

Additional file 2. Collection and refinement statistics for RORy structures.

Data Collection	EBI96/BIO592	BIO399
Space Group	P2 ₁	C2
Cell Dimensions		
a (Å)	85	126
b (Å)	68	56
c (Å)	96	78
Wavelength (Å)	0.98	0.98
Resolution (Å)	2.63	2.35
R _{sym} ^a	0.109 (0.449)	0.10 (0.437)
I/σ	9.9 (2.7)	16.2 (2.8)
Multiplicity	3.7 (3.7)	3.3 (3.3)
Total No. reflections/ No. unique reflections	114,149/31,077	36,027/18,850
Mean I/σ	9.9/2.7	16.2/2.8
Completeness (%)	99.6 (99.7)	99.5 (99.9)
Rwork/Rfree	19.9/25.5	21.1/26.3
CC _{1/2}	0.95 (0.58)	0.97 (0.66)
No. Molecules per asymmetric unit	4	2
R.m.s.d. bond distance (Å)	0.016	0.021
R.m.s.d bond angle (deg)	1.65	2.1
Total no. of non-H atoms in ASU	8,528	3,574
No. of solvent molecules	171	12
Avg. protein B-value (Å ²)	32.5	49.7
Avg. solvent B-value (Å ²)	34.2	54.5
Ramachandran Plot		
Preferred	977	417
Generous	23	13
Disallowed	1	1

***The value in parentheses is for the highest resolution bin (approximate interval, 0.1 Å)**

^aR_{sym} = $\sum_i |f_i^{\text{hkl}} - \langle f^{\text{hkl}} \rangle| / \sum_i f_i^{\text{hkl}}$

^bR_{work} = $\sum_i |f_i^{\text{hkl}} - |F_o| |F_c| | / \sum_i |f_i^{\text{hkl}}| |F_o|$ for all data except 5% which is used for the R_{free} calculation