



# Viewing RP1\_sm\_35-107H-multi.table

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All-Atom Contacts	Clashscore, all atoms:	33.56		12 <sup>th</sup> percentile* (N=1784, all resolutions)
	Clashscore is the number of serious steric overlaps (> 0.4 Å) per 1000 atoms.			
Protein Geometry	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	3	4.23%	Goal: <0.05%
	Ramachandran favored	67	94.37%	Goal: >98%
	MolProbity score^	2.39		53 <sup>rd</sup> percentile* (N=27675, 0Å - 99Å)
	Cβ deviations >0.25Å	1	1.49%	Goal: 0
	Bad backbone bonds:	2 / 592	0.34%	Goal: 0%
	Bad backbone angles:	5 / 797	0.63%	Goal: <0.1%

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

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

<sup>^</sup> 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: Clashscore:		Outliers: 3 of	Poor rotamers: 0 of	Outliers:	Outliers: 2	Outliers: 2
		56.85		71	65	1 of 67	of 73	of 73
A 35	ALA	50	-	-	-	0.098Å	-	-
A 36	LYS	50	-	Favored (31.41%) General / -75.4,126.6	35.6% ( <i>ttpt</i> ) chi angles: 175.8,169.4,60.3,188.6	0.176Å	-	-
A 37	ARG	99.99	0.462Å HA with A 53 VAL O	Favored (51.89%) General / -104.7,131.7	95.6% ( <i>mtt-85</i> ) chi angles: 291.1,181.6,178.7,276.2	0.083Å	-	-
A 38	ILE	50	0.652Å CD1 with A 98 LEU HB3	Favored (26.07%) Isoleucine or valine / -139.8,157.0	76.2% ( <i>mt</i> ) chi angles: 292.3,176.3	0.168Å	-	-
A 39	SER	50	-	Favored (43.97%) General / -107.4,138.2	24.5% ( <i>t</i> ) chi angles: 186.1	0.065Å	-	-
A			0.792Å HE2 with A	Favored	77.8% ( <i>m-85</i> )			

40	PHE	50	53 VAL HG11	(56.08%) General / -118.9,132.1 Favored	chi angles: 290.5,283.8	0.022Å	-	-
A 41	TYR	50	-	(9.67%) General / -110.6,168.2 Favored	92.3% ( <i>m-85</i> ) chi angles: 291.5,89.7	0.089Å	-	-
A 42	LYS	50	-	(48.69%) General / -113.3,139.6 Favored	53.8% ( <i>mtmt</i> ) chi angles: 297.8,179,293.2,178.3	0.022Å	-	-
A 43	SER	50	-	(24.62%) General / -53.6,127.2 Favored	14.8% ( <i>t</i> ) chi angles: 190.1	0.045Å	-	-
A 44	GLY	50	-	(69.92%) Glycine / 64.8,24.5 Favored	-	-	-	-
A 45	ASP	50	-	(17.05%) Pre-proline / -107.9,96.2 Favored	50% ( <i>t0</i> ) chi angles: 189,335.8	0.062Å	-	-
A 46	PRO	50	-	(39.69%) Trans-proline / -69.2,-18.1 Favored	92.4% ( <i>Cg_endo</i> ) chi angles: 32.1	0.053Å	-	-
A 47	GLN	50	-	(9.39%) General / -97.1,-39.3 Favored	19.1% ( <i>mm100</i> ) chi angles: 296.4,298.9,97.4	0.016Å	-	-
A 48	PHE	50	0.464Å HZ with A 51 VAL HG23	(27.7%) General / -65.0,126.3 Favored	75.1% ( <i>t80</i> ) chi angles: 185,72.7	0.047Å	-	-
A 49	GLY	50	-	(62.66%) Glycine / -92.8,15.4 Favored	-	-	-	-
A 50	GLY	50	-	(6.73%) Glycine / 74.4,159.6 Favored	-	-	-	-
A 51	VAL	50	0.464Å HG23 with A 48 PHE HZ	(44.22%) Isoleucine or valine / -120.6,140.6 Favored	92.4% ( <i>t</i> ) chi angles: 178	0.034Å	-	-
A 52	ARG	50	-	(34.74%) General / -90.2,133.7 Favored	30.6% ( <i>ptt-85</i> ) chi angles: 60.7,175.7,179.5,281.9	0.025Å	-	-

A 53	VAL	50	0.792Å HG11 with A 40 PHE HE2	Favored (20.46%) Isoleucine or valine / -118.3,152.6	13.4% ( <i>p</i> ) chi angles: 62.8	0.113Å	-	-
A 54	VAL	99.99	-	Favored (30.76%) Isoleucine or valine / -103.6,110.7	89.8% ( <i>t</i> ) chi angles: 177.1	0.171Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 56.85	Clashscore: 33.56	Outliers: 3 of 71	Poor rotamers: 0 of 65	Outliers: 1 of 67	Outliers: 2 of 73	Outliers: 2 of 73
A 55	VAL	50	0.443Å HG11 with A 95 LEU HD22	Favored (53.94%) Isoleucine or valine / -106.3,132.2	58.2% ( <i>t</i> ) chi angles: 181.8	0.028Å	-	-
A 56	ASN	50	0.544Å OD1 with A 57 PRO HD2	Favored (7.52%) Pre-proline / -167.1,153.0	48.7% ( <i>t30</i> ) chi angles: 186.4,61.1	0.058Å	-	-
A 57	PRO	50	0.544Å HD2 with A 56 ASN OD1	Favored (33.53%) Trans-proline / -49.9,-33.4	46.6% ( <i>Cg_exo</i> ) chi angles: 326.4	0.062Å	-	-
A 58	ARG	50	0.517Å H with A 56 ASN ND2	Favored (95.61%) General / -61.1,-40.9	54.8% ( <i>mmm-85</i> ) chi angles: 296,293.3,291,277.9	0.06Å	-	-
A 59	SER	50	-	Favored (17.36%) General / -92.6,-27.4	63.3% ( <i>p</i> ) chi angles: 56.6	0.076Å	-	-
A 60	PHE	50	-	Favored (7.73%) General / -132.9,106.5	70.1% ( <i>m-85</i> ) chi angles: 305,283.7	0.02Å	-	-
A 61	LYS	50	-	Favored (66.18%) General / -66.5,-22.2	55.9% ( <i>mtmt</i> ) chi angles: 293.6,181.5,295.7,177.9	0.053Å	-	-
A 62	SER	50	-	Favored (40.33%) General / -149.6,162.4	84.2% ( <i>p</i> ) chi angles: 68.6	0.016Å	-	-
A 63	PHE	50	-	Favored (89.11%) General / -64.0,-37.9	67.7% ( <i>t80</i> ) chi angles: 186.8,71.9	0.031Å	-	-

A 64	ASP	50	-	Favored (64.04%) General / -69.8,-26.1	76.4% ( <i>m-20</i> ) chi angles: 294.5,321.6	0.091Å	-	-
A 65	ALA	50	-	Favored (82.94%) General / -67.5,-37.6	-	0.027Å	-	-
A 66	LEU	50	0.478Å HD22 with A 95 LEU CD2	Favored (78.65%) General / -65.6,-46.6	54.3% ( <i>tp</i> ) chi angles: 176.1,67.2	0.025Å	-	-
A 67	LEU	50	0.431Å HD22 with A 80 VAL HG12	Favored (77.28%) General / -62.6,-34.5	62.2% ( <i>mt</i> ) chi angles: 299.9,185.1	0.071Å	-	-
A 68	ASP	50	-	Favored (82.18%) General / -68.3,-39.1	41.3% ( <i>t0</i> ) chi angles: 190.6,328.8	0.023Å	-	-
A 69	ASN	50	-	Favored (74.52%) General / -70.2,-36.2	21.6% ( <i>t-20</i> ) chi angles: 188.5,294.5	0.035Å	-	-
A 70	LEU	99.99	0.729Å HD23 with A 80 VAL HG21	Favored (53.19%) General / -94.3,5.0	6.2% ( <i>tt</i> ) chi angles: 194.2,166.1	0.11Å	-	-
A 71	SER	99.99	-	Favored (55.48%) General / -66.3,136.2	27.9% ( <i>t</i> ) chi angles: 185.4	0.117Å	-	-
A 72	ARG	99.99	0.886Å HB3 with A 76 LEU HD12	Favored (10.89%) General / -127.1,172.0	26.4% ( <i>tpt180</i> ) chi angles: 179.5,68.8,184.6,184.4	0.133Å	-	-
A 73	LYS	99.99	0.779Å HG3 with A 74 VAL H	Allowed (0.75%) General / -115.9,-71.2	20.7% ( <i>pttp</i> ) chi angles: 57.1,175.1,187.6,68.7	0.172Å	-	-
A 74	VAL	99.99	0.779Å H with A 73 LYS HG3	OUTLIER (0%) Pre-proline / -58.5,-127.9	8% ( <i>p</i> ) chi angles: 59.5	0.347Å	OUTLIER(S) worst is N-- CA: 4.038 σ	OUTLIER(S) worst is CA- C-N: 12.602 σ
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 56.85	Clashscore: 33.56	Outliers: 3 of 71	Poor rotamers: 0 of 65	Outliers: 1 of 67	Outliers: 2 of 73	Outliers: 2 of 73
A	PRO	50	0.701Å HD2 with A	OUTLIER (0.02%)	10.1% ( <i>Cg_endo</i> )	0.142Å	-	OUTLIER(S) worst is CA-

				74 VAL HG13	Trans-proline / -32.2,97.7	chi angles: 13.3	N-CD: 4.152 $\sigma$	
A 75								
A 76	LEU	50	0.886Å HD12 with A 72 ARG HB3	OUTLIER (0%) Pre-proline / 103.3,71.5	24.6% ( <i>mt</i> ) chi angles: 311.3,170.9	0.206Å	-	-
A 77	PRO	50	0.436Å HA with A 73 LYS O	Favored (87.49%) Trans-proline / -57.2,-30.5	57.1% ( <i>Cg_endo</i> ) chi angles: 26.2	0.147Å	-	-
A 78	PHE	50	-	Favored (10.31%) General / -119.8,24.9	1.6% ( <i>m-85</i> ) chi angles: 291.3,37.6	0.024Å	-	-
A 79	GLY	50	0.636Å HA2 with A 72 ARG O	Favored (43.04%) Glycine / 66.9,-164.6	-	-	-	-
A 80	VAL	50	0.729Å HG21 with A 70 LEU HD23	Favored (28.45%) Isoleucine or valine / -91.5,114.3	62.4% ( <i>t</i> ) chi angles: 180	0.078Å	-	-
A 81	ARG	50	-	Favored (7.13%) General / -119.9,-21.5	60.4% ( <i>mtm180</i> ) chi angles: 303.5,192.6,303.9,185.7	0.034Å	-	-
A 82	ASN	50	-	Favored (43.64%) General / -137.6,146.1	36.2% ( <i>m120</i> ) chi angles: 297,111.4	0.034Å	-	-
A 83	ILE	50	-	Favored (70.59%) Isoleucine or valine / -123.6,132.9	71.7% ( <i>mt</i> ) chi angles: 299.4,177.9	0.027Å	-	-
A 84	SER	50	-	Favored (38.49%) General / -119.4,151.5	59.8% ( <i>m</i> ) chi angles: 299.2	0.065Å	-	-
A 85	THR	50	0.624Å HB with A 86 PRO HD2	Favored (10.57%) Pre-proline / -59.3,161.1	80.8% ( <i>p</i> ) chi angles: 60.4	0.05Å	-	-
A 86	PRO	50	0.624Å HD2 with A 85 THR HB	Favored (74.7%) Trans-proline / -56.0,-29.6	63.4% ( <i>Cg_endo</i> ) chi angles: 27.6	0.093Å	-	-
A 87	ARG	99.99	0.666Å HH11 with A 89 ARG NH2	Favored (44.92%) General / -99.2,8.3	99.5% ( <i>mtt180</i> ) chi angles: 292.7,183.8,180,180.6	0.017Å	-	-
				Favored				

A 88	GLY	50	-	(60.42%) Glycine / 57.1,30.3	-	-	-	-	
A 89	ARG	99.99	0.666Å NH2 with A 87 ARG HH11	Favored (76.56%) General / -69.5,-36.4	99.6% ( <i>mtt180</i> ) chi angles: 291.5,180.8,178.6,178.7	0.029Å	-	-	
A 90	HIS	50	-	Favored (35.21%) General / -154.5,165.8	80.4% ( <i>m80</i> ) chi angles: 293.9,87.9	0.026Å	OUTLIER(S) worst is CG-- ND1: 4.792 σ	-	
A 91	SER	50	-	Favored (20.78%) General / -98.7,151.4	48.4% ( <i>m</i> ) chi angles: 301.9	0.066Å	-	-	
A 92	ILE	50	-	Favored (52.88%) Isoleucine or valine / -102.3,130.0	47.1% ( <i>mm</i> ) chi angles: 298.9,300.5	0.085Å	-	-	
A 93	THR	50	-	Favored (13.79%) General / -111.3,-14.5	68.1% ( <i>p</i> ) chi angles: 64.5	0.054Å	-	-	
A 94	ARG	50	-	Favored (43.54%) General / -148.9,157.6	32.2% ( <i>ptt-85</i> ) chi angles: 61.9,176.6,180.4,279.4	0.033Å	-	-	
#	Alt	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 56.85	Clashscore: 33.56	Outliers: 3 of 71	Poor rotamers: 0 of 65	Outliers: 1 of 67	Outliers: 2 of 73	Outliers: 2 of 73
A 95	LEU	50	0.501Å O with A 98 LEU HB2	Favored (69.24%) General / -58.3,-33.3	92.1% ( <i>mt</i> ) chi angles: 296.7,179.1	0.032Å	-	-	
A 96	GLU	50	-	Favored (70.66%) General / -64.2,-29.6	53.5% ( <i>mt-10</i> ) chi angles: 295.3,183.7,296.2	0.052Å	-	-	
A 97	GLU	50	-	Favored (67.94%) General / -69.1,-29.8	44.2% ( <i>mt-10</i> ) chi angles: 287,176.1,279.5	0.024Å	-	-	
A 98	LEU	50	0.652Å HB3 with A 38 ILE CD1	Favored (51.1%) General / -59.4,131.5	36.5% ( <i>mt</i> ) chi angles: 290.2,186.2	0.127Å	-	-	
A	GLU	50	-	Favored (56.09%)	80.5% ( <i>mm-40</i> ) chi angles:	0.008Å	-	-	

99				General / -113.9,132.0	290.9,299.4,314.8			
A 100	ASP	50	-	Favored (15.77%) General / -53.2,124.9	38.5% ( <i>t70</i> ) chi angles: 183.5,59.5	0.07Å	-	-
A 101	GLY	50	-	Favored (87.28%) Glycine / 78.2,9.0	-	-	-	-
A 102	GLU	50	0.59Å O with A 38 ILE HG23	Favored (12.96%) General / -99.5,162.5	66.9% ( <i>mt-10</i> ) chi angles: 290.1,186.3,24.8	0.028Å	-	-
A 103	SER	50	0.441Å O with A 86 PRO HD3	Favored (33.64%) General / -109.8,147.2	69.8% ( <i>m</i> ) chi angles: 297.8	0.061Å	-	-
A 104	TYR	50	0.426Å CD2 with A 38 ILE HG21	Favored (49.77%) General / -136.9,152.0	99% ( <i>m-85</i> ) chi angles: 296.5,275.9	0.011Å	-	-
A 105	LEU	50	-	Favored (45.33%) General / -115.8,122.4	9.5% ( <i>tt</i> ) chi angles: 181.5,155.2	0.108Å	-	-
A 106	CYS	50	-	Favored (29.79%) General / -95.2,140.7	36.3% ( <i>m</i> ) chi angles: 308.3	0.09Å	-	-
A 107	SER	99.99	-	-	33.3% ( <i>t</i> ) chi angles: 183.6	0.041Å	-	-

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