PDBePISA: Side Chain Interactions as per PDB: 1IRA

Salt Bridges:

	IL-1R1		IL-1Ra
1	Y:ARG 268[NH1]	3.88	X:GLU 150[OE2]
2	Y:ARG 268[NE]	3.89	X:GLU 150[OE2]
3	Y:ARG 268[NH2]	3.32	X:GLU 150[OE2]
4	Y:GLU 8[OE2]	3.07	X:ARG 26[NE]
5	Y:GLU 8[OE1]	3.89	X:ARG 26[NH2]

show sticks, /1ira/B/Y/ARG`268/
show sticks, /1ira/A/X/GLU`150/
distance saltbridge1, /1ira/B/Y/ARG`268/NH1, /1ira/A/X/GLU`150/OE2
distance saltbridge2, /1ira/B/Y/ARG`268/NE, /1ira/A/X/GLU`150/OE2
distance saltbridge3, /1ira/B/Y/ARG`268/NH2, /1ira/A/X/GLU`150/OE2
hide labels, saltbridge1
hide labels, saltbridge2
hide labels, saltbridge3

show sticks, /1ira/B/Y/GLU`8/
show sticks, /1ira/A/X/ARG`26/
distance saltbridge4, /1ira/B/Y/GLU`8/OE2, /1ira/A/X/ARG`26/NE
distance saltbridge5, /1ira/B/Y/GLU`8/OE1, /1ira/A/X/ARG`26/NH2
hide labels, saltbridge4
hide labels, saltbridge5

Hydrogen Bonding:

	IL-1R1		IL-1Ra
9	Y:TYR 124[OH]	3.43	X:ASP 128[OD1]
1	Y:SER 235[OG]	3.42	X:GLN 11[OE1]

show sticks, /1ira/B/Y/TYR`124/
show sticks, /1ira/A/X/ASP`128/
show sticks, /1ira/B/Y/SER`235/
show sticks, /1ira/A/X/GLN`11/
distance hbond, /1ira/B/Y/TYR`124/OH, /1ira/A/X/ASP`128/OD1
distance hbond2, /1ira/B/Y/SER`235/OG, /1ira/A/X/GLN`11/OE1
hide labels, hbond
hide labels, hbond2

PDBePISA: Main Chain Interactions as per PDB: 1IRA

Receptor side chain to antagonist main chain:

	IL-1R1		IL-1Ra
24	Y:GLU 126[OE2]	3.27	X:ALA 127[N]
18	Y:TYR 124[OH]	3.75	X:TYR 34[N]
2	Y:ARG 160[NH2]	3.06	X:VAL 18[O]

*Lys9 and Leu25 are missing from PDBePISA. Now, corrected from structural analysis.

show sticks, /1ira/B/Y/GLU`126/
show sticks, /1ira/A/X/ALA`127/
show sticks, /1ira/B/Y/TYR`124/
show sticks, /1ira/A/X/TYR`34/
show sticks, /1ira/B/Y/ARG`160/
show sticks, /1ira/A/X/VAL`18/
distance hbond1, /1ira/B/Y/GLU`126/OE2, /1ira/A/X/ALA`127/N
distance hbond2, /1ira/B/Y/TYR`124/OH, /1ira/A/X/TYR`34/N
distance hbond3, /1ira/B/Y/ARG`160/NH2, /1ira/A/X/VAL`18/O
distance hbond4, /1ira/A/X/LEU`25/O, /1ira/B/Y/LYS`9/NZ
hide labels, hbond1
hide labels, hbond2
hide labels, hbond3

Receptor main chain to antagonist main chain:

21	Y:ILE 107[O]	3.09	X:GLY 37[N]
23	Y:THR 297[O]	2.81	X:HIS 54[N]

*Asn296 and Pro53 are missing. Now corrected from structural analysis.

show sticks, /1ira/B/Y/ILE`107/
show sticks, /1ira/A/X/GLY`37/
show sticks, /1ira/B/Y/THR`297/
show sticks, /1ira/A/X/HIS`54/
distance hbond5,/1ira/B/Y/ILE`107/O, /1ira/A/X/GLY`37/N
distance hbond6, /1ira/B/Y/THR`297/O, /1ira/A/X/HIS`54/N
distance hbond7, /1ira/B/Y/ASN`296/O, /1ira/A/X/PRO`53/CA

Receptor main chain antagonist side chain:

	IL-1R1			IL-1Ra	
8	Y:ILE 11[N]	3.24		X:ASN 39[OD1]	
22	Y:ILE 11[O]	2.94		X:ASN 39[ND2]	
8	Y:ILE 11[N]	3.24		X:ASN 39[OD1]	
7	Y:VAL 13[N]	2.84		X:GLN 36[OE1]	
19	Y:VAL 13[O]	2.95		X:GLN 36[NE2]	
20	Y:ALA 106[O]	3.09		X:GLN 36[NE2]	
15	Y:LYS 111[O]	2.95		X:GLN 20[NE2]	
4	Y:LYS 111[N]	3.06		X:GLN 20[OE1]	
13	Y:LYS 111[O]	3.32		X:TRP 16[NE1]	
14	Y:GLY 119[O]	3.36		X:GLN 20[NE2]	

show sticks, /1ira/B/Y/ILE`11/
show sticks, /1ira/A/X/ASN`39/
show sticks, /1ira/B/Y/VAL`13/
show sticks, /1ira/A/X/GLN`36/
show sticks, /1ira/B/Y/ALA`106/
show sticks, /1ira/B/Y/LYS`111/
show sticks, /1ira/B/Y/GLN`20/
show sticks, /1ira/A/X/TRP`16/
show sticks, /1ira/B/Y/GLY`119/
distance hbond1, /1ira/B/Y/ILE`11/N, /1ira/A/X/ASN`39/OD1
distance hbond2, /1ira/B/Y/ILE`11/O, /1ira/A/X/ASN`39/ND2
distance hbond3, /1ira/B/Y/ILE`11/N, /1ira/A/X/ASN`39/OD1
distance hbond4, /1ira/B/Y/VAL`13/N, /1ira/A/X/GLN`36/OE1
distance hbond5, /1ira/B/Y/VAL`13/O, /1ira/A/X/GLN`36/NE2
distance hbond6, /1ira/B/Y/ALA`106/O, /1ira/A/X/GLN`36/NE2
distance hbond7, /1ira/B/Y/LYS`111/O, /1ira/B/Y/GLN`20/NE2
distance hbond8, /1ira/B/Y/LYS`111/N, /1ira/B/Y/GLN`20/OE1
distance hbond9, /1ira/B/Y/LYS`111/O, /1ira/A/X/TRP`16/NE1
distance hbond10,/1ira/B/Y/GLY`119/O, /1ira/B/Y/GLN`20/NE2

Hydrogen bonds XML

##	Structure 1	Dist. [Å]	Structure 2
1	Y:SER 235[OG]	3.42	X:GLN 11[OE1]
2	Y:ARG 160[NH2]	3.06	X:VAL 18[O]
3	Y:ARG 160[NH2]	3.70	X:ASN 19[OD1]
4	Y:LYS 111[N]	3.06	X:GLN 20[OE1]
5	Y:ASN 27[ND2]	3.78	X:GLN 29[OE1]
6	Y:TYR 124[OH]	3.18	X:TYR 34[O]
7	Y:VAL 13[N]	2.84	X:GLN 36[OE1]
8	Y:ILE 11[N]	3.24	X:ASN 39[OD1]
9	Y:TYR 124[OH]	3.43	X:ASP 128[OD1]
10	Y:GLN 233[NE2]	3.54	X:GLU 150[OE2]
11	Y:LYS 267[NZ]	3.87	X:ASP 151[O]
12	Y:SER 235[O]	3.85	X:SER 8[OG]
13	Y:LYS 111[O]	3.32	X:TRP 16[NE1]
14	Y:GLY 119[O]	3.36	X:GLN 20[NE2]
15	Y:LYS 111[O]	2.95	X:GLN 20[NE2]
16	Y:GLU 8[OE2]	3.07	X:ARG 26[NE]
17	Y:GLU 8[OE1]	3.89	X:ARG 26[NH2]
18	Y:TYR 124[OH]	3.75	X:TYR 34[N]
19	Y:VAL 13[O]	2.95	X:GLN 36[NE2]
20	Y:ALA 106[O]	3.09	X:GLN 36[NE2]
21	Y:ILE 107[O]	3.09	X:GLY 37[N]
22	Y:ILE 11[O]	2.94	X:ASN 39[ND2]
23	Y:THR 297[O]	2.81	X:HIS 54[N]
24	Y:GLU 126[OE2]	3.27	X:ALA 127[N]

Salt bridges XML

##	Structure 1	Dist. [Å]	Structure 2
1	Y:ARG 268[NH1]	3.88	X:GLU 150[OE2]
2	Y:ARG 268[NE]	3.89	X:GLU 150[OE2]
3	Y:ARG 268[NH2]	3.32	X:GLU 150[OE2]
4	Y:GLU 8[OE2]	3.07	X:ARG 26[NE]
5	Y:GLU 8[OE1]	3.89	X:ARG 26[NH2]

No disulfide bonds found

No covalent bonds found