

## Viewing pax6-val126asp\_FFX1Hmulti.table

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All-Atom	Clashscore, all atoms:	0.92		99 <sup>th</sup> percentile* (N=1784, all resolutions)		
Contacts	Clashscore is the number	of serious :	steric ove	rlaps (> 0.4 Å) per 1000 atoms.		
	Poor rotamers	4	3.48%	Goal: <1%		
	Ramachandran outliers	5	3.82%	Goal: <0.05%		
	Ramachandran favored	113	86.26%	Goal: >98%		
Protein Geometry	MolProbity score <sup>^</sup>	1.82		84 <sup>th</sup> percentile* (N=27675, 0Å - 99Å)		
	Cβ deviations >0.25Å	4	3.28%	Goal: 0		
-	Bad backbone bonds:	0 / 1039	0.00%	Goal: 0%		
	Bad backbone angles:	10 / 1404	0.71%	Goal: <0.1%		

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

<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: 54.96	Clashscore: 0.92	Outliers: 5 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122		
A 4		SER	50	-	-	6% ( <i>p</i> ) chi angles: 44	0.152Å	-	-
A 5		HIS	50	-	Favored (38.08%) General / -95.8,135.0	46.6% ( <i>p-80</i> ) chi angles: 64.9,270.8	0.1Å	-	OUTLIER(S) worst is CA- CB-CG: 4.742 σ
A 6		SER	50	-	Favored (43.76%) General / -67.1,153.4	74.3% ( <i>m</i> ) chi angles: 294.1	0.06Å	-	-
A 7		GLY	50	-	Favored (21.19%) Glycine / -130.6,170.1	-	-	-	-

**Favored** 

<sup>\* 100&</sup>lt;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.

A 10 GLN 50									
A 19 ASN 50 20437Å Favored (4.78%)	A 8	VAL	50	-	Isoleucine or valine /		0.077Å	-	-
A 10 GLN 50	A 9	ASN	50	HB2 with C2019 DGU	Favored (4.78%) General /	•	0.098Å	-	OUTLIER(S) worst is CA- CB-CG: 4.28 σ
A 11 LEU 50 - (50.09%)	A 10	GLN	50	-	(61.79%) General /	chi angles:	0.077Å	-	-
A 12 GLY 50	A 11	LEU	50	-	(50.09%) General /		0.102Å	-	-
A 13 GLY 50 - (45.57%) Glycine / 89.7,-176.4 Favored (34.46%) Soleucine or valine / -128.6,150.7 Favored (47.75%) General / -136.9,136.6 Favored (47.75%) Soleucine or valine / -136.9,136.6 Favored (47.75%) General / -136.9,136.6 Favored (47.75%)	A 12	GLY	50	-	(55.69%)	-	-	-	-
A 14 VAL 50 - (34.46%)   6.6% (m)   chi angles: 286.2   0.04Å   -   -   -   -   -   -   -   -   -	A 13	GLY	50	-	(45.57%) Glycine /	-	-	-	-
A 15 PHE 50 - (2.74%)	A 14	VAL	50	-	(34.46%) Isoleucine or valine /		0.04Å	-	-
A 16 VAL 50 - \( \begin{array}{c} (47.75\%) \\ 76.4\% (t) \\ \text{chi angles: } 174.2 \\ \ \text{A 17} \\ \text{ASN} \\ \text{50} \\ \text{50} \\ \text{70} \\ \text{20} \\ \	A 15	PHE	50	-	(2.74%) General /		0.068Å	-	-
A 17 ASN 50 - Favored (35.85%) 18.4% (t30) chi angles: 203.6,58.9	A 16	VAL	50	-	(47.75%) Isoleucine or valine /		0.072Å	-	-
A 18 GLY 50 - (34.19%) Glycine / 55.1,24.0  A 19 ARG 50 - (34.75%) 26.9% (mmm180) chi angles: 0.037Å Pre-proline / 293.6,302.4,292.3,178	A 17	ASN	50	-	Favored (35.85%) General /		0.028Å	-	-
A 19 ARG 50 - (34.75%) 20.37% (IIIIII 1760) chi angles: 0.037Å Pre-proline / 293.6,302.4,292.3,178	A 18	GLY	50	-	(34.19%) Glycine /	-	-	-	-
Pre-proline / 293.6,302.4,292.3,178	A 19	ARG	50	-			0.037Å	-	-
•					Pre-proline / -149.0,160.6	<u> </u>			

A 20	PRO	50	-	Favored (18.07%) Trans-proline / -80.0,146.2	4.8% ( <i>Cg_exo</i> ) chi angles: 356	0.044Å	-	-
A 21	LEU	50	-	Favored (70.36%) Pre-proline / -57.1,125.5	18.6% ( <i>tp</i> ) chi angles: 193,70.6	0.058Å	-	-
A 22	PRO	50	-	Favored (45.49%) Trans-proline / -52.5,143.5	0.1% chi angles: 316.7	0.052Å	-	-
A 23	ASP	50	-	Allowed (0.66%) General / -47.5,-23.6	7.5% ( <i>m-20</i> ) chi angles: 305.6,3.3	0.134Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	Bond angles
		Avg: 54.96	Clashscore: 0.92	Outliers: 5 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122		Outliers: 10 of 133
A 24	SER	50	-	Favored (70.01%) General / -53.5,-46.3	57.4% (p) chi angles: 55.6	0.074Å	-	-
A 25	THR	50	-	Favored (20.9%) General / -87.9,-29.4	2.1% ( <i>m</i> ) chi angles: 322.3	0.111Å	-	-
A 26	ARG	50	-	Favored (77.84%) General / -64.4,-34.3	11.5% ( <i>mtp85</i> ) chi angles: 312,182.9,102.7,89.4	0.128Å	-	-
A 27	GLN	50	-	Favored (83.48%) General / -60.6,-38.0	1.3% ( <i>tp60</i> ) chi angles: 170.3,69,113.6	0.059Å	-	-
A 28	LYS	50	-	Favored (72.28%) General / -71.0,-35.8	25.6% (mmmt) chi angles: 309.2,315.3,301.9,180.1	0.167Å	-	-
A 29	ILE	50	-	Favored (97.8%) Isoleucine or valine / -63.0,-42.7	61.7% ( <i>mt</i> ) chi angles: 304,177.5	0.209Å	-	-
A 30	VAL	50	-	Favored (67.6%)	1.9% ( <i>p</i> ) chi angles: 83.2	0.244Å	-	-

				Isoleucine or valine / -69.2,-35.3				
A 31	GLU	50	-	Favored (95.34%) General / -60.4,-42.1	30.9% ( <i>mt-10</i> ) chi angles: 276.2,178.5,48.6	0.086Å	-	-
A 32	LEU	50	-	Favored (2.58%) General / -86.2,-58.6	28.1% ( <i>mt</i> ) chi angles: 305.6,189.7	0.141Å	-	-
A 33	ALA	50	-	Favored (99.2%) General / -63.2,-41.6	-	0.104Å	-	-
A 34	HIS	50	-	Favored (38.3%) General / -71.6,-6.1	2.2% ( <i>t-80</i> ) chi angles: 212.6,313.8	0.061Å	-	-
A 35	SER	50	-	Favored (19.98%) General / -102.8,-9.4	58% ( <i>m</i> ) chi angles: 291.3	0.059Å	-	-
A 36	GLY	50	-	Allowed (0.62%) Glycine / 131.6,28.5	-	-	-	-
A 37	ALA	50	-	Favored (48.09%) General / -124.6,148.1	-	0.05Å	-	-
A 38	ARG	50	-	Favored (20.02%) Pre-proline / -82.0,169.0	72.8% ( <i>mtm180</i> ) chi angles: 298.8,180.4,300,155	0.071Å	-	-
A 39	PRO	50	-	Favored (11.98%) Trans-proline / -53.1,-51.0	3% ( <i>Cg_exo</i> ) chi angles: 321.7	0.044Å	-	-
A 40	CYS	50	-	Favored (72.95%) General / -66.2,-31.9	1.2% ( <i>p</i> ) chi angles: 87.9	0.212Å	-	-
A 41	ASP	50	-	Favored (90.41%) General /	31.8% ( <i>m-20</i> ) chi angles: 308.4,322	0.166Å	-	-
A 40	пе	F0		-66.0,-39.8 Favored (10.64%)	5.9% (pt)	0 227 %		

A 42	ILE	50	-	Isoleucine or valine / -81.4,-29.0 Favored	chi angles: 64.6,148.7	U.32/A	-	-
A 43	SER	50	-	(91.02%) General / -64.8,-44.1	78.6% (p) chi angles: 59.3	0.102Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	<b>C</b> β <b>deviation</b>	Bond lengths	Bond angles
		Avg: 54.96	Clashscore: 0.92	Outliers: 5 of 131	Poor rotamers: 4 of 115	Outliers: 4 of 122		Outliers: 10 of 133
A 44	ARG	50	-	Favored (61.18%) General / -73.2,-18.8	33.4% ( <i>ttp-105</i> ) chi angles: 197.9,179.4,66.7,249.8	0.06Å	-	-
A 45	ILE	50	-	Favored (8.57%) Isoleucine or valine / -109.8,-17.0	18.5% ( <i>mt</i> ) chi angles: 305,188.1	0.265Å	-	-
A 46	LEU	50	-	Favored (20.8%) General / -99.0,-12.3	74.2% ( <i>mt</i> ) chi angles: 297.8,168.9	0.13Å	-	-
A 47	GLN	50	-	Allowed (0.77%) General / 70.8,42.6	35.5% ( <i>mt-30</i> ) chi angles: 305.9,181.1,252.9	0.152Å	-	-
A 48	VAL	50	-	Favored (24.75%) Isoleucine or valine / -121.1,154.1	55% ( <i>t</i> ) chi angles: 169.9	0.127Å	-	-
A 49	SER	50	-	Favored (21.32%) General / -64.9,160.1	82.9% ( <i>p</i> ) chi angles: 69.3	0.05Å	-	-
A 50	ASN	50	-	Favored (87.9%) General / -66.2,-43.0	20.3% ( <i>m-20</i> ) chi angles: 316.4,306	0.101Å	-	-
A 51	GLY	50	0.42Å HA3 with C2019 DGU O6	Favored (56.14%) Glycine / -75.5,-31.7	-	-	-	-
A 52	CYS	50	-	Favored (99.69%) General / -62.6,-42.7	42.1% ( <i>t</i> ) chi angles: 175.9	0.058Å	-	-

A 53	VAL	50	<del>-</del>	Allowed (1.61%) Isoleucine or valine / -46.3,-55.3	2.2% ( <i>t</i> ) chi angles: 150.6	0.171Å	-	-
A 54	SER	50	-	Favored (48.62%) General / -85.6,-13.5	69.9% ( <i>m</i> ) chi angles: 297.2	0.215Å	-	-
A 55	LYS	50	-	Favored (58.86%) General / -73.3,-9.6	49.6% ( <i>mtmt</i> ) chi angles: 286.5,187.3,283.2,196.3	0.202Å	-	-
A 56	ILE	50	-	Favored (3.13%) Isoleucine or valine / -90.6,-59.0	3.3% ( <i>mp</i> ) chi angles: 291.1,77.2	0.151Å	-	-
A 57	LEU	50	-	Favored (75.73%) General / -56.1,-41.9	81.8% ( <i>mt</i> ) chi angles: 299.3,181.9	0.221Å	-	-
A 58	GLY	50	-	Favored (93.58%) Glycine / -60.6,-37.6	-	-	-	-
A 59	ARG	50	-	Favored (55.09%) General / -78.7,-18.0	75% (mtm180) chi angles: 295.3,183.4,278.2,183.5	0.135Å	-	-
A 60	TYR	50	-	Favored (62.05%) General / -75.0,-36.4	80% ( <i>t80</i> ) chi angles: 184.3,76.6	0.135Å	-	-
A 61	TYR	50	-	Favored (72.46%) General / -60.4,-33.4	19.6% ( <i>m-30</i> ) chi angles: 299.9,338.8	0.126Å	-	-
A 62	GLU	50	-	Allowed (0.12%) General / -91.2,-96.7	10.7% ( <i>tm-20</i> ) chi angles: 191.5,282.7,314.5	0.208Å	-	OUTLIER(S) worst is C-CA- CB: 4.049 σ
A 63	THR	50	-	Favored (81.83%)	2.4% (m)	0.119Å	_	-
				General / -64.0,-35.8	chi angles: 280.8			
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles

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		Avg. 54.96	Ciastiscore. 0.92	Outriers, 5 or 131	rooi iolameis. 4 oi 115		Outriers. 0 of 133	of 133
A 64	GLY	50	-	Favored (7.9%) Glycine / 107.7,21.4	-	-	-	-
A 65	SER	50	-	Favored (29.33%) General / -76.5,125.5	23.2% (t) chi angles: 187.3	0.051Å	-	-
A 66	ILE	50	-	Favored (8.32%) Isoleucine or valine / -85.1,-20.4	45.4% ( <i>pt</i> ) chi angles: 62.8,168.2	0.198Å	-	-
A 67	ARG	50	-	Favored (95.4%) Pre-proline / -70.7,151.4	12.4% (mmm180) chi angles: 270.2,293.7,305.3,173.9	0.095Å	-	-
A 68	PRO	50	-	Allowed (0.86%) Trans-proline / -85.9,-171.4	0.5% chi angles: 42.9	0.112Å	-	-
A 69	ARG	50	-	OUTLIER (0.02%) General / -74.2,-149.0	83.1% ( <i>mtm180</i> ) chi angles: 295.8,178.9,280.2,174.4	0.161Å	-	-
A 70	ALA	50	-	Favored (47.94%) General / -128.7,132.2	-	0.091Å	-	-
A 71	ILE	50	-	Favored (4.64%) Isoleucine or valine / -80.0,152.0	42.1% ( <i>mt</i> ) chi angles: 292.6,155.3	0.114Å	-	-
A 72	GLY	50	0.46Å HA2 with C2013 DAD H2	Favored (40.94%) Glycine / 80.1,170.3	-	-	-	-
A 73	GLY	50	-	Favored (3.14%) Glycine / 97.3,113.9	-	-	-	-
A 74	SER	50	-	Allowed (0.11%) General / -82.1,-153.7	14.3% ( <i>p</i> ) chi angles: 82.1	0.236Å	-	-
				Favored	28.7% ( <i>mmtm</i> )	•		

A 75	LYS	50	-	(39.93%) Pre-proline / -142.0,163.5	chi angles: 308.1,298.8,161.3,307.3	0.047A	-	-
A 76	PRO	50	-	Allowed (0.35%) Trans-proline / -54.9,109.1	0.1% chi angles: 318	0.07Å	-	-
A 77	ARG	50	-	Favored (14.91%) General / -93.4,-30.8	83.8% (mtm180) chi angles: 283.2,175.3,283.7,177.2	0.179Å	-	-
A 78	VAL	50	-	Allowed (0.98%) Isoleucine or valine / -125.9,-32.3	10.1% ( <i>m</i> ) chi angles: 308.5	0.182Å	-	-
A 79	ALA	50	-	Allowed (1.89%) General / -80.5,53.7	-	0.056Å	-	-
A 80	THR	50	-	Favored (6.52%) Pre-proline / -57.9,161.5	71.1% (p) chi angles: 63.4	0.072Å	-	-
A 81	PRO	50	-	Favored (31.4%) Trans-proline / -48.7,-35.9	0.1% chi angles: 318.4	0.092Å	-	-
A 82	GLU	50	-	Favored (31.37%) General / -81.8,-32.1	46.8% (tt0) chi angles: 185.3,156.3,352.8	0.239Å	-	-
A 83	VAL	50	-	Favored (84.95%) Isoleucine or valine / -58.4,-42.7	24.6% ( <i>t</i> ) chi angles: 163.8	0.11Å	-	-
#	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg: 54.96	Clashscore: 0.92	Outliers: 5 of 131	Poor rotamers: 4 of 115		Outliers:	_
				Favored				
A 84	VAL	50	-	(89.66%) Isoleucine or valine / -60.1,-48.0 Favored	95.8% ( <i>t</i> ) chi angles: 176	0.072Å	-	-
A 85	SER	50	-	(71.96%)	55.4% ( <i>m</i> ) chi angles: 299 7	0.079Å	-	-

				General / -57.2,-37.3	em ungles. 2557			
A 86	LYS	50	-	Favored (58.36%) General / -73.3,-44.7	70.3% ( <i>mmtt</i> ) chi angles: 285.4,293.1,176.5,186.7	0.094Å	-	-
A 87	ILE	50	-	Favored (69.92%) Isoleucine or valine / -68.3,-35.2	25.1% ( <i>mt</i> ) chi angles: 303.6,154.8	0.215Å	-	-
A 88	ALA	50	-	Favored (78.61%) General / -56.5,-47.8	-	0.07Å	-	-
A 89	GLN	50	-	Favored (75.52%) General / -55.3,-47.5	25.7% (tt0) chi angles: 189.8,198.1,309.9	0.064Å	-	-
A 90	TYR	50	-	Favored (41.74%) General / -72.7,-48.1	4.3% ( <i>m-30</i> ) chi angles: 315.5,325	0.117Å	-	-
A 91	LYS	50	-	Favored (60.64%) General / -74.8,-17.4	64.8% ( <i>mmtt</i> ) chi angles: 290.6,280.7,181.8,170.5	0.106Å	-	-
A 92	ARG	50	-	Favored (14.19%) General / -108.3,-16.7	27.4% ( <i>mtp180</i> ) chi angles: 303,153.9,74.1,162.1	0.176Å	-	-
A 93	GLU	50	-	Favored (12.87%) General / -92.7,-36.5	7.4% ( <i>pt-20</i> ) chi angles: 89.7,181,341.6	0.145Å	-	-
A 94	CYS	50	-	Favored (29.25%) Pre-proline / -138.6,79.4	35.9% ( <i>t</i> ) chi angles: 188.5	0.047Å	-	-
A 95	PRO	50	-	Favored (7.16%) Trans-proline /	11.4% ( <i>Cg_exo</i> ) chi angles: 323.1	0.11Å	-	-
A 96	SER	50	-	-46.0,-30.3 Favored (9.34%) General / -86.2,78.6	91.2% (p) chi angles: 65.9	0.062Å	-	-
. 07				Favored (21.25%)	20.7% (mt)	0 00 å		

A 9/	ILE	50	-	Isoleucine or valine / -145.2,137.9	chi angles: 287.2,185.1	0.08A	-	-
A 98	PHE	50	-	Favored (9.91%) General / -92.3,170.3	49.6% ( <i>m-85</i> ) chi angles: 307.1,293.5	0.049Å	-	-
A 99	ALA	50	-	Favored (87.73%) General / -60.5,-39.4	-	0.091Å	-	-
A 100	TRP	50	-	Favored (77.09%) General / -68.8,-35.5	63.8% ( <i>p</i> -90) chi angles: 54,271.4	0.179Å	-	-
A 101	GLU	50	-	Favored (81.81%) General / -61.7,-36.7	47.6% ( <i>mt-10</i> ) chi angles: 292.6,188.2,281.8	0.106Å	-	-
A 102	ILE	50	-	Favored (40.61%) Isoleucine or valine / -71.1,-30.4	51.2% ( <i>mt</i> ) chi angles: 303.7,181	0.32Å	-	-
				Favored				
A 103	ARG	50	-	(87.75%) General / -60.9,-39.1	31.6% ( <i>ttt180</i> ) chi angles: 202.6,169.5,184.7,151.6		-	-
	ARG <b>Alt Res</b>		- Clash > 0.4Å	(87.75%) General /	chi angles: 202.6,169.5,184.7,151.6	Сβ	Bond lengths	- Bond angles
		High B	<b>0.4Å</b> Clashscore:	(87.75%) General / -60.9,-39.1  Ramachandran	chi angles: 202.6,169.5,184.7,151.6	Cβ deviation Outliers:	lengths	<b>angles</b> Outliers: 10
		<b>High B</b> Avg:	<b>0.4Å</b> Clashscore:	(87.75%) General / -60.9,-39.1  Ramachandran  Outliers: 5 of	chi angles: 202.6,169.5,184.7,151.6 <b>Rotamer</b> Poor rotamers: 4 of	Cβ deviation Outliers:	<b>lengths</b> Outliers: 0	<b>angles</b> Outliers: 10
#	Alt Res	<b>High B</b> Avg: 54.96	<b>0.4Å</b> Clashscore:	(87.75%) General / -60.9,-39.1  Ramachandran  Outliers: 5 of 131  Favored (52.64%) General /	chi angles: 202.6,169.5,184.7,151.6 <b>Rotamer</b> Poor rotamers: 4 of 115  26.1% ( <i>m</i> -20)	Cβ deviation Outliers: 4 of 122 0.157Å	<b>lengths</b> Outliers: 0	<b>angles</b> Outliers: 10
# A 104	Alt Res	High B Avg: 54.96	<b>0.4Å</b> Clashscore:	(87.75%) General / -60.9,-39.1  Ramachandran  Outliers: 5 of 131 Favored (52.64%) General / -80.8,-16.8 Favored (99.1%) General /	chi angles: 202.6,169.5,184.7,151.6  Rotamer  Poor rotamers: 4 of 115  26.1% (m-20) chi angles: 282.7,13.3	Cβ deviation Outliers: 4 of 122 0.157Å	<b>lengths</b> Outliers: 0	<b>angles</b> Outliers: 10

A 108	SER	50	-	Favored (11.82%) General / -99.1,-31.3	82.6% ( <i>p</i> ) chi angles: 60.7	0.167Å	-	-
A 109	GLU	50	-	Favored (54.84%) General / -77.0,-27.6	21.7% ( <i>mt-10</i> ) chi angles: 284.2,205.1,26.4	0.114Å	-	-
A 110	GLY	50	-	Favored (7.85%) Glycine / 90.5,34.5	-	-	-	-
A 111	VAL	50	-	Favored (19.51%) Isoleucine or valine / -82.3,-44.2	95.5% ( <i>t</i> ) chi angles: 176	0.081Å	-	-
A 112	CYS	50	-	Favored (11.41%) General / -97.2,166.8	84.4% ( <i>m</i> ) chi angles: 300.2	0.024Å	-	-
A 113	THR	50	-	Allowed (0.16%) General / -98.7,-112.6	49.5% ( <i>m</i> ) chi angles: 305	0.243Å	-	OUTLIER(S) worst is C-CA- CB: 4.349 σ
A 114	ASN	50	-	Allowed (1.5%) General / -142.5,31.0	8.5% ( <i>m120</i> ) chi angles: 291.5,164.4	0.046Å	-	OUTLIER(S) worst is CA- CB-CG: 9.274
A 115	ASP	50	-	OUTLIER (0.04%) General / -166.0,20.7	1.3% ( <i>p30</i> ) chi angles: 36.3,16.2	0.057Å	-	OUTLIER(S) worst is CA- CB-CG: 5.121 σ
A 116	ASN	50	-	OUTLIER (0.01%) General / -172.4,35.4	23% ( <i>p30</i> ) chi angles: 49.5,15.1	0.03Å	-	-
A 117	ILE	50	-	Favored (53.4%) Pre-proline/	7.6% ( <i>tp</i> ) chi angles: 184.7,72	0.077Å	-	-
A 118	PRO	50	-	-97.1,123.3 Favored (92.48%) Trans-proline / -61.3,148.6	54% ( <i>Cg_exo</i> ) chi angles: 326.8	0.103Å	-	-
A 119	SER	50	-	Favored (4.84%) General / -96.7,179.8	46.4% ( <i>m</i> ) chi angles: 302.2	0.158Å	-	-

A 120	V	/AL	50	-	Favored (23.43%) Isoleucine or valine / -73.8,-51.7	48.2% (t) chi angles: 182.8	0.131Å	-	-
A 121	S	SER	50	-	Favored (92.39%) General / -64.6,-38.8	8% ( <i>t</i> ) chi angles: 195.4	0.087Å	-	-
A 122	S	SER	50	-	Favored (97.76%) General / -61.9,-41.4	68.8% ( <i>m</i> ) chi angles: 298	0.079Å	-	-
A 123	I	ILE	50	-	Favored (76.64%) Isoleucine or valine / -64.8,-36.0	20.6% ( <i>mt</i> ) chi angles: 298.2,189	0.256Å	-	-
#	Alt I	Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
			Avg: 54.96	Clashscore: 0.92	Outliers: 5 of 131	Poor rotamers: 4 of 115		Outliers:	Outliers: 10
A 124	A	SN	50	-	Favored (54.54%) General / -77.0,-27.8	7.8% ( <i>m-20</i> ) chi angles: 288.2,23.5	0.133Å	-	-
A 125	A	ĸRG	50	-	Favored (93.75%) General / -59.9,-45.0	35.8% ( <i>ttp85</i> ) chi angles: 183.4,160.9,51.3,63.8	0.106Å	-	-
A 126	A	ASP	50	-	Favored (89.18%) General / -62.3,-46.4	47.7% ( <i>t0</i> ) chi angles: 176.8,9.4	0.077Å	-	OUTLIER(S) worst is CA- CB-CG: 4.492 σ
A 127	L	.EU	50	-	Favored (62.72%) General / -53.4,-37.8	95.9% ( <i>mt</i> ) chi angles: 298.6,177.7	0.174Å	-	-
A 128	A	ĸRG	50	-	Favored (54.45%) General / -76.4,-25.4	81% ( <i>mtm-85</i> ) chi angles: 296.9,197.6,295,291	0.233Å	-	-
A 129	A	SN	50	-	Favored (90.14%) General / -66.0,-39.3	87.5% ( <i>m-20</i> ) chi angles: 295.5,317.9	0.081Å	-	-
					Favored	20 50/ (mt)	٥		

A 130	LEU	50	-	(61.23%) General / -73.1,-19.0	30.3 /o (IIII) chi angles: 300.9,163.3	0.105Å	-	-
A 131	ALA	50	-	Favored (68.37%) General / -62.5,-26.1	-	0.105Å	-	-
A 132	SER	50	-	OUTLIER (0.01%) General / -76.9,-126.9	11.5% (p) chi angles: 83.1	0.239Å	-	OUTLIER(S) worst is C-CA- CB: 4.288 σ
A 133	GLU	50	-	Allowed (0.34%) General / 56.4,-106.6	1.8% (tt0) chi angles: 190.4,226.6,288.2	0.198Å	-	OUTLIER(S) worst is C-N- CA: 7.21 σ
A 134	LYS	50	-	OUTLIER (0%) General / -48.9,14.8	1.3% ( <i>pttm</i> ) chi angles: 60.6,230.5,171.8,284.7	0.05Å	-	-
A 135	GLN	50	-	Favored (12.25%) General / -118.1,7.8	20.7% ( <i>mt-30</i> ) chi angles: 288,159.1,112.2	0.068Å	-	-
A 136	GLN	99.99	-	-	5% ( <i>tp-100</i> ) chi angles: 177,47,205.3	0.082Å	-	OUTLIER(S) worst is CB- CG-CD: 4.138 σ
B1001	DAD	100.5	-	-	-	-	_	-
B1002	DAD	102.72	-	-	-	-	-	-
B1003	DGU	95.24	-	-	-	-	-	-
B1004	DCY	83.06	-	-	-	-	-	-
B1005	DAD	74.41	-	-	-	-	-	-
B1006	DTY	64.72	-	-	-	-	-	-
B1007	DTY	55.15	-	-	-	-	-	-
# /	Alt Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg:	Clashscore:	Outliers: 5 of	Poor rotamers: 4 of	Outliers:	Outliers:	Outliers: 10
		54.96	0.92	131	115	4 of 122	0 of 133	of 133
B1008	DTY	63.52	-	-	-	-	-	-
B1009	DTY	50.43	-	-	-	-	-	-
B1010	DCY	60.49	-	-	-	-	-	-
B1011	DAD	62.65	-	-	-	-	-	-
B1012	DCY	60.46	-	-	-	-	-	-
B1013	DGU	62.87	-	-	-	-	-	-
B1014	DCY	66.18	-	-	-	-	-	-
D101F		F2 02						

RIUI2	UAU	53.92	-	-	-	-	-	-
B1016	DTY	60.67	-	-	-	-	-	-
B1017	DGU	53.38	-	-	-	-	-	-
B1018	DAD	45.88	-	-	-	-	-	-
B1019	DGU	45.01	-	-	-	-	-	-
B1020	DTY	47.07	-	-	-	-	-	-
B1021	DGU	57.3	-	-	-	-	-	-
B1022	DCY	69.79	-	-	-	-	-	-
B1023	DAD	85.8	-	-	-	-	-	-
B1024	DCY	89.37	-	-	-	-	-	-
B1025	DAD	84.51	-	-	-	-	-	-
B1026	DGU	87.98	-	-	-	-	-	-
C2001	DTY	75.67	-	-	-	-	-	-
# A	It Res	High B	Clash > 0.4Å	Ramachandran	Rotamer	Cβ deviation	Bond lengths	Bond angles
		Avg:			Poor rotamers: 4 of			
		54.96	0.92	131	115	4 of 122	0 of 133	of 133
C2002		77.07	-	-	-	-	-	-
C2003		78.78	-	-	-	-	-	-
C2004		48.81	-	-	-	-	-	-
C2005		57.01	-	-	-	-	-	-
C2006		69.23	-	-	-	-	-	-
C2007		76.12	-	-	-	-	-	-
C2008		80.78	-	-	-	-	-	-
C2009		74.88	-	-	-	-	-	-
C2010		75.39	-	-	-	-	-	-
C2011		73.29	-	-	-	-	-	-
C2012	DCY	61.25	-	-	-	-	-	-
C2013	DAD	63.28	0.46Å H2 with A 72 GLY HA2	-	-	-	-	-
C2014	DTY	61.51	-	-	-	-	-	-
C2015	DGU	43.87	-	-	-	-	-	-
C2016	DCY	43.32	-	-	-	-	-	-
C2017	DGU	43.75	-	-	-	-	-	-
C2018	DTY	44.55	-	-	-	-	-	-
C2019	DGU	51.15	0.437Å OP2 with A 9 ASN HB2	-	-	-	-	-
C2020	DAD	67.99	-	-	-	-	-	-
C2021	DAD	76 69	-	-	-	_	-	-

Сβ **Bond Bond** Clash > Ramachandran Alt Res High B # **Rotamer** deviation lengths angles Avg: Clashscore: Outliers: 5 of Poor rotamers: 4 of Outliers: Outliers: 0 4 of 122 0 of 133 54.96 0.92 131 115 of 133 DAD 70.65 C2022 C2023 DAD 68.53 C2024 DTY 68.92 C2025 DGU 68.54 C2026 DCY 62.68

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