

Table 1. Data collection and refinement statistics

	<i>T</i> -p53C V143A	<i>T</i> -p53C Y220C	<i>T</i> -p53C G245S	<i>T</i> -p53C F270L	<i>T</i> -p53C R273C	<i>T</i> -p53C R282W
Data Collection						
Space group	<i>P</i> ₂ ₁ ₂ ₁	<i>P</i> ₂ ₁ ₂ ₁	<i>P</i> ₂ ₁	<i>P</i> ₂ ₁ ₂ ₁	<i>P</i> ₂ ₁ ₂ ₁	<i>P</i> ₂ ₁ ₂ ₁
Cell, Å, °						
<i>a</i>	64.66	64.50	68.51	64.71	64.72	64.81
<i>b</i>	71.07	71.11	73.08	71.04	70.98	71.40
<i>c</i>	105.00	104.90	84.76	104.92	105.18	104.98
β	90.00	90.00	90.05	90.00	90.00	90.00
Molecules/a.u.	2	2	4	2	2	2
Resolution, Å	29.4–1.80 (1.90–1.80)	26.8–1.65 (1.74–1.65)	37.4–1.69 (1.78–1.69)	41.1–1.80 (1.90–1.80)	31.4–1.80 (1.90–1.80)	29.2–1.60 (1.69–1.60)
Unique reflections	43,176	55,177	93,315	45,350	44,922	64,960
Completeness, %	95.2 (90.8)	94.2 (89.2)	99.6 (98.4)	99.6 (99.2)	98.5 (95.4)	99.9 (100)
Multiplicity	6.9 (6.7)	8.1 (7.9)	3.7 (3.5)	5.4 (5.4)	7.0 (5.8)	6.3 (6.1)
<i>R</i> _{merge} , %*	7.3 (28.5)	5.9 (19.0)	6.7 (27.3)	7.2 (33.0)	6.8 (19.9)	6.1 (36.4)
< <i>I</i> / <i>σ</i> _{<i>i</i>} >	21.2 (5.7)	24.4 (8.2)	15.4 (4.0)	16.1 (4.7)	22.5 (6.1)	18.3 (4.3)
Wilson <i>B</i> value, Å ²	20.5	16.1	18.4	17.8	20.8	19.9
Refinement						
Number of atoms						
Protein [†]	3,094	3,098	6,072	3,092	3,070	3,006
Water	391	393	754	389	382	354
Ions [‡]	2	2	8	2	12	2
<i>R</i> _{cryst} , % [§]	18.5	18.5	18.9	18.4	18.8	19.8
<i>R</i> _{free} , % [§]	20.6	20.6	21.8	21.3	20.6	22.4
rmsd bonds, Å	0.008	0.008	0.009	0.009	0.008	0.009
rmsd angles, °	1.5	1.5	1.5	1.5	1.5	1.5
Mean <i>B</i> value, Å ²	23.6	18.7	20.6	21.8	24.0	23.3
Ramachandran plot						
Most favored, %	91.3	90.7	90.0	91.3	91.2	92.1
Additional allowed, %	8.7	9.3	9.1	8.7	8.8	7.9
Generously allowed, %	0	0	0.9	0	0	0
Disallowed, %	0	0	0	0	0	0
PDB ID code	2J1W	2J1X	2J1Y	2J1Z	2J20	2J21

Values in parentheses are for the highest resolution shell.

$$*R_{\text{merge}} = \sum(I_{h,i} - \langle I_h \rangle) / \sum I_{h,i}$$

[†]Numbers include alternative conformations.

[‡]In addition to the bound zinc ion, each chain of *T*-p53C-G245S has a surface-bound calcium ion, and each chain of *T*-p53C-R273C has a surface-bound sulfate ion, which were present at high concentration in the corresponding crystallization buffer.

[§]*R*_{cryst} and *R*_{free} = $\sum ||F_{\text{obs}}| - |F_{\text{calc}}|| / \sum |F_{\text{obs}}|$, where *R*_{free} was calculated over 5% of the amplitudes chosen at random and not used in the refinement.