wwPDB EM Validation Summary Report (i)

Jan 14, 2024 – 12:09 AM JST

PDB ID	:	8IYD
EMDB ID	:	EMD-35818
Title	:	Tail cap of phage lambda tail
Authors	:	Wang, J.W.; Wang, C.
Deposited on	:	2023-04-04
Resolution	:	3.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

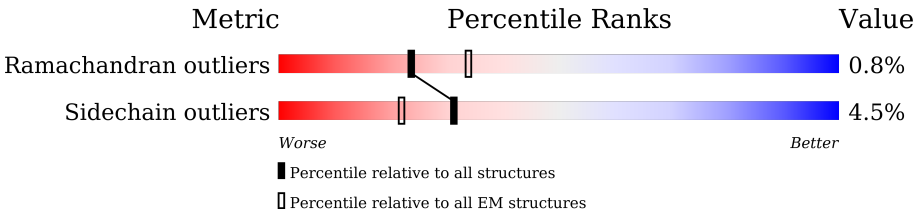
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	246	96%
1	B	246	96%
1	C	246	95%
1	D	246	94% 5%
1	E	246	96%
1	F	246	95%
1	H	246	97%
1	I	246	95%
1	J	246	94%
1	L	246	93% 6%

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Mol	Chain	Length	Quality of chain
1	M	246	97%
1	N	246	93% 6%
1	O	246	95%
1	P	246	93% 6%
1	R	246	96%
1	S	246	96%
1	T	246	96%
1	V	246	93% 6%
1	X	246	93% 6%
1	Y	246	95%
1	a	246	97%
1	b	246	93% 5%
1	c	246	95%
1	v	246	96%
2	G	131	97%
2	K	131	96%
2	Q	131	93% 5%
2	U	131	95% 5%
2	W	131	96%
2	u	131	95%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 49344 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tail tube protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	B	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	C	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	a	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	b	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	c	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	V	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	v	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	D	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	E	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	F	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	H	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	I	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	J	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	L	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	M	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	N	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	P	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	R	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	S	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	T	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	X	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		
1	Y	244	Total	C	N	O	S	0	0
			1799	1124	303	367	5		

- Molecule 2 is a protein called Tail tube terminator protein.

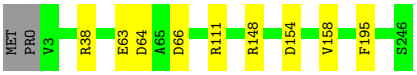
Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	131	Total	C	N	O	S	0	0
			1032	655	159	213	5		
2	u	130	Total	C	N	O	S	0	0
			1024	650	158	212	4		
2	G	131	Total	C	N	O	S	0	0
			1032	655	159	213	5		
2	K	130	Total	C	N	O	S	0	0
			1024	650	158	212	4		
2	Q	131	Total	C	N	O	S	0	0
			1032	655	159	213	5		
2	W	130	Total	C	N	O	S	0	0
			1024	650	158	212	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

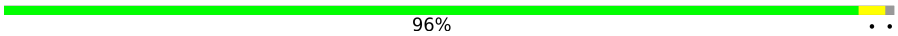
• Molecule 1: Tail tube protein

Chain A:



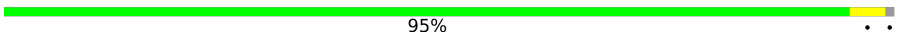
• Molecule 1: Tail tube protein

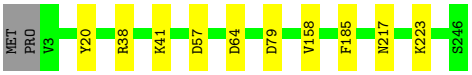
Chain B:



• Molecule 1: Tail tube protein

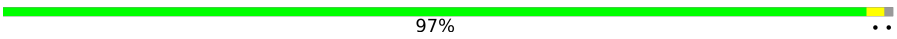
Chain C:





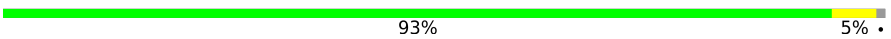
• Molecule 1: Tail tube protein

Chain a:



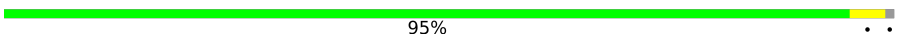
• Molecule 1: Tail tube protein

Chain b:



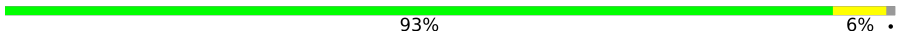
• Molecule 1: Tail tube protein

Chain c:



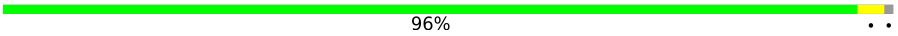
• Molecule 1: Tail tube protein

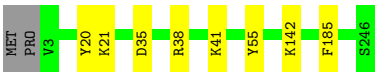
Chain V:



• Molecule 1: Tail tube protein

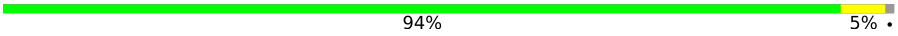
Chain v:

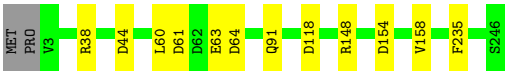




• Molecule 1: Tail tube protein

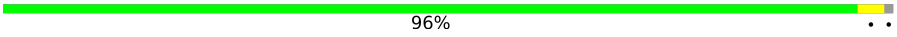
Chain D:

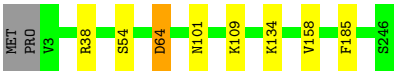




• Molecule 1: Tail tube protein

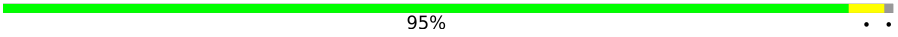
Chain E:





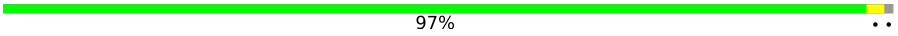
• Molecule 1: Tail tube protein

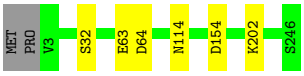
Chain F:



• Molecule 1: Tail tube protein

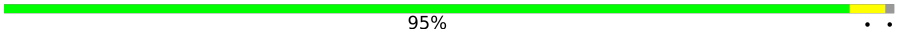
Chain H:





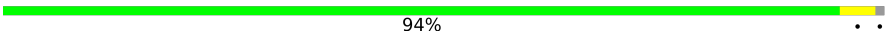
• Molecule 1: Tail tube protein

Chain I:



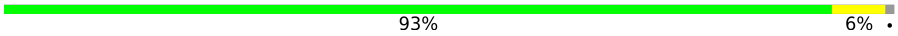
• Molecule 1: Tail tube protein

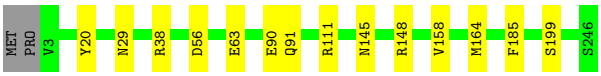
Chain J:



• Molecule 1: Tail tube protein

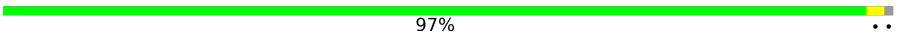
Chain L:

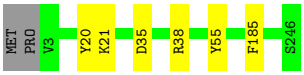




• Molecule 1: Tail tube protein

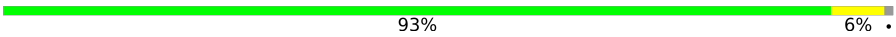
Chain M:





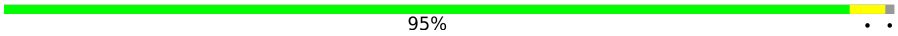
• Molecule 1: Tail tube protein

Chain N:



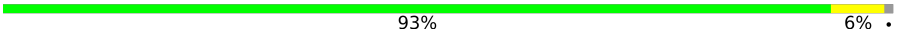
• Molecule 1: Tail tube protein

Chain O:



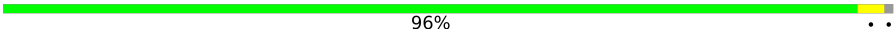
• Molecule 1: Tail tube protein

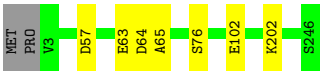
Chain P:



• Molecule 1: Tail tube protein

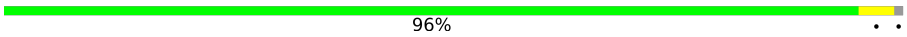
Chain R:

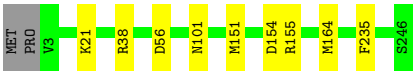




• Molecule 1: Tail tube protein

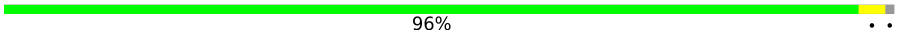
Chain S:





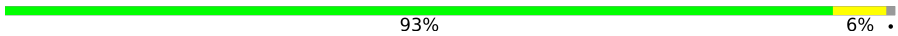
• Molecule 1: Tail tube protein

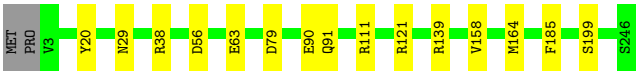
Chain T:



• Molecule 1: Tail tube protein

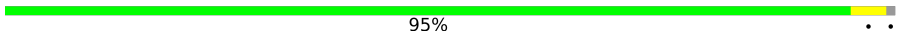
Chain X:





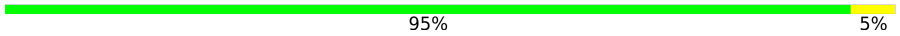
• Molecule 1: Tail tube protein

Chain Y:



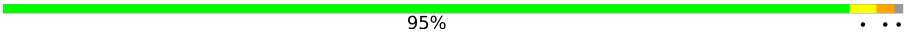
• Molecule 2: Tail tube terminator protein

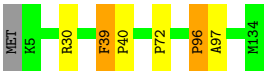
Chain U:



• Molecule 2: Tail tube terminator protein

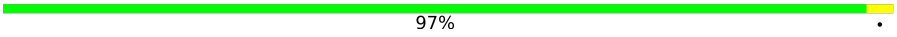
Chain u:

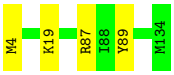




• Molecule 2: Tail tube terminator protein

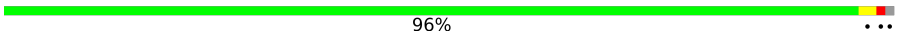
Chain G:

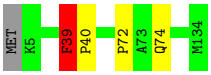




• Molecule 2: Tail tube terminator protein

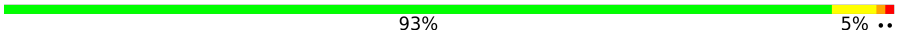
Chain K:

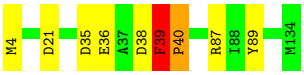




• Molecule 2: Tail tube terminator protein

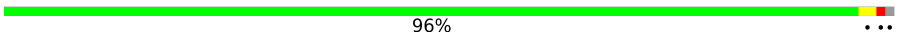
Chain Q:





• Molecule 2: Tail tube terminator protein

Chain W:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15959	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.29	0/1834	0.58	0/2505
1	B	0.29	0/1834	0.58	0/2505
1	C	0.30	0/1834	0.57	0/2505
1	D	0.30	0/1834	0.57	0/2505
1	E	0.28	0/1834	0.57	0/2505
1	F	0.31	0/1834	0.59	0/2505
1	H	0.29	0/1834	0.56	0/2505
1	I	0.30	0/1834	0.59	0/2505
1	J	0.30	0/1834	0.59	0/2505
1	L	0.29	0/1834	0.54	0/2505
1	M	0.27	0/1834	0.54	0/2505
1	N	0.29	0/1834	0.58	0/2505
1	O	0.29	0/1834	0.58	0/2505
1	P	0.30	0/1834	0.58	0/2505
1	R	0.30	0/1834	0.56	0/2505
1	S	0.30	0/1834	0.58	0/2505
1	T	0.31	0/1834	0.58	0/2505
1	V	0.29	0/1834	0.55	0/2505
1	X	0.30	0/1834	0.55	0/2505
1	Y	0.29	0/1834	0.58	0/2505
1	a	0.29	0/1834	0.54	0/2505
1	b	0.31	0/1834	0.58	0/2505
1	c	0.31	0/1834	0.59	1/2505 (0.0%)
1	v	0.27	0/1834	0.54	0/2505
2	G	0.32	0/1058	0.59	0/1444
2	K	0.32	0/1050	0.59	0/1434
2	Q	0.33	0/1058	0.63	1/1444 (0.1%)
2	U	0.30	0/1058	0.58	0/1444
2	W	0.33	0/1050	0.58	0/1434
2	u	0.32	0/1050	0.61	0/1434
All	All	0.30	0/50340	0.57	2/68754 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	1
2	U	0	1
2	W	0	1
2	u	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	39	PHE	CB-CA-C	5.61	121.63	110.40
1	c	187	PRO	N-CA-C	-5.40	98.05	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	39	PHE	Peptide
2	U	39	PHE	Peptide
2	W	39	PHE	Peptide
2	u	39	PHE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/246 (98%)	209 (86%)	32 (13%)	1 (0%)	34	69
1	B	242/246 (98%)	217 (90%)	24 (10%)	1 (0%)	34	69
1	C	242/246 (98%)	220 (91%)	20 (8%)	2 (1%)	19	54
1	D	242/246 (98%)	210 (87%)	31 (13%)	1 (0%)	34	69
1	E	242/246 (98%)	218 (90%)	22 (9%)	2 (1%)	19	54
1	F	242/246 (98%)	220 (91%)	19 (8%)	3 (1%)	13	44
1	H	242/246 (98%)	216 (89%)	25 (10%)	1 (0%)	34	69
1	I	242/246 (98%)	215 (89%)	27 (11%)	0	100	100
1	J	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	19	54
1	L	242/246 (98%)	222 (92%)	18 (7%)	2 (1%)	19	54
1	M	242/246 (98%)	226 (93%)	16 (7%)	0	100	100
1	N	242/246 (98%)	208 (86%)	32 (13%)	2 (1%)	19	54
1	O	242/246 (98%)	218 (90%)	21 (9%)	3 (1%)	13	44
1	P	242/246 (98%)	221 (91%)	19 (8%)	2 (1%)	19	54
1	R	242/246 (98%)	223 (92%)	17 (7%)	2 (1%)	19	54
1	S	242/246 (98%)	214 (88%)	28 (12%)	0	100	100
1	T	242/246 (98%)	216 (89%)	23 (10%)	3 (1%)	13	44
1	V	242/246 (98%)	224 (93%)	16 (7%)	2 (1%)	19	54
1	X	242/246 (98%)	219 (90%)	20 (8%)	3 (1%)	13	44
1	Y	242/246 (98%)	224 (93%)	18 (7%)	0	100	100
1	a	242/246 (98%)	224 (93%)	18 (7%)	0	100	100
1	b	242/246 (98%)	213 (88%)	28 (12%)	1 (0%)	34	69
1	c	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	19	54
1	v	242/246 (98%)	225 (93%)	17 (7%)	0	100	100
2	G	129/131 (98%)	109 (84%)	20 (16%)	0	100	100
2	K	128/131 (98%)	120 (94%)	5 (4%)	3 (2%)	6	28
2	Q	129/131 (98%)	108 (84%)	18 (14%)	3 (2%)	6	28
2	U	129/131 (98%)	107 (83%)	21 (16%)	1 (1%)	19	54
2	W	128/131 (98%)	117 (91%)	8 (6%)	3 (2%)	6	28
2	u	128/131 (98%)	113 (88%)	10 (8%)	5 (4%)	3	18
All	All	6579/6690 (98%)	5906 (90%)	623 (10%)	50 (1%)	24	54

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	VAL
1	B	158	VAL
1	C	158	VAL
2	u	39	PHE
2	u	40	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/196 (99%)	186 (96%)	8 (4%)	30	64
1	B	194/196 (99%)	188 (97%)	6 (3%)	40	70
1	C	194/196 (99%)	186 (96%)	8 (4%)	30	64
1	D	194/196 (99%)	183 (94%)	11 (6%)	20	52
1	E	194/196 (99%)	187 (96%)	7 (4%)	35	67
1	F	194/196 (99%)	186 (96%)	8 (4%)	30	64
1	H	194/196 (99%)	189 (97%)	5 (3%)	46	74
1	I	194/196 (99%)	184 (95%)	10 (5%)	23	55
1	J	194/196 (99%)	183 (94%)	11 (6%)	20	52
1	L	194/196 (99%)	182 (94%)	12 (6%)	18	49
1	M	194/196 (99%)	188 (97%)	6 (3%)	40	70
1	N	194/196 (99%)	181 (93%)	13 (7%)	16	46
1	O	194/196 (99%)	186 (96%)	8 (4%)	30	64
1	P	194/196 (99%)	181 (93%)	13 (7%)	16	46
1	R	194/196 (99%)	189 (97%)	5 (3%)	46	74
1	S	194/196 (99%)	185 (95%)	9 (5%)	27	59
1	T	194/196 (99%)	187 (96%)	7 (4%)	35	67
1	V	194/196 (99%)	182 (94%)	12 (6%)	18	49
1	X	194/196 (99%)	182 (94%)	12 (6%)	18	49
1	Y	194/196 (99%)	183 (94%)	11 (6%)	20	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	194/196 (99%)	189 (97%)	5 (3%)	46	74
1	b	194/196 (99%)	180 (93%)	14 (7%)	14	44
1	c	194/196 (99%)	185 (95%)	9 (5%)	27	59
1	v	194/196 (99%)	186 (96%)	8 (4%)	30	64
2	G	109/109 (100%)	105 (96%)	4 (4%)	34	66
2	K	108/109 (99%)	106 (98%)	2 (2%)	57	81
2	Q	109/109 (100%)	101 (93%)	8 (7%)	14	43
2	U	109/109 (100%)	105 (96%)	4 (4%)	34	66
2	W	108/109 (99%)	106 (98%)	2 (2%)	57	81
2	u	108/109 (99%)	106 (98%)	2 (2%)	57	81
All	All	5307/5358 (99%)	5067 (96%)	240 (4%)	31	60

5 of 240 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	118	ASP
1	X	90	GLU
1	L	164	MET
1	X	38	ARG
1	Y	150	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	c	74	GLN
1	H	177	GLN
1	S	94	GLN
1	X	94	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.