Table S1: Topological properties of (3, -1) CPs on the intermolecular interactions: distances (Å), electron density (e/Å^3), Laplacian (e/Å^5), Hessian eigenvalues (e/Å^5), ellipticity.

Contact	D_{12}	d_{1cp}	d_{2cp}	$\rho(r_b)$	$\nabla^2\rho(r_{cp})$	λ_1	λ_2	λ_3	ε	$G(r_{cp})$	$V(r_{cp})$
O1⋯ H2^{i}	1.769	1.151	0.619	0.289	1.29	-1.92	-1.91	5.12	0	62.95	-90.73
O3⋯H2W^{ii}	1.818	1.158	0.662	0.284	1.3	-1.86	-1.83	4.99	0.02	61.83	-88.35
O2⋯H3W^{iii}	1.928	1.202	0.727	0.228	1.25	-1.38	-1.35	3.98	0.02	49.24	-64.46
O2⋯H4W^{iv}	2.046	1.244	0.803	0.177	1.16	-0.99	-0.94	3.09	0.04	38.43	-45.37
H7B⋯H16A^{v}	2.158	1.083	1.075	0.049	0.57	-0.2	-0.16	0.93	0.28	12.33	-9.2
H4A⋯H14A^{vi}	2.328	1.156	1.174	0.033	0.41	-0.11	-0.09	0.61	0.17	8.57	-5.87
H12A⋯H16B^{vii}	2.367	1.184	1.184	0.031	0.34	-0.11	-0.1	0.56	0.04	7.2	-5.03
H8A⋯H1B^{viii}	2.384	1.193	1.191	0.028	0.43	-0.1	-0.06	0.59	0.68	8.6	-5.52
H11A⋯H18A^{vii}	2.391	1.195	1.196	0.029	0.35	-0.11	-0.08	0.54	0.39	7.16	-4.86
H1B⋯H15B^{vii}	2.418	1.211	1.207	0.028	0.31	-0.1	-0.08	0.5	0.26	6.51	-4.49
H9A⋯H15B^{vii}	2.497	1.255	1.247	0.023	0.24	-0.08	-0.07	0.39	0.16	4.96	-3.37
H7A⋯H4A^{ix}	2.512	1.258	1.259	0.023	0.29	-0.07	-0.05	0.42	0.4	5.83	-3.79
O1⋯H6B^{vii}	2.564	1.512	1.058	0.052	0.7	-0.16	-0.14	1.01	0.14	14.97	-10.85
H7A⋯H20A^{vi}	2.652	1.289	1.381	0.017	0.31	-0.05	-0.03	0.39	0.6	5.95	-3.5
H11B⋯O2W^{ii}	2.689	1.110	1.582	0.042	0.57	-0.15	-0.1	0.82	0.56	12.02	-8.42
O1⋯H15A^{vi}	2.730	1.568	1.162	0.035	0.41	-0.12	-0.12	0.66	0.05	8.68	-6.11
H12B⋯O2W^{iii}	2.832	1.210	1.625	0.026	0.39	-0.08	-0.07	0.53	0.17	7.76	-4.91
H15A⋯H6A^{x}	2.922	1.490	1.441	0.009	0.17	-0.02	-0.01	0.2	0.31	3.22	-1.78
C11⋯H18B^{xi}	2.936	1.796	1.153	0.033	0.48	-0.11	-0.06	0.65	0.92	9.83	-6.49
O2W⋯H18C^{xii}	2.985	1.702	1.300	0.022	0.27	-0.06	-0.03	0.36	1.19	5.37	-3.48
O1W⋯H1A^{xiii}	2.995	1.703	1.292	0.018	0.29	-0.05	-0.03	0.38	0.59	5.64	-3.38
H18C⋯H12B^{xiv}	2.995	1.529	1.470	0.008	0.14	-0.02	-0.01	0.17	0.71	2.65	-1.47
O3⋯H2C^{viii}	3.063	1.722	1.344	0.018	0.21	-0.05	-0.05	0.31	0.03	4.25	-2.69
H2B⋯O1W^{xii}	3.080	1.420	1.700	0.016	0.31	-0.04	-0.03	0.38	0.17	6	-3.49
C4⋯H20A^{vi}	3.152	1.856	1.307	0.022	0.24	-0.05	-0.03	0.32	0.79	4.85	-3.24
C4⋯H20B^{xv}	3.310	1.920	1.457	0.014	0.23	-0.03	-0.02	0.28	1.12	4.51	-2.65
C6⋯H20C^{xv}	3.430	2.025	1.443	0.011	0.15	-0.03	-0.02	0.19	0.65	2.89	-1.68
H6A⋯C15^{v}	3.448	1.436	2.076	0.009	0.17	-0.02	-0.01	0.2	0.23	3.24	-1.79
O1W⋯C2	3.554	1.703	1.888	0.016	0.31	-0.04	-0.03	0.38	0.21	5.92	-3.44
O2W⋯C12	3.696	1.624	2.152	0.025	0.39	-0.08	-0.07	0.53	0.16	7.69	-4.86
O2W⋯C11	3.729	1.566	2.175	0.041	0.52	-0.14	-0.11	0.78	0.18	10.97	-7.72

(i) *x+1 ; y-1 ; z* (ii) *x-1/2 ; -y+3/2 ; -z* (iii) *x ; y+1 ; z* (iv) *x-1 ; y+1 ; z* (v) *-x+2 ; y-1/2 ; -z+1/2* (vi) *-x+1 ; y-1/2 ; -z+1/2* (vii) *x+1 ; y ; z* (viii) *x-1 ; y ; z* (ix) *-x+1 ; y+1/2 ; -z+1/2* (x) *-x+2 ; y+1/2 ; -z+1/2* (xi) *x+1/2 ; -y+1/2 ; -z* (xii) *x+1/2 ; -y+3/2 ; -z* (xiii) *x-1/2 ; -y+3/2 ; -z* (xiv) *x-1/2 ; -y+1/2 ; -z* (xv) *x ; y-1 ; z.*

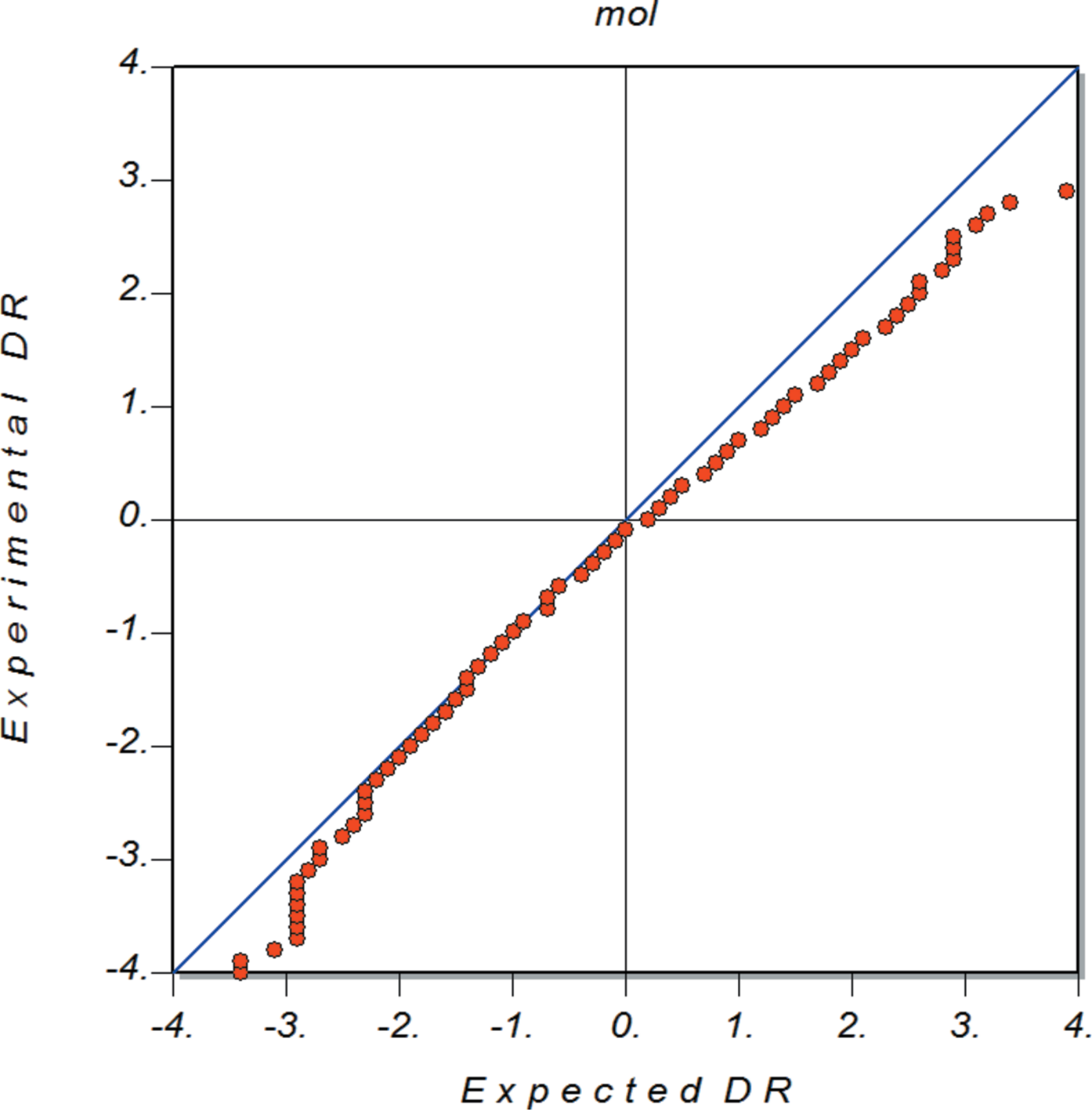

Figure S1. A normal probability plot showing the quality of the data used for the refinement.

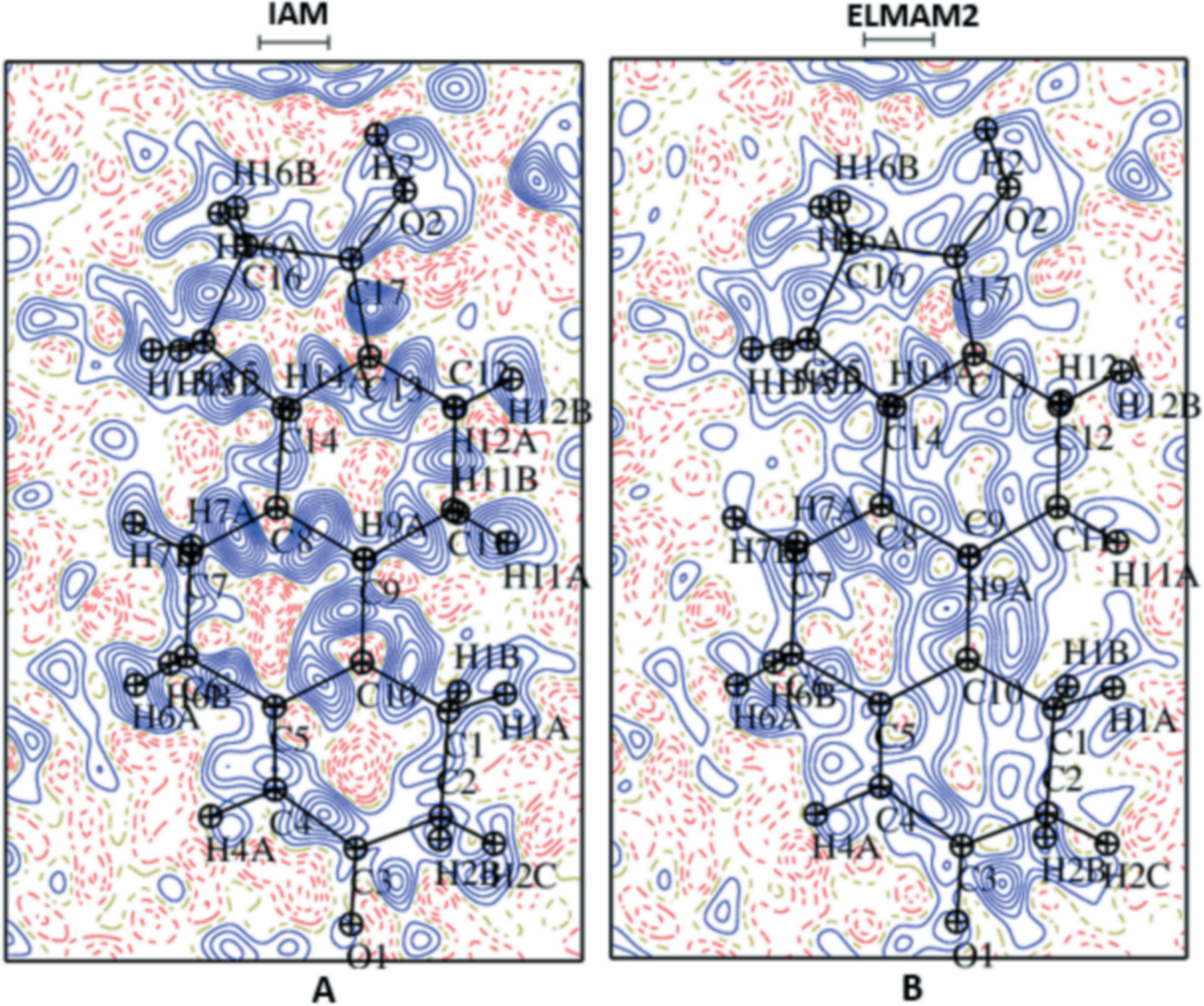

Figure S2. A comparison of the residual electron-density maps after IAM (A) and ELMAM2 (B) refinements using all data. The contour levels are drawn at e/Å^3. The blue contours represent the positive electron density, whereas the red ones show the negative density. The yellow lines show the zero regions.