Supplementary Table 1: Interacting residues, polar contacts and hydrophobic contacts between IL-6 and olokizumab

	4CNI_BEFORE DOCKING			ClusPro_AFTER DOCKING			ZDOCK_AFTER DOCKING			Rosetta_AFTER DOCKING		
	H	**L**	**IL-6**	**H**	**L**	**IL-6**	**H**	**L**	**IL-6**	**H**	**L**	**IL-6**
Interface Residue	Asp31 Phe33 Arg52 Asn53 Asn55 Tyr56 Gln57 Tyr61 Glu101 Ser102 Tyr103 Tyr104 Gly105	Gln27 Asp28 Gly30 Ile31 Ser32 Asn50 Ser67 His91 Asn92 Ser93 Ala94 Tyr96	Ser47 Asn48 Lys54 Leu57 Asn60 Asn61 Asn103 Arg104 Glu106 Thr149 Lys150 Gln152 Ala153 Gln154 Asn155 Gln156 Trp157 Leu158 Gln159 Asp160	Asp31 Tyr32 Phe33 Gln50 Arg52 Lys54 Asn55 Tyr56 Gln57 Tyr61 Glu101 Ser102 Tyr103 Tyr104 Gly105	Asp28 Gly30 Ile31 Ser32 Asn50 His91 Asn92 Ser93 Ala94 Tyr96	Ser47 Asn48 Lys54, Leu57 Asn103 Arg104 Glu106 Gln152 Ala153 Gln154 Asn155 Gln156 Trp157 Leu158 Gln159 Asp160	Asp31 Tyr32 Phe33 Gln50 Arg52 Asn53 Lys54 Asn55 Tyr56 Gln57 Tyr61 Glu101 Ser102 Tyr103 Tyr104 Gly105	Gln27 Asp28 Gly30 Ile31 Ser32 Asn50 Asn52 Asn53 Ser67 His91 Asn92 Ser93 Ala94 Tyr96	Ser47 Asn48 Lys54 Leu57 Asn60 Asn61 Asn103 Arg104 Glu106 Thr149 Lys150 Gln152 Ala153 Gln154 Asn155 Gln156 Trp157 Leu158 Gln159 Asp160	Phe33 Gln50 Arg52 Asn53 Lys54 Asn55 Tyr56 Gln57 Tyr61 Glu101 Ser102 Tyr103 Tyr104 Gly105	Gln27 Asp28 Gly30 Ile31 Ser32 Ser67 His91 Asn92 Ser93 Ala94 Tyr96	Ser47 Lys54 Leu57 Asn60 Asn61 Asn103 Arg104 Gln106 Thr149 Lys150 Gln152 Ala153 Gln154 Asn155 Gln156 Trp157 Leu158 Gln159 Asp160
Surface Area	4781.886 Å²			4481.597 Å²			5025.286 Å			5236.795 Å²		
Hydrogen Bond	Gln152::O---NH2: :Arg52:H Gln152::O---NH1: :Arg52:H Arg104::NH1---O::Asn55:H Arg104::NH1---O::Asn55:H Asn103::O---NE_2::Gln57:H Asp160:: OD2--O::Tyr103:H Trp157::N---O::Tyr103:H Ala153::O---N::Ala94:L Asn155::N---O::Asn92:L Asn155::ND2---O::His91:L Asn155::ND2---O::Ser32:L			Ala153::O---NH2::Arg52:H Gln154::O---NH1::Arg52:H Gln154::O---NH2::Arg52:H Gln152::NE2---OE1::Gln57:H Gln152::O---NH1::Arg52:H Asn103::O---DH22::Asn55:H Arg104::HH1--OD1::Asn55:H Arg104::NH1---HO::Tyr56:H Gln156::NE2---O::Ser102:H Gln156::NE2-OE2::Glu101:H Gln156::O---HO::Tyr103:H Asp160::OD2--HO::Tyr103:H Trp157::H---O::Tyr103:H Asn155::O---ND2::His91:L Asn155::O---ND1::Asn92:L			Arg104::NH1---O::Asn55:H Arg104::NH2---O::Asn55:H Gln152::O---NH1::Arg52:H Gln152::O---NH2::Agr52:H Trp157::N---O::Tyr103:H Asn155::ND2---O::Asn92:L Asn155::N---O::Asn92:L Ala153::O---N::Ala94:L			Ser47::O---HO::Tyr103:H Gln159::OE1---HO::Tyr156:H Gln152::O---NH1::Arg52:H Gln152::O---NH2::Arg52:H Asn103::O---NE2::Gln57:H Asn155::ND2---O::His91:L Asn155::NH----O::Asn92:L Asn155::ND2---OG::Asn92:L Ala153::O---HN::Ala94:L		
Hydrophobic Bond	Gln152 --- H: Gln57 Asn155 --- H: Gly105 Glu106 --- H: Lys54 Glu106 --- H: Asn55 (2) Asn103 --- H: Asn55 Arg104 --- H: Asn55 (2) Arg104 --- H: Tyr56 (2) Gln159 --- H: Tyr56 (4) Gln156 --- H: Tyr56 (2) Gln156 --- H: Ser102 (3) Gln156 --- H: Phe33 (3) Gln156 --- H: Glu101 (2) Gln156 --- H: Tyr103 (*) Asp160 --- H: Tyr103 (5) Ser47 --- H: Tyr103 (4) Trp157 --- H: Tyr103 (8) Trp157 --- H: Tyr104 (6) Asn48 --- H: Tyr103 (2) Trp157 --- L: Ser32 Asn155 --- L: Tyr96 (2) Asn155 --- L: Asn92 Asn158 --- L: Asn92 Lys54 --- L: Ile31			Ala153 --- H: Tyr61 (2) Ala153 --- H: Arg52 (3) Gln154 --- H: Arg52 (3) Gln152 --- H: Gln57 Asn155 --- H: Gly105 Glu106 --- H: Lys54 Glu106 --- H: Asn55 (2) Asn103 --- H: Asn155 Arg104 --- H: Asn55_A (2) Arg104---H: Tyr56_A (2) Gln159---H: Tyr56_A (4) Gln156---H: Tyr56_A (2) Gln156---H: Ser102_A (3) Gln156---H: Phe33_A (3) Gln156---H: Glu101_A (2) Gln156---H: Tyr103_A (*) Asp160---H: Tyr103_A (5) Ser47---H: Tyr103_A (4) Trp157---H: Tyr103_A (8) Trp157---H: Tyr104_A (6) Asn48---H: Tyr103_A (2) Trp157---L: Ser32_B Asn155---L: Tyr96_B (2) Asn155---L: Asn92_B Leu158---L: Asn92_B Lys54---L: Ile31_B			Asn103---H: Gln57 Asn103---H: Asn55 (3) Arg104---H: Asn55 (7) Arg104—H: Tyr56 (5) Gln159---H: Tyr56 Gln159---H: Arg52 Gln154---H: Arg52 (2) Gln152---H: Arg52 (6) Gln152---H: Tyr61 Ala153---H: Arg52 (3) Ala153---H: Tyr61 Asn155---H: Gly105 Asn155---H: Tyr104 Asn155---H: Glu101 ASn155---H: Tyr103 Trp157---H: Tyr104 (9) Trp157---H: Tyr103 (5) ASn48---H: Tyr103 (7) Asp160---H: Tyr103 (7) Ser47---H: Tyr103 (5) Gln156---H: Tyr103 (7) Gln156---H: Phe33 Gln156---H: Ser102 Asn155---L: Tyr96 (3) Asn155---L: His91 (4) Asn155---L: Asn92 (3)			Asp160---H: Tyr103 (2) Trp157---H: Tyr103 Ser47---H: Tyr103 Gln156---H: Tyr103 (8) Gln156---H: Phe33 Gln156---H: Tyr56 Arg104---H: Tyr56 (2) Gln156---H: Tyr56 (5) Gln152---H: Arg52 Gln152---H: Tyr61 Ala153---H: Arg52 Ala153---H: Tyr61 Asn103---H: Gln157 Asn155---H: Tyr104 Leu57---L: Ile31 ASn60---L: Asp28 Asn155---L: His91 Asn155---L: Ser32 Asn155---L: Asn92 Leu158---L: Ser32 Leu158---L: Asn92 (3) Gln154---L: Ser93 Ala153---L: Ser93 (2) Ala153---L: Ala94 (3)		

	Gln154---L: Ser93 (2) Leu158---L: Asn92 (7) Leu158---L: Ser32 Trp157---L: Ser32 Trp157---L: ASn50 Trp157---L: Ile31 Lys54---L: Ile31 Leu57---L: Ile31 Leu57---L: Gly30 Leu57---L: Ile29 Ala153---L: Ala(4)