

PDB Entry	7Q98	7Q99
Details	HLA A*02:01-NLSALGIFST	MEL5:HLA A*02:01-NLSALGIFST
Data Collection		
Diamond Beamline	I04-1	I04
Date	08/09/2018	02/03/2020
Wavelength	0.91587	0.97951
Crystal Data (outer shell statistics in brackets)		
Crystallisation	25% PEG 8000, 0.2M NH ₄ ⁺ SO ₄ ²⁻ , 0.1M Na Cacodylate, pH 6.5	0.1M HEPES, 25% PEG 4000, 15% Glycerol, pH 7.5
<i>a,b,c</i> (Å)	118.27, 169.55, 248.75	121.28, 121.28, 81.314
α,β,γ (°)	90.0, 90.0, 90.0	90.0, 90.0, 90.0
Space group	I 2 2 2	P 4 ₃
Resolution (Å)	2.50 – 84.85	2.55 – 60.65
Outer shell	2.50 – 2.55	2.55 – 2.59
<i>R</i> -merge (%)	8.7 (52.3)	19.7 (386.4)
<i>R</i> -pim	4.0 (24.1)	7.5 (152.1)
<i>R</i> -meas (%)	9.6 (57.7)	21.1 (415.7)
CC1/2	0.998 (0.874)	0.995 (0.221)
I / σ (I)	10.0 (3.0)	7.2 (0.4)
Completeness (%)	99.2 (97.2)	100 (100)
Multiplicity	5.6 (5.6)	7.8 (7.4)
Total Measurements	479,533 (24,803)	303,254 (14,105)
Unique Reflections	85,745 (4,408)	38,671(1,909)
Wilson B-factor(Å ²)	33.4	53.5
Refinement Statistics		
Non-H Atoms	16,557	6,664
R-work reflections	81,381	36,363
R-free reflections	4,344	1,905
R-work/R-free (%)	23.5 / 27.4	21.8 / 27.2
rms deviations (ML target in brackets)		
Bond lengths (Å)	0.011 (0.013)	0.010 (0.013)
Bond Angles (°)	1.404 (1.655)	1.454 (1.648)
^l Coordinate error	0.239	0.375
Mean B value (Å ²)	46.2	72.4
Ramachandran Statistics		
Favoured/allowed/Outlier	1873 / 32 / 0	745 / 66 / 7
%	98 / 2 / 0	91 / 8 / 1

7Q9A	7Q9B	7ZUC
MEL5:HLA A*02:01-LLLGIGILVL	MEL8:HLA A*02:01-EAAGIGILTV	HLA A*02:01-LLLGIGILV 9mer
I04	I03	I04
02/03/2020	17/01/2019	28/04/2022
0.97951	0.97625	0.9795
0.1M TRIS, 15% PEG 8000, 15% Glycerol, pH 7.5	0.1M HEPES, 25% PEG 4000, 0.2 M (NH ₄) ₂ SO ₄	20% PEG 3,350, 0.2 M Potassium Thiocyanate, 0.1 M BIS-TRIS Propane pH 7.5
122.02, 122.02, 82.418	99.97, 53.65, 203.51	85.26, 83.26, 213.49
90.0, 90.0, 90.0	90.0, 94.33, 90.0	90.0, 90.0, 120.0
P 4 ₃	P 1 2 ₁ 1	P 3 ₂ 1 2
2.1 – 61.02	3.24 – 99.67	1.89 – 71.18
2.10 – 2.14	3.24 – 3.32	1.89 – 1.92
10.5 (260.3)	28.0 (94.9)	8.4 (25.2)
4.0 (98.9)	22.0 (71.9)	1.9 (5.6)
11.3 (278.6)	32.8 (110.2)	8.6 (25.8)
0.998 (0.312)	0.995 (0.686)	0.999 (0.998)
10.6 (0.3)	2.7 (1.1)	31.7 (6.5)
100 (100)	100.0 (99.9)	100 (100)
7.7 (7.8)	3.7 (3.8)	20.8 (20.9)
541,775 (27,332)	128,197 (9,847)	1,494,858 (78,458)
70,731 (3,512)	34,992 (2,579)	71,594 (3768)
44	36.7	31.2
6,911	13,221	6615
67,098	33,241	71521
3,454	1,742	3417
20.4 / 24.3	22.6 / 27.7	21.1/24.7
0.010 (0.013)	0.011 (0.013)	0.012 (0.013)
1.676 (1.647)	1.452 (1.651)	1.408 (1.656)
0.193	0.636	0.162
63.4	56.4	39
773 / 42 / 7	1440 / 159 / 24	734 / 25 / 0
94 / 5 / 1	89 / 10 / 2	97 / 3 / 0
