

Table S1: Composing residues of each pocket extracted from 32 complex structures. The first column gives PDB IDs of 32 MHC-II HLA-peptide complex structures from PDB. The next 9 columns give extracted composing residues of nine pockets of the HLA-DR molecule in the corresponding complex, respectively. Each element, e.g. 82N, consists of an index number and the residue on that site. The last row gives a union set of composing residue indexes.

| PDB | Pocket1 | Pocket2 | Pocket3 | Pocket4 | Pocket5 | Pocket6 | Pocket7 | Pocket8 | Pocket9 |
|-------|-----------------|-----------------|---------|-----------------------------|-------------------|-------------------|-------------------------|---------|------------------|
| 1AQD | 82N 85V 86G | 77T 78Y 81H 82N | 78Y | 13F 74 A 78Y | 13F 71R | 11L | 47Y 61W 67L 70 Q 71R | 60Y 61W | 9W 57D 61W |
| 1PYW | 82N 85V 86G 89F | 77T 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 13F 71R | 11L | 11L 28E 61W 71R | 60Y 61W | 57D 61W |
| 1KLG | 82N 85V | 78Y 81H 82N | 78Y | 13F 71R 78Y | 13F 71R | 11L | 61W | 60Y 61W | 57D 61W |
| 2FES | 82N 85V 86G 89F | 77T 78Y 82N | | 13F 28E 70Q 71R 74A 78Y | 13F 71R | 71R | 28E 47Y 61W 67L 71R | 61W | 57D |
| 1KLU | 82N 85V | 78Y 81H 82N | | 13F 71R 78Y | 13F 71R | 11L | 61W | 60Y 61W | 57D 61W |
| 1SJH | 82N | 78Y 81H 82N | | 13F 26L 70Q 71R 74A 78Y | 71R | 11L | 61W | 60Y 61W | 57D 61W |
| 1SJE | 82N | 78Y 81H 82N | 78Y | 13F 26L 70Q 71R 74A 78Y | 71R | 11L | 61W | 60Y 61W | 57D 60Y 61W |
| 1T5W | 82N 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 13F 71R | 11L | 61W 71R | 60Y 61W | 9W 57D 61W |
| 1T5X | 82N 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 71R | 11L | 61W 71R | 61W | 57D 61W |
| 2IAN | 82N 85V | 78Y 81H 82N | 78Y | 13F 70Q 74A 78Y | 13F 70Q 71R | 11L | 61W 71R | 61W | 57D 61W |
| 2IPK | 82N 85V 86G 89F | 77T 78Y 81H 82N | | 13F 70Q 71R 74A 78Y | 71R | 11L | 47Y 61W 67L 71R | 60Y 61W | 9W 57D 61W |
| 1FYT | 82N 85V 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 13F 71R | 11L | 28E 47Y 61W 67L 71R | 60Y 61W | 9W 57D 61W |
| 1R5I | 82N 85V 86G 89F | 77T 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 70Q 71R | 11L | 47Y 61W 67L 71R | 61W | 9W 57D 61W |
| 1HXY | 82N 85V 86G 89F | 78Y 81H 82N | | 13F 70Q 71R 74A 78Y | 71R | 11L | 28E 47Y 61W 67L 71R | 60Y 61W | 9W 57D 61W |
| 1JWM | 82N 85V 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 71R | 11L | 28E 47Y 61W 67L 71R | 61W | 57D 61W |
| 1JWS | 82N 85V 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 13F 71R | 11L | 47Y 61W 67L 71R | 61W | 9W 57D 61W |
| 1JWU | 82N 85V 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 13F 71R | 11L | 28E 47Y 61W 67L 71R | 61W | 9W 57D 61W |
| 1LO5 | 82N 85V 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 78Y | 13F 71R | 11L | 47Y 61W 67L 71R | 61W | 9W 57D 60Y 61W |
| 2ICW | 82N 85V 86G 89F | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 13F 71R | 11L | 28E 47Y 61W 67L 71R | 61W | 9W 57D 61W |
| 2OJE | 82N 85V 86G | 77T 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 70Q 71R | 11L | 28E 47Y 61W 67L 71R | 61W | 9W 57D 61W |
| 2G9H | 82N 85V 86G 89F | 77T 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 71R | 11L 13F | 28E 47Y 61W 67L 71R | 60Y 61W | 9W 57D 61W |
| 2IAM | 82N | 78Y 81H 82N | 78Y | 13F 70Q 71R 74A 78Y | 70Q 71R | 11L | 61W 67L 71R | 60Y 61W | 57D 61W |
| 1A6A | 82N 85V 86V | 77N 78Y 81H 82N | 78Y | 13S 26Y 74R 78Y | 71K 74R | 11S 30Y | 30Y 47F 61W 67L 71K | 61W | 9E 30Y 57D 61W |
| 1J8H | 82N 85V 86G 89F | 77T 78Y 81H 82N | 78Y | 13H 26F 28D 70Q 71K 78Y | 13H 70Q 71K | 11V 13H 30Y | 30Y 47Y 61W 67L | 60Y 61W | 37Y 57D 61W |
| 2SEB | 82N | 77T 78Y 81H 82N | | 13H 26F 71K 78Y | 13H 71K | 30Y | 30Y 47Y 61W | 60Y 61W | 61W |
| 1BX2 | 82N 85V | 77T 78Y 81H 82N | 78Y | 13R 26F 28D 70Q 74A 78Y | 70Q | 13R | | | 57D 60Y 61W |
| 1YMM | 82N | 77T 78Y 81H 82N | 78Y | 13R 26F 28D 70Q 71A 78Y | 70Q | 13R | 61W 67I | 61W | 57D 61W |
| 2Q6W | 82N 85V 86G | 77N 78Y 81H 82N | 78Y | 11R 13S 26Y 28D 71K 74R 78Y | 11R 70Q 71K | 11R | 30Y 47Y 61W 67L 71K | 61W | 37F 57V 61W |
| 3C5J | 82N 85V 86V | 77N 78Y 81H 82N | 78Y | 13S 26F 28E 71K 74Q 78Y | 28E 71K | 11L 30Y | 30Y 61W | 61W | 61W |
| 1FV1 | 82N 85V 86G 89F | 78Y 81H 82N | 78Y | 13Y 71R 78Y | 71R | 13Y | 61W 67F 71R | 61W | 57D |
| 1H15 | 82N 89F | 77T 78Y 81H 82N | 78Y | 13Y 71R 78Y | 71R | 11D 13Y 30D | 61W | | 57D 60Y |
| 1ZGL | 82N 85V 89F | 77T 78Y 81H 82N | | 13Y 26F 71R 78Y | 13Y | 13Y 28H 61W 71R | 61W | | 57D 60Y 61W |
| Union | 82 85 86 89 | 77 78 81 82 | 78 | 11 13 26 28 70 71 74 78 | 11 13 28 70 71 74 | 11 13 28 30 61 71 | 11 28 30 47 61 67 70 71 | 60 61 | 9 30 37 57 60 61 |