Supplementary Materials

Structural perspective of gliadin peptides active in Celiac disease

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Table S1 (A-F)

Quantitative measure of the similarity, i.e. Root Mean Square Deviation (RMSD, Å) between superimposed atomic coordinates of peptides. Superimpositions obtained by using PyMOL software (http://www.PyMOL.org). The row and column headers refer to the PDB codes of the gliadin peptides bound to HLA-DQ in binary or ternary complexes. P3143-PPII refers to P31-43 peptide modelled in polyproline II (PPII).

Table S1A. DQ2.5-glia-α1 vs. other gluten peptides. Sequence based alignment (RMSD Å)

	6mfg_pepF	**4ozi-pepI**	**6mmf_pepC**	**6u3m-pepE**	**P3143-PPII**
1s9v-pepC	0.265	0.562	0.299	0.403	2.441
6mfg_pepF		0.345	0.219	0.280	2.484 (ω1)
4ozi-pepI			0.404	0.385	2.560
6mmf_pepC				0.230	2.438
6u3m-pepE					2.454

Table S1B. DQ2.5-glia-α1 vs. other gluten peptides. Structure based alignment (RMSD Å)

	6mfg_pepF	**4ozi-pepI**	**6mmf_pepC**	**6u3m-pepE**	**P3143- PPII**
1s9v-pepC	0.178	0.518	0.343	0.344	1.30
6mfg_pepF		0.337	0.289	0.172	1.14 (ω1)
4ozi-pepI			0.400	0.425	1.28
6mmf_pepC				0.290	1.01
6u3m-pepE					0.951

Table S1C. DQ2.5-glia-α2 vs. other gluten peptides. Sequence based alignment (RMSD Å)

	4ozg-pepI	**4ozh-pepJ**	**6u3o-pepI**	**P3143- PPII**
4ozf-pepJ	0.519	0.308	0.150	0.793
4ozg-pepI		0.279	0.165	0.834
4ozh-pepJ			0.240	0.753
6u3o-pepI				1.029

Table S1D. DQ2.5-glia-α2 vs. other gluten peptides. Structure based alignment (RMSD Å)

	4ozg-pepI	**4ozh-pepJ**	**6u3o-pepI**	**P3143-PPII**
4ozf-pepJ	0.610	0.369	2.150	1.314
4ozg-pepI		0.322	0.414	1.440
4ozh-pepJ			0.526	1.352
6u3o-pepI				2.148

Table S1E. DQ8-glia-α1 vs. other gluten peptides. Sequence based alignment (RMSD Å)

	5ks9-pep	**4z7v-pepI**	**4z7u-pepI**	**4z7w-pepI**	**4gg6-pepI**	**5ksb-pepI**	**P3143-PPII**
2nna-pepC	0.350	0.360	0.315	0.237	0.389	2.086	0.529
5ks9-pepI		0.356	0.338	0.416	0.346	0.981	0.417
4z7v-pepI			0.209	0.297	0.313	2.077	0.366
4z7u-pepI				0.315	0.297	0.978	0.368
4z7w-pepI					0.391	0.943	0.555
4gg6-pepI						2.050	0.372
5ksb-pepI							1.522 (γ1)

Table S1F. DQ8-glia-α1 vs. other gluten peptides. Structure based alignment (RMSD Å)

	5ks9-pep	**4z7v-pepI**	**4z7u-pepI**	**4z7w-pepI**	**4gg6-pepI**	**5ksb-pepI**	**P3143-PPII**
2nna-pepC	0.303	0.422	0.312	0.258	0.378	1.253	1.155
5ks9-pepI		0.274	0.320	0.436	0.445	0.501	1.792
4z7v-pepI			0.214	0.358	0.296	1.286	1.002
4z7u-pepI				0.380	0.348	1.439	1.355
4z7w-pepI					0.321	0.420	1.626
4gg6-pepI						1.207	0.856
5ksb-pepI							1.874 (γ1)