Viewing RD3_mb_77-191-FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	0		100th percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	5	4.72%	Goal: <1%
	Ramachandran outliers	2	1.77%	Goal: <0.05%
	Ramachandran favored	102	90.27%	Goal: >98%
	MolProbity score^	1.55		94th percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	0.88%	Goal: 0
	Bad backbone bonds:	0 / 970	0.00%	Goal: 0%
	Bad backbone angles:	7 / 1311	0.53%	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: 109.32	Clashscore: 0	Outliers: 2 of 113	Poor rotamers: 5 of 106	Outliers: 1 of 113	Outliers: 0 of 115	Outliers: 7 of 115
77		GLU	50.66	-	-	3.7% (*mp0*) chi angles: 295.8,73.8,313.8	0.112Å	-	OUTLIER(S) worst is CB-CG-CD: 5.305 σ
78		ARG	160.75	-	Allowed (0.21%) General / -57.8,-3.5	71.9% (*mtm-85*) chi angles: 307.8,182.6,305.2,283.8	0.092Å	-	-
79		LEU	235.06	-	Allowed (0.76%) General / -60.3,172.8	10.7% (*mp*) chi angles: 278.4,67.2	0.041Å	-	-
80		GLN	173.91	-	Favored (19.85%) General /	8.8% (*tp-100*) chi angles: 185.7,49.4,219.2	0.11Å	-	-

81	LEU	57.9	-	-52.8,-27.8 Favored (65.56%) General / -54.3,-38.1	83.3% (*mt*) chi angles: 298.2,181.8	0.14Å	-	-
82	GLU	94.21	-	Favored (61.44%) General / -63.3,-52.6	13.5% (*tm-20*) chi angles: 185,284.5,323.1	0.028Å	-	-
83	ASP	89.21	-	Favored (79.85%) General / -62.1,-35.8	22% (*t70*) chi angles: 179.8,45.6	0.124Å	-	-
84	VAL	34.28	-	Favored (94.85%) Isoleucine or valine / -65.3,-44.6	51.1% (*t*) chi angles: 168.8	0.163Å	-	-
85	CYS	83.13	-	Favored (76.63%) General / -59.0,-37.3	2.1% (*m*) chi angles: 271	0.116Å	-	-
86	VAL	40.64	-	Favored (84.85%) Isoleucine or valine / -61.7,-39.9	84.2% (*t*) chi angles: 177.5	0.106Å	-	-
87	LYS	85.68	-	Favored (17.99%) General / -87.0,-36.8	36.6% (*mtmm*) chi angles: 290.2,179.1,292.3,297	0.098Å	-	-
88	ILE	101.11	-	Favored (8.58%) Isoleucine or valine / -82.8,-23.8	29.2% (*pt*) chi angles: 68.2,166.9	0.177Å	-	-
89	HIS	72.47	-	Favored (9.15%) Pre-proline / -142.9,60.3	38.1% (*m-70*) chi angles: 299.8,318.1	0.045Å	-	OUTLIER(S) worst is CA-CB-CG: 4.645 σ
90	PRO	84.27	-	Favored (29.2%) Trans-proline / -68.7,-29.8	66% (*Cg_endo*) chi angles: 27.8	0.104Å	-	-
91	SER	84.26	-	Favored (10.56%) General / -88.4,-44.7	68.1% (*p*) chi angles: 57.3	0.062Å	-	-
92	TYR	83.32	-	Favored (71.81%) General /	42.1% (*t80*) chi angles: 191.1,91.8	0.171Å	-	-

-71.2,-36.2

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
93		CYS	72.4	-	Favored (22.36%) General / -74.4,-49.5	90.8% (*m*) chi angles: 293.4	0.113Å	-	-
94		GLY	101.99	-	Favored (22.31%) Glycine / 55.9,-121.1	-	-	-	-
95		PRO	73.9	-	Favored (20.33%) Trans-proline / -54.1,-20.9	88.1% (*Cg_exo*) chi angles: 328.9	0.074Å	-	-
96		ALA	42.56	-	Favored (61.06%) General / -72.6,-12.4	-	0.08Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 109.32	Clashscore: 0	Outliers: 2 of 113	Poor rotamers: 5 of 106	Outliers: 1 of 113	Outliers: 0 of 115	Outliers: 7 of 115
97		ILE	59.59	-	Favored (24.03%) Isoleucine or valine / -52.2,-38.2	78.4% (*mt*) chi angles: 291.7,164	0.096Å	-	-
98		LEU	129.14	-	Favored (64.92%) General / -52.2,-48.5	3.2% (*tm?*) chi angles: 189.9,280.1	0.084Å	-	-
99		ARG	149.8	-	Favored (63.33%) General / -73.9,-32.0	45.8% (*tpt85*) chi angles: 184.9,62.6,193.7,91.4	0.13Å	-	-
100		PHE	60.42	-	Favored (81.57%) General / -60.6,-37.5	37% (*m-85*) chi angles: 283.4,298.2	0.046Å	-	-
101		ARG	78.31	-	Favored (57.14%) General / -78.3,-17.1	31% (*mmm180*) chi angles: 297.9,299.6,298.3,169.4	0.131Å	-	-
102		GLN	251.23	-	Favored (7.4%) General / -78.3,101.9	98.8% (*mt-30*) chi angles: 291.3,175.3,324.4	0.079Å	-	-
103		LEU	261.05	-	Favored (2.65%) General /	21.6% (*mt*) chi angles: 314.4,180	0.065Å	-	-

-65.1,173.0

104	LEU	145.2	-	Favored (23.83%) General / -102.1,111.5	2.5% (*tt*) chi angles: 205.9,177.3	0.065Å	-	-
105	ALA	47.21	-	Favored (82.24%) General / -65.2,-35.8	-	0.05Å	-	-
106	GLU	120.37	-	Favored (63.47%) General / -53.1,-50.9	70.6% (*mt-10*) chi angles: 298.2,162.9,331	0.033Å	-	-
107	GLN	186.21	-	Favored (2.88%) General / -90.5,55.0	96.1% (*mt-30*) chi angles: 291.7,182.7,331.7	0.081Å	-	-
108	GLU	87.13	-	Favored (57.3%) Pre-proline / -57.9,-37.6	5.2% (*tm-20*) chi angles: 185.5,299.9,315.3	0.191Å	-	-
109	PRO	129.3	-	Favored (68.55%) Trans-proline / -63.9,-23.6	26.9% (*Cg_exo*) chi angles: 324.8	0.068Å	-	-
110	GLU	76.26	-	Favored (15.88%) General / -91.7,-31.3	59.8% (*mm-40*) chi angles: 297.7,284.5,318.6	0.08Å	-	-
111	VAL	51.45	-	Favored (92.49%) Isoleucine or valine / -59.2,-45.8	38.8% (*t*) chi angles: 166	0.147Å	-	-
112	GLN	103.7	-	Favored (96.26%) General / -60.7,-44.7	4.2% (*pt20*) chi angles: 68.9,183.7,237.1	0.154Å	-	-
113	GLU	124.08	-	Favored (63.61%) General / -74.2,-34.1	76.4% (*mt-10*) chi angles: 287.9,188.1,328.7	0.1Å	-	-
114	VAL	114.59	-	Favored (10.17%) Isoleucine or valine / -83.2,-18.9	2.9% (*p*) chi angles: 80.6	0.215Å	-	-
				Favored (70.97%)	8.3% (*t*)			

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
115		SER	84	-	General / -62.8,-29.8	chi angles: 194.7	0.136Å	-	-
116		GLN	108.9	-	Favored (75.85%) General / -60.9,-35.1	12.1% (*tp-100*) chi angles: 185,62.7,240	0.068Å	-	-
			Avg: 109.32	Clashscore: 0	Outliers: 2 of 113	Poor rotamers: 5 of 106	Outliers: 1 of 113	Outliers: 0 of 115	Outliers: 7 of 115
117		LEU	232.16	-	Allowed (0.38%) General / -167.5,92.1	0.9% chi angles: 205.6,290.9	0.04Å	-	-
118		PHE	331.89	-	Favored (56.31%) General / -62.9,134.5	43.6% (*m-85*) chi angles: 309.6,274.8	0.07Å	-	-
119		ARG	355.68	-	Allowed (0.59%) General / -152.2,-155.1	13.9% (*mtp180*) chi angles: 256.8,188.2,67.5,175.1	0.117Å	-	-
120		SER	77.46	-	Favored (9.85%) General / -64.2,-7.7	54.2% (*p*) chi angles: 55.1	0.028Å	-	-
121		VAL	45.65	-	Favored (2.87%) Isoleucine or valine / -46.6,-36.0	92.4% (*t*) chi angles: 178	0.093Å	-	-
122		LEU	153.19	-	Favored (56.59%) General / -76.7,-30.2	2.9% (*mm?*) chi angles: 293.5,312.3	0.125Å	-	-
123		GLN	48.27	-	Favored (58.83%) General / -73.8,-43.5	20.6% (*tp60*) chi angles: 182.6,60.8,92.1	0.037Å	-	-
124		GLU	62.5	-	Favored (61.59%) General / -73.5,-27.9	32.5% (*mt-10*) chi angles: 301,169.1,80.8	0.078Å	-	-
125		VAL	99.92	-	Favored (33.54%) Isoleucine or valine / -73.1,-31.0	1.7% (*p*) chi angles: 83.8	0.209Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
126		LEU	126.04	-	Favored (39.36%) General / -79.9,-33.8	64.2% (*mt*) chi angles: 299.8,168.9	0.11Å	-	-
127		GLU	82.41	-	Favored (59.08%) General / -80.3,-13.6	62.6% (*mm-40*) chi angles: 296.6,304.2,298	0.135Å	-	-
128		ARG	111.84	-	Favored (68.21%) General / -61.5,-26.9	12.6% (*ttp180*) chi angles: 210.6,173.4,91.2,217.8	0.134Å	-	-
129		MET	52.7	-	Favored (58.03%) General / -78.5,-8.0	61.6% (*mtm*) chi angles: 296.7,171,281	0.111Å	-	-
130		LYS	79.49	-	Favored (8.16%) General / -119.1,-20.2	41.2% (*mtmt*) chi angles: 301.7,169.4,292.6,171.3	0.051Å	-	-
131		GLN	116.43	-	Favored (2.16%) General / -113.2,-172.9	0% chi angles: 69.6,126.9,202	0.089Å	-	OUTLIER(S) worst is CB-CG-CD: 5.95 σ
132		GLU	80.52	-	Favored (40.09%) General / -60.8,148.1	49.3% (*tt0*) chi angles: 184.8,186,320.2	0.075Å	-	-
133		GLU	132.72	-	Allowed (1.43%) General / -76.9,58.2	6.9% (*mt-10*) chi angles: 289.7,217.3,78.6	0.094Å	-	-
134		GLU	110.54	-	Favored (35.33%) General / -80.9,-30.9	10.7% (*tp10*) chi angles: 188.6,46.5,69.2	0.086Å	-	-
135		ALA	56.37	-	Favored (72.62%) General / -61.6,-32.5	-	0.133Å	-	-
136		HIS	49.22	-	Favored (60.34%) General / -75.7,-14.8	11.6% (*t-80*) chi angles: 211.3,289.2	0.179Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg:	Clashscore:	Outliers: 2 of	Poor rotamers: 5 of	Outliers:	Outliers:	Outliers: 7

		109.32	0	113	106	1 of 113	0 of 115	of 115
137	LYS	75.5	-	Favored (15.05%) General / -86.5,-40.7	46.9% (*mtmt*) chi angles: 296.9,171.3,289.4,173.6	0.08Å	-	-
138	LEU	46.43	-	Favored (72.27%) General / -61.6,-50.5	81.4% (*mt*) chi angles: 301.7,180.7	0.143Å	-	-
139	THR	44.46	-	Favored (73.12%) General / -57.9,-37.0	11.5% (*m*) chi angles: 312.7	0.134Å	-	-
140	ARG	141.27	-	Favored (22.83%) General / -82.3,-39.4	36.5% (*mmt180*) chi angles: 293.2,295.7,178.8,172.7	0.169Å	-	-
141	GLN	79.06	-	Favored (10.88%) General / -109.7,-24.5	48.3% (*mm-40*) chi angles: 287.8,287.2,349.6	0.114Å	-	-
142	TRP	119.1	-	Favored (13.47%) General / -103.5,-24.3	82.5% (*m95*) chi angles: 295.5,83.7	0.08Å	-	OUTLIER(S) worst is CE3-CD2-CG: 4.51 σ
143	SER	95.53	-	Favored (5.73%) General / -100.9,-44.5	70.6% (*m*) chi angles: 297.6	0.122Å	-	-
144	LEU	141.71	-	Favored (49.23%) General / -75.3,-43.7	50.3% (*tp*) chi angles: 183.9,64.1	0.065Å	-	-
145	ARG	157.59	-	Favored (4.86%) Pre-proline / -74.9,-43.4	57.5% (*ttp180*) chi angles: 181.9,177.8,64.3,177.9	0.188Å	-	-
146	PRO	153.21	-	Favored (18.44%) Trans-proline / -68.0,128.9	85.8% (*Cg_exo*) chi angles: 331.1	0.057Å	-	-
147	ARG	112.31	-	Favored (71.01%) General / -59.5,-33.1	38.6% (*mmt180*) chi angles: 291.1,298.2,180.2,183.8	0.156Å	-	-
148	GLY	33.79	-	Favored (76.94%)	-	-	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					Glycine / -77.4,-19.1				
149		SER	95.93	-	Favored (14.55%) General / -82.7,-45.4	50.3% (*m*) chi angles: 289.7	0.106Å	-	-
150		LEU	139.49	-	Favored (77.04%) General / -69.5,-40.2	58.8% (*tp*) chi angles: 180.2,64.7	0.047Å	-	-
151		ALA	55.07	-	Favored (42.86%) General / -68.2,130.4	-	0.041Å	-	-
152		THR	129.4	-	Favored (18.02%) General / -49.8,136.4	86.1% (*m*) chi angles: 302.7	0.049Å	-	-
153		PHE	120.33	-	Favored (3.16%) General / -56.4,116.6	55% (*t80*) chi angles: 178.4,92.8	0.068Å	-	-
154		LYS	189.06	-	Allowed (1.65%) General / -144.6,81.1	58.9% (*tttm*) chi angles: 180.8,186.9,178.4,295.5	0.094Å	-	-
155		THR	145.73	-	Favored (10.54%) General / -135.3,174.5	4.8% (*t*) chi angles: 198.3	0.13Å	-	-
156		ARG	163.42	-	Favored (58.32%) General / -65.8,139.8	13.3% (*ptm180*) chi angles: 57.1,174.8,289.8,140.3	0.032Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 109.32	Clashscore: 0	Outliers: 2 of 113	Poor rotamers: 5 of 106	Outliers: 1 of 113	Outliers: 0 of 115	Outliers: 7 of 115
157		ALA	54.82	-	Favored (24.66%) General / -93.3,-16.5	-	0.066Å	-	-
158		ARG	232.54	-	Favored (35.09%) General / -81.3,140.0	42.5% (*ttm105*) chi angles: 188.6,176.1,294.7,104.4	0.029Å	-	OUTLIER(S) worst is C-N-CA: 4.09 σ
					Allowed (1%)				

159	ILE 194.89	-	Isoleucine or valine / -45.1,-56.1	38.7% (*mm*) chi angles: 301.2,306.6	0.118Å	-	-
160	SER 131.43	-	OUTLIER (0.1%) Pre-proline / 86.5,161.7	13.3% (*t*) chi angles: 190.6	0.052Å	-	-
161	PRO 73.63	-	Favored (71%) Trans-proline / -57.4,148.6	1.1% (*Cg_exo*) chi angles: 321.1	0.069Å	-	-
162	PHE 92.3	-	Favored (64.75%) General / -57.7,-29.5	56.2% (*m-85*) chi angles: 308,279.2	0.129Å	-	-
163	ALA 29.58	-	Favored (58.33%) General / -75.9,-9.1	-	0.067Å	-	-
164	SER 89.35	-	Favored (4.58%) General / -96.8,88.3	67.6% (*p*) chi angles: 71	0.08Å	-	-
165	ASP 183.88	-	Favored (7.47%) General / -81.2,97.1	56.3% (*t0*) chi angles: 187.1,9.1	0.15Å	-	-
166	ILE 142.5	-	Favored (5.08%) Isoleucine or valine / -150.8,158.4	8.7% (*tp*) chi angles: 198.9,70.8	0.128Å	-	-
167	ARG 107.6	-	Favored (20.52%) General / -94.8,-19.2	84.3% (*mmt-85*) chi angles: 299.2,293.1,172.3,275	0.136Å	-	-
168	THR 111	-	Favored (7.7%) General / -151.6,122.8	22.2% (*p*) chi angles: 49.2	0.113Å	-	-
169	ILE 103.88	-	Favored (42.04%) Isoleucine or valine / -118.8,140.6	75.8% (*mt*) chi angles: 301.4,167.5	0.077Å	-	-
170	SER 80.43	-	Favored (28.63%) General / -73.8,125.7	13.3% (*t*) chi angles: 190.6	0.05Å	-	-
171	GLU 81.97	-	Favored (30.42%) General /	4.4% (*tp10*) chi angles: 197.3,83.5,71.1	0.09Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
					-82.1,-32.2				
172		ASP	95.87	-	Favored (28.13%) General / -83.5,146.9	6% (*p-10*) chi angles: 50,294.5	0.027Å	-	-
173		VAL	102.72	-	Favored (8.43%) Isoleucine or valine / -88.5,-17.4	9.2% (*p*) chi angles: 72.9	0.131Å	-	-
174		GLU	60.06	-	Favored (68.96%) General / -60.5,-29.3	44.6% (*mt-10*) chi angles: 290.9,192.1,35.9	0.086Å	-	-
175		ARG	132.11	-	Allowed (0.48%) General / -60.5,-2.3	0% chi angles: 81.7,116.7,206.4,202.8	0.072Å	-	OUTLIER(S) worst is CD-NE-CZ: 4.661 σ
176		ASP	51.12	-	Favored (33.48%) General / -105.2,6.9	59.9% (*m-20*) chi angles: 301.4,341.7	0.109Å	-	-
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 109.32	Clashscore: 0	Outliers: 2 of 113	Poor rotamers: 5 of 106	Outliers: 1 of 113	Outliers: 0 of 115	Outliers: 7 of 115
177		THR	136.17	-	Allowed (0.21%) Pre-proline / -99.3,-20.8	2.1% (*t*) chi angles: 202.3	0.304Å	-	-
178		PRO	132.66	-	Favored (11.38%) Trans-proline / -75.2,-25.7	87.1% (*Cg_exo*) chi angles: 331.6	0.126Å	-	-
179		PRO	146.25	-	Favored (17.94%) Trans-proline / -56.1,157.2	0.1% chi angles: 316.4	0.083Å	-	-
180		PRO	168.87	-	Favored (49.77%) Trans-proline / -72.9,150.6	55.5% (*Cg_endo*) chi angles: 34.8	0.041Å	-	-
181		LEU	201.83	-	OUTLIER (0.04%) General / 87.0,133.4	60.8% (*mt*) chi angles: 306.4,180.1	0.121Å	-	-
					Favored (3.27%)	32.3% (*mmm180*)			

182	ARG	99.52	-	General / -108.6,90.4	chi angles: 298.3,297,295.9,167.4	0.029Å	-	-
183	SER	36.49	-	Favored (74.87%) General / -59.4,-35.9	24.4% (*m*) chi angles: 304.7	0.065Å	-	-
184	TRP	72.73	-	Favored (37.88%) General / -70.2,-6.9	23.2% (*m-90*) chi angles: 297.9,276.7	0.061Å	-	-
185	SER	88.42	-	Favored (21.95%) General / -91.8,-20.0	63.7% (*m*) chi angles: 292.3	0.083Å	-	-
186	MET	152.75	-	Favored (87.81%) Pre-proline / -59.7,130.0	15.7% (*tpt*) chi angles: 186.2,58.2,189.7	0.061Å	-	-
187	PRO	66.37	-	Favored (5.49%) Trans-proline / -43.2,-35.8	0.2% chi angles: 319.1	0.147Å	-	-
188	GLU	76.78	-	Favored (60.98%) General / -72.8,-24.7	17% (*mp0*) chi angles: 303,74.1,334.7	0.107Å	-	OUTLIER(S) worst is CB-CG-CD: 6.485 σ
189	PHE	61.1	-	Favored (8.82%) General / -90.4,16.4	79.2% (*m-85*) chi angles: 297.9,289	0.077Å	-	-
190	ARG	135.36	-	Favored (41.06%) General / -100.2,0.7	97.8% (*mtt180*) chi angles: 300.1,174.5,187.3,183.7	0.096Å	-	-
191	ALA	11.72	-	-	-	0.05Å	-	-

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