

**Table 1 Data collection and refinement statistics**

	5SW8	5SWG	5SWO	5SWP	5SWR	5SWT	5SX8
Fragments	7, 12	5, 21	4, 16	6, 24	20, 26	17, 27	13, 15
<b>Data collection</b>							
Space group	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Cell dimensions <i>a</i> , <i>b</i> , <i>c</i> (Å)	115.6, 117.8, 152.9	114.5, 116.7, 149.5	114.8, 116.4, 149.4	114.1, 116.1, 148.3	114.2, 116.3, 149.3	114.5, 115.9, 149.3	113.9, 116.3, 148.0
Resolution (Å)	50-3.30 (3.37-3.30)	50-3.12 (3.23-3.12)	50-3.50 (3.63-3.50)	50-3.40 (3.52-3.40)	50.00-3.30 (3.42-3.30)	50.00- 3.50(3.56- 3.50)	50-3.45 (3.57-3.45)
<i>R</i> <sub>sym</sub>	0.101 (0.734)	0.085 (0.709)	0.130 (0.601)	0.121 (0.875)	0.097 (0.639)	0.123 (0.973)	0.098 (0.925)
<i>I</i> / $\sigma$ <i>I</i>	26.5 (2.4)	27.1 (2.1)	15.2 (2.0)	17.3 (2.0)	27.5 (2.5)	19.2 (1.8)	24.2 (1.8)
Completeness (%)	99.9 (99.7)	99.9 (98.8)	99.7 (98.1)	99.9 (99.9)	99.7 (98.8)	100 (100)	99.9 (100)
Redundancy	7.1 (6.7)	7.2 (6.1)	6.8 (5.0)	6.7 (6.3)	7.2 (6.5)	7.3 (7.5)	7.3 (7.4)
Unique reflections	31,971	36,555	25,700	27,455	30,235	25,886	25,993
Total reflections	226,811	263,120	174,299	184,879	216,686	188,483	188,731
X-ray Source wavelength	1.0	1.0	1.0	1.0	1.0	1.0	1.0
<b>Refinement</b>							
Resolution (Å)	93.24-3.30	49.14-3.11	48.73-3.50	48.91-3.41	48.54-3.31	92.57-3.50	91.49-3.47
No. reflections	30,096	34,630	24,324	25,928	28,638	24,456	24,618
<i>R</i> <sub>work</sub> / <i>R</i> <sub>free</sub>	0.225/0.298	0.206/0.261	0.188/0.274	0.215/0.296	0.197/0.272	0.208/0.284	0.207/0.275
No. atoms							
Protein	10,166	10,695	10,864	10,852	10,748	10,781	10,657
Ligand	57	28	35	67	44	37	38
<i>B</i> -factors							
Protein	124	101	117	118	121	142	149
Ligand	187	116	142	142	153	155	180
R.m.s. deviations							
Bond lengths (Å)	0.011	0.009	0.011	0.009	0.010	0.009	0.009
Bond angles (°)	1.61	1.46	1.54	1.36	1.45	1.34	1.31

	5SX9	5SXA	5SXB	5SXC	5SXD	5SXE	5SXF
Fragment	14	10	23	8	22	19, 28	9
<b>Data collection</b>							
Space group	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Cell dimensions <i>a</i> , <i>b</i> , <i>c</i> (Å)	113.4, 116.1, 148.0	115.2, 117.4, 152.1	114.6, 116.8, 150.1	114.7, 117.3, 150.3	114.9, 116.4, 150.0	113.8, 116.3, 149.0	112.3, 115.9, 147.2
Resolution (Å)	50-3.50 (3.63-3.50)	50-3.35 (3.42-3.30)	50-3.30 (3.42-3.30)	50.00-3.55 (3.68-3.55)	50-3.50 (3.63-3.50)	50-3.50 (3.63-3.50)	50-3.45 (3.51-3.45)
<i>R</i> <sub>sym</sub>	0.108 (0.874)	0.104 (0.862)	0.107 (0.988)	0.113 (0.848)	0.111 (0.883)	0.112 (0.952)	0.112 (0.938)
<i>I</i> / $\sigma$ <i>I</i>	19.2 (2.3)	24.4 (2.3)	23.7 (2.1)	19.9 (2.3)	18.2 (1.8)	15.7 (1.5)	21.1 (2.0)
Completeness (%)	100 (100)	100 (100)	100 (100)	100 (100)	100 (100)	99.9 (100)	100 (100)
Redundancy	7.2 (7.3)	7.3 (7.4)	7.3 (7.5)	7.3 (7.5)	7.2 (7.2)	6.5 (6.6)	7.3 (7.4)
Unique reflections	24,477	30,528	31,023	25,308	25,936	25,370	25,565
Total reflections	177,395	221,875	226,528	184,302	186,212	165,094	186,277
X-ray Source wavelength	1.0	1.0	1.0	1.0	1.0	1.0	1.0
<b>Refinement</b>							
Resolution (Å)	91.34-3.52	92.91-3.35	92.16-3.30	92.46-3.54	91.97-3.5	91.65-3.51	91.07-3.46
No. reflections	23,166	28,743	29,298	23,959	24,555	24,018	24,200
<i>R</i> <sub>work</sub> / <i>R</i> <sub>free</sub>	0.192/0.277	0.221/0.274	0.204/0.278	0.193/0.267	0.194/0.277	0.191/0.271	0.194/0.266
No. atoms							
Protein	10,583	10,476	10,475	10,305	10,659	10,483	9,960
Ligand	19	44	29	29	31	35	22
<i>B</i> -factors							
Protein	134	136	121	138	138	139	129
Ligand	145	188	146	168	159	181	157
R.m.s. deviations							
Bond lengths (Å)	0.011	0.009	0.010	0.011	0.010	0.011	0.010
Bond angles (°)	1.56	1.33	1.50	1.53	1.52	1.54	1.48

	5SXI 25	5SXJ 29	5SXX 18
<b>Data collection</b>			
Space group	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	p2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>
Cell dimensions <i>a</i> , <i>b</i> , <i>c</i> (Å)	114.2, 116.8, 150.5	114.8, 117.9, 151.0	113.3, 115.8, 149.0
Resolution (Å)	50-3.40 (3.52-3.40)	50-3.45 (3.57-3.45)	50-3.55 (3.61-3.55)
<i>R</i> <sub>sym</sub>	0.133 (0.907)	0.129 (0.955)	0.137 (0.934)
<i>I</i> / $\sigma I$	18.8 (1.7)	25.8 (2.5)	18.7 (1.7)
Completeness (%)	98.6 (96.8)	99.7 (99.8)	99.7 (99.6)
Redundancy	5.1 (3.6)	7.0 (5.7)	5.0 (6.4)
Unique reflections	28,264	28,041	24,161
Total reflections	144,489	197,575	155,578
X-ray Source wavelength	1.0	1.0	1.0
<b>Refinement</b>			
Resolution (Å)	92.27-3.38	92.94-3.42	91.45-3.55
No. reflections	26,461	26,321	22,868
<i>R</i> <sub>work</sub> / <i>R</i> <sub>free</sub>	0.201/0.278	0.212/0.279	0.193/0.277
No. atoms			
Protein	10,332	10,370	10,791
Ligand	28	50	19
<i>B</i> -factors			
Protein	132	138	142
Ligand	161	188	147
R.m.s. deviations			
Bond lengths (Å)	0.010	0.010	0.011
Bond angles (°)	1.50	1.43	1.54