Viewing RP1_sm_35-107-FFX1H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	1.72		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	1.54%	Goal: <1%
	Ramachandran outliers	3	4.23%	Goal: <0.05%
	Ramachandran favored	64	90.14%	Goal: >98%
	MolProbity score^	1.61		92nd percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	2	2.99%	Goal: 0
	Bad backbone bonds:	0 / 592	0.00%	Goal: 0%
	Bad backbone angles:	6 / 797	0.75%	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: 56.85	Clashscore: 1.72	Outliers: 3 of 71	Poor rotamers: 1 of 65	Outliers: 2 of 67	Outliers: 0 of 73	Outliers: 5 of 73
A 35		ALA	50	-	-	-	0.052Å	-	-
A 36		LYS	50	-	Favored (38.08%) General / -77.9,133.4	96.1% (*mttt*) chi angles: 300.5,183.3,176.9,183.8	0.035Å	-	-
A 37		ARG	99.99	-	Allowed (1.4%) General / -105.2,78.6	0% chi angles: 58.6,225.3,145.5,295.5	0.129Å	-	-
A 38		ILE	50	-	Favored (6.21%) Isoleucine or valine / -101.4,150.0	59.8% (*mt*) chi angles: 288.4,176.6	0.141Å	-	-
A 39		SER	50	-	Favored (16.16%)	8.4% (*t*)	0.022Å	-	-

				General / -101.2,158.3	chi angles: 194.3			
A 40	PHE	50	-	Favored (25.65%) General / -144.4,135.8	72% (*m-85*) chi angles: 286.9,278	0.067Å	-	-
A 41	TYR	50	-	Favored (3.57%) General / -121.8,-177.5	82.6% (*m-85*) chi angles: 298.9,82.5	0.053Å	-	-
A 42	LYS	50	-	Favored (48.41%) General / -136.4,149.7	28.5% (*mtmt*) chi angles: 303.5,160.9,305.2,194.2	0.155Å	-	-
A 43	SER	50	-	Favored (48.64%) General / -63.5,131.6	8.1% (*t*) chi angles: 195	0.04Å	-	-
A 44	GLY	50	-	Favored (69.96%) Glycine / 83.8,15.6	-	-	-	-
A 45	ASP	50	-	Favored (2.49%) Pre-proline / -155.1,96.5	43.9% (*t0*) chi angles: 194.1,348.5	0.046Å	-	-
A 46	PRO	50	-	Favored (3.54%) Trans-proline / -92.7,-3.5	10.2% (*Cg_endo*) chi angles: 40.2	0.014Å	-	-
A 47	GLN	50	-	Favored (19.23%) General / -88.1,-31.5	24.4% (*mm100*) chi angles: 307.4,309.4,120.6	0.094Å	-	-
A 48	PHE	50	-	Favored (7.28%) General / -48.6,123.8	88% (*t80*) chi angles: 179.8,80.8	0.106Å	-	-
A 49	GLY	50	-	Favored (73.7%) Glycine / -70.1,-17.2	-	-	-	-
A 50	GLY	50	-	Favored (12.35%) Glycine / 105.6,144.3	-	-	-	-
A 51	VAL	50	-	Favored (69.16%) Isoleucine or valine / -112.0,127.4	2.9% (*t*) chi angles: 155	0.081Å	-	-
A 52	ARG	50	-	Favored (34.56%) General / -99.3,139.7	86.5% (*mtt-85*) chi angles: 280.5,181.9,175,278.8	0.045Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 53		VAL	50	-	Favored (20.73%) Isoleucine or valine / -141.1,154.0	4.6% (*p*) chi angles: 77.1	0.109Å	-	-
A 54		VAL	99.99	-	Favored (15.06%) Isoleucine or valine / -95.7,103.8	85% (*t*) chi angles: 177.4	0.065Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.85	Clashscore: 1.72	Outliers: 3 of 71	Poor rotamers: 1 of 65	Outliers: 2 of 67	Outliers: 0 of 73	Outliers: 5 of 73
A 55		VAL	50	-	Favored (18.41%) Isoleucine or valine / -84.5,110.0	83.3% (*t*) chi angles: 174.8	0.057Å	-	-
A 56		ASN	50	-	Favored (46.48%) Pre-proline / -147.2,155.8	21.7% (*t30*) chi angles: 204.8,55	0.126Å	-	-
A 57		PRO	50	-	Favored (74.57%) Trans-proline / -62.7,-23.5	40.1% (*Cg_exo*) chi angles: 325.9	0.06Å	-	-
A 58		ARG	50	-	Favored (40.14%) General / -81.9,-19.8	45.9% (*tpt85*) chi angles: 188.2,59.8,188.9,83.5	0.146Å	-	-
A 59		SER	50	-	Favored (14.16%) General / -95.9,-29.5	16.5% (*p*) chi angles: 49.3	0.171Å	-	-
A 60		PHE	50	-	Favored (28.74%) General / -138.0,130.1	76.1% (*m-85*) chi angles: 302.8,286.2	0.093Å	-	-
A 61		LYS	50	-	Favored (81.63%) General / -66.8,-36.1	17.9% (*pttp*) chi angles: 62.2,169,192.3,73.1	0.122Å	-	-
A 62		SER	50	-	Favored (3.58%) General / -167.7,-177.7	37.2% (*p*) chi angles: 53.4	0.092Å	-	-
A 63		PHE	50	-	Favored (97.89%) General / -60.8,-42.6	30.3% (*t80*) chi angles: 191.8,60.6	0.072Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 64		ASP	50	-	Favored (69.44%) General / -56.6,-36.5	6.2% (*p-10*) chi angles: 49.6,298.7	0.121Å	-	-
A 65		ALA	50	-	Favored (86.2%) General / -62.6,-37.5	-	0.1Å	-	-
A 66		LEU	50	-	Favored (67.08%) General / -73.0,-36.8	59.2% (*tp*) chi angles: 177.5,58.5	0.08Å	-	-
A 67		LEU	50	-	Favored (92.59%) General / -61.0,-40.2	14.8% (*mt*) chi angles: 309.9,192.6	0.151Å	-	-
A 68		ASP	50	0.522Å HA with A 71 SER HB2	Favored (31.57%) General / -84.7,-20.2	34.4% (*m-20*) chi angles: 288.4,294.9	0.399Å	-	-
A 69		ASN	50	-	Favored (68.72%) General / -58.7,-31.9	11.6% (*t30*) chi angles: 183.9,84.1	0.075Å	-	-
A 70		LEU	99.99	-	Favored (27.77%) General / -108.3,10.2	68.1% (*mt*) chi angles: 305.3,176.6	0.064Å	-	-
A 71		SER	99.99	0.522Å HB2 with A 68 ASP HA	Favored (3.18%) General / -76.5,77.4	42.6% (*t*) chi angles: 181.1	0.118Å	-	-
A 72		ARG	99.99	-	Favored (5.93%) General / -62.4,165.5	15.6% (*tpt180*) chi angles: 202.7,61.5,195.7,169.7	0.064Å	-	-
A 73		LYS	99.99	-	Favored (2.66%) General / -136.2,40.8	35.3% (*mmtm*) chi angles: 301.2,289.9,162.8,290.5	0.036Å	-	-
A 74		VAL	99.99	0.723Å HG13 with A 75 PRO HD2	OUTLIER (0%) Pre-proline / -155.4,-91.2	2.7% (*p*) chi angles: 49.9	0.51Å	-	OUTLIER(S) worst is C-CA-CB: 7.069 σ
#	Alt	Res	**High B**	**Clash > 0.4Å**	**Ramachandran**	**Rotamer**	**Cβ deviation**	**Bond lengths**	**Bond angles**
			Avg: 56.85	Clashscore: 1.72	Outliers: 3 of 71	Poor rotamers: 1 of 65	Outliers: 2 of 67	Outliers: 0 of 73	Outliers: 5 of 73
A 75		PRO	50	0.723Å HD2 with A 74 VAL HG13	Favored (3.93%) Trans-proline / -71.8,114.3 OUTLIER	28.1% (*Cg_endo*) chi angles: 20.7	0.052Å	-	-

A 76	LEU	50	-	(0.04%) Pre-proline / 73.9,97.1	30.1% (*mt*) chi angles: 311.7,181	0.108Å	-	-
A 77	PRO	50	-	Allowed (1.03%) Trans-proline / -84.4,-28.7	86.3% (*Cg_endo*) chi angles: 31.3	0.086Å	-	-
A 78	PHE	50	-	Favored (14.48%) General / -91.7,-34.8	11.6% (*m-85*) chi angles: 318.9,118.8	0.081Å	-	-
A 79	GLY	50	-	Favored (27.5%) Glycine / 143.0,-160.1	-	-	-	-
A 80	VAL	50	-	Favored (61.57%) Isoleucine or valine / -106.0,125.8	62.1% (*t*) chi angles: 180.1	0.04Å	-	-
A 81	ARG	50	-	Favored (2.96%) General / -137.5,10.8	33.3% (*mmt180*) chi angles: 294.7,297.9,172.3,236.3	0.139Å	-	-
A 82	ASN	50	-	Favored (29.84%) General / -154.9,152.5	27.2% (*t30*) chi angles: 174.9,34.4	0.118Å	-	-
A 83	ILE	50	-	Favored (48.2%) Isoleucine or valine / -136.1,137.7	46.4% (*mt*) chi angles: 284.4,172.1	0.064Å	-	-
A 84	SER	50	-	Favored (25.6%) General / -114.0,155.6	30.6% (*t*) chi angles: 184.8	0.034Å	-	-
A 85	THR	50	-	Favored (94.25%) Pre-proline / -64.8,150.7	8.6% (*p*) chi angles: 43.7	0.05Å	-	-
A 86	PRO	50	-	Favored (5.85%) Trans-proline / -80.2,5.7	6.2% (*Cg_endo*) chi angles: 41	0.012Å	-	-
A 87	ARG	99.99	-	Favored (7.47%) General / -126.8,15.6	37.4% (*mmt-85*) chi angles: 307.8,299.2,173.9,241.1	0.109Å	-	-
A 88	GLY	50	-	Favored (96.36%) Glycine / 65.3,42.2	-	-	-	-
A 89	ARG	99.99	-	Favored (8.27%) General / -125.4,16.2	94.5% (*mtt180*) chi angles: 296.9,188.4,178.6,192.3	0.138Å	-	-

OUTLIER(S)

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
A 90		HIS	50	-	OUTLIER (0.03%) General / 170.6,142.4	46.4% (*m-70*) chi angles: 280.5,304.5	0.177Å	-	worst is CA-CB-CG: 4.994 σ
A 91		SER	50	-	Favored (15.74%) General / -78.6,171.0	3.7% (*m*) chi angles: 276.5	0.029Å	-	-
A 92		ILE	50	-	Favored (48.55%) Isoleucine or valine / -124.6,140.2	50.8% (*mm*) chi angles: 302.3,299	0.117Å	-	-
A 93		THR	50	-	Favored (9.69%) General / -120.6,-6.9	6.2% (*t*) chi angles: 195.5	0.176Å	-	-
A 94		ARG	50	-	Favored (29.75%) General / -149.9,166.4	14.6% (*ptt-85*) chi angles: 87.1,196.2,192.9,257.2	0.129Å	-	-

#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.85	Clashscore: 1.72	Outliers: 3 of 71	Poor rotamers: 1 of 65	Outliers: 2 of 67	Outliers: 0 of 73	Outliers: 5 of 73
A 95		LEU	50	-	Favored (78.78%) General / -62.7,-35.1	90.5% (*mt*) chi angles: 298.7,174.1	0.112Å	-	-
A 96		GLU	50	-	Favored (79.78%) General / -68.6,-37.4	26% (*mt-10*) chi angles: 311,189.6,285.1	0.082Å	-	-
A 97		GLU	50	-	Favored (70.66%) General / -65.7,-30.1	40.5% (*mt-10*) chi angles: 289.4,157.8,29	0.045Å	-	-
A 98		LEU	50	-	Allowed (0.77%) General / -65.8,102.6	15.1% (*mt*) chi angles: 308.1,161.8	0.061Å	-	-
A 99		GLU	50	-	Favored (25.5%) General / -91.2,144.6	5.1% (*tp10*) chi angles: 201.9,43.3,77.4	0.124Å	-	OUTLIER(S) worst is C-N-CA: 4.412 σ
A 100		ASP	50	-	Favored (5.85%) General / -53.7,151.7	12.4% (*t0*) chi angles: 210.3,355.6	0.04Å	-	-
A 101		GLY	50	-	Favored (2.57%) Glycine / 76.1,-49.5	-	-	-	-

A 102	GLU	50	-	Allowed (0.59%) General / -52.2,161.7	5.1% (*tp10*) chi angles: 181.6,54.8,118.3	0.068Å	-	OUTLIER(S) worst is C-N-CA: 4.406 σ
A 103	SER	50	-	Favored (29.33%) General / -105.0,146.2	74.2% (*m*) chi angles: 295.1	0.134Å	-	-
A 104	TYR	50	-	Favored (33.18%) General / -131.6,161.2	58.7% (*m-85*) chi angles: 304.2,262.3	0.036Å	-	-
A 105	LEU	50	-	Favored (55.53%) General / -110.5,130.6	3% (*tt*) chi angles: 179.2,132.5	0.058Å	-	-
A 106	CYS	50	-	Favored (30.32%) General / -88.6,139.6	96.9% (*m*) chi angles: 294.7	0.047Å	-	OUTLIER(S) worst is C-N-CA: 4.855 σ
A 107	SER	99.99	-	-	5.6% (*t*) chi angles: 161.1	0.095Å	-	-

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