

References

- [1] Spek, A. L. 2003. *J. Appl. Cryst.*, **36**, 7–13.

Table 4. Supplementary information: Data used for the calculation of Cruickshanks DPI value

#	Compound	Formula Sum	n _{obs}	n _{pred}	n _{par}	R(F) _{IAM}	R(F) _{inv}	d	cpl.(%)	DPI _{IAM}	DPI _{inv}
1	N-Acetyl-L-tyrosine ethyl ester·H ₂ O	C ₁₃ H ₁₉ NO ₅	5534	8194	248	2.25	1.09	0.46	0.675	0.068	0.033
2	Cis-[5-oxo-L-prolyl-L-prolinamide·H ₂ O	C ₁₀ H ₁₇ N ₃ O ₄	1202	1253	221	2.29	1.95	0.81	0.959	0.271	0.231
3	L-Alanyl-L-threonine	C ₇ H ₁₄ N ₂ O ₄	2069	2187	174	2.76	1.53	0.62	0.946	0.162	0.090
4	L-Phenylalanyl-L-valine	C ₁₄ H ₂₀ N ₂ O ₃	1613	1902	252	2.77	1.48	0.76	0.848	0.268	0.143
5	L-Threonyl-L-Alanine	C ₇ H ₁₄ N ₂ O ₄	1041	1219	174	2.84	1.93	0.76	0.854	0.302	0.205
6	Bis(L-tyrosinium) sulfate·H ₂ O	C ₁₈ H ₂₆ N ₂ O ₁₁ S	1969	2083	405	2.87	2.27	0.85	0.945	0.427	0.338
7	L-Seryl-L-valine	C ₈ H ₁₆ N ₂ O ₄	1179	1256	190	2.91	2.16	0.78	0.939	0.306	0.227
8	N-Methyl-DL-aspartic acid·H ₂ O	C ₅ H ₁₁ NO ₅	890	940	141	2.97	2.27	0.75	0.947	0.315	0.241
9	L-Alanyl-L-tryptophan·H ₂ O	C ₁₄ H ₁₉ N ₃ O ₄	1542	1625	266	3.01	2.28	0.82	0.949	0.345	0.262
10	L-Valyl-L-phenylalanine	C ₁₄ H ₂₄ N ₂ O ₅	2046	2107	286	3.05	2.12	0.77	0.971	0.285	0.198
11	L-Valyl-L-serine·3 H ₂ O	C ₈ H ₂₂ N ₂ O ₇	3180	3573	241	3.05	2.25	0.58	0.890	0.156	0.115
12	L-tryptophan formic acid	C ₁₂ H ₁₄ N ₂ O ₄	10655	14132	219	3.10	2.48	0.36	0.754	0.051	0.041
13	L-Cysteine	C ₆ H ₁₄ N ₂ O ₄ S ₂	2850	3038	169	3.11	2.91	0.58	0.938	0.191	0.179
14	L-Isoleucyl-L-isoleucine	C ₁₂ H ₂₈ N ₂ O ₅	3586	3875	284	3.15	2.00	0.62	0.925	0.167	0.106
15	L-Asparagyl-L-valine·1 $\frac{1}{2}$ H ₂ O	C ₂₇ H ₅₉ N ₉ O ₁₆	8623	10592	705	3.18	2.09	0.59	0.814	0.175	0.115
16	Bis(L-glutamic acid) sulfate· $\frac{1}{2}$ H ₂ O	C ₂₀ H ₄₂ N ₄ O ₂₅ S ₂	5542	5940	1237	3.27	3.02	0.85	0.933	0.391	0.361
17	Cyclo-(D,L-Proline) ₂ -(L-Alanine) ₄ ·H ₂ O	C ₂₂ H ₃₆ N ₆ O ₇	21478	25177	460	3.38	2.69	0.38	0.853	0.058	0.046
18	L-Asparaginium nitrate	C ₈ H ₁₅ N ₃ O ₁₁	836	1409	259	3.40	3.33	0.85	0.593	0.681	0.667
19	DL-Arginine·H ₂ O	C ₆ H ₁₆ N ₄ O ₃	1830	1870	182	3.47	2.06	0.81	0.979	0.285	0.169
20	DL-Alanyl-methionine	C ₈ H ₁₆ N ₂ O ₃ S	6466	8853	190	3.49	2.45	0.50	0.730	0.106	0.074
21	Glycyl-L-aspartic acid·2 H ₂ O	C ₆ H ₁₄ N ₂ O ₇	4115	7903	192	3.52	2.79	0.42	0.521	0.108	0.086
22	L-Isoleucyl-L-leucine·H ₂ O	C ₂₄ H ₄₂ N ₄ O ₈	2797	3426	524	3.55	3.01	0.81	0.816	0.405	0.343
23	L-Seryl-L-phenylalanine	C ₁₂ H ₁₆ N ₂ O ₄	1358	1607	227	3.59	3.25	0.79	0.845	0.396	0.358
24	L-Leucyl-L-alanine·4 H ₂ O	C ₉ H ₂₆ N ₂ O ₇	4243	4792	267	3.62	2.84	0.57	0.885	0.160	0.126
25	Glycyl-L-threonine·2 H ₂ O	C ₆ H ₁₆ N ₂ O ₆	4312	7100	191	3.73	2.96	0.43	0.607	0.109	0.086
26	L-Alanyl-L-methionine· $\frac{1}{2}$ H ₂ O	C ₁₆ H ₃₄ N ₄ O ₇ S ₂	2288	2867	398	3.74	3.38	0.78	0.798	0.470	0.425
27	L-Argininium chloride	C ₆ H ₁₅ ClN ₄ O ₂	3734	4570	352	3.85	3.56	0.61	0.817	0.194	0.179
28	Glycyl-L-tryptophan·2 H ₂ O	C ₁₃ H ₁₉ N ₃ O ₅	1364	1441	265	4.04	3.39	0.82	0.947	0.510	0.428
29	L-Phenylalanyl-L-alanine·2 H ₂ O	C ₁₂ H ₂₀ N ₂ O ₅	3196	3691	252	4.05	3.81	0.62	0.866	0.227	0.213
30	L-Valyl-L-glutamine	C ₁₀ H ₁₉ N ₃ O ₄	1281	2045	230	4.43	3.98	0.71	0.626	0.445	0.399
31	Glycyl-DL-Leucine	C ₈ H ₁₆ N ₂ O ₃	1496	1657	183	4.62	4.13	0.86	0.903	0.439	0.392
32	L-tryptophan formic acid	C ₁₂ H ₁₄ N ₂ O ₄	1947	2610	219	4.71	3.83	0.65	0.746	0.345	0.281
33	Bis(L-proline) nitrate	C ₁₀ H ₁₉ N ₃ O ₇	1242	1481	257	4.74	4.29	0.82	0.839	0.644	0.582
34	L-Glutamyl-L-valine	C ₁₀ H ₁₈ N ₂ O ₅	1419	1902	225	4.82	4.45	0.71	0.746	0.465	0.429
35	L-Tyrosyl-glycyl-glycine·H ₂ O	C ₁₃ H ₁₉ N ₃ O ₆	4766	9701	275	4.83	3.71	0.43	0.491	0.164	0.126
36	L-Histidinyl-L-histidine glutarate	C ₁₇ H ₂₆ N ₆ O ₈	3908	4197	556	5.49	5.50	0.79	0.945	0.470	0.470
37	N-Acetyl-L-glutamic acid	C ₇ H ₁₁ NO ₅	1074	1214	162	5.51	5.33	0.77	0.885	0.579	0.560
38	L-Leucyl-L-phenylalanine·2-proOH	C ₁₈ H ₃₀ N ₂ O ₄	6263	10731	676	5.54	5.07	0.58	0.584	0.227	0.208
39	Hippuryl-L-histidinyl-L-leucine·5 H ₂ O	C ₂₁ H ₃₇ N ₅ O ₁₀	1439	1991	325	5.55	5.42	0.93	0.723	1.049	1.024
40	L-Seryl-L-alanine	C ₆ H ₁₂ N ₂ O ₄	1738	1838	156	5.92	4.93	0.62	0.946	0.369	0.307
41	L-Aspartic acid monohydrate	C ₄ H ₉ NO ₅	669	693	128	6.14	5.73	0.85	0.965	0.840	0.783
42	L-Lysine L-lysium dichloride nitrate	C ₁₂ H ₃₁ Cl ₂ N ₅ O ₇	1406	2197	389	6.15	6.02	0.85	0.640	1.136	1.112

For structures marked with ∇ data were not merged by the authors. To calculate the completeness (cpl.) for these structures, we have divided the number of unique reflections with $I > 2\sigma(I)$ by the number of predicted reflections n_{pred} as calculated with PLATON [1].