

Viewing crb1_sm_36-148Hmulti.table

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All-Atom	Clashscore, all atoms:	33.46		12 th percentile* (N=1784, all resolutions)
Contacts	Clashscore is the number	r of serious	steric ove	erlaps (> 0.4 Å) per 1000 atoms.
	Poor rotamers	0	0.00%	Goal: <1%
	Ramachandran outliers	6	5.41%	Goal: <0.05%
	Ramachandran favored	94 84.68%		Goal: >98%
Protein Geometry	MolProbity score [^]	2.67		38 th percentile* (N=27675, 0Å - 99Å)
geometry	Cβ deviations >0.25Å	3	2.91%	Goal: 0
	Bad backbone bonds:	5 / 841	0.59%	Goal: 0%
	Bad backbone angles:	20 / 1139	1.76%	Goal: <0.1%

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

[^] 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	$\begin{array}{c} C\beta \\ \text{deviation} \end{array}$	Bond lengths	Bond angles
		Avg: 56.19		Outliers: 6 of 111	Poor rotamers: 0 of 99	Outliers: 3 of 103	Outliers: 4 of 113	Outliers: 9 of 113
A 36	SER	50	-	-	39.3% (t) chi angles: 181.6	0.038Å	-	-
A 37	ASN	50	-	Favored (15.78%) General / -77.8,113.6	48.7% (<i>t30</i>) chi angles: 184.3,20	0.049Å	-	-
A 38	SER	50	-	Favored (63.91%) General / -62.5,-19.8	80.7% (p) chi angles: 60.3	0.048Å	-	-
A 39	CYS	50	0.732Å HB3 with A 43 SER HB3	Favored (23.61%) General / -87.3,114.1	58.3% (<i>m</i>) chi angles: 305.3	0.074Å	-	-

^{* 100&}lt;sup>th</sup> 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.

A 40	GLN 9	9.99	0.551Å HG3 with A 68 ASP OD1	Favored (34.53%) General / -74.4,158.1	86.3% (<i>mm-40</i>) chi angles: 296.4,291,326.7	0.02Å	-	-
A 41	ASN	50	-	Favored (9.61%) General / 61.6,43.9	32.8% (<i>m120</i>) chi angles: 292.4,116.5	0.054Å	-	-
A 42	ASN	50	-	Favored (20.01%) General / 56.8,31.8	20.3% (<i>t-20</i>) chi angles: 188.6,291.8	0.039Å	-	OUTLIER(S) worst is OD1- CG-ND2: 4.573 σ
A 43	SER	50	0.732Å HB3 with A 39 CYS HB3	Favored (43.43%) General / -73.9,147.2	30.8% (t) chi angles: 174.9	0.075Å	-	-
A 44	THR	50	0.684Å OG1 with A 55 SER HB3	Favored (36.41%) General / -78.8,131.2	69.5% (<i>p</i>) chi angles: 64.2	0.029Å	-	-
A 45	CYS	50	-	Favored (41.4%) General / -95.8,126.9	46.8% (t) chi angles: 185.2	0.045Å	-	-
A 46	LYS	50	-	Favored (27.6%) General / -118.9,117.0	27% (<i>tptp</i>) chi angles: 187.9,61.9,183.1,67.1	0.065Å	-	-
A 47	ASP	50	0.42Å HA with A 52 ASN OD1	Favored (35.54%) General / -77.9,129.6	41.8% (<i>t0</i>) chi angles: 189.4,328.2	0.026Å	-	-
A 48	РНЕ	50	0.49Å CE2 with A 53 ASP OD2	Favored (21.27%) General / -118.2,160.6	1.5% (<i>m-85</i>) chi angles: 291.7,39.8	0.027Å	-	-
A 49	SER	50	-	Favored (8.14%) General / -77.1,105.4	70.7% (<i>m</i>) chi angles: 297.6	0.098Å	-	-
A 50	LYS	50	-	OUTLIER (0.01%) General / 113.1,-33.5	28.3% (<i>tptp</i>) chi angles: 182.8,65.8,181.5,62.2	0.071Å	-	-
A 51	ASP 9	9.99	_	Allowed (0.28%) General / -144.7,-149.6	55.8% (<i>m-20</i>) chi angles: 297.6,297.8	0.054Å	-	-

A 52	ASN	99.99	0.42Å OD1 with A 47 ASP HA	Favored (32.38%) General / -159.3,158.4	69.4% (<i>m-80</i>) chi angles: 296.5,285.5	0.055Å	-	-
A 53	ASP	50	0.49Å OD2 with A 48 PHE CE2	Favored (47.8%) General / -129.6,153.7	56.8% (<i>m-20</i>) chi angles: 294.6,299.8	0.016Å	-	-
A 54	CYS	50	-	Favored (55.45%) General / -113.0,132.3	97.2% (<i>m</i>) chi angles: 290.8	0.051Å	-	-
A 55	SER	50	0.684Å HB3 with A 44 THR OG1	Favored (5.2%) General / -102.6,93.6	35.3% (<i>t</i>) chi angles: 175.7	0.044Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	$\begin{array}{c} C\beta \\ \text{deviation} \end{array}$	Bond lengths	Bond angles
		Avg: 56.19	Clashscore: 33.46	Outliers: 6 of 111	Poor rotamers: 0 of 99	Outliers: 3 of 103	Outliers: 4 of 113	Outliers: 9 of 113
A 56	CYS	50	-	Favored (49.5%) General / -70.1,147.9	55.5% (<i>m</i>) chi angles: 306.5	0.013Å	-	-
A 57	SER	50	-	Favored (32.76%) General / -74.0,159.4	70.6% (<i>m</i>) chi angles: 297.4	0.017Å	-	-
A 58	ASP	50	-	Favored (7.29%) General / -59.4,119.4	43.6% (<i>t0</i>) chi angles: 187.5,328.3	0.084Å	-	-
A 59	THR	50	1.119Å HG21 with A 89 PRO HA	OUTLIER (0.01%) General / 110.7,-5.9	46.2% (<i>m</i>) chi angles: 305.2	0.076Å	-	-
A 60	ALA	50	-	Favored (54.06%) General / -116.9,135.0	-	0.053Å	-	-
A 61	ASN	50	0.407Å CG with A 62 ASN H	Favored (12.22%) General / -130.6,172.2	57.6% (<i>t30</i>) chi angles: 186.5,48.7	0.038Å	-	-
A 62	ASN	99.99	0.766Å HB2 with A 65 LYS O	Favored (6.78%) General / -127.3,102.1	22.6% (<i>p-10</i>) chi angles: 78.2,358	0.3Å	-	OUTLIER(S) worst is N-CA-CB: 6.747σ

 $http://molprobity.biochem.duke.edu/viewtable.php? MolProbSID=m8e...mhda 9160d6lq3ojgim8qst8ej/raw_data/crb1_sm_36-148H-multi.table$

A 63	LEU 9	99.99	-	Favored (54.5%) General / -74.2,-44.1	7.7% (tt) chi angles: 188.3,161.4	0.084Å	-	-
A 64	ASP 9	99.99	-	Favored (4.17%) General / -133.0,9.6	28.9% (<i>p30</i>) chi angles: 59.5,26.9	0.021Å	-	-
A 65	LYS 9	99.99	0.868Å HB3 with A 66 ASP HB2	Allowed (0.08%) General / -161.3,-142.2	5.2% (<i>mmtm</i>) chi angles: 272.3,329.5,163.5,299.2	0.287Å	-	OUTLIER(S) worst is C-N- CA: 10.021 σ
A 66	ASP	50	0.868Å HB2 with A 65 LYS HB3	OUTLIER (0%) General / 136.8,14.3	74.5% (<i>m</i> -20) chi angles: 297.3,348.2	0.395Å	-	OUTLIER(S) worst is N-CA-CB: 7.936σ
A 67	CYS	50	-	Favored (27.52%) General / 55.8,36.6	31.7% (<i>m</i>) chi angles: 309.8	0.036Å	-	-
A 68	ASP 9	99.99	0.551Å OD1 with A 40 GLN HG3	Favored (54.71%) General / -86.6,-10.0	87.2% (<i>m</i> -20) chi angles: 294.4,346.6	0.092Å	-	-
A 69	ASN	50	-	Favored (31.64%) General / -103.6,116.0	27.9% (<i>t-20</i>) chi angles: 184.9,301.5	0.032Å	-	-
A 70	MET	50	-	Favored (6.48%) General / -79.3,98.0	61.7% (<i>tpp</i>) chi angles: 183.6,63.7,70.5	0.043Å	-	-
A 71	LYS	50	-	Favored (24.96%) General / -51.1,130.0	28.9% (<i>tptp</i>) chi angles: 184.4,64.3,180.4,64.6	0.064Å	-	-
A 72	ASP	50	0.516Å HA with A 87 ASN OD1	Allowed (0.98%) Pre-proline / -93.3,94.6	50.1% (<i>t0</i>) chi angles: 187.3,333.8	0.052Å	-	-
A 73	PRO	50	0.793Å HD2 with A 87 ASN OD1	Favored (6.52%) Trans-proline / -69.3,-0.4	92.2% (<i>Cg_endo</i>) chi angles: 32.1	0.05Å	-	-
A 74	CYS	50	-	Favored (23.96%) General / -108.5,4.2	93.2% (<i>m</i>) chi angles: 291.4	0.064Å	-	-
				Favored	/	^		

A 75	PHE	50	-	(71.14%) General / -66.2,-30.6	80.8% (<i>t80</i>) chi angles: 183.4,80.5	0.029Å	-	-
#	Alt Res	High B	Clash > 0.4 Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 56.19	Clashscore: 33.46	Outliers: 6 of 111	Poor rotamers: 0 of 99	Outliers: 3 of 103	Outliers: 4 of 113	Outliers: 9 of 113
A 76	SER	50	-	Favored (30.69%) General / -96.2,12.5	78.1% (p) chi angles: 59	0.026Å	-	-
A 77	ASN	50	-	Favored (3.81%) Pre-proline / 48.9,68.2	26.7% (<i>m120</i>) chi angles: 298.9,132.8	0.031Å	-	-
A 78	PRO	50	0.668Å O with A 106 ILE HG23	Favored (12.66%) Trans-proline / -72.1,-31.0	92.2% (<i>Cg_endo</i>) chi angles: 32.1	0.057Å	-	-
A 79	CYS	50	0.474Å HB3 with A 83 ALA HB3	Favored (35.44%) General / -78.6,130.0	62.5% (<i>m</i>) chi angles: 303.2	0.054Å	-	-
A 80	GLN	50	-	Favored (17.36%) General / -107.8,158.4	86.5% (<i>mt-30</i>) chi angles: 296.9,178.5,0.6	0.075Å	-	-
A 81	GLY	50	0.776Å O with A 99 PRO HG3	Favored (25.42%) Glycine / 66.2,54.2	-	-	-	-
A 82	SER	50	-	Favored (9.4%) General / 58.7,21.9	55.2% (<i>m</i>) chi angles: 299.7	0.028Å	-	-
A 83	ALA	50	0.474Å HB3 with A 79 CYS HB3	Favored (41.11%) General / -73.1,152.6	-	0.04Å	-	-
A 84	THR	50	-	Favored (33.91%) General / -94.7,137.3	13.7% (<i>m</i>) chi angles: 312.1	0.065Å	-	-
A 85	CYS	50	-	Favored (50.63%) General / -108.2,134.7	25% (<i>t</i>) chi angles: 190.6	0.059Å	-	-
			~ · - ~ ⁹	Favored	40 .0/ / \			

A 86	VAL	50	0.459A CG1 with A 95 LEU H	(42.39%) Isoleucine or valine / -108.1,112.9	12.4% (<i>p</i>) chi angles: 65.8	0.126Å	-	-
A 87	ASN	50	0.793Å OD1 with A 73 PRO HD2	Favored (2.5%) General / -73.1,98.1	48.1% (<i>t30</i>) chi angles: 184.4,61.6	0.074Å	-	-
A 88	THR	50	0.482Å HB with A 89 PRO HD2	Favored (15.44%) Pre-proline / -110.0,164.2	67.8% (p) chi angles: 62.1	0.018Å	-	-
A 89	PRO	99.99	1.119Å HA with A 59 THR HG21	Favored (5.54%) Trans-proline/ -75.9,58.7	39.3% (<i>Cg_endo</i>) chi angles: 36.6	0.069Å	-	-
A 90	GLY	99.99	-	Favored (20.44%) Glycine / -162.5,150.9	-	-	-	-
A 91	GLU	99.99	-	Favored (14.96%) General / -106.9,-14.4	12.3% (<i>pt-20</i>) chi angles: 65.4,178.7,58.4	0.025Å	-	-
A 92	ARG	99.99	-	Favored (64.95%) General / -55.2,-35.5	24.1% (<i>ptt-85</i>) chi angles: 62.5,170.3,177.3,287.7	0.059Å	-	-
A 93	SER	99.99	0.814Å O with A 95 LEU HD12	OUTLIER (0.02%) General / -171.3,45.5	5.5% (<i>m</i>) chi angles: 279.9	0.063Å		OUTLIER(S) worst is CA-C- N: 12.112 σ
A 94	PHE	50	0.634Å CD2 with A 94 PHE O	OUTLIER (0%) General / -1.4,130.3	44.9% (<i>p</i> 90) chi angles: 57.1,274.3	0.233Å	OUTLIER(S) worst is N CA: 5.275 σ	OUTLIER(S) worst is O-C- N: 4.791 σ
A 95	LEU	50	0.814Å HD12 with A 93 SER O	Favored (36.54%) General / -103.8,141.2	8.1% (<i>mp</i>) chi angles: 286.4,63.9	0.249Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	C β deviation	Bond lengths	Bond angles
		0			Poor rotamers: 0 of			Outliers: 9
A 96	CYS	56.19 50	33.46	111 Favored (50.18%) General / -102.8,127.0	99 73.4% (<i>m</i>) chi angles: 298.3	3 of 103 0.024Å	of 113 -	of 113 -
				Favored	39.1% (<i>ttpt</i>)			
A	11/0			(0.000/)	ahi analaa.	0.0568		

A 97	LYS	50	-	(9.08%) General / -101.5,98.8	cm angles: 183,181.7,64.4,181.4	U.U56A	-	-
A 98	CYS	50	-	Favored (97.69%) Pre-proline / -65.2,139.7	60.5% (<i>m</i>) chi angles: 304.2	0.04Å	-	-
A 99	PRO	50	0.776Å HG3 with A 81 GLY O	Favored (41.63%) Trans-proline / -71.0,142.0	79.2% (<i>Cg_endo</i>) chi angles: 33.2	0.033Å	-	-
A 100	PRO	50	-	Favored (12.67%) Trans-proline / -46.9,127.7	63.9% (<i>Cg_exo</i>) chi angles: 327.4	0.031Å	-	-
A 101	GLY	50	0.629Å O with A 111 ILE HG12	Favored (21.29%) Glycine / 113.7,-16.4	-	-	-	-
A 102	TYR	50	0.598Å CE1 with A 110 THR HG22	Favored (41.12%) General / -118.9,149.7	99% (<i>m</i> -85) chi angles: 296.8,275.2	0.044Å	-	-
A 103	SER	50	-	Favored (20.4%) General / -143.5,168.2	84.7% (p) chi angles: 61	0.032Å	-	-
A 104	GLY	50	-	Favored (16.31%) Glycine / 114.9,170.0	-	-	-	-
A 105	THR	50	-	Favored (74.56%) General / -64.0,-32.9	77.6% (p) chi angles: 60.2	0.031Å	-	-
A 106	ILE	50	0.668Å HG23 with A 78 PRO O	Favored (9.52%) Isoleucine or valine / -109.4,0.7	55.7% (<i>mt</i>) chi angles: 288.1,177.6	0.151Å	-	-
A 107	CYS	50	-	Favored (22.59%) General / 59.5,38.0	49% (<i>m</i>) chi angles: 306.9	0.022Å	-	-
A 108	GLU	50	-	Favored (32.27%) General / -83.4,-23.8	17.9% (pm0) chi angles: 68.8,285.8,358.6	0.087Å	-	-

A 109	THR	50	-	Favored (35.28%) General / -91.5,124.0	58.2% (p) chi angles: 65.2	0.021Å	-	-
A 110	THR	50	0.598Å HG22 with A 102 TYR CE1	Favored (9.28%) General / -82.8,98.7	68.9% (p) chi angles: 57.5	0.027Å	-	-
A 111	ILE	50	0.629Å HG12 with A 101 GLY O	Allowed (0.95%) Isoleucine or valine / -44.8,124.9	37.7% (<i>pt</i>) chi angles: 66.8,172.2	0.052Å	-	-
A 112	GLY	50	0.909Å HA2 with A 127 GLN NE2	Allowed (0.46%) Glycine / -71.8,88.0	-	-	-	-
A 113	SER	50	-	Favored (64.55%) General / -68.2,-18.4	51.3% (<i>m</i>) chi angles: 300.2	0.05Å	-	-
A 114	CYS	50	-	Favored (59.5%) General / -81.9,-9.8	73.3% (<i>m</i>) chi angles: 296.9	0.021Å	-	-
A 115	GLY	50	-	Favored (95.65%) Glycine / -62.1,-38.1	-	-	-	-
115	GLY	50 High B	- Clash > 0.4Å	(95.65%) Glycine /	- Rotamer	<u>-</u> Cβ deviation	- Bond lengths	Bond angles
115		High B	0.4Å Clashscore:	(95.65%) Glycine / -62.1,-38.1 Ramachandran	Rotamer Poor rotamers: 0 of 99	deviation	lengths	angles
115		High B Avg:	0.4Å Clashscore:	(95.65%) Glycine / -62.1,-38.1 Ramachandran Outliers: 6 of	Poor rotamers: 0 of	deviation Outliers:	lengths Outliers: 4	angles Outliers: 9
115 # A	Alt Res	High B Avg: 56.19	0.4Å Clashscore:	(95.65%) Glycine / -62.1,-38.1 Ramachandran Outliers: 6 of 111 Favored (52.58%) General /	Poor rotamers: 0 of 99 32.7% (mmmt) chi angles:	deviation Outliers: 3 of 103	lengths Outliers: 4	angles Outliers: 9
115 # A A 116	Alt Res	High B Avg: 56.19	0.4Å Clashscore:	(95.65%) Glycine / -62.1,-38.1 Ramachandran Outliers: 6 of 111 Favored (52.58%) General / -81.3,-3.4 Allowed (0.57%) General /	Poor rotamers: 0 of 99 32.7% (mmmt) chi angles: 296.2,294.5,293.4,181.2	deviation Outliers: 3 of 103 0.026Å	lengths Outliers: 4	angles Outliers: 9

119				-74.8,110.5				
A 120	GLN	50	0.503Å OE1 with A 146 GLU HB3	Favored (39.42%) General / -70.8,156.5	86.2% (<i>mt-30</i>) chi angles: 294.7,181.1,298.3	0.017Å	-	-
A 121	HIS	50	0.557Å CG with A 140 TYR HE2	Favored (19.62%) General / 61.0,33.8	27.1% (<i>m80</i>) chi angles: 309,115.4	0.049Å	OUTLIER(S) worst is CG ND1: 4.597 σ	OUTLIER(S) worst is CA- CB-CG: 6.216 σ
A 122	GLY	50	-	Favored (7.28%) Glycine / 56.3,61.6	-	-	-	-
A 123	GLY	50	-	Favored (18.7%) Glycine / -94.7,147.7	-	-	-	-
A 124	ILE	50	0.754Å CG1 with A 135 ILE HB	Favored (32.54%) Isoleucine or valine / -70.0,133.0	41.4% (<i>pt</i>) chi angles: 65.7,172.5	0.081Å	-	-
A 125	CYS	50	-	Favored (54.58%) General / -113.1,134.3	44.4% (<i>t</i>) chi angles: 183.1	0.062Å	-	-
A 126	HIS	50	0.822Å HB3 with A 133 VAL HG13	Favored (26.13%) General / -122.3,117.4	13.9% (<i>t-160</i>) chi angles: 174.1,208.1	0.124Å	OUTLIER(S) worst is CD2NE2: 4.615 σ	OUTLIER(S) worst is CB- CG-CD2: 4.721 σ
A 127	GLN	50	0.909Å NE2 with A 112 GLY HA2	Favored (48.02%) General / -71.1,136.1	52.2% (<i>tt0</i>) chi angles: 182.9,185,56.9	0.059Å	-	-
A 128	ASP	50	0.66Å HB3 with A 129 PRO HD2	Allowed (0.13%) Pre-proline / -128.5,-167.4	56.1% (<i>m-20</i>) chi angles: 293.9,299.8	0.129Å	-	-
A 129	PRO	50	0.66Å HD2 with A 128 ASP HB3	Allowed (1.57%) Trans-proline / -88.8,124.7	94.9% (<i>Cg_endo</i>) chi angles: 32.6	0.045Å	-	-
A 130	ILE	50	0.505Å HG23 with A 101 GLY N	Allowed (0.14%) Isoleucine or valine / 50.6,28.6	21.1% (<i>pt</i>) chi angles: 51.2,176.4	0.134Å	-	-
٨			0 49 Å	Envored	70 F0/ /(00)			

131	TYR	50	U.4UA HE1 with A 143 ARG HH12	1 avoieu (2.37%) Pre-proline / -165.5,133.3	/2.5% (töU) chi angles: 183.9,84.6	0.042Å	-	-
A 132	PRO	50	-	OUTLIER (0.08%) Trans-proline / -108.7,155.4	25.3% (<i>Cg_endo</i>) chi angles: 37.9	0.083Å	-	-
A 133	VAL	50	0.822Å HG13 with A 126 HIS HB3	Favored (33.52%) Isoleucine or valine / -126.9,113.6	2.6% (p) chi angles: 49.6	0.161Å	-	-
A 134	CYS	50	-	Favored (36.28%) General / -89.9,129.3	96.1% (<i>m</i>) chi angles: 294	0.076Å	-	-
A 135	ILE	50	0.754Å HB with A 124 ILE CG1	Favored (8.44%) Isoleucine or valine / -110.9,99.3	14.2% (<i>mm</i>) chi angles: 313.4,291.4	0.04Å	-	-
# /	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Clashscore:	Outliers: 6 of	Poor rotamers: 0 of	Outliers:	Outliers: 4	Outliers: 9
		56.19	33.46	111	99	3 of 103	of 113	of 113
A 136	CYS	56.19 50	33.46	111 Favored (98.71%) Pre-proline / -65.6,147.4	99 61.3% (<i>m</i>) chi angles: 303.8	3 of 103 0.031Å	of 113 -	of 113 -
	CYS PRO		33.46	Favored (98.71%) Pre-proline /	61.3% (<i>m</i>)		of 113 - -	of 113 - -
136 A		50	33.46 - - 0.44Å HA with A 139 GLY HA2	Favored (98.71%) Pre-proline / -65.6,147.4 Favored (15.98%) Trans-proline /	61.3% (<i>m</i>) chi angles: 303.8 67.2% (<i>Cg</i> _endo)	0.031Å	of 113 - -	of 113 - -
136 A 137	PRO	50 50	- 0.44Å HA with A	Favored (98.71%) Pre-proline / -65.6,147.4 Favored (15.98%) Trans-proline / -73.8,172.4 Favored (28.32%) General /	61.3% (<i>m</i>) chi angles: 303.8 67.2% (<i>Cg</i> _endo)	0.031Å 0.025Å	of 113 - -	of 113 - -
136 A 137 A 138	PRO ALA	50 50 50	- 0.44Å HA with A 139 GLY HA2 0.444Å C with A 140 TYR HD1 0.557Å HE2 with A 121 HIS CG	Favored (98.71%) Pre-proline / -65.6,147.4 Favored (15.98%) Trans-proline / -73.8,172.4 Favored (28.32%) General / -81.3,123.2 Allowed (0.35%) Glycine /	61.3% (<i>m</i>) chi angles: 303.8 67.2% (<i>Cg</i> _endo)	0.031Å 0.025Å	of 113	of 113 - OUTLIER(S) worst is CD2- CE2-CZ: 4.989 σ
136 A 137 A 138 A 139	PRO ALA GLY	505050	- 0.44Å HA with A 139 GLY HA2 0.444Å C with A 140 TYR HD1 0.557Å HE2 with A	Favored (98.71%) Pre-proline / -65.6,147.4 Favored (15.98%) Trans-proline / -73.8,172.4 Favored (28.32%) General / -81.3,123.2 Allowed (0.35%) Glycine / -124.6,82.8 Favored (17.51%) General /	61.3% (<i>m</i>) chi angles: 303.8 67.2% (<i>Cg_endo</i>) chi angles: 33.8 - 1.5% (<i>m-30</i>)	0.031Å 0.025Å 0.03Å	of 113	- OUTLIER(S) worst is CD2- CE2-CZ:

141	/ \L / \	JU	<u></u> HD11	(12.77 /0) General / -167.4,169.3	-	U.134/1	-	-
A 142	GLY	50	-	Allowed (0.29%) Glycine / -125.0,-43.5	-	-	-	-
A 143	ARG	50	0.48Å HH12 with A 131 TYR HE1	Favored (8.89%) General / -96.9,-40.5	57.1% (ttm-85) chi angles: 187.4,183,286.1,280	0.105Å	-	-
A 144	PHE	50	-	Favored (12.54%) General / -115.0,-5.8	1.6% (<i>m</i> -30) chi angles: 292.4,33.5	0.025Å	-	-
A 145	CYS	50	-	Favored (16.94%) General / 61.5,36.7	39.7% (<i>m</i>) chi angles: 307.6	0.025Å	-	-
A 146	GLU	50	0.503Å HB3 with A 120 GLN OE1	Favored (21.29%) General / -87.1,-30.2	11.2% (<i>pt-20</i>) chi angles: 56.1,179.7,71.4	0.044Å	-	-
A 147	ILE	50	0.878Å HD11 with A 141 ALA HB3	Favored (14.08%) Isoleucine or valine / -71.2,117.2	14% (pt) chi angles: 73.4,179.4	0.107Å	-	-
A 148	ASP 9	99.99) -	-	41.4% (<i>t0</i>) chi angles: 185,24.3	0.048Å	-	-

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