

	zVDR LBD – 1,4 α ,25D ₃	zVDR LBD – 1,4 β ,25D ₃
PDB ID	9EZ1	9EZ2
Data collection		
Beamline	PX2	PX2
Space group	P6 ₅ 22	P6 ₅ 22
Unit-cell parameters (Å, °)	65.98, 65.98, 263.47 90, 90, 120	66.14, 66.14, 263.74 90, 90, 120
Resolution range (Å)	43.16-1.95	43.96-1.8
Unique reflections	25896	32871
I/ σ (I)	22.96	23.45
CC _{1/2}	1	1
Completeness	99.30	99.30
Refinement		
Resolution range (Å)	43.16-1.95	43.96-1.8
R _{work} / R _{free} (%)	20.58 / 25.52	20.16 / 22.98
Ramachandran		
Allowed (%)	1.23	0.82
Favored (%)	98.77	99.18
Mean B factors (Å ²)		
Protein	61.31	58.52
Ligand	42.56	39.18

Supplementary Table S1. Crystallographic data and refinement.