

(a) Hydrogen bonding network in the type I and II ligand-receptor interface of wildtype BMP-2 bound to BMPR-IA_{ECD} and ActR-IIB_{ECD} (ternary complex 1:1:1)

H-bonds between BMP-2 and BMPR-IA_{ECD} in the ternary complex (1:1:1)
wtBMP-2:BMPR-IA:ActR-IIB

BMP-2	BMPR-IA	Distance Å	Angle NOC ^a	H-bond ^b
Ser24 _A (O)	Lys92 (NZ)	3.06	152	MC-SC
Val26 _A (O)	Ser90 (OG)	2.59	133	MC-SC
Trp28 _A (NE1)	Asp89 (O)	2.79	136	SC-MC
Leu51 _B (N)	Gln86 (OE1)	2.86	128	MC-SC
Leu51 _B (O)	Gln86 (NE2)	2.98	135	MC-SC
Asp53 _B (N)	Cys77 (O)	2.80	129	MC-MC
Asp53 _B (OD1)	Lys79 (NZ)	3.01	111	SC-SC
Asp53 _B (OD2)	Thr55 (OG1)	2.61	132	SC-SC
Ser69 _B (O)	Gln94 (N)	2.86	151	MC-MC
Ser69 _B (OG)	Arg97 (NH2)	3.07	92	SC-SC
Ser72 _B (OG)	Gln94 (OE1)	2.97	129	SC-SC
Lys101 _A (NZ)	Asp84 (OD2)	2.95	146	SC-SC
Tyr103 _A (OH)	Asp84 (OD2)	2.97	116	SC-SC

H-bonds between BMP-2 and ActR-IIB_{ECD} in the ternary complex (1:1:1)
wtBMP-2:BMPR-IA:ActR-IIB

BMP-2	ActR-IIB	Distance Å	Angle NOC ^a	H-bond ^b
Ala86 _A (N)	Glu34 (OE2)	3.24	147	MC-SC
Ser88 _A (OG)	Leu61 (N)	2.82	131	SC-MC
Glu96 _A (O)	Arg46 (NH2)	2.96	171	MC-SC
Glu96 _A (OE1)	Gln80 (NE2)	3.05	147	SC-SC
Glu109 _A (OE2)	Lys37 (NZ)	2.62	140	SC-SC

- a) N, O, C are the donor-acceptor atoms; from general statistics this angle is $149^\circ \pm 15^\circ$ for MC-MC hydrogen bonds and $129^\circ \pm 18^\circ$ for SC-MC and SC-SC H-bonds;
b) MC (main chain) and SC (side chain) donor/acceptor atoms;

(b) Hydrogen bonding network in the type I and II ligand-receptor interface of the BMP-2 double variant L100K/N102D bound to BMPR-IA_{ECD} and ActR-IIB_{ECD} (ternary complex 1:2:2)

H-bonds between BMP-2 and BMPR-IA _{ECD} in the ternary complex (1:2:2)				
BMP-2L100K/N102D:(BMPR-IA _{ECD}) ₂ :(ActR-IIB _{ECD}) ₂				
BMP-2	BMPR-IA	Distance Å	Angle NOC ^a	H-bond ^b
Val26 _A (O)	Ser90 (OG)	2.88	128	MC-SC
Trp28 _A (NE1)	Asp89 (O)	2.89	135	SC-MC
Leu51 _B (N)	Gln86 (OE1)	2.83	123	MC-SC
Leu51 _B (O)	Gln86 (NE2)	3.00	132	MC-SC
Asp53 _B (N)	Cys77 (O)	2.90	124	MC-MC
Asp53 _B (OD2)	Thr55 (OG1)	2.80	125	SC-SC
Asn59 _B (N)	Glu81 (OE2)	3.00	127	MC-SC
Asn59 _B (OD1)	Gly82 (N)	3.09	147	SC-MC
Ser69 _B (O)	Gln94 (N)	2.87	148	MC-MC
Ser69 _B (OG)	Arg97 (NH2)	2.70	116	SC-SC
Val70 _B (O)	Gln94 (NE2)	2.87	94	MC-SC
Ser72 _B (OG)	Gln94 (NE2)	3.10	117	SC-SC
Tyr103 _A (OH)	Asp84 (OD2)	2.76	113	SC-SC

H-bonds between BMP-2 and ActR-IIB _{ECD} in the ternary complex (1:2:2)				
BMP-2L100K/N102D:(BMPR-IA _{ECD}) ₂ :(ActR-IIB _{ECD}) ₂				
BMP-2	ActR-IIB	Distance Å	Angle NOC ^a	H-bond ^b
Ser88 (OG)	Leu61 (N)	2.90	128	SC-MC
Glu96 (O)	Arg46 (NH2)	3.24	161	MC-SC
Val98 (O)	Lys56 (NZ)	3.02	145	MC-SC

- a) N, O, C are the donor-acceptor atoms; from general statistics this angle is $149^\circ \pm 15^\circ$ for MC-MC hydrogen bonds and $129^\circ \pm 18^\circ$ for SC-MC and SC-SC H-bonds;
- b) MC (main chain) and SC (side chain) donor/acceptor atoms;