Viewing crx_sm_34-95_FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.87		99th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	1	1.79%	Goal: <1%
	Ramachandran outliers	2	3.33%	Goal: <0.05%
	Ramachandran favored	52	86.67%	Goal: >98%
	MolProbity score^	1.77		87th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad backbone bonds:	0 / 538	0.00%	Goal: 0%
	Bad backbone angles:	8 / 722	1.11%	Goal: <0.1%

In the two column results, the left column gives the raw count, right column gives the percentage.

* 100th percentile is the best among structures of comparable resolution; 0th percentile is the worst. For clashscore the comparative set of structures was selected in 2004, for MolProbity score in 2006.

^ MolProbity score combines the clashscore, rotamer, and Ramachandran evaluations into a single score, normalized to be on the same scale as X-ray resolution.

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.81	Clashscore: 1.87	Outliers: 2 of 60	Poor rotamers: 1 of 56	Outliers: 0 of 62	Outliers: 0 of 62	Outliers: 7 of 62
A 34		SER	50	-	-	15.7% (*m*) chi angles: 308.2	0.045Å	-	-
A 35		ALA	50	-	Favored (94.46%) Pre-proline / -64.7,129.8	-	0.063Å	-	-
A 36		PRO	50	-	Favored (38.41%) Trans-proline / -67.4,-29.2	33.5% (*Cg_exo*) chi angles: 325.4	0.065Å	-	-
A 37		ARG	50	-	Favored (15.45%) General / 63.0,32.6	53.9% (*mmm-85*) chi angles: 299.5,288.8,292.5,275.9	0.09Å	-	-
					Favored	96.3% (*mttt*)			

A 38	LYS	50	-	(46.06%) General / -141.0,156.4	chi angles: 300.2,183.8,183.8,180.8	0.069Å	-	-
A 39	GLN	50	-	Favored (4.81%) General / -166.9,144.4	19.2% (*tt0*) chi angles: 179.9,184.1,113.7	0.113Å	-	-
A 40	ARG	50	-	Favored (2.5%) General / -99.1,80.8	3.9% (*tpm_?*) chi angles: 172,63.7,257.2,206.3	0.045Å	-	-
A 41	ARG	50	-	Favored (22.92%) General / -68.8,164.0	8.9% (*tpt180*) chi angles: 176.3,64.4,215.7,169.2	0.077Å	-	-
A 42	GLU	50	-	OUTLIER (0.01%) General / -65.0,-90.2	1.1% (*tm-20*) chi angles: 155.4,267.5,350.7	0.189Å	-	OUTLIER(S) worst is C-N-CA: 5.279 σ
A 43	ARG	50	-	Favored (8.82%) General / -130.8,175.7	44.3% (*mtt85*) chi angles: 308.2,171.6,192.6,115.8	0.072Å	-	-
A 44	THR	50	-	Allowed (0.16%) General / -96.7,-107.0	33% (*p*) chi angles: 51.8	0.177Å	-	-
A 45	THR	50	-	Favored (45.36%) General / -63.4,149.7	15.2% (*m*) chi angles: 311.8	0.034Å	-	-
A 46	PHE	50	-	Favored (19.86%) General / -60.6,124.3	33.8% (*m-85*) chi angles: 309.4,265.1	0.118Å	-	-
A 47	THR	50	-	Favored (5.99%) General / -75.2,178.1	7.8% (*t*) chi angles: 193.5	0.208Å	-	-
A 48	ARG	50	-	Favored (56.76%) General / -52.9,-52.6	16.3% (*tpt180*) chi angles: 165.1,61.3,196.9,184.4	0.135Å	-	-
A 49	SER	50	-	Favored (82.07%) General / -61.9,-36.7	69.9% (*p*) chi angles: 57.6	0.097Å	-	-
A				Favored (88.25%)	51.1% (*mt-30*)			

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
50	GLN	50	-	General / -66.0,-38.3	chi angles: 301.7,177.8,271.7	0.122Å	-	-
A 51	LEU	50	-	Favored (85.49%) General / -67.4,-40.4	48.9% (*mt*) chi angles: 298.1,164.9	0.074Å	-	OUTLIER(S) worst is C-N-CA: 4.274 σ
A 52	GLU	50	-	Favored (92.23%) General / -65.4,-42.8	23.6% (*tt0*) chi angles: 194.9,165.7,55.5	0.083Å	-	-
A 53	GLU	50	-	Favored (67.98%) General / -71.2,-31.7	1% chi angles: 230.6,278.8,299.4	0.081Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 50.81	Clashscore: 1.87	Outliers: 2 of 60	Poor rotamers: 1 of 56	Outliers: 0 of 62	Outliers: 0 of 62	Outliers: 7 of 62
A 54		LEU	50	-	Favored (80.93%) General / -67.1,-36.0	39% (*mt*) chi angles: 290.9,160.6	0.116Å	-	-
A 55		GLU	50	-	Favored (96.16%) General / -64.8,-41.1	72.2% (*mm-40*) chi angles: 283.8,300.2,317.4	0.092Å	-	-
A 56		ALA	50	-	Favored (91.11%) General / -59.5,-41.9	-	0.073Å	-	-
A 57		LEU	50	-	Favored (89.85%) General / -58.6,-44.3	20.6% (*tp*) chi angles: 186.3,50.4	0.106Å	-	-
A 58		PHE	50	-	Favored (79.05%) General / -60.3,-36.9	53% (*t80*) chi angles: 188.3,89.6	0.108Å	-	-
A 59		ALA	50	-	Favored (84.8%) General / -67.6,-38.9	-	0.075Å	-	-
A 60		LYS	50	-	Favored (40.41%) General / -82.1,-19.4	17.1% (*ptmt*) chi angles: 47.5,182.2,281.3,180.1	0.243Å	-	-

A 61	THR	50	-	Allowed (0.18%) General / -176.9,131.6	4.8% (*t*) chi angles: 175.3	0.087Å	-	-
A 62	GLN	50	-	Favored (59.3%) General / -84.7,-5.3	64.9% (*mt-30*) chi angles: 308.4,181,359.2	0.12Å	-	-
A 63	TYR	50	-	Favored (31.1%) Pre-proline / -137.0,82.2	96.1% (*m-85*) chi angles: 292.4,95.8	0.041Å	-	-
A 64	PRO	50	-	Favored (3.94%) Trans-proline / -84.5,128.1	71.6% (*Cg_endo*) chi angles: 29.5	0.06Å	-	-
A 65	ASP	50	-	Favored (10.78%) General / -78.8,175.1	32.7% (*t0*) chi angles: 199.5,10.2	0.102Å	-	OUTLIER(S) worst is C-N-CA: 4.405 σ
A 66	VAL	50	-	Allowed (1.14%) Isoleucine or valine / -42.6,-45.6	22% (*m*) chi angles: 293	0.164Å	-	-
A 67	TYR	50	-	Favored (89.29%) General / -58.9,-45.9	1.3% (*m-85*) chi angles: 328.4,278.7	0.119Å	-	-
A 68	ALA	50	-	Favored (28.8%) General / -83.1,-29.4	-	0.081Å	-	-
A 69	ARG	50	-	Favored (95.4%) General / -64.5,-43.0	89.2% (*mtm-85*) chi angles: 295.4,200.4,300.8,283.7	0.19Å	-	-
A 70	GLU	50	0.418Å HA with A 73 ALA HB3	Favored (30.66%) General / -84.3,-22.2	2.8% (*mm-40*) chi angles: 297.9,315,73.1	0.242Å	-	-
A 71	GLU	50	-	Favored (45.98%) General / -50.6,-51.8	10.5% (*tt0*) chi angles: 182.9,208.5,294.3	0.045Å	-	-
A 72	VAL	50	-	Favored (12%) Isoleucine or valine / -80.8,-30.5	56% (*t*) chi angles: 169.6	0.192Å	-	-
			0.433Å	Favored				

# Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 73	ALA	50	HB1 with A 78 LEU O	(77.87%) General / -60.0,-36.8	-	0.06Å	-	-
		Avg: 50.81	Clashscore: 1.87	Outliers: 2 of 60	Poor rotamers: 1 of 56	Outliers: 0 of 62	Outliers: 0 of 62	Outliers: 7 of 62
A 74	LEU	50	-	Favored (76.83%) General / -64.9,-47.7	38.9% (*mt*) chi angles: 289.2,160.7	0.077Å	-	-
A 75	LYS	50	-	Favored (85.6%) General / -67.4,-40.1	38% (*mtmt*) chi angles: 290.7,169.8,277.5,167.2	0.099Å	-	-
A 76	ILE	50	-	Favored (10.68%) Isoleucine or valine / -83.8,-17.2	5.8% (*pt*) chi angles: 72.6,190.7	0.216Å	-	-
A 77	ASN	50	-	Allowed (0.28%) General / 74.1,43.8	0.1% chi angles: 336.6,124.9	0.169Å	-	OUTLIER(S) worst is CA-CB-CG: 4.295 σ
A 78	LEU	50	0.433Å O with A 73 ALA HB1	Favored (4.79%) Pre-proline / -124.0,173.2	98.4% (*mt*) chi angles: 296.8,177.3	0.067Å	-	-
A 79	PRO	50	-	Allowed (0.34%) Trans-proline / -101.9,161.7	19.4% (*Cg_endo*) chi angles: 38.7	0.109Å	-	OUTLIER(S) worst is C-N-CA: 6.508 σ
A 80	GLU	50	-	OUTLIER (0.01%) General / -16.0,-65.4	4.7% (*tm-20*) chi angles: 188.8,297.6,307.6	0.106Å	-	-
A 81	SER	50	-	Favored (11.33%) General / -46.7,-39.4	38.5% (*t*) chi angles: 181.8	0.089Å	-	-
A 82	ARG	50	-	Favored (89.51%) General / -65.1,-38.1	28.4% (*mmm-85*) chi angles: 289.8,286.4,291,253.8	0.081Å	-	-
A 83	VAL	50	-	Favored (43.42%) Isoleucine or valine / -75.3,-41.2	24.3% (*t*) chi angles: 187	0.054Å	-	-
				Favored	5.4% (*tp-100*)			

# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 84	GLN 50	-	(69.71%) General / -53.9,-49.0	chi angles: 190.1,78.2,253.8	0.031Å	-	-
A 85	VAL 50	-	Favored (69.23%) Isoleucine or valine / -71.9,-42.8	63.8% (*t*) chi angles: 171.3	0.105Å	-	-
A 86	TRP 50	-	Favored (94.41%) General / -59.9,-44.1	78.8% (*t90*) chi angles: 188.5,85.5	0.112Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.461 σ
A 87	PHE 50	-	Favored (74.7%) General / -63.7,-33.0	14.4% (*m-85*) chi angles: 272,76.6	0.166Å	-	OUTLIER(S) worst is CA-CB-CG: 4.321 σ
A 88	LYS 50	-	Favored (95.66%) General / -64.3,-40.3	33.9% (*mmtm*) chi angles: 309.6,303.7,164.3,284.5	0.163Å	-	-
A 89	ASN 50	-	Favored (52.55%) General / -77.0,-38.8	38.7% (*m-80*) chi angles: 288.4,269	0.079Å	-	-
A 90	ARG 50	-	Favored (83.38%) General / -64.8,-36.1	45.9% (*tpt85*) chi angles: 181.5,61.8,179.7,73.1	0.088Å	-	-
A 91	ARG 50	-	Favored (21.31%) General / -92.3,-20.2	18.4% (*ttt-85*) chi angles: 218,179,189,264.7	0.175Å	-	-
A 92	ALA 50	-	Favored (69.55%) General / -59.8,-31.3	-	0.103Å	-	-
A 93	LYS 50	-	Allowed (0.49%) General / -64.0,2.8	4.2% (*tptp*) chi angles: 196.1,62.5,233.8,67.2	0.124Å	-	-
# Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
	Avg: 50.81	Clashscore: 1.87	Outliers: 2 of 60	Poor rotamers: 1 of 56	Outliers: 0 of 62	Outliers: 0 of 62	Outliers: 7 of 62
A 94	CYS 50	-	Favored (41.85%) General / -69.3,-8.0	25.2% (*p*) chi angles: 67.4	0.131Å	-	-
A				47.1% (*tpt85*)			

| 95 | ARG 99.99 | - | - | chi angles:
181.8,64.1,192.9,79.8 | 0.048Å | - | - |