90.00	424.09	106.02
11	$P2_12_12_1$	13.41	5.319	7.010	12.085	90.00	90.00	90.00	450.61	112.65
12	*C*2	13.42	7.621	5.919	11.427	90.00	104.63	90.00	498.71	124.68
13	*C*2	13.53	5.387	9.224	10.458	90.00	93.99	90.00	518.32	129.58
14	$P2_12_12_1$	14.33	5.273	5.987	15.141	90.00	90.00	90.00	477.95	119.49
15	*C*2	14.72	13.094	6.828	5.397	90.00	91.03	90.00	482.50	120.63

[a] All energies are relative to the lowest energy predicted *racemic* crystal structure (Table S1).

Table S3. Unit cells and relative energies of the predicted crystal structures of DL-valine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	*P*-1	0.00	5.257	5.365	11.337	89.79	82.03	71.83	300.58	150.29
2	$P2_1/c$	1.64	5.235	22.101	5.360	90.00	106.96	90.00	593.16	148.29
3	*C*2/*c*	2.62	24.917	5.297	10.056	90.00	111.41	90.00	1235.59	154.45
4	*P*-1	2.72	5.294	5.364	12.774	81.07	85.57	71.48	339.65	169.83
5	*C*2/*c*	3.43	23.595	5.368	9.966	90.00	91.42	90.00	1261.89	157.74
6	$P2_1/c$	4.22	5.339	21.880	6.217	90.00	125.22	90.00	593.26	148.32
7	*C*2/*c*	4.94	25.417	5.383	9.992	90.00	112.46	90.00	1263.27	157.91
8	*Pbca*	5.25	7.171	9.713	19.369	90.00	90.00	90.00	1348.92	168.62
9	*Pbcn*	5.53	24.143	5.331	9.993	90.00	90.00	90.00	1286.18	160.77
10	$P2_1/c$	5.54	9.739	7.213	9.534	90.00	98.56	90.00	662.31	165.58
11	$P2_1/c$	6.29	11.258	5.346	10.127	90.00	92.05	90.00	609.10	152.28
12	*C*2/*c*	6.46	25.776	4.892	10.104	90.00	106.54	90.00	1221.43	152.68
13	*P*-1	6.96	5.373	6.555	9.198	91.00	99.39	95.38	317.99	159.00

[a] All energies are relative to the lowest energy predicted crystal structure.

Table S4. Unit cells and relative energies of the predicted crystal structures of L-valine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	$P2_12_12_1$	8.31	7.333	8.797	10.140	90.00	90.00	90.00	654.15	163.54
2	$P2_12_12_1$	9.77	5.391	6.478	18.636	90.00	90.00	90.00	650.76	162.69
3	*C*2	10.01	5.372	10.224	11.715	90.00	95.22	90.00	640.79	160.20
4	$P2_1$	10.13	5.037	5.156	11.644	90.00	91.70	90.00	302.28	151.14
5	*C*2	10.44	10.173	5.370	11.927	90.00	106.55	90.00	624.53	156.13
6	$P2_12_12_1$	11.01	5.854	6.362	18.290	90.00	90.00	90.00	681.11	170.28
7	$P2_1$	11.16	6.496	5.838	9.073	90.00	94.19	90.00	343.10	171.55
8	$P2_1$	11.93	6.471	5.387	9.521	90.00	90.71	90.00	331.88	165.94
9	*C*2	12.01	10.528	5.327	11.254	90.00	91.78	90.00	630.83	157.71
10	*C*2	13.85	10.060	5.335	12.486	90.00	109.13	90.00	633.05	158.26

[a] All energies are relative to the lowest energy predicted *racemic* crystal structure (Table S3).

Table S5. Unit cells and relative energies of the predicted crystal structures of DL-leucine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	*P*-1	0.00	5.149	5.329	13.997	85.03	82.88	71.09	360.05	180.03
2	$P2_1/c$	0.61	5.132	28.044	6.125	90.00	124.29	90.00	728.40	182.10
3	*C*2/*c*	0.92	8.567	6.155	27.781	90.00	98.68	90.00	1448.02	181.00
4	*P*-1	1.18	5.135	5.334	15.218	94.19	91.10	108.73	393.31	196.66
5	*C*2/*c*	1.50	8.608	6.109	27.858	90.00	98.04	90.00	1450.62	181.33

6	*C*2/*c*	1.70	6.153	8.566	27.868	90.00	93.24	90.00	1466.58	183.32
7	$P2_1/c$	2.68	5.108	28.549	5.339	90.00	107.96	90.00	740.59	185.15
8	$P2_1/c$	4.51	5.330	29.469	5.139	90.00	108.76	90.00	764.28	191.07
9	$P2_1/c$	5.02	5.330	29.447	5.154	90.00	108.48	90.00	767.30	191.83
10	$P2_1/c$	7.90	13.676	6.006	9.523	90.00	90.18	90.00	782.17	195.54
11	*C*2/*c*	8.72	27.340	6.012	9.541	90.00	90.48	90.00	1568.30	196.04
12	*Pbca*	9.13	5.955	9.674	27.007	90.00	90.00	90.00	1555.76	194.47
13	$P2_1/c$	9.19	13.915	5.108	9.922	90.00	91.66	90.00	704.96	176.24
14	*C*2/*c*	9.61	28.229	5.950	9.724	90.00	108.64	90.00	1547.63	193.45

[a] All energies are relative to the lowest energy predicted crystal structure.

Table S6. Unit cells and relative energies of the predicted crystal structures of L-leucine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	*C*2	7.70	9.434	5.448	14.769	90.00	93.38	90.00	757.73	189.43
2	*C*2	8.41	8.647	6.011	13.989	90.00	94.64	90.00	724.63	181.16
3	*C*2	8.79	9.551	5.373	15.586	90.00	107.58	90.00	762.55	190.64
4	*C*2	12.91	5.344	9.780	15.697	90.00	96.56	90.00	815.04	203.76
5	*C*2	13.75	6.111	8.634	14.137	90.00	94.07	90.00	743.97	185.99
6	*C*2	20.66	10.153	5.343	14.671	90.00	96.67	90.00	790.45	197.61
7	$P2_12_12_1$	20.94	5.409	6.752	21.533	90.00	90.00	90.00	786.41	196.60
8	*C*2	21.94	10.085	5.340	14.773	90.00	97.18	90.00	789.28	197.32
9	$P2_1$	21.99	5.351	6.640	11.172	90.00	93.33	90.00	396.27	198.13

[a] All energies are relative to the lowest energy predicted *racemic* crystal structure (Table S5).

Table S7. Unit cells and relative energies of the predicted crystal structures of DL-isoleucine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	$P2_1/c$	0.00	5.340	26.795	5.233	90.00	107.53	90.00	714.02	178.51
2	*P*-1	0.09	5.207	5.348	13.582	98.05	96.60	107.38	352.45	176.23
3	$P2_1/c$	0.46	5.223	26.908	6.267	90.00	125.53	90.00	716.73	179.18
4	*C*2/*c*	0.99	8.601	6.223	26.609	90.00	91.36	90.00	1423.78	177.97
5	$P2_1/c$	1.97	5.243	26.877	5.351	90.00	108.60	90.00	714.72	178.68
6	*C*2/*c*	2.12	8.564	6.262	26.816	90.00	93.92	90.00	1434.59	179.32
7	*P*-1	3.00	5.341	6.511	10.530	89.46	85.96	85.38	364.11	182.06
8	*P*-1	3.58	5.341	6.556	10.891	93.19	90.14	95.09	379.27	189.64
9	$P2_1/c$	3.99	5.255	26.449	6.227	90.00	125.32	90.00	706.13	176.53
10	$P2_1/c$	5.77	11.972	6.102	10.998	90.00	111.81	90.00	745.98	186.50
11	$P2_1/c$	6.03	6.586	5.334	21.086	90.00	91.70	90.00	740.49	185.12
12	$P2_1/c$	6.66	11.350	7.118	9.810	90.00	101.08	90.00	777.70	194.43
13	$P2_1/c$	6.71	10.793	6.481	10.641	90.00	95.71	90.00	740.59	185.15
14	$P2_1/c$	6.82	13.958	5.399	10.025	90.00	101.01	90.00	741.54	185.39
15	$P2_1/c$	7.00	11.413	6.990	9.896	90.00	103.39	90.00	768.07	192.02
16	*C*2/*c*	7.30	23.149	7.016	9.744	90.00	100.32	90.00	1557.12	194.64
17	$P2_1/c$	7.45	12.636	5.318	13.004	90.00	120.30	90.00	754.47	188.62
18	*C*2/*c*	7.85	26.282	6.065	9.679	90.00	103.56	90.00	1499.81	187.48
19	*C*2/*c*	8.32	22.509	7.154	9.834	90.00	105.00	90.00	1529.65	191.21
20	*C*2/*c*	8.37	27.734	5.465	10.006	90.00	98.73	90.00	1498.99	187.37
21	*Pbca*	8.87	5.496	9.965	27.196	90.00	90.00	90.00	1489.43	186.18

22	*Pbca*	9.30	6.185	10.871	22.717	90.00	90.00	90.00	1527.43	190.93
23	$P2_1/c$	9.37	12.348	5.326	12.875	90.00	120.32	90.00	730.91	182.73
24	$P2_1/c$	9.48	14.052	5.476	9.813	90.00	100.60	90.00	742.27	185.57
25	$P2_1/c$	10.07	10.515	5.792	12.834	90.00	97.33	90.00	775.16	193.79
26	$P2_1/c$	10.07	5.344	6.498	21.763	90.00	94.49	90.00	753.39	188.35
27	*Pbca*	10.42	6.998	9.858	24.093	90.00	90.00	90.00	1662.01	207.75

[a] All energies are relative to the lowest energy predicted crystal structure.

Table S8. Unit cells and relative energies of the predicted crystal structures of L-isoleucine.

rank	spcgrp	E_{rel} [a] (kJ/mol)	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	unit cell volume (Å^3)	Vol per molecule (Å^3)
1	$P2_1$	9.61	6.468	5.827	10.360	90.00	91.79	90.00	390.29	195.15
2	$P2_12_12_1$	9.92	5.359	6.497	21.985	90.00	90.00	90.00	765.41	191.35
3	$P2_12_12_1$	12.51	7.080	10.075	10.189	90.00	90.00	90.00	726.75	181.69
4	*C*2	13.08	6.239	8.645	13.676	90.00	98.29	90.00	729.95	182.49
5	$P2_1$	14.45	6.229	5.877	11.149	90.00	103.86	90.00	396.22	198.11
6	*C*2	14.58	8.785	6.068	13.701	90.00	90.00	90.00	730.25	182.56
7	$P2_12_12_1$	14.71	5.931	6.171	20.443	90.00	90.00	90.00	748.24	187.06
8	$P2_1$	15.10	6.029	5.436	11.749	90.00	103.90	90.00	373.81	186.91
9	$P2_1$	15.75	6.207	5.951	10.257	90.00	96.06	90.00	376.72	188.36
10	$P2_12_12_1$	21.50	5.461	6.786	19.599	90.00	90.00	90.00	726.29	181.57
11	$P2_1$	22.24	5.481	6.709	10.272	90.00	97.60	90.00	374.40	187.20

[a] All energies are relative to the lowest energy predicted *racemic* crystal structure (Table S7).