Manuscript no. HAEMATOL/2010/030924 entitled "The impact of human leucocyte antigen (HLA) micropolymorphism on ligand specificity within the HLA-B*41 allotypic family"

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Information about the contributions of each person named as having participated in the study

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The guarantors of this manuscript confirm that all persons designated as authors qualify for authorship, and that each author has participated sufficiently in the work to take public responsibility for appropriate portions of the content.

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3) **Design & Methods**. The following authors were responsible for specific investigations:

• Christina Bade-Doeding was responsible for eukaryotic and prokaryotic vector design, cloning, eukaryotic and prokaryotic protein expression, mass spectrometric analysis of the peptides, refolding, crystal seeding

• Alex Theodossis was responsible for crystallographic data collection, refinement of the structures, computational analysis

• Stephanie Gras was responsible for refolding, crystal seeding, crystallographic data collection

• Lars Kjer-Nielsen was responsible for prokaryotic vector design, cloning, prokaryotic protein expression

• Trevor Huyton was responsible for statistical analysis

4) **Results**. The following authors were responsible for specific portions of the results, including figures and tables:

• Christina Bade-Doeding was responsible for peptide analysis, Table 3: Polymorphic positions and corresponding peptide anchors within in the B*41 group, Supplementary Table 1: Ligands of the HLA-B*41 variants, Supplementary Table 2: List of promiscuous peptides, Supplementary Table 3: Differentially selected peptides by B*41 subtypes

• Alex Theodossis was responsible for crystallographic analysis, Table 1: Data collection and refinement statistics, Figure 1: The Crystal structures of B*41:03/AEMYGSVTEHPSPSPL and B*41:04/HEEAVSVDRVL, Figure 2: Peptides bound to B*41:03 and B*41:04, Figure 3: A conserved network of interactions in the B*41:03/16mer and B*41:04/11mer complexes, Supplementary Fig. 1: Stereographic representations of the Ag-binding cleft of B*41:03/AEMYGSVTEHPSPSPL and B*41:04/HEEAVSVDRVL, Supplementary Figure 2: Polymorphism alters the size and charge of the Ag-binding cleft in B*41:03 and B*41:04, Supplementary Table 4: Peptide contacts in the B*41:03/16-mer and B*41:04/11-mer structures, , Supplementary Table 5: Theoretically calculated ionisation states for selected titratable groups in the B*41:03 and B*41:04 structures • Trevor Huyton was responsible for statistical analysis of the peptides, Table 2: Statistical analysis of the length of HLA-B*41-derived ligands

5) Writing the manuscript. The following authors were responsible for writing the manuscript:

- Christina Bade-Doeding was responsible for writing the manuscript
- Alex Theodossis was responsible for writing the manuscript
- Jamie Rossjohn was responsible for writing the manuscript
- Stephanie Gras was responsible for critically reviewing the manuscript
- Lars Kjer-Nielsen was responsible for critically reviewing the manuscript
- Britta Eiz-Vesper was responsible for critically reviewing the manuscript
- Axel Seltsam was responsible for critically reviewing the manuscript
- Trevor Huyton was responsible for critically reviewing the manuscript

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The authors would like to thank Susanne Aufderbeck and Nicole Neumann for their excellent technical assistance and the beamline staff at the Standford Synchrotron Radiation Lightsource (SSRL) and the Argonne Advanced Proton Source (APS) for valuable assistance.

The atomic coordinates and structure factors (codes 3LN4 and 3LN5) have been deposited in the Protein Data Bank Japan (http://www.pdbj.org/).

This work was supported by the German José Carreras Leukemia Foundation (DJCLS R05/27f) and the German Federal Ministry of Education and Research (reference number: 01E00802).