

Supplementary Information

Electron densities by the maximum entropy method for various types of prior densities: a case study on three amino acids and a tripeptide

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Supplementary tables and figures

As discussed in Section 2.7 of the main text, local maxima in different density maps of a single compound are found at nearly equal positions. Tables 1–4 compare the exact coordinates of corresponding local maxima within the eight density maps for each compound, α -Glycine, D , L -Serine, L -Alanine and Ala-Tyr-Ala(*etho*), respectively. A good agreement is also found between positions of bond critical points (BCPs) of the covalent and hydrogen bonds in different density maps of a single compound (Tables 5–8).

The values of the electron density, ρ_{BCP} , and the Laplacian, $\nabla^2\rho_{BCP}$, at the BCPs in the static and dynamic model density maps of the INV and MP models are compared in Tables 9–12 for α -Glycine, D , L -Serine, L -Alanine and Ala-Tyr-Ala(*etho*), respectively. A comparison of these quantities between all four dynamic model densities and all four MEM densities of each compound is incorporated in the main text.

The number of electrons in and volumes of the atomic basins are given for the four MEM density maps of each compound in Tables 13–16. Atomic charges derived from these values are given in Tables 17–20.

Finally, the values of the electron density and the Laplacian at the the local maxima in the four dynamic model density maps of each compound are compiled in Tables 21–24.

Figures are provided of selected sections of the residual density (difference Fourier map), dynamic deformation density (Eq. 4 in the main text) and MEM density for each of the four MEM densities for D , L -Serine, L -Alanine and Ala-Tyr-Ala(*etho*) (Figs. 1–6). Difference density maps (Eq. 3 in the main text) for the MEM densities with INV and MP priors are provided for each compound in Fig. 7. The main text includes similar figures for α -Glycine.

Table 1. *Coordinates of atomic maxima in eight different density maps of α -Glycine: Dynamic model densities and MEM density maps for IAM (first line), IAM-HO(second line), INV (third line) and MP (fourth line).*

Atom	Dynamic model density			MEM density		
	x	y	z	x	y	z
C1	0.069390	0.125125	0.065821	0.069390	0.125130	0.065823
	0.069372	0.125146	0.065893	0.069377	0.125146	0.065878
	0.069391	0.125151	0.065832	0.069393	0.125152	0.065826
	0.069332	0.125159	0.065784	0.069334	0.125160	0.065782
C2	0.942035	0.854144	0.214085	0.942046	0.854147	0.214091
	0.942084	0.854141	0.214142	0.942085	0.854143	0.214138
	0.942104	0.854123	0.214122	0.942098	0.854127	0.214122
	0.942053	0.854140	0.214081	0.942049	0.854140	0.214080
O1	0.302380	0.093779	0.236580	0.302382	0.093776	0.236580
	0.302145	0.093783	0.236464	0.302179	0.093782	0.236476
	0.302167	0.093765	0.236447	0.302172	0.093769	0.236449
	0.302167	0.093777	0.236481	0.302169	0.093778	0.236482
O2	0.844485	0.142350	0.106570	0.844475	0.142362	0.106564
	0.844629	0.142380	0.106527	0.844605	0.142384	0.106524
	0.844639	0.142382	0.106533	0.844631	0.142385	0.106529
	0.844662	0.142400	0.106559	0.844657	0.142401	0.106559
N	0.795040	0.411631	0.240529	0.795048	0.411633	0.240526
	0.794975	0.411620	0.240512	0.795000	0.411624	0.240513
	0.795096	0.411617	0.240492	0.795096	0.411620	0.240496
	0.794968	0.411614	0.240447	0.794970	0.411617	0.240451
H4	0.933848	0.767334	0.243315	-	-	-
	0.934178	0.767362	0.242926	-	-	-
	0.929145	0.779652	0.236394	-	-	-
	-	-	-	-	-	-
H5	0.362661	0.384024	0.143026	0.375856	0.382268	0.153181
	0.361074	0.384233	0.141443	0.371727	0.382925	0.149768
	0.386129	0.382193	0.162571	0.385648	0.380739	0.162145
	-	-	-	0.386866	0.380316	0.162572

Table 2: Coordinates of atomic maxima in eight different density maps of *D, L*-Serine: Dynamic model densities and MEM density maps for IAM (first line), IAM-HO(second line), INV (third line) and MP (fourth line).

Atom	Dynamic model density			MEM density		
	x	y	z	x	y	z
C1	0.253576	0.589520	0.333834	0.253577	0.589526	0.333839
	0.253548	0.589542	0.333933	0.253555	0.589547	0.333936
	0.253550	0.589540	0.333844	0.253554	0.589542	0.333848
	0.253558	0.589541	0.333882	0.253560	0.589542	0.333884
C2	0.245520	0.716450	0.121080	0.245528	0.716450	0.121086
	0.245561	0.716493	0.121096	0.245560	0.716481	0.121095
	0.245533	0.716443	0.121097	0.245540	0.716444	0.121098
	0.245565	0.716475	0.121194	0.245566	0.716474	0.121194
C3	0.610519	0.716383	0.030168	0.610513	0.716372	0.030175
	0.610500	0.716301	0.030268	0.610498	0.716308	0.030263
	0.610495	0.716355	0.030117	0.610494	0.716352	0.030122
	0.610497	0.716364	0.030201	0.610496	0.716362	0.030199
O1	0.158577	0.092971	0.427202	0.158578	0.092969	0.427197
	0.158703	0.092979	0.427398	0.158682	0.092978	0.427375
	0.158631	0.092962	0.427373	0.158631	0.092962	0.427375
	0.158652	0.092965	0.427469	0.158651	0.092964	0.427468
O2	0.671165	0.011055	0.248263	0.671163	0.011058	0.248260
	0.671245	0.010977	0.248463	0.671229	0.010990	0.248432
	0.671221	0.010993	0.248349	0.671219	0.010994	0.248343
	0.671227	0.010981	0.248313	0.671225	0.010983	0.248308
O3	0.571156	0.675502	0.278788	0.571151	0.675500	0.278782
	0.571181	0.675350	0.278308	0.571173	0.675379	0.278371
	0.571219	0.675377	0.278529	0.571219	0.675378	0.278537
	0.571198	0.675417	0.278510	0.571199	0.675421	0.278519
N	0.846779	0.673434	0.256313	0.846779	0.673433	0.256310
	0.846814	0.673435	0.256397	0.846806	0.673434	0.256377
	0.846786	0.673423	0.256272	0.846785	0.673425	0.256276
	0.846780	0.673451	0.256247	0.846779	0.673451	0.256250
H2	0.234045	0.173591	0.062048	0.236067	0.181518	0.039990
	0.234364	0.173112	0.063144	0.235762	0.180555	0.043167
	0.234592	0.178119	0.051320	0.235563	0.180487	0.047280
	0.233839	0.178646	0.048953	0.235232	0.180545	0.046420
H31	0.890659	0.130541	0.105515	0.891397	0.141085	0.087573
	0.890440	0.130197	0.106778	0.891437	0.141308	0.087666
	0.891875	0.135934	0.095748	0.891651	0.138198	0.092383
	0.892385	0.135398	0.096592	0.891861	0.136761	0.094732

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Table 2: Continued

Atom	x	y	z	x	y	z
H32	0.454322	0.205393	0.082627	0.448972	0.212465	0.075857
	0.454745	0.205613	0.082854	0.447660	0.213459	0.073316
	0.450510	0.212512	0.078741	0.449080	0.212821	0.076061
	0.451025	0.211501	0.078006	0.448986	0.212913	0.074810

Table 3: Coordinates of atomic maxima in eight different density maps of *L*-Alanine: Dynamic model densities and MEM density maps for IAM (first line), IAM-HO(second line), INV (third line) and MP (fourth line).

Atom	Dynamic model density			MEM density		
	x	y	z	x	y	z
C1	0.945850	0.859160	0.099790	0.945846	0.859162	0.099796
	0.945860	0.859256	0.099934	0.945858	0.859250	0.099928
	0.946011	0.859187	0.099903	0.946000	0.859187	0.099899
	0.945876	0.859192	0.099843	0.945874	0.859192	0.099845
C2	0.533760	0.661039	0.145358	0.533756	0.661040	0.145376
	0.533777	0.661036	0.145645	0.533771	0.661038	0.145639
	0.533709	0.661103	0.145488	0.533705	0.661101	0.145500
	0.533610	0.661040	0.145627	0.533613	0.661040	0.145631
C3	0.740148	0.590708	0.196736	0.740153	0.590707	0.196733
	0.740279	0.590721	0.196686	0.740272	0.590719	0.196685
	0.740068	0.590612	0.196675	0.740080	0.590616	0.196675
	0.740116	0.590654	0.196639	0.740123	0.590658	0.196642
O1	0.772976	0.916264	0.124390	0.772979	0.916268	0.124390
	0.773204	0.916249	0.124376	0.773190	0.916252	0.124374
	0.773169	0.916228	0.124389	0.773169	0.916230	0.124391
	0.773084	0.916259	0.124432	0.773087	0.916261	0.124435
O2	0.940810	0.315831	0.238711	0.940807	0.315836	0.238707
	0.940725	0.315943	0.238781	0.940731	0.315938	0.238774
	0.940992	0.315968	0.238711	0.940983	0.315965	0.238715
	0.940802	0.315931	0.238720	0.940802	0.315930	0.238719
N	0.647303	0.137507	0.182925	0.647287	0.137509	0.182931
	0.647093	0.137554	0.182978	0.647098	0.137550	0.182980
	0.647197	0.137513	0.182939	0.647195	0.137516	0.182940
	0.647045	0.137559	0.183065	0.647052	0.137560	0.183067
H1	-	-	-	-	-	-
	-	-	-	-	-	-
	0.699641	0.066084	0.195466	0.697789	0.067485	0.195108
	-	-	-	-	-	-
H2	-	-	-	-	-	-
	-	-	-	-	-	-
	0.771971	0.182726	0.202565	0.767466	0.181950	0.201976
	-	-	-	-	-	-
H3	-	-	-	-	-	-
	-	-	-	-	-	-
	0.596012	0.146460	0.031858	0.595304	0.146737	0.032253
	-	-	-	-	-	-

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Table 3: Continued

Atom	x	y	z	x	y	z
H4	0.577405	0.744212	0.155646	0.575900	0.742427	0.157484
	0.577988	0.744321	0.154381	0.575935	0.742185	0.156484
	0.576860	0.743427	0.160754	0.576489	0.743306	0.161313
	0.576758	0.742557	0.160070	0.576409	0.742554	0.160313
H5	0.200461	0.108222	0.147062	0.202089	0.107187	0.150748
	0.200428	0.108261	0.146743	0.202295	0.107346	0.150505
	0.199299	0.109386	0.150184	0.199719	0.109445	0.149785
	0.201157	0.108694	0.150891	0.201060	0.108777	0.150395
H6	0.857305	0.606328	0.078529	0.858167	0.605675	0.079191
	0.857147	0.606231	0.079780	0.857970	0.605589	0.080230
	0.859371	0.603354	0.081606	0.860837	0.603441	0.080464
	0.856299	0.605074	0.081669	0.858150	0.604562	0.080908
H7	0.703098	0.517972	0.192167	-	-	-
	0.701820	0.515855	0.191471	0.698291	0.513361	0.193263
	0.697739	0.513028	0.193434	0.700434	0.514726	0.192399
	0.699264	0.513757	0.192623			

Table 4: Coordinates of atomic maxima in eight different density maps of Ala-Tyr-Ala_(eth): Dynamic model densities and MEM density maps for IAM (first line), IAM-HO(second line), INV (third line) and MP (fourth line).

Atom	Dynamic model density			MEM density		
	x	y	z	x	y	z
C1	0.497196	0.199084	0.392133	0.497197	0.199084	0.392127
	0.497255	0.199099	0.392074	0.497246	0.199101	0.392075
	0.497167	0.200705	0.392081	0.497163	0.200704	0.392080
	0.497103	0.199141	0.392049	0.497104	0.199141	0.392050
C2	0.456573	0.284119	0.492763	0.456570	0.284114	0.492767
	0.456519	0.284173	0.492798	0.456519	0.284168	0.492797
	0.456616	0.285760	0.492787	0.456615	0.285756	0.492788
	0.456624	0.284094	0.492787	0.456622	0.284094	0.492786
C3	0.563182	0.774969	0.310572	0.563182	0.774963	0.310573
	0.563164	0.774933	0.310595	0.563162	0.774933	0.310592
	0.563136	0.776555	0.310571	0.563134	0.776552	0.310569
	0.563165	0.774917	0.310604	0.563161	0.774915	0.310598
C4	0.504642	0.668297	0.220255	0.504645	0.668298	0.220250
	0.504687	0.668269	0.220235	0.504688	0.668275	0.220234
	0.504606	0.669884	0.220210	0.504609	0.669887	0.220210
	0.504652	0.668337	0.220218	0.504653	0.668338	0.220218
C5	0.431252	0.639958	0.025754	0.431256	0.639961	0.025751
	0.431323	0.639992	0.025764	0.431322	0.639994	0.025762
	0.431265	0.641611	0.025734	0.431268	0.641611	0.025738
	0.431310	0.640035	0.025737	0.431310	0.640035	0.025739
C6	0.440601	0.140179	0.052094	0.440599	0.140181	0.052099
	0.440587	0.140236	0.052143	0.440588	0.140236	0.052142
	0.440652	0.141879	0.052111	0.440648	0.141878	0.052113
	0.440622	0.140222	0.052099	0.440620	0.140224	0.052102
C7	0.665752	0.217945	0.374128	0.665752	0.217942	0.374127
	0.665766	0.217833	0.374107	0.665764	0.217843	0.374108
	0.665699	0.219470	0.374110	0.665698	0.219471	0.374109
	0.665713	0.217885	0.374097	0.665711	0.217884	0.374098
C8	0.716645	0.195377	0.034786	0.716653	0.195372	0.034791
	0.716640	0.195509	0.034861	0.716649	0.195489	0.034855
	0.716671	0.196985	0.034731	0.716675	0.196984	0.034736
	0.716723	0.195314	0.034741	0.716722	0.195316	0.034746
C20	0.735276	0.808490	0.302077	0.735277	0.808489	0.302076
	0.735299	0.808529	0.302060	0.735297	0.808529	0.302060
	0.735165	0.809852	0.302093	0.735171	0.809863	0.302088
	0.735232	0.808503	0.302064	0.735232	0.808503	0.302062

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Table 4: Continued

Atom	x	y	z	x	y	z
C21	0.833970	0.671628	0.306256	0.833971	0.671630	0.306262
	0.834023	0.671631	0.306307	0.834018	0.671635	0.306305
	0.833967	0.673243	0.306294	0.833964	0.673243	0.306296
	0.833959	0.671674	0.306280	0.833957	0.671674	0.306282
C22	0.860036	0.595837	0.210194	0.860038	0.595840	0.210193
	0.860032	0.595933	0.210231	0.860031	0.595932	0.210227
	0.860089	0.597475	0.210249	0.860088	0.597475	0.210241
	0.860056	0.595946	0.210200	0.860057	0.595945	0.210195
C23	0.944744	0.465170	0.213030	0.944751	0.465169	0.213026
	0.944887	0.465223	0.213017	0.944882	0.465222	0.213016
	0.944820	0.466762	0.213034	0.944822	0.466762	0.213032
	0.944812	0.465193	0.213036	0.944813	0.465193	0.213035
C24	0.004006	0.407942	0.313306	0.004015	0.407933	0.313309
	0.004054	0.407884	0.313362	0.004056	0.407886	0.313360
	0.004019	0.409436	0.313321	0.004022	0.409438	0.313322
	0.004004	0.407856	0.313352	0.004011	0.407858	0.313351
C25	0.983706	0.484692	0.409660	0.983710	0.484690	0.409666
	0.983765	0.484701	0.409706	0.983763	0.484698	0.409707
	0.983727	0.486180	0.409664	0.983728	0.486179	0.409666
	0.983733	0.484609	0.409686	0.983734	0.484609	0.409688
C26	0.898679	0.615365	0.405659	0.898678	0.615371	0.405667
	0.898629	0.615522	0.405714	0.898630	0.615519	0.405715
	0.898572	0.617003	0.405646	0.898573	0.617006	0.405655
	0.898567	0.615508	0.405704	0.898569	0.615508	0.405709
C31	0.080712	0.980068	0.132979	0.080700	0.980085	0.132971
	0.080697	0.980397	0.132941	0.080690	0.980381	0.132940
	0.080574	0.981795	0.132935	0.080575	0.981806	0.132931
	0.080596	0.980384	0.132875	0.080597	0.980390	0.132876
C32	0.133342	0.917075	0.244005	0.133342	0.917072	0.243991
	0.133427	0.917093	0.243897	0.133418	0.917099	0.243911
	0.133309	0.918671	0.243954	0.133306	0.918666	0.243932
	0.133261	0.917053	0.243913	0.133266	0.917055	0.243902
O1	0.420374	0.416475	0.485673	0.420369	0.416477	0.485673
	0.420399	0.416393	0.485692	0.420391	0.416402	0.485691
	0.420433	0.417859	0.485679	0.420422	0.417864	0.485677
	0.420283	0.416461	0.485686	0.420280	0.416463	0.485684
O2	0.496395	0.533827	0.239354	0.496404	0.533825	0.239356
	0.496478	0.533942	0.239387	0.496478	0.533936	0.239387
	0.496290	0.535608	0.239389	0.496305	0.535604	0.239390

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Table 4: Continued

Atom	x	y	z	x	y	z
	0.496480	0.533879	0.239366	0.496486	0.533879	0.239367
O3	0.328407	0.224410	0.032948	0.328410	0.224416	0.032949
	0.328459	0.224390	0.032950	0.328456	0.224402	0.032952
	0.328539	0.225978	0.033000	0.328535	0.225986	0.032999
	0.328463	0.224524	0.032917	0.328462	0.224530	0.032917
O4	0.461388	0.055827	0.134932	0.461379	0.055829	0.134933
	0.461288	0.055927	0.134888	0.461292	0.055924	0.134893
	0.461358	0.057495	0.134897	0.461353	0.057493	0.134895
	0.461261	0.055910	0.134908	0.461259	0.055908	0.134906
O5	0.081570	0.275741	0.320058	0.081569	0.275741	0.320056
	0.081516	0.275932	0.319941	0.084063	0.139045	0.132918
	0.081512	0.277602	0.320075	0.081510	0.277594	0.320072
	0.081561	0.275868	0.319956	0.081561	0.275866	0.319956
O6	0.083880	0.138995	0.132871	0.083890	0.139008	0.132870
	0.084080	0.139028	0.132930	0.081519	0.275915	0.319955
	0.084178	0.140499	0.132836	0.084171	0.140506	0.132831
	0.084021	0.139095	0.132898	0.084018	0.139095	0.132894
N1	0.401506	0.257518	0.296121	0.401509	0.257513	0.296121
	0.401566	0.257524	0.296203	0.401562	0.257521	0.296194
	0.401531	0.259076	0.296152	0.401530	0.259074	0.296151
	0.401581	0.257438	0.296194	0.401578	0.257439	0.296193
N2	0.533848	0.706918	0.414000	0.533856	0.706919	0.414002
	0.533983	0.706947	0.414027	0.533977	0.706949	0.414026
	0.533909	0.708447	0.414010	0.533909	0.708447	0.414009
	0.533949	0.707026	0.413980	0.533948	0.707024	0.413979
N3	0.470975	0.729202	0.122503	0.470968	0.729196	0.122504
	0.470926	0.729211	0.122500	0.470924	0.729209	0.122501
	0.470950	0.730795	0.122500	0.470946	0.730791	0.122500
	0.470921	0.729111	0.122498	0.470918	0.729109	0.122498
H1	0.466973	0.088421	0.399666	0.469238	0.092698	0.398650
	0.466527	0.087528	0.399488	0.468929	0.091796	0.398627
	-	-	-	-	-	-
	0.474136	0.101019	0.398634			
H3	0.503368	0.876081	0.302821	0.504744	0.872930	0.302718
	0.502923	0.877111	0.302438	0.504160	0.874013	0.302388
	-	-	-	-	-	-
	0.503507	0.868868	0.301588	0.504560	0.868389	0.301552
H5	0.422554	0.531827	0.052165	0.421944	0.535456	0.050956
	0.421354	0.532044	0.052257	0.421147	0.536357	0.050708

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Table 4: Continued

Atom	x	y	z	x	y	z
	-	-	-	-	-	-
	-	-	-	-	-	-
H7a	0.727208	0.179502	0.434827		-	
	0.728581	0.179227	0.435938	0.724130	0.179756	0.433438
	-	-	-	-	-	-
	-	-	-	-	-	-
H7c	0.691372	0.161528	0.311783	0.692694	0.164847	0.313386
	0.691878	0.160261	0.310405	0.692734	0.163460	0.311823
	-	-	-	-	-	-
	-	-	-	-	-	-
H8c	0.199347	0.686821	0.009733	0.204354	0.689247	0.008357
	0.197304	0.686170	0.010015	0.202775	0.688659	0.008633
	-	-	-	-	-	-
	-	-	-	-	-	-
H20a	0.745775	0.866299	0.232937	0.743992	0.859828	0.236953
	0.747823	0.867143	0.232513	0.745241	0.860755	0.236284
	0.737620	0.858250	0.231937	0.738741	0.858375	0.234747
	-	-	-	-	-	-
H20b	0.768171	0.878509	0.358995	0.766595	0.873800	0.357570
	0.768652	0.878068	0.357588	0.766558	0.873204	0.356658
	0.766258	0.876263	0.364512	0.766779	0.876606	0.362988
	0.764961	0.874705	0.356844	0.765863	0.874583	0.357066
H23	0.959281	0.407779	0.143650	0.961762	0.412373	0.146347
	0.958603	0.407470	0.143978	0.961079	0.412093	0.147045
	-	-	-	-	-	-
	-	-	-	-	-	-
H25	0.028095	0.437260	0.481237	0.026427	0.441059	0.477764
	0.027868	0.437597	0.481441	0.025828	0.441853	0.477141
	-	-	-	-	-	-
	-	-	-	-	-	-
H26	0.883548	0.669923	0.473015	-	-	-
	0.884681	0.670642	0.473775	-	-	-
	-	-	-	-	-	-
	-	-	-	-	-	-
H32a	0.072694	0.954239	0.297032	-	-	-
	0.073174	0.955142	0.298346	0.078246	0.952233	0.292653
	-	-	-	-	-	-
	-	-	-	-	-	-

Table 5: Coordinates of BCPs in eight different density maps of α -Glycine: Dynamic model densities and MEM density maps for IAM (first line), IAM-HO(second line), INV (third line) and MP (fourth line).

Bond	Dynamic model density			MEM density		
	x	y	z	x	y	z
C1-O1	0.657408	0.386761	0.630687	0.648703	0.386088	0.626674
	0.657033	0.386717	0.630434	0.651657	0.386523	0.629810
	0.659444	0.386958	0.630902	0.653695	0.386856	0.629442
	0.657760	0.386791	0.630732	0.653586	0.386850	0.629295
C1-O2	0.484688	0.368389	0.581224	0.490142	0.369824	0.576308
	0.484927	0.368385	0.581207	0.488714	0.369727	0.576990
	0.480953	0.367791	0.577757	0.486222	0.368888	0.577433
	0.484096	0.368255	0.580609	0.486748	0.368909	0.577618
C1-C2	0.936507	0.864409	0.074176	0.938724	0.864633	0.078175
	0.936522	0.864384	0.074149	0.938892	0.864724	0.075687
	0.933796	0.865582	0.073966	0.936274	0.864043	0.081525
	0.936113	0.864794	0.077312	0.936259	0.864132	0.080471
C2-N1	0.335786	0.619986	0.734730	0.345158	0.624579	0.729474
	0.335843	0.619981	0.734758	0.344735	0.624528	0.729197
	0.341426	0.620439	0.735514	0.348500	0.624846	0.727875
	0.341260	0.621531	0.734130	0.349217	0.624758	0.728171
O1...H1-N	0.287851	0.096922	0.431046	0.282769	0.098066	0.430689
	0.288923	0.096729	0.431216	0.280350	0.097364	0.429801
	0.288530	0.096904	0.440504	0.290774	0.095772	0.441037
	0.284803	0.098200	0.438897	0.291673	0.095888	0.441407
O2...H2-N	0.626369	0.126627	0.957301	0.622006	0.124782	0.943587
	0.626236	0.126860	0.957554	0.626193	0.121417	0.944594
	0.617238	0.125914	0.947182	0.610202	0.132617	0.944052
	0.616335	0.127703	0.949144	0.610045	0.133175	0.943302
O2...H3-N	0.729323	0.554116	0.326691	0.709478	0.544571	0.330367
	0.728788	0.554142	0.326576	0.708793	0.545040	0.329762
	0.732188	0.549069	0.320558	0.705215	0.543244	0.314054
	0.741749	0.552335	0.319642	0.711619	0.543801	0.317147
O1...H3-N	0.480057	0.969027	0.770940	0.433766	0.969596	0.709516
	0.479968	0.968992	0.770807	0.437843	0.969455	0.711125
	0.476806	0.975798	0.765836	0.465346	0.963081	0.776867
	0.478775	0.976299	0.764862	0.463283	0.961372	0.773295
O1...H4-C2	0.558636	0.806807	0.758849	0.503885	0.811812	0.700627
	0.558768	0.806922	0.758657	0.503537	0.812762	0.699015
	0.553111	0.803733	0.755632	0.530902	0.803714	0.725127
	0.546795	0.802582	0.755536	0.520915	0.803992	0.723085

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Table 5: Continued

Bond	x	y	z	x	y	z
O2...H4-C2	0.310559	0.787342	0.811623	0.364051	0.793558	0.835732
	0.310683	0.787469	0.811493	0.364255	0.794240	0.837189
	0.307033	0.784185	0.807335	0.344850	0.790686	0.824033
	0.311258	0.783065	0.805644	0.340828	0.790776	0.817615

Table 6: Coordinates of BCPs in eight different density maps of *D,L*-Serine: Dynamic model densities and MEM density maps for IAM (first line), IAM-HO(second line), INV (third line) and MP (fourth line).

Bond	Dynamic model density			MEM density		
	x	y	z	x	y	z
C1-O1	0.712326	0.409322	0.574065	0.713941	0.409760	0.579469
	0.712763	0.409322	0.574989	0.712943	0.409077	0.573776
	0.711973	0.408760	0.573699	0.712906	0.409284	0.575100
	0.711978	0.409521	0.572458	0.712254	0.409490	0.572233
C1-O2	0.778355	0.449341	0.699340	0.775175	0.446907	0.697864
	0.778063	0.449003	0.698882	0.777025	0.450098	0.699742
	0.779451	0.448853	0.702909	0.776808	0.448760	0.700473
	0.779159	0.450022	0.700500	0.778031	0.450178	0.700969
C3-O3	0.906238	0.198651	0.866576	0.902097	0.200004	0.868565
	0.906204	0.198580	0.866871	0.901057	0.200321	0.873061
	0.906847	0.198334	0.869129	0.902439	0.199695	0.870208
	0.905430	0.198843	0.869956	0.903155	0.199473	0.868697
C1-C2	0.750535	0.347225	0.772676	0.751335	0.344934	0.775004
	0.750543	0.347208	0.772643	0.751115	0.345024	0.773883
	0.750308	0.346840	0.770767	0.751452	0.345113	0.774632
	0.751245	0.346113	0.774225	0.751239	0.345181	0.773551
C2-C3	0.822185	0.250119	0.925017	0.822263	0.247387	0.923965
	0.822187	0.250080	0.925009	0.822489	0.247404	0.924510
	0.821683	0.249764	0.923100	0.821986	0.247535	0.923465
	0.821600	0.249377	0.922031	0.821671	0.247971	0.923863
C2-N1	0.709015	0.234279	0.818951	0.711650	0.235429	0.822288
	0.708934	0.234203	0.818866	0.711545	0.235647	0.821977
	0.710767	0.235426	0.818709	0.711984	0.235107	0.823200
	0.711017	0.236348	0.821271	0.712217	0.235728	0.823671
O1...H4-O3	0.620782	0.514700	0.357884	0.616842	0.519317	0.361644
	0.620812	0.514492	0.356961	0.616524	0.518317	0.362790
	0.620130	0.519163	0.362311	0.614753	0.519600	0.357172
	0.619486	0.519025	0.361269	0.616364	0.519327	0.359358
O3...H11-N1	0.513889	0.261887	0.706253	0.515352	0.259349	0.704093
	0.513754	0.261747	0.707038	0.514702	0.260361	0.703735
	0.517740	0.260268	0.706162	0.514675	0.256749	0.701384
	0.519808	0.261055	0.714965	0.516858	0.258752	0.703372
O2...H12-N1	0.660840	0.064049	1.032432	0.669064	0.067041	1.031131
	0.660820	0.063934	1.032508	0.670227	0.069100	1.033184
	0.659473	0.066835	1.023642	0.670204	0.068057	1.030896
	0.660410	0.069911	1.027448	0.668500	0.068091	1.030240

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Table 6: Continued

Bond	x	y	z	x	y	z
O2...H13-N1	0.667638	0.079853	0.441572	0.668098	0.078269	0.458068
	0.667544	0.080061	0.440898	0.670561	0.076058	0.464196
	0.668383	0.081621	0.453809	0.668385	0.079425	0.456363
	0.666745	0.080841	0.453148	0.665911	0.078051	0.456870
O1...H2-C2	0.703359	0.360992	0.222035	0.698564	0.354457	0.213788
	0.703710	0.361144	0.222477	0.695661	0.349612	0.208309
	0.703997	0.358691	0.217757	0.694611	0.353610	0.205922
	0.701021	0.356350	0.207473	0.698502	0.351689	0.207334

Table 7. Coordinates of BCPs in eight different density maps of L-Alanine: Dynamic model densities and MEM density maps for IAM (first line), IAM-HO (second line), INV (third line) and MP (fourth line).

Bond	Dynamic model density			MEM density		
	x	y	z	x	y	z
C1-O1	0.379900	0.619095	0.890871	0.382181	0.621809	0.891579
	0.380574	0.619125	0.890689	0.381066	0.622117	0.891934
	0.379707	0.618887	0.891658	0.381079	0.619418	0.891373
	0.379628	0.618893	0.892229	0.379707	0.619366	0.891208
C1-O2	0.489291	0.657296	0.838495	0.486292	0.656137	0.844221
	0.488939	0.657183	0.838767	0.486873	0.656172	0.843155
	0.492007	0.658168	0.839466	0.490007	0.656304	0.841755
	0.489286	0.657245	0.839861	0.489677	0.656652	0.840657
C1-C2	0.489805	0.650952	0.022630	0.488646	0.649456	0.023133
	0.489843	0.650911	0.022666	0.489314	0.649663	0.023254
	0.488264	0.650664	0.023077	0.488145	0.649244	0.020995
	0.489379	0.651015	0.027438	0.489337	0.649488	0.025197
C2-C3	0.362644	0.125916	0.328983	0.365881	0.125859	0.329864
	0.362570	0.125917	0.328873	0.364943	0.125457	0.329400
	0.360695	0.125782	0.328419	0.362414	0.126274	0.327629
	0.361243	0.125894	0.328064	0.363904	0.126391	0.329216
C2-N1	0.452242	0.650452	0.222782	0.454839	0.650252	0.216369
	0.452402	0.650494	0.222844	0.454474	0.650102	0.218705
	0.454246	0.650092	0.220215	0.454230	0.650440	0.216409
	0.462722	0.651241	0.212319	0.459727	0.650495	0.210943
O2...H3-N	0.531104	0.161516	0.921143	0.513733	0.154647	0.928108
	0.531737	0.161567	0.920832	0.515545	0.155493	0.928672
	0.538053	0.160542	0.928523	0.526902	0.158641	0.931362
	0.537108	0.161713	0.929909	0.526213	0.158309	0.931043
O2...H2-N	0.156026	0.736867	0.274552	0.169842	0.737578	0.264715
	0.156001	0.736847	0.273523	0.169585	0.737325	0.263201
	0.163245	0.734411	0.281284	0.166682	0.733281	0.270840
	0.167788	0.736241	0.278019	0.169505	0.733725	0.265316
O1...H1-N	0.230221	0.496251	0.834100	0.223945	0.493289	0.833780
	0.231499	0.496035	0.832843	0.222061	0.494150	0.832297
	0.229447	0.492072	0.833069	0.221262	0.490439	0.847632
	0.226989	0.492208	0.837202	0.227572	0.489683	0.843353

Table 8: Coordinates of BCPs in eight different density maps of Ala-Tyr-Ala(*etoh*): Dynamic model densities and MEM density maps for IAM (first line), IAM-HO(second line), INV (third line) and MP (fourth line).

Bond	Dynamic model density			MEM density		
	x	y	z	x	y	z
C2-O1	0.442350	0.335203	0.490091	0.443275	0.331966	0.489942
	0.442488	0.334874	0.490101	0.443095	0.332300	0.489972
	0.441433	0.337161	0.493357	0.442406	0.335182	0.491190
	0.440878	0.335236	0.489386	0.441286	0.334399	0.488705
C4-O2	0.498716	0.116704	0.772497	0.500082	0.120948	0.772847
	0.498599	0.117039	0.772575	0.500128	0.120642	0.772826
	0.501197	0.117037	0.775671	0.500513	0.120147	0.774309
	0.499342	0.116097	0.772100	0.499630	0.116797	0.772107
C6-O3	0.395649	0.173137	0.044615	0.397880	0.171104	0.043910
	0.395925	0.173063	0.044690	0.397276	0.171463	0.044152
	0.395894	0.175194	0.044279	0.397156	0.174779	0.043873
	0.395520	0.174175	0.043808	0.395997	0.174107	0.043466
C6-O4	0.448543	0.107590	0.083999	0.447131	0.109834	0.081143
	0.448496	0.107779	0.083904	0.447229	0.109498	0.081210
	0.450824	0.107995	0.083964	0.449210	0.109820	0.082467
	0.450112	0.106878	0.084081	0.448979	0.107767	0.083077
C24-O5	0.035509	0.354012	0.315751	0.032121	0.355423	0.313787
	0.035549	0.354146	0.315758	0.031860	0.354917	0.313835
	0.035575	0.355390	0.315844	0.035788	0.356697	0.315232
	0.035799	0.356409	0.315095	0.035027	0.356349	0.314585
C31-O6	0.918304	0.546113	0.867404	0.918087	0.542393	0.867135
	0.918250	0.546273	0.867427	0.918979	0.541940	0.867766
	0.918499	0.546792	0.868560	0.918413	0.543921	0.869773
	0.915991	0.540559	0.866697	0.916795	0.540066	0.868715
C1-N1	0.454279	0.225229	0.348926	0.456219	0.225923	0.352893
	0.454328	0.225219	0.348928	0.455967	0.226623	0.352098
	0.455780	0.226972	0.350372	0.455632	0.227299	0.351066
	0.458081	0.224373	0.350908	0.456643	0.225769	0.351270
C2-N2	0.460583	0.251815	0.531821	0.460369	0.256263	0.526389
	0.460481	0.251883	0.531839	0.460839	0.255764	0.527397
	0.460278	0.254834	0.531565	0.459606	0.257089	0.528964
	0.460328	0.252871	0.531950	0.459566	0.255080	0.529758
C3-N2	0.449976	0.244720	0.643260	0.446935	0.249091	0.646764
	0.449933	0.244746	0.643236	0.447340	0.248685	0.646642
	0.449943	0.246664	0.644068	0.447971	0.249325	0.645438
	0.450468	0.246392	0.644168	0.447518	0.248202	0.645766

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Table 8: Continued

Bond	x	y	z	x	y	z
C4-N3	0.509315	0.193660	0.820585	0.508499	0.192221	0.815161
	0.509312	0.193642	0.820580	0.508814	0.193294	0.817353
	0.509523	0.193765	0.820187	0.508825	0.192947	0.817586
	0.509739	0.193091	0.820992	0.509218	0.193137	0.819592
C5-N3	0.551194	0.179590	0.931073	0.551398	0.179308	0.932937
	0.551179	0.179626	0.931074	0.551432	0.179005	0.932749
	0.551257	0.181643	0.932363	0.553053	0.180206	0.933777
	0.552727	0.177434	0.931608	0.553676	0.176674	0.933465
C1-C2	0.476963	0.241510	0.442545	0.477155	0.240847	0.440940
	0.477003	0.241566	0.442543	0.477343	0.240920	0.441154
	0.478061	0.241129	0.439301	0.477868	0.242262	0.440220
	0.478784	0.241493	0.441228	0.478600	0.240350	0.440532
C1-C7	0.581985	0.208272	0.383124	0.587827	0.207451	0.384667
	0.582007	0.208247	0.383099	0.586279	0.207107	0.384981
	0.583464	0.209256	0.382942	0.587768	0.208796	0.383503
	0.588169	0.207232	0.384617	0.589954	0.207504	0.384752
C3-C4	0.466119	0.221618	0.734657	0.466095	0.221450	0.733620
	0.466079	0.221559	0.734651	0.466068	0.221198	0.733390
	0.463433	0.225113	0.731624	0.464887	0.223141	0.732680
	0.466023	0.222532	0.734660	0.466075	0.221810	0.733954
C3-C20	0.350702	0.291961	0.693687	0.349885	0.294747	0.691981
	0.350716	0.291974	0.693710	0.350810	0.294259	0.691703
	0.352156	0.294231	0.692502	0.351625	0.294676	0.693539
	0.348921	0.290312	0.693429	0.350169	0.291685	0.694047
C5-C6	0.495345	0.639906	0.986780	0.493834	0.641960	0.987042
	0.495360	0.639948	0.986748	0.493847	0.642138	0.986616
	0.496878	0.642464	0.987800	0.496238	0.643080	0.987596
	0.494706	0.641369	0.988256	0.495126	0.640652	0.987861
C5-C8	0.643664	0.167475	0.004623	0.646820	0.168627	0.002207
	0.643630	0.167558	0.004659	0.646766	0.167964	0.001726
	0.645562	0.168979	0.004788	0.646729	0.169434	0.003061
	0.647257	0.169105	0.005174	0.647643	0.169550	0.003254
C20-C21	0.215145	0.240093	0.695897	0.216785	0.238784	0.695598
	0.215038	0.240145	0.695870	0.216601	0.238402	0.695714
	0.213789	0.241217	0.695897	0.213945	0.239059	0.696478
	0.216665	0.239068	0.697112	0.215897	0.236991	0.697327
C21-C22	0.847247	0.633605	0.258153	0.848381	0.633895	0.257011
	0.847268	0.633660	0.258182	0.848979	0.634932	0.257938
	0.847527	0.634786	0.256709	0.847496	0.637261	0.258368

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Table 8: Continued

Bond	x	y	z	x	y	z
	0.846956	0.634113	0.258246	0.847288	0.636842	0.259701
C22-C23	0.902487	0.530412	0.211814	0.899852	0.532005	0.212943
	0.902553	0.530501	0.211818	0.900120	0.531582	0.213369
	0.903307	0.530842	0.211679	0.901911	0.531899	0.212048
	0.903009	0.529929	0.212217	0.901519	0.530766	0.212140
C23-C24	0.025741	0.936716	0.736881	0.026448	0.937941	0.739426
	0.025675	0.936740	0.736845	0.025820	0.936717	0.738339
	0.025265	0.937086	0.738151	0.024416	0.937567	0.738320
	0.025283	0.935493	0.738176	0.024452	0.936304	0.738118
C24-C25	0.006175	0.446497	0.361543	0.004358	0.948583	0.635930
	0.006142	0.946525	0.638450	0.003846	0.947739	0.636663
	0.005688	0.948117	0.636458	0.005869	0.947890	0.636396
	0.005569	0.945868	0.637358	0.006668	0.946228	0.636755
C25-C26	0.941273	0.549915	0.407527	0.944665	0.547518	0.406904
	0.941221	0.549986	0.407560	0.942450	0.550172	0.407025
	0.941224	0.551392	0.407285	0.943085	0.549665	0.406691
	0.941196	0.549664	0.406938	0.942531	0.547680	0.406633
C21-C26	0.133374	0.143324	0.643937	0.132101	0.144767	0.648174
	0.133387	0.143376	0.643901	0.130978	0.142998	0.645952
	0.132922	0.144818	0.642277	0.131460	0.144363	0.642858
	0.133243	0.143157	0.643762	0.132267	0.141914	0.643942
C31-C32	0.892794	0.446602	0.811691	0.892030	0.446116	0.807725
	0.892847	0.446654	0.811763	0.891922	0.446136	0.808197
	0.892154	0.449579	0.810211	0.891387	0.448142	0.806993
	0.890883	0.445786	0.808715	0.890713	0.445311	0.806622
O6...H15-O5	0.923020	0.695865	0.791484	0.919681	0.697438	0.789344
	0.923174	0.696077	0.791751	0.921008	0.698509	0.789557
	0.926055	0.699033	0.788316	0.920827	0.699058	0.788099
	0.921278	0.697886	0.788607	0.922026	0.696112	0.788750
O3...H16-O6	0.228251	0.191813	0.074025	0.219262	0.197918	0.069950
	0.227799	0.191902	0.073519	0.219213	0.198338	0.070244
	0.226132	0.189608	0.075662	0.221864	0.192608	0.072045
	0.223542	0.189660	0.075317	0.220098	0.191072	0.071052
O4...H11A-N1	0.572706	0.636794	0.804376	0.563723	0.636007	0.798198
	0.573089	0.637080	0.804620	0.566339	0.635142	0.798619
	0.571853	0.642828	0.802137	0.565053	0.640933	0.799304
	0.570375	0.640100	0.800716	0.564137	0.641697	0.800891
O2...H11C-N1	0.538706	0.924267	0.737640	0.528375	0.918559	0.741725
	0.538030	0.924161	0.737760	0.527373	0.918240	0.740719

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Table 8: Continued

Bond	x	y	z	x	y	z
	0.543933	0.923938	0.738905	0.542012	0.921933	0.743490
	0.543063	0.921167	0.737786	0.539060	0.918609	0.742551
O5...H11B-N1	0.790481	0.770586	0.688206	0.785246	0.783856	0.690806
	0.790752	0.771036	0.688500	0.785924	0.784119	0.691336
	0.784948	0.770561	0.688001	0.784140	0.779780	0.690413
	0.783717	0.772121	0.688849	0.782769	0.774291	0.689324
O4...H13-N3	0.528896	0.426287	0.874845	0.522166	0.423565	0.869348
	0.528565	0.426368	0.874538	0.515899	0.424298	0.868964
	0.526379	0.421480	0.878474	0.532087	0.420959	0.880359
	0.533732	0.413578	0.872910	0.534780	0.414932	0.879162
O1...H1-C1	0.484217	0.515423	0.549344	0.477121	0.509178	0.557819
	0.484320	0.515404	0.549453	0.476513	0.509454	0.559228
	0.480972	0.517937	0.550882	0.473004	0.514264	0.559118
	0.471371	0.528451	0.548196	0.474756	0.522184	0.558145
O1...H12-N2	0.473777	0.524778	0.445766	0.478535	0.520195	0.435444
	0.473915	0.524700	0.446013	0.480407	0.517217	0.433326
	0.472861	0.533974	0.443349	0.480550	0.531861	0.443750
	0.468080	0.537786	0.448390	0.472431	0.531265	0.440547

Table 9. *Topological properties of covalent and hydrogen bonds of α -Glycine: ρ_{BCP} ($e/\text{\AA}^3$; first line) and $\nabla^2\rho_{BCP}$ ($e/\text{\AA}^5$; second line) for the static and dynamic model densities of the INV and MP models. See tables in the main text for values in other dynamic model densities*

as well as in MEM densities.

Bond	Dynamic		Static	
	INV	MP	INV	MP
C1-O1	2.636	2.701	2.699	2.770
	-17.18	-19.44	-31.82	-36.57
C1-O2	2.598	2.648	2.680	2.733
	-21.83	-23.61	-31.23	-35.07
C1-C2	1.696	1.698	1.735	1.735
	-14.28	-13.28	-13.89	-12.80
C2-N	1.749	1.657	1.788	1.691
	-11.65	-10.21	-11.54	-10.42
O1...H1-N	0.256	0.289	0.239	0.283
	3.46	2.51	3.81	2.68
O2...H2-N	0.209	0.249	0.194	0.240
	3.61	2.77	3.19	2.29
O2...H3-N	0.127	0.158	0.116	0.151
	2.01	1.61	1.93	1.51
O1...H3-N	0.069	0.072	0.062	0.065
	1.24	1.29	1.18	1.24
O1...H4-C2	0.082	0.070	0.075	0.063
	1.11	1.04	1.03	0.95
O2...H4-C2	0.086	0.077	0.080	0.070
	1.16	1.13	1.14	1.09

Table 10. Topological properties of covalent and hydrogen bonds of D,L-Serine: ρ_{BCP} ($e/\text{\AA}^3$; first line) and $\nabla^2\rho_{BCP}$ ($e/\text{\AA}^5$; second line) for the static and dynamic model densities of the INV and MP models. See tables in the main text for values in other dynamic model densities

as well as in MEM densities.

Bond	Dynamic		Static	
	INV	MP	INV	MP
C1-O1	2.632	2.723	2.709	2.810
	-19.44	-23.40	-32.04	-32.18
C1-O2	2.585	2.693	2.666	2.791
	-16.79	-24.15	-30.75	-35.32
C3-O3	1.752	1.807	1.804	1.869
	-6.83	-9.02	-12.26	-16.64
C1-C2	1.674	1.669	1.719	1.710
	-12.67	-11.23	-13.28	-11.77
C2-C3	1.707	1.684	1.752	1.726
	-14.28	-13.60	-13.01	-12.29
C2-N	1.746	1.664	1.769	1.684
	-12.33	-12.20	-9.83	-10.06
O1...H4-O3	0.287	0.279	0.266	0.258
	3.94	3.91	4.24	4.29
O3...H11-N	0.235	0.237	0.218	0.219
	3.93	4.10	3.65	3.89
O2...H12-N	0.220	0.218	0.203	0.200
	3.61	3.71	3.29	3.47
O2...H13-N	0.210	0.202	0.194	0.185
	3.65	3.84	3.13	3.42
O1...H2-C2	0.119	0.086	0.110	0.075
	1.88	1.97	1.41	1.53

Table 11. Topological properties of covalent and hydrogen bonds of L-Alanine: ρ_{BCP} ($e/\text{\AA}^3$; first line) and $\nabla^2\rho_{BCP}$ ($e/\text{\AA}^5$; second line) for the static and dynamic model densities of the INV and MP models. See tables in the main text for values in other dynamic model densities

Bond	<i>as well as in MEM densities.</i>			
	Dynamic		Static	
	INV	MP	INV	MP
C1-O1	2.656	2.807	2.727	2.902
	-17.82	-27.51	-32.18	-43.72
C1-O2	2.577	2.649	2.657	2.743
	-20.13	-24.01	-30.46	-38.20
C1-C2	1.673	1.696	1.714	1.736
	-12.90	-12.51	-13.24	-12.78
C2-C3	1.642	1.611	1.680	1.649
	-11.16	-10.67	-11.17	-10.67
C2-N	1.736	1.614	1.769	1.650
	-10.06	-11.52	-9.93	-13.45
O2...H3-N	0.231	0.258	0.222	0.249
	3.61	3.52	3.56	3.54
O2...H2-N	0.195	0.215	0.186	0.206
	3.19	3.22	3.10	3.19
O1...H1-N	0.188	0.206	0.179	0.197
	3.05	3.00	2.96	2.97

Table 12: Topological properties of covalent and hydrogen bonds of Ala-Tyr-Ala(*etho*): ρ_{BCP} (e/ \AA^3 ; first line) and $\nabla^2\rho_{BCP}$ (e/ \AA^5 ; second line) for the static and dynamic model densities of the INV and MP models. See tables in the main text for values in other dynamic model densities as well as in MEM densities.

Bond	Dynamic		Static	
	INV	MP	INV	MP
C2-O1	2.495	2.711	2.595	2.829
	-8.97	-14.97	-30.11	-35.54
C4-O2	2.462	2.807	2.587	2.984
	-12.46	-24.86	-30.09	-42.60
C6-O3	2.609	2.728	2.683	2.812
	-7.73	-11.58	-31.74	-30.01
C6-O4	2.473	2.594	2.599	2.741
	-16.32	-20.73	-28.34	-34.27
C24-O5	1.904	1.954	1.992	2.052
	-10.25	-11.12	-14.10	-19.35
C31-O6	1.656	1.607	1.759	1.730
	-5.30	-3.16	-10.81	-20.40
C1-N1	1.700	1.665	1.742	1.703
	-8.81	-8.40	-9.51	-9.15
C2-N2	2.203	2.319	2.304	2.428
	-19.98	-21.60	-22.94	-24.24
C3-N2	1.732	1.779	1.788	1.842
	-10.38	-12.35	-10.30	-12.60
C4-N3	2.222	2.416	2.319	2.530
	-20.09	-24.30	-23.64	-26.85
C5-N3	1.720	1.797	1.783	1.874
	-9.30	-12.99	-10.08	-14.39
C1-C2	1.744	1.692	1.803	1.753
	-12.23	-13.48	-12.05	-13.63
C1-C7	1.613	1.733	1.655	1.788
	-11.39	-13.90	-10.85	-13.73
C3-C4	1.742	1.708	1.793	1.760
	-11.46	-12.48	-11.80	-13.01
C3-C20	1.628	1.603	1.648	1.625
	-11.08	-11.57	-10.03	-10.90
C5-C6	1.634	1.715	1.681	1.770
	-13.51	-14.84	-12.70	-14.25
C5-C8	1.580	1.614	1.642	1.681
	-9.78	-9.99	-10.61	-10.95
C20-C21	1.700	1.636	1.752	1.679
	-11.31	-9.61	-11.15	-9.23
C21-C22	1.955	1.999	2.046	2.094
	-16.61	-17.94	-16.93	-18.49
C22-C23	1.984	2.011	2.074	2.103
	-16.57	-16.92	-17.02	-17.32
C23-C24	2.019	2.029	2.100	2.110
	-16.01	-16.00	-16.42	-16.42
C24-C25	1.997	2.021	2.095	2.122

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Table 12: Continued

Bond	Dynamic		Static	
	INV	MP	INV	MP
C25-C26	-17.07	-18.06	-17.38	-18.45
C21-C26	1.999	1.984	2.091	2.069
O6...H15-O5	-16.04	-15.02	-16.37	-15.01
O3...H16-O6	1.957	1.995	2.038	2.073
O4...H11A-N1	-15.97	-15.40	-16.80	-16.01
O2...H11C-N1	1.670	1.680	1.704	1.704
O5...H11B-N1	-11.02	-10.37	-11.52	-10.99
O4...H13-N3	0.308	0.310	0.269	0.270
O1...H1-C1	3.54	4.48	4.36	5.22
O1...H12-N2	0.284	0.285	0.253	0.262
O1...H12-N2	3.66	3.63	4.09	4.04
O1...H12-N2	0.246	0.251	0.220	0.236
O1...H12-N2	3.33	3.28	3.52	3.44
O1...H12-N2	0.250	0.268	0.230	0.252
O1...H12-N2	3.61	3.59	3.80	3.94
O1...H12-N2	0.198	0.210	0.175	0.189
O1...H12-N2	2.98	3.43	2.82	3.41
O1...H12-N2	0.150	0.104	0.136	0.091
O1...H12-N2	2.19	2.50	2.01	2.38
O1...H12-N2	0.118	0.105	0.107	0.095
O1...H12-N2	1.70	1.63	1.53	1.48
O1...H12-N2	0.119	0.107	0.109	0.095
O1...H12-N2	1.84	2.09	1.76	2.02

Table 13. Number of electrons in atomic basins and volumes of the atomic basins in MEM-electron-density maps of α -Glycine obtained with different prior densities as indicated. Hydrogen atoms in the brackets indicate that they are included in the atomic basin of the corresponding parent atom.

Atom	prior: IAM		prior: IAM-HO		prior: INV		prior: MP	
	Electrons	Volume	Electrons	Volume	Electrons	Volume	Electrons	Volume
C1	4.40	5.11	4.48	5.33	4.47	4.66	4.46	4.69
C2(+H4)	6.76	13.79	6.77	13.79	6.72	13.71	6.76	13.82
O1	9.11	14.94	9.07	14.77	9.20	15.72	9.19	15.69
O2	9.11	15.13	9.10	15.05	9.24	15.78	9.26	15.95
N1(+H1+H2+H3)	9.74	20.85	9.73	21.00	9.65	20.20	9.64	20.30
H5	0.88	5.79	0.85	5.71	0.72	5.72	0.69	5.34
Total	40.00	75.61	40.00	75.65	40.00	75.79	40.00	75.79

Table 14. Number of electrons in atomic basins and volumes of the atomic basins in MEM-electron-density maps of D,L-Serine obtained with different prior densities as indicated. Hydrogen atoms in the brackets indicate that they are included in the atomic basin of the corresponding parent atom.

Atom	prior: IAM		prior: IAM-HO		prior: INV		prior: MP	
	Electrons	Volume	Electrons	Volume	Electrons	Volume	Electrons	Volume
C1	4.25	4.91	4.43	5.18	4.33	4.77	4.41	4.97
C2	5.73	7.97	5.73	7.76	5.63	7.42	5.63	7.22
C3	6.15	9.42	6.11	9.17	6.15	9.07	6.16	9.10
O1	9.28	16.16	9.28	16.13	9.35	17.14	9.27	16.18
O2	9.16	16.94	9.08	16.71	9.23	17.92	9.12	16.89
O3(+H4)	9.16	16.57	9.24	16.88	9.17	16.62	9.23	17.07
N1(+H11+H12+H13)	9.23	20.98	9.23	21.04	9.15	19.57	9.29	21.47
H2	0.78	4.85	0.82	5.20	0.87	5.58	0.86	5.67
H31	0.97	6.36	0.93	6.38	0.93	6.25	0.94	6.50
H32	1.23	8.86	1.15	8.83	1.17	8.92	1.09	8.21
Spurious maxima-1	0.05	0.27	-	-	-	-	-	-
Total	55.99	113.29	56.00	113.28	55.98	113.26	56.00	113.28

Table 15. Number of electrons in atomic basins and volumes of the atomic basins in MEM-electron-density maps of L-Alanine obtained with different prior densities as indicated. Hydrogen atoms in the brackets indicate that they are included in the atomic basin of the corresponding parent atom.

Atom	prior: IAM		prior: IAM-HO		prior: INV		prior: MP	
	Electrons	Volume	Electrons	Volume	Electrons	Volume	Electrons	Volume
C1	4.58	5.98	4.62	5.87	4.57	5.51	4.56	5.16
C2	5.84	8.42	5.84	8.06	5.85	7.48	5.82	8.00
C3(+H7)	7.32	17.88	7.29	17.93	7.23	17.17	7.38	18.20
O1	8.91	15.20	8.90	15.18	9.11	18.00	9.04	16.63
O2	8.96	14.01	8.95	13.95	9.14	16.13	9.15	15.78
N1(+H1+H2+H3)	9.89	25.49	9.86	25.62	9.58	21.39	9.76	23.22
H4	0.83	5.46	0.84	5.64	0.83	5.82	0.75	5.42
H5	0.87	6.75	0.88	6.86	0.91	8.05	0.83	7.31
H6	0.81	6.06	0.82	6.16	0.78	5.73	0.71	5.55
Total	48.01	105.25	48.00	105.27	48.00	105.28	48.00	105.27
H1	-	-	-	-	0.35	2.00	-	-
H2	-	-	-	-	0.33	1.80	-	-
H3	-	-	-	-	0.40	1.92	-	-
H7	-	-	-	-	0.76	5.67	0.68	5.41

Table 16. Number of electrons in atomic basins and volumes of the atomic basins in MEM-electron-density maps of Ala-Tyr-Ala_(eth) obtained with different prior densities as indicated. Hydrogen atoms in the brackets indicate that they are included in the atomic basin of the corresponding parent atom.

Atom	prior: IAM		prior: IAM-HO		prior: INV		prior: MP	
	Electrons	Volume	Electrons	Volume	Electrons	Volume	Electrons	Volume
C1(+H1)	6.59	13.15	6.58	13.31	6.65	13.21	6.61	12.45
C2	4.76	6.14	4.82	6.37	4.82	6.44	4.85	6.28
C3(+H3)	6.66	12.82	6.68	13.06	6.71	12.82	6.65	13.04
C4	4.73	6.07	4.81	6.25	4.86	6.14	4.84	6.04
C5(+H5)	6.81	18.24	6.82	17.63	6.68	16.14	6.60	14.38
C6	4.55	6.05	4.59	5.97	4.61	6.63	4.66	6.70
C7(+H7a+H7b+H7c)	8.25	29.74	8.75	36.73	8.70	34.08	8.72	34.29
C8(+H8a+H8b+H8c)	8.98	36.33	8.96	36.15	8.94	35.81	9.03	36.51
C20(+H20a)	7.38	17.87	7.40	17.76	7.41	17.68	7.36	18.02
C21	6.01	9.44	6.05	9.10	6.02	9.93	5.96	9.69
C22(+H22)	6.77	18.27	6.79	18.19	7.01	20.48	7.01	20.50
C23(+H23)	7.05	21.44	7.03	21.31	7.05	22.22	7.00	22.28
C24	5.80	12.76	5.78	12.89	5.68	10.34	5.68	10.73
C25(+H25)	6.89	21.61	6.91	21.74	6.95	21.62	6.93	22.70
C26(+H26)	7.17	22.79	7.09	22.93	7.04	21.15	7.03	21.83
C31(+H31a+H31b)	7.49	26.93	7.44	26.86	7.61	25.48	7.42	24.37
C32(+H32a+H32b+H32c)	8.84	38.96	8.78	39.56	9.06	39.82	8.75	37.68
O1	9.13	16.84	9.13	16.85	9.04	18.74	9.04	18.76
O2	9.28	17.07	9.30	17.20	9.10	19.09	9.22	20.11
O3	8.85	16.96	8.85	17.62	8.83	17.91	8.91	19.97
O4	9.07	13.51	9.09	13.97	9.13	16.02	9.17	16.01
O5(+H15)	9.56	18.03	9.46	18.16	9.57	20.75	9.72	20.45
O6(+H16)	9.44	18.30	9.58	18.15	9.35	18.48	9.54	18.99
N1(+H11a+H11b+H11c)	9.71	23.48	9.72	23.59	9.40	21.08	9.64	22.58
N2(+H12)	8.47	17.69	8.46	17.53	8.45	17.21	8.47	16.60
N3(+H13)	8.43	16.08	8.37	15.35	8.47	15.89	8.41	15.68
H20b	0.74	6.57	0.72	6.42	0.84	6.34	0.74	6.04
Spurious maxima-1	0.01	0.51	0.01	0.59	0.00	0.31	0.01	0.54
Spurious maxima-2	0.00	1.36	0.00	1.49	0.02	1.81	0.00	0.22
Spurious maxima-3	0.02	0.45	-	-	-	-	-	-
Spurious maxima-4	0.00	0.19	-	-	-	-	-	-
Spurious maxima-5	0.01	0.18	-	-	-	-	-	-
Total	197.45	485.83	197.97	492.73	198.00	493.62	197.97	493.44
H1	0.75	5.86	0.76	6.13	-	-	-	-
H3	0.88	5.98	0.90	6.32	-	-	0.72	5.12
H5	0.79	9.85	0.75	8.99	-	-	-	-
H7a	-	-	0.61	7.44	-	-	-	-
H7c	0.75	8.16	0.77	8.33	-	-	-	-
H8c	0.65	7.79	0.68	7.59	-	-	-	-
H20a	0.76	7.48	0.77	7.42	0.75	6.68	-	-
H23	0.72	6.50	0.70	6.49	-	-	-	-
H25	0.67	7.01	0.63	6.93	-	-	-	-
H32a	-	-	0.59	7.82	-	-	-	-

Table 17. *Atomic charges (Q) obtained from the integrated number of electrons in atomic basins for MEM-electron-density maps of α -Glycine as obtained with different prior densities as indicated.*

Atom	dynamic model density as prior:			
	IAM	IAM-HO	INV	MP
C1	+1.60	+1.52	+1.53	+1.54
C2(+H4)	+0.24	+0.23	+0.28	+0.24
O1	-1.11	-1.07	-1.20	-1.19
O2	-1.11	-1.10	-1.24	-1.26
N1(+H1+H2+H3)	+0.26	+0.27	+0.35	+0.36
H5	+0.12	+0.15	+0.28	+0.31
Total	0.00	0.00	0.00	0.00

Table 18. *Atomic charges (Q) obtained from the integrated number of electrons in atomic basins for MEM-electron-density maps of D,L-Serine as obtained with different prior densities as indicated.*

Atom	dynamic model density as prior:			
	IAM	IAM-HO	INV	MP
C1	+1.75	+1.57	+1.67	+1.59
C2	+0.27	+0.27	+0.37	+0.37
C3	-0.15	-0.11	-0.15	-0.16
O1	-1.28	-1.28	-1.35	-1.27
O2	-1.16	-1.08	-1.23	-1.12
O3(+H4)	-0.16	-0.24	-0.17	-0.23
N1(+H11+H12+H13)	+0.73	+0.77	+0.85	+0.71
H2	+0.22	+0.18	+0.13	+0.14
H31	+0.03	+0.07	+0.07	+0.06
H32	-0.23	-0.15	-0.17	-0.09
Total	+0.02	0.00	+0.02	0.00

Table 19. *Atomic charges (Q) obtained from the integrated number of electrons in atomic basins for MEM-electron-density maps of L-Alanine as obtained with different prior densities as indicated.*

Atom	dynamic model density as prior:			
	IAM	IAM-HO	INV	MP
C1	+1.42	+1.38	+1.43	+1.44
C2	+0.16	+0.16	+0.15	+0.18
C3(+H7)	-0.32	-0.29	-0.23	-0.38
O1	-0.91	-0.90	-1.11	-1.04
O2	-0.96	-0.95	-1.14	-1.15
N1(+H1+H2+H3)	+0.11	+0.14	+0.42	+0.24
H4	+0.17	+0.16	+0.17	+0.25
H5	+0.13	+0.12	+0.09	+0.17
H6	+0.19	+0.18	+0.22	+0.29
Total	-0.01	0.00	0.00	0.00

Table 20. *Atomic charges (Q) obtained from the integrated number of electrons in atomic basins for MEM-electron-density maps of Ala-Tyr-Ala_(eth) as obtained with different prior densities as indicated.*

Atom	dynamic model density as prior:			
	IAM	IAM-HO	INV	MP
C1(+H1)	+0.41	+0.42	+0.35	+0.39
C2	+1.24	+1.18	+1.18	+1.15
C3(+H3)	+0.34	+0.32	+0.29	+0.35
C4	+1.27	+1.19	+1.14	+1.16
C5(+H5)	+0.19	+0.18	+0.32	+0.40
C6	+1.45	+1.41	+1.39	+1.34
C7(+H7a+H7b+H7c)	+0.75	+0.25	+0.30	+0.28
C8(+H8a+H8b+H8c)	+0.02	+0.04	+0.06	-0.03
C20(+H20a)	-0.38	-0.40	-0.41	-0.36
C21	-0.01	-0.05	-0.02	+0.04
C22(+H22)	+0.23	+0.21	-0.01	-0.01
C23(+H23)	-0.05	-0.03	-0.05	0.00
C24	+0.20	+0.22	+0.32	+0.32
C25(+H25)	+0.11	+0.09	+0.05	+0.07
C26(+H26)	-0.17	-0.09	-0.04	-0.03
C31(+H31a+H31b)	+0.51	+0.56	+0.39	+0.58
C32(+H32a+H32b+H32c)	+0.16	+0.22	-0.06	+0.25
O1	-1.13	-1.13	-1.04	-1.04
O2	-1.28	-1.30	-1.10	-1.22
O3	-0.85	-0.85	-0.83	-0.91
O4	-1.07	-1.09	-1.13	-1.17
O5(+H15)	-0.56	-0.46	-0.57	-0.72
O6(+H16)	-0.44	-0.58	-0.35	-0.54
N1(+H11a+H11b+H11c)	+0.29	+0.28	+0.60	+0.36
N2(+H12)	-0.47	-0.46	-0.45	-0.47
N3(+H13)	-0.43	-0.37	-0.47	-0.41
H20b	+0.26	+0.28	+0.16	+0.26
Spurious maxima-1	0.01	0.01	0.00	0.01
Spurious maxima-2	0.00	0.00	0.02	0.00
Spurious maxima-3	0.02	-	-	-
Spurious maxima-4	0.00	-	-	-
Spurious maxima-5	0.01	-	-	-
Total	+0.59	+0.04	+0.02	+0.04

Table 21. *Topological properties at atomic maxima of α -Glycine: ρ_{max} ($e/\text{\AA}^3$; first line) and $\nabla^2\rho_{max}$ ($e/\text{\AA}^5$; second line) for four different dynamic model density maps.*

Atom	Dynamic Model density			
	IAM	IAM-HO	INV	MP
C1	136.2	140.0	136.2	135.5
	-52150.4	-54944.0	-52163.2	-51750.0
C2	116.3	119.4	116.2	115.9
	-39152.9	-41073.7	-39014.8	-38877.7
O1	153.1	158.4	154.6	153.9
	-54940.5	-58613.4	-55843.0	-55455.3
O2	146.6	151.9	148.4	147.4
	-51329.6	-54837.0	-52332.5	-51672.7
N	138.7	143.0	138.7	138.0
	-48984.0	-51862.2	-48920.5	-48494.5

Table 22. *Topological properties at atomic maxima of D, L-Serine: ρ_{max} ($e/\text{\AA}^3$; first line) and $\nabla^2\rho_{max}$ ($e/\text{\AA}^5$; second line) for four different dynamic model density maps.*

Atom	Dynamic Model density			
	IAM	IAM-HO	INV	MP
C1	98.1	107.9	101.4	104.9
	-28694.3	-34177.2	-30419.6	-32453.4
C2	97.3	107.1	101.1	104.8
	-28200.6	-33731.5	-30279.2	-32405.8
C3	83.2	90.0	85.4	88.3
	-20998.5	-24215.2	-21961.7	-23311.1
O1	109.3	120.9	113.4	117.0
	-29024.6	-35166.2	-31306.1	-32939.7
O2	107.4	118.1	111.3	114.2
	-28472.9	-34024.2	-30342.7	-31738.9
O3	105.5	114.0	107.8	110.8
	-28525.7	-32710.3	-29358.3	-30701.1
N	109.5	119.9	113.1	116.5
	-31706.1	-37420.4	-33562.0	-35401.7

Table 23. *Topological properties at atomic maxima of L-Alanine: ρ_{max} ($e/\text{\AA}^3$; first line) and $\nabla^2 \rho_{max}$ ($e/\text{\AA}^5$; second line) for four different dynamic model density maps.*

Atom	Dynamic Model density			
	IAM	IAM-HO	INV	MP
C1	121.5	123.8	128.9	127.2
	-42105.9	-43623.4	-47042.8	-45974.2
C2	116.5	120.0	123.4	121.9
	-39081.9	-41347.7	-43539.0	-42630.1
C3	83.7	85.3	86.4	86.2
	-21372.4	-22122.9	-22607.3	-22500.2
O1	128.1	132.7	136.5	136.0
	-39491.8	-42377.1	-44409.7	-44276.0
O2	134.3	138.6	144.2	140.8
	-43572.9	-46270.5	-49810.1	-47475.4
N	130.1	131.9	135.0	134.8
	-43358.6	-44383.9	-46255.1	-45968.4

Table 24. Topological properties at atomic maxima of Ala-Tyr-Ala_(eth): ρ_{max} ($e/\text{\AA}^3$; first line) and $\nabla^2\rho_{max}$ ($e/\text{\AA}^5$; second line) for four different dynamic model density maps.

Atom	Dynamic Model density			
	IAM	IAM-HO	INV	MP
C1	82.7	85.7	86.3	87.4
	-20911.4	-22299.9	-22631.2	-23092.6
C2	88.3	91.6	92.7	93.8
	-23537.1	-25227.0	-25957.9	-26469.3
C3	89.0	91.5	93.1	94.6
	-23922.5	-25085.6	-25936.7	-26645.1
C4	90.4	93.2	94.5	96.1
	-24576.6	-26093.0	-26853.0	-27770.8
C5	79.9	81.6	83.0	84.2
	-19665.0	-20396.6	-21052.0	-21527.1
C6	84.8	87.4	88.1	89.6
	-21806.4	-23027.1	-23388.9	-24108.8
C7	53.5	54.9	55.2	55.9
	-9460.5	-9909.3	-9960.9	-10194.6
C8	47.5	48.3	48.7	49.3
	-7988.3	-8254.9	-8329.9	-8523.2
C20	75.2	77.2	78.9	79.1
	-17378.9	-18279.1	-19024.5	-19029.0
C21	76.1	77.6	79.3	80.2
	-17733.9	-18423.9	-19132.2	-19542.7
C22	67.8	68.8	70.5	71.1
	-14561.4	-15000.6	-15653.4	-15886.4
C23	64.1	65.7	66.7	67.5
	-13172.0	-13815.3	-14194.1	-14508.1
C24	70.0	71.7	72.5	73.3
	-15282.2	-15938.3	-16278.6	-16596.3
C25	62.4	64.8	65.2	66.0
	-12600.4	-13502.8	-13669.3	-13996.8
C26	66.1	68.0	69.1	69.8
	-13953.9	-14685.3	-15146.0	-15434.2
C31	41.3	41.9	42.3	42.6
	-6135.6	-6302.7	-6351.5	-6435.0
C32	34.9	35.4	35.7	36.1
	-4534.6	-4687.6	-4686.6	-4807.8
O1	95.1	99.4	99.3	100.4
	-23467.2	-25627.8	-25595.7	-25914.1
O2	87.7	90.8	92.2	92.6
	-20830.2	-22418.5	-23169.1	-23022.0
O3	79.9	82.0	83.4	84.5
	-16522.9	-17363.5	-17916.6	-18324.9
O4	100.5	104.0	105.0	106.0
	-25709.4	-27242.7	-27730.3	-28094.3
O5	79.8	82.7	82.5	84.0
	-16528.6	-17640.7	-17568.9	-18037.6
O6	70.8	73.3	73.2	74.9
	-13108.4	-13991.6	-13864.9	-14495.3
N1	93.2	96.4	96.6	98.5
	-23708.7	-25194.9	-25314.5	-26095.4
N2	102.7	105.2	106.9	108.6
	-29014.5	-30283.6	-31080.9	-32022.4
N3	101.4	104.1	106.0	107.7
	-28295.5	-29728.2	-30634.4	-31557.2

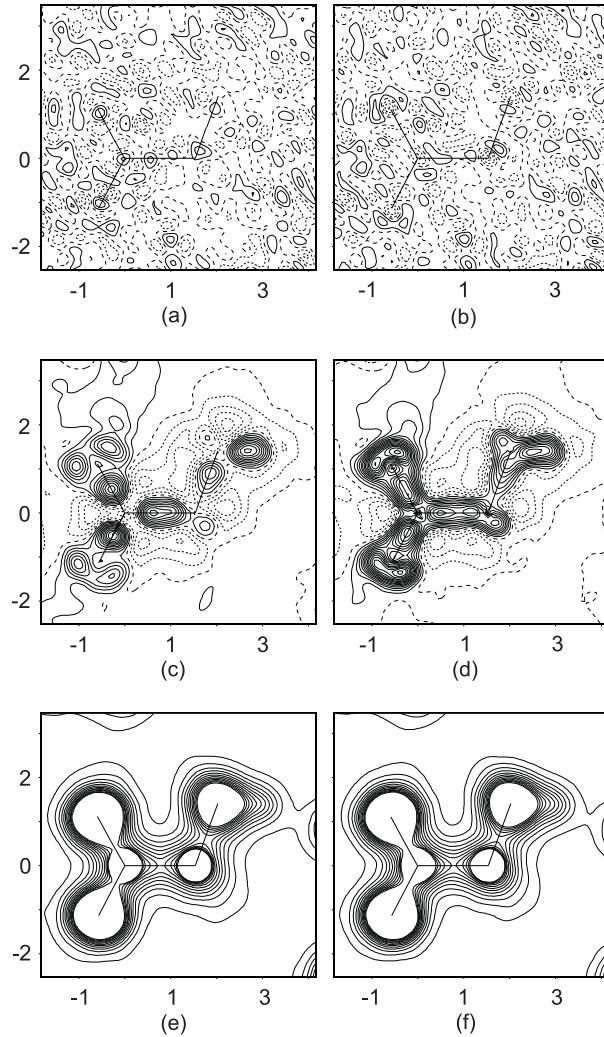


Fig. 1. C1-C2-N plane of density maps of *D, L*-serine. (a, b) residual density (difference Fourier map) with contours at $0.05 \text{ e}/\text{\AA}^3$; (c, d) dynamic deformation density (Eq. 4) with contours at $0.05 \text{ e}/\text{\AA}^3$; and (e, f) MEM density with contours at $0.2 \text{ e}/\text{\AA}^3$ up to $2.5 \text{ e}/\text{\AA}^3$. For (a, c, e) the IAM prior, and for (b, d, f) the IAM-HO prior has been used. Solid lines denote positive values, dotted values denote negative values and dashed lines are the zero contour.

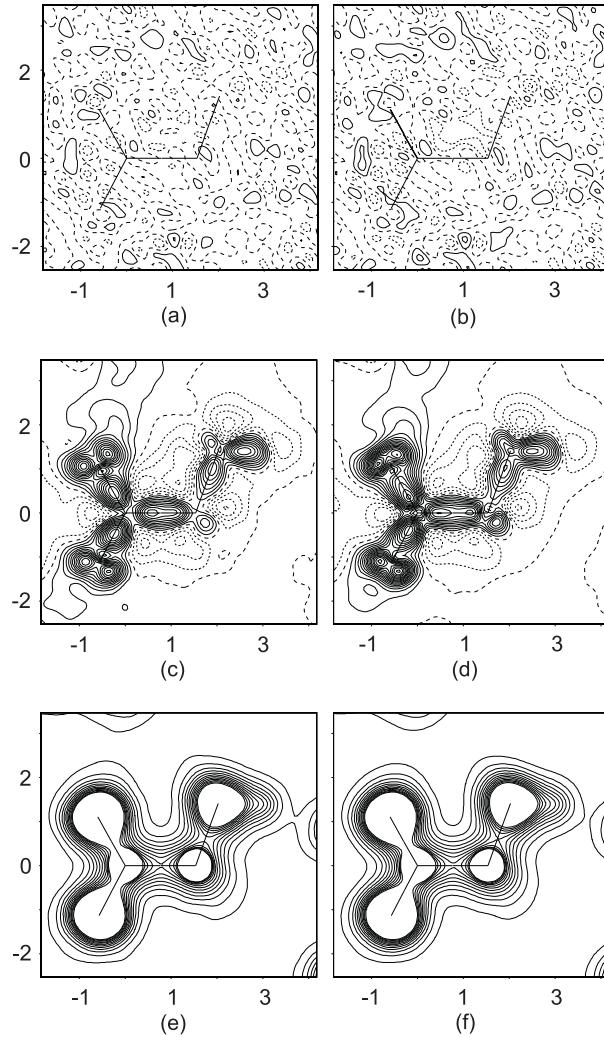


Fig. 2. C1-C2-N plane of density maps of *D, L*-serine. (a, b) residual density (difference Fourier map) with contours at $0.05 \text{ e}/\text{\AA}^3$; (c, d) dynamic deformation density (Eq. 4) with contours at $0.05 \text{ e}/\text{\AA}^3$; and (e, f) MEM density with contours at $0.2 \text{ e}/\text{\AA}^3$ up to $2.5 \text{ e}/\text{\AA}^3$. For (a, c, e) the INV prior, and for (b, d, f) the MP prior has been used. Solid lines denote positive values, dotted values denote negative values and dashed lines are the zero contour.

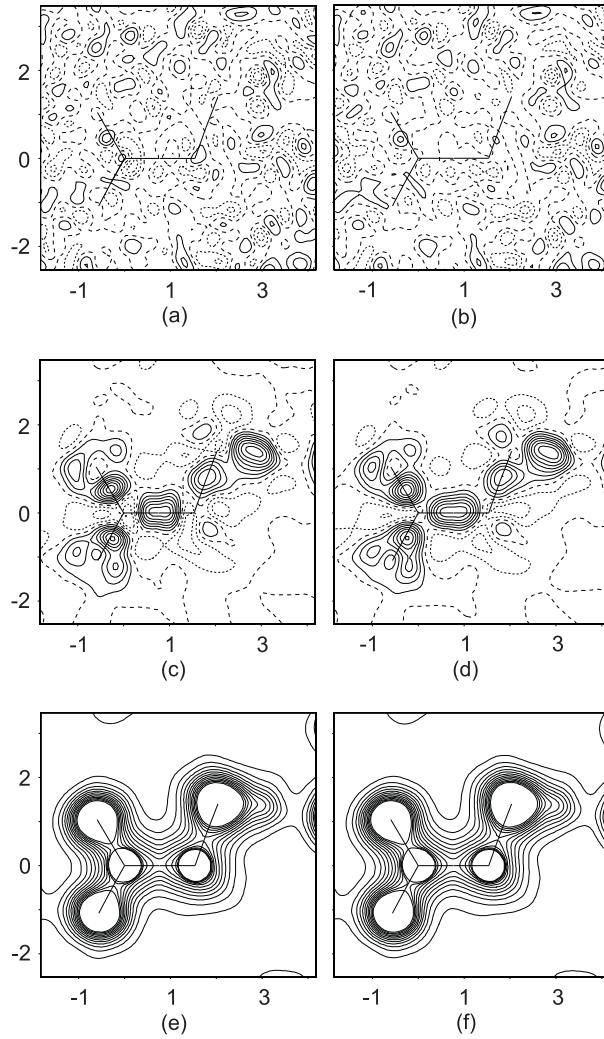


Fig. 3. C1-C2-N plane of density maps of *L*-alanine. (a, b) residual density (difference Fourier map) with contours at $0.05 \text{ e}/\text{\AA}^3$; (c, d) dynamic deformation density (Eq. 4) with contours at $0.05 \text{ e}/\text{\AA}^3$; and (e, f) MEM density with contours at $0.2 \text{ e}/\text{\AA}^3$ up to $2.5 \text{ e}/\text{\AA}^3$. For (a, c, e) the IAM prior, and for (b, d, f) the IAM-HO prior has been used. Solid lines denote positive values, dotted values denote negative values and dashed lines are the zero contour.

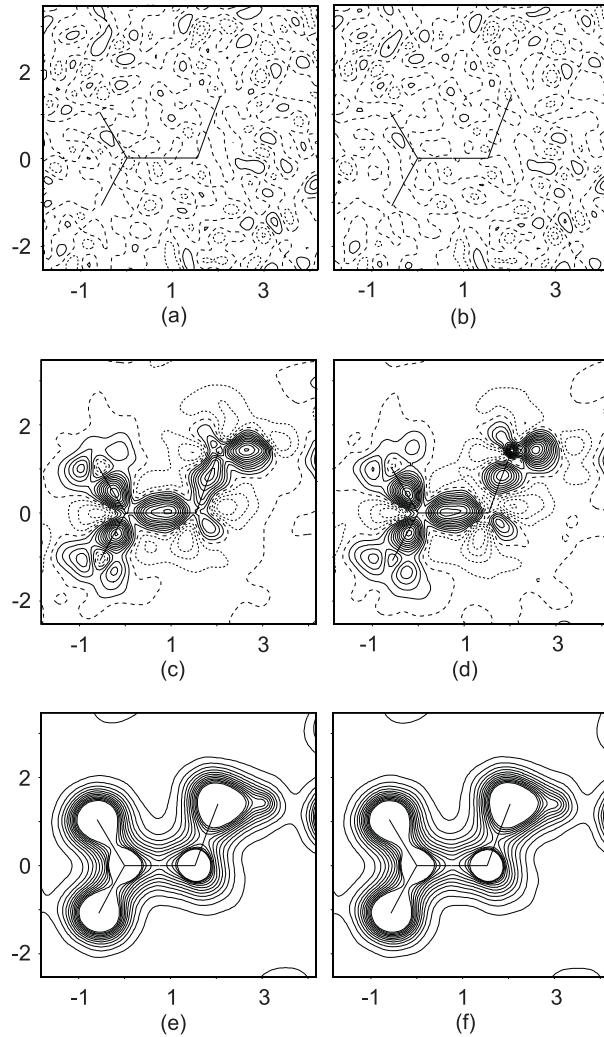


Fig. 4. C1-C2-N plane of density maps of *L*-alanine. (a, b) residual density (difference Fourier map) with contours at $0.05 \text{ e}/\text{\AA}^3$; (c, d) dynamic deformation density (Eq. 4) with contours at $0.05 \text{ e}/\text{\AA}^3$; and (e, f) MEM density with contours at $0.2 \text{ e}/\text{\AA}^3$ up to $2.5 \text{ e}/\text{\AA}^3$. For (a, c, e) the INV prior, and for (b, d, f) the MP prior has been used. Solid lines denote positive values, dotted lines denote negative values and dashed lines are the zero contour.

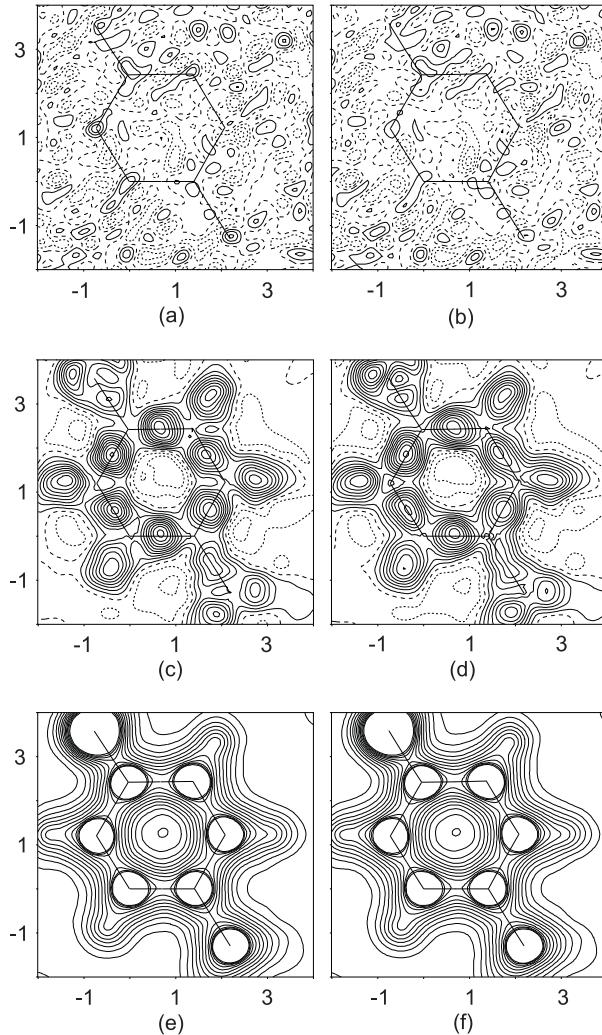


Fig. 5. Phenyl ring plane of density maps of Ala-Tyr-Ala(*etho*). (a, b) residual density (difference Fourier map) with contours at $0.05 \text{ e}/\text{\AA}^3$; (c, d) dynamic deformation density (Eq. 4) with contours at $0.05 \text{ e}/\text{\AA}^3$; and (e, f) MEM density with contours at $0.2 \text{ e}/\text{\AA}^3$ up to $2.5 \text{ e}/\text{\AA}^3$. For (a, c, e) the IAM prior, and for (b, d, f) the IAM-HO prior has been used. Solid lines denote positive values, dotted values denote negative values and dashed lines are the zero contour.

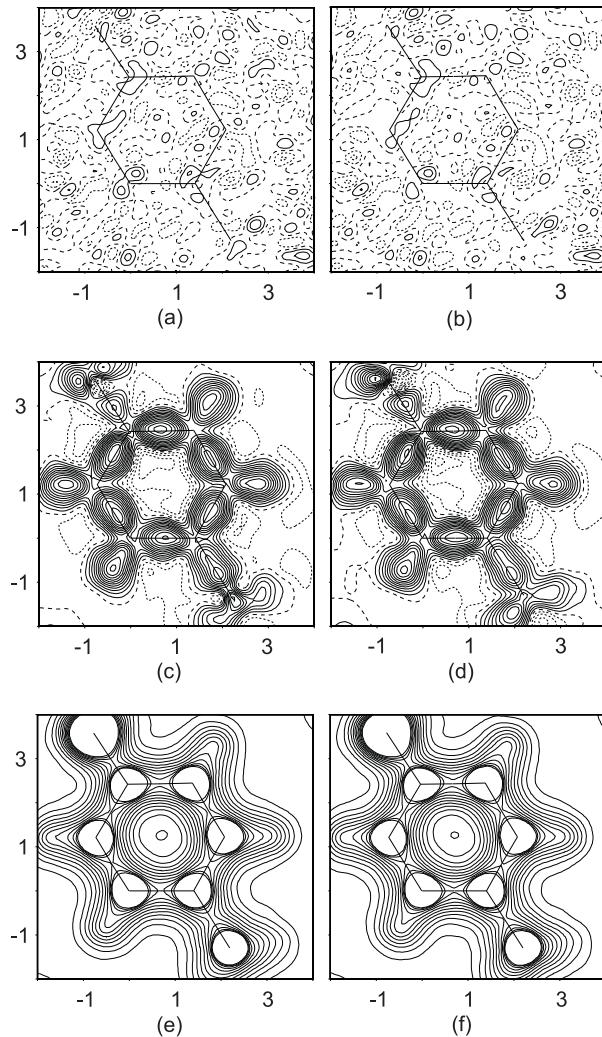


Fig. 6. Phenyl ring plane of density maps of Ala-Tyr-Ala(*etho*). (a, b) residual density (difference Fourier map) with contours at $0.05 \text{ e}/\text{\AA}^3$; (c, d) dynamic deformation density (Eq. 4) with contours at $0.05 \text{ e}/\text{\AA}^3$; and (e, f) MEM density with contours at $0.2 \text{ e}/\text{\AA}^3$ up to $2.5 \text{ e}/\text{\AA}^3$. For (a, c, e) the INV prior, and for (b, d, f) the MP prior has been used. Solid lines denote positive values, dotted values denote negative values and dashed lines are the zero contour.

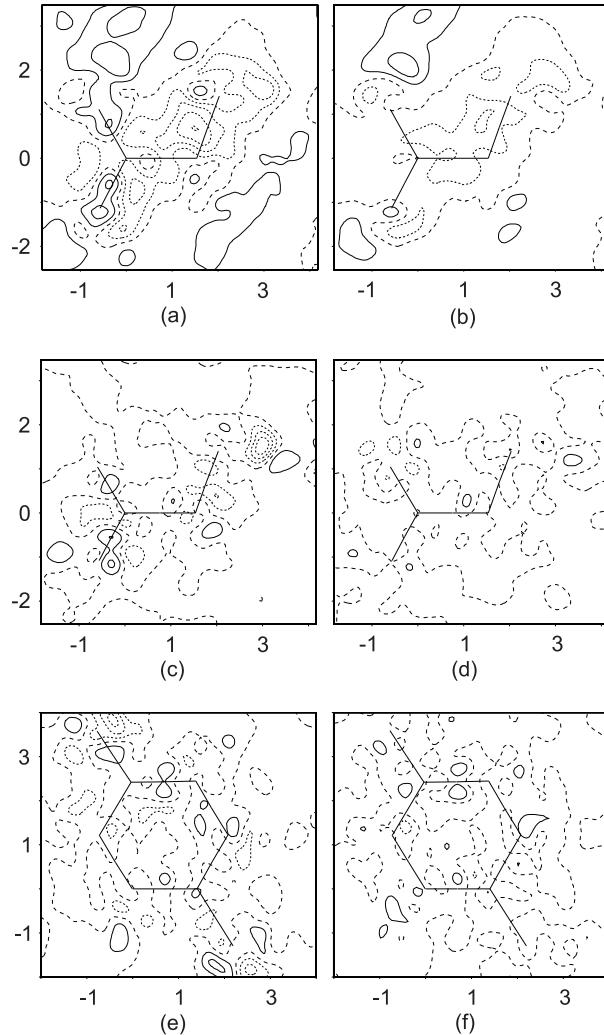


Fig. 7. C1-C2-N plane of difference density maps (Eq. 3) with contours at $0.05 \text{ e}/\text{\AA}^3$. (a) INV prior and (b) MP prior of *D, L*-serine; (c) INV prior and (d) MP prior of *L*-alanine; (e) INV prior and (f) MP prior of Ala-Tyr-Ala_(etho). Solid lines denote positive values, dotted values denote negative values and dashed lines are the zero contour.