Table 1

Crystallographic data and refinement parameters.

Data-collection details	Compound 1 (PDB ID:4X0M)	Compound 2 (PDB ID:4X2F)
Space group	P212121	P212121
Unit-Cell parameters [Å, °]	a=41.99 b= 76.88 c= 89.59 α = 90.0 β = 90.0 γ = 90.0	a=42.25 b=77.53 c=89.85 α = 90.0 β = 90.0 γ = 90.0
Resolution [Å]	1.68	1.49
Data collection wavelength [Å]	1.0000	1.0000
Number of measurements	102541	337198
Number of unique reflections	32312	48030
Completeness[%] [a]	95.3 (84.5)	98.5 (91.3)
R_{merge} [%]	8.5 (42.9)	7.4 (35.9)
$<I/\sigma(I)>$ [a]	9.2 (4.2)	19.8 (5.0)
Refinement		
Nr. of molecules / asymmetric unit	1	1
R_{work}/R_{free} [b]	0.184/0.239	0.161/0.180
Rmsd bond length [Å]	0.010	0.010
Rmsd bond angle [°]	1.09	1.04
Average B-factor [Å^2]		
Protein	15.3	17.8
Ligand	15.9	18.2
Water	20.2	27.0
Other entities	17.8	17.6
All atoms	15.6	18.7
Number of atoms		
Protein atoms	2439	2475
Ligand	12	19
Water	173	263
Sulfate ion	5	5
All atoms	2629	2762
Ramachandran		
G-factor	0.11	0.14
Core [%]	92.3	92.3
Allowed [%]	7.3	7.3
Generously allowed [%]	0.4	0.4
Dissallowed [%]	0.0	0.0

Data-collection details	Compound 3 (PDB ID:4X2G)	Compound 4 (PDB ID:4X2J)
Space group	P212121	P212121
Unit-Cell parameters [Å, °]	a=42.22 b=77.68 c=90.16 α = 90.0 β = 90.0 γ = 90.0	a=42.31 b=77.51 c=90.20 α = 90.0 β = 90.0 γ = 90.0
Resolution [Å]	1.51	1.69
Data collection wavelength [Å]	1.0000	1.0000
Number of measurements	331417	233410
Number of unique reflections	46334	33372
Completeness[%] [a]	97.4 (92.8)	99.0 (95.3)
R_{merge} [%]	4.6 (16.3)	7.2 (32.1)
$<I/\sigma(I)>$[a]	30.4 (12.5)	21.4 (6.9)
Refinement		
Nr. of molecules / asymmetric unit	1	1
R_{work}/R_{free}[b]	0.164/0.182	0.154/0.184
Rmsd bond length [Å]	0.010	0.010
Rmsd bond angle [°]	1.06	1.02
Average B-factor [Å^2]		
Protein	17.3	18.7
Ligand	16.5	21.6
Water	26.3	28.9
Other entities	27.9	21.8
All atoms	18.2	19.7
Number of atoms		
Protein atoms	2459	2475
Ligand	19	19
Water	266	250
Sulfate ion	13	5
All atoms	2757	2749
Ramachandran		
G-factor	0.13	0.15
Core [%]	93.0	92.3
Allowed [%]	6.6	7.3
Generously allowed [%]	0.4	0.4
Dissallowed [%]	0.0	0.0

Data-collection details	Compound 5 (PDB ID:4X2K)	TGF1B apo structure (PDB ID: 4X2N)
Space group	P212121	P212121
Unit-Cell parameters [Å, °]	a=41.85 b=76.90 c=89.10 α = 90.0 β = 90.0 γ = 90.0	a=41.81 b=77.89 c=90.26 α = 90.0 β = 90.0 γ = 90.0
Resolution [Å]	1.68	1.80
Data collection wavelength [Å]	1.0000	1.5418
Number of measurements	407692	82877
Number of unique reflections	32921	26362
Completeness[%] [a]	98.2 (88.7)	94.6 (84.9)
R_{merge} [%]	15.5 (68.1)	5.2 (28.5)
$<I/\sigma(I)>$[a]	19.0 (4.9)	17.2 (4.9)
Refinement		
Nr. of molecules / asymmetric unit	1	1
R_{work}/R_{free}[b]	0.167/0.196	0.161/0.201
Rmsd bond length [Å]	0.011	0.010
Rmsd bond angle [°]	1.10	0.98
Average B-factor [Å^2]		
Protein	17.6	15.9
Ligand	22.1	n.a.
Water	25.5	26.1
Other entities	21.8	22.8
All atoms	18.2	17.1
Number of atoms		
Protein atoms	2444	2444
Ligand	18	0
Water	209	320
Sulfate ion	6	5
All atoms	2676	2769
Ramachandran		
G-factor	0.16	0.14
Core [%]	92.7	93.4
Allowed [%]	6.6	6.2
Generously allowed [%]	0.7	0.4
Dissallowed [%]	0.0	0.0

Data-collection details	Tie2 (PDB ID: 4X3J)
Space group	P41212
Unit-Cell parameters [Å, °]	a=62.46 b=62.46 c=178.45 $\alpha = 90.0$ $\beta = 90.0$ $\gamma = 90.0$
Resolution [Å]	2.5
Data collection wavelength [Å]	1.0000
Number of measurements	176802
Number of unique reflections	12936
Completeness[%] [a]	99.2 (97.5)
R_{merge} [%]	5.7 (81.0)
$<I/\sigma(I)>$ [a]	12.2 (2.0)
Refinement	
Nr. of molecules / asymmetric unit	1
R_{work}/R_{free} [b]	0.255/0.293
Rmsd bond length [Å]	0.010
Rmsd bond angle [°]	1.12
Average B-factor [Å^2]	
Protein	76.0
Ligand	80.5
Water	51.2
Other entities	n.a.
All atoms	75.9
Number of atoms	
Protein atoms	1887
Ligand	33
Water	17
Sulfate ion	0
All atoms	1937
Ramachandran	
G-factor	0.03
Core [%]	91.7
Allowed [%]	9.3
Generously allowed [%]	0.0
Dissallowed [%]	0.0