



## wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 13, 2016 – 03:52 PM EST

PDB ID : 5FIK  
EMDB ID: : EMD-3169  
Title : Bovine mitochondrial ATP synthase state 3a  
Authors : Zhou, A.; Rohou, A.; Schep, D.G.; Bason, J.V.; Montgomery, M.G.; Walker, J.E.; Grigorieff, N.; Rubinstein, J.L.  
Deposited on : 2015-09-28  
Resolution : 6.40 Å(reported)  
Based on PDB ID : 2CLY, 2XND, 2WSS

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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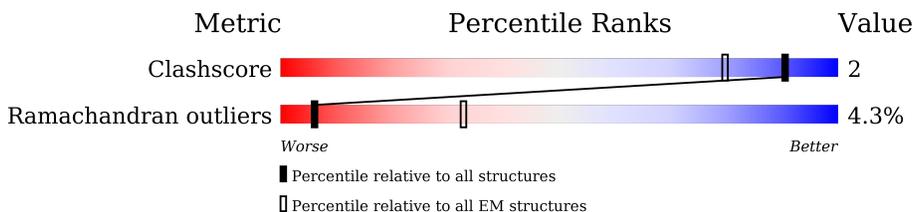
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

# 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 6.40 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)
Clashscore	114402	924
Ramachandran outliers	111179	726

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	510	89% 10% .
1	B	510	85% 9% . 6%
1	C	510	88% 7% . 5%
2	D	482	89% 8% .
2	E	482	88% 8% . .
2	F	482	85% 11% . .
3	G	273	78% 17% . .
4	H	146	71% 19% 10%
5	I	50	86% 8% 6%
6	J	72	97% .
6	K	72	99% .

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Mol	Chain	Length	Quality of chain
6	L	72	100%
6	M	72	97% .
6	N	72	100%
6	O	72	99% .
6	P	72	99% .
6	Q	72	97% .
7	S	190	64% 22% . . 12%
8	T	174	83% 13% . .
9	U	124	82% 11% . . .
10	V	77	74% 10% . 13%
11	W	217	92% 7% .

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 18545 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	A	509	2035	1018	509	508	0	0
1	B	480	1918	960	480	478	0	0
1	C	487	1947	974	487	486	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CONFLICT	UNP P19483
B	481	GLY	SER	CONFLICT	UNP P19483
C	481	GLY	SER	CONFLICT	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	D	467	1867	934	467	466	0	0
2	E	466	1863	932	466	465	0	0
2	F	466	1863	932	466	465	0	0

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	G	264	1053	528	264	261	0	0

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	H	131	523	262	131	130	0	0

- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	I	47	187	94	47	46	0	0

- Molecule 6 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	J	72	288	144	72	72	0	0
6	K	72	288	144	72	72	0	0
6	L	72	288	144	72	72	0	0
6	M	72	288	144	72	72	0	0
6	N	72	288	144	72	72	0	0
6	O	72	288	144	72	72	0	0
6	P	72	288	144	72	72	0	0
6	Q	72	288	144	72	72	0	0

- Molecule 7 is a protein called ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	S	168	669	334	168	167	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	129	THR	ALA	CONFLICT	UNP P13621

- Molecule 8 is a protein called ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	T	174	697	348	174	175	0	0

- Molecule 9 is a protein called ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	U	122	485	242	122	121	0	1

- Molecule 10 is a protein called ATP SYNTHASE-COUPPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	V	67	265	132	67	66	0	1

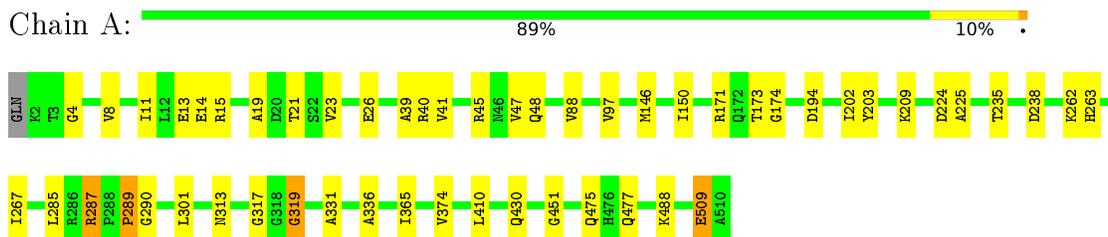
- Molecule 11 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	W	217	869	434	217	218	0	0

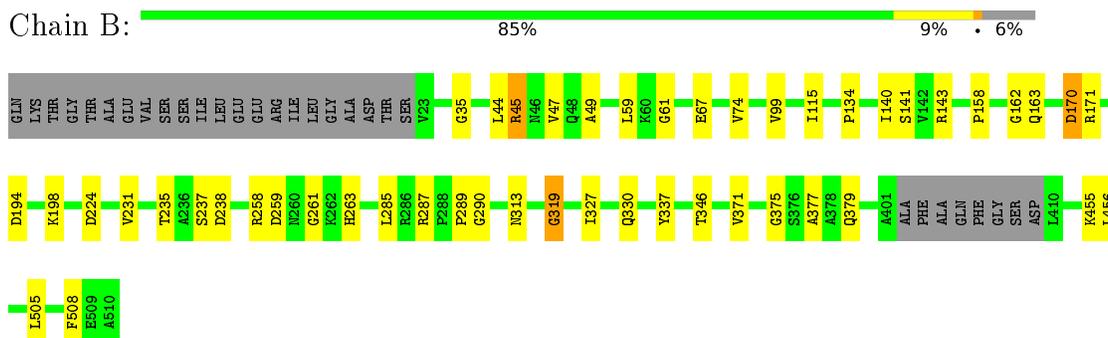
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

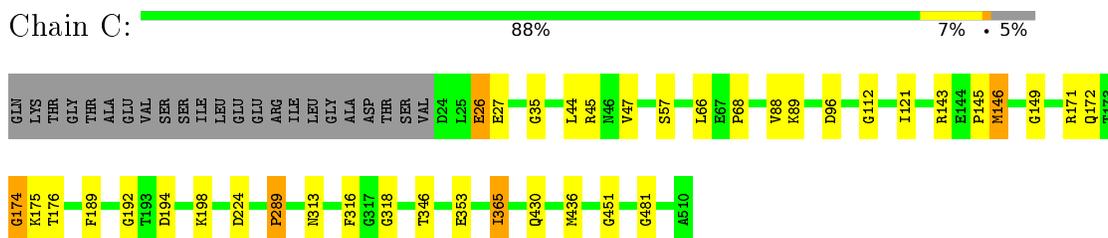
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



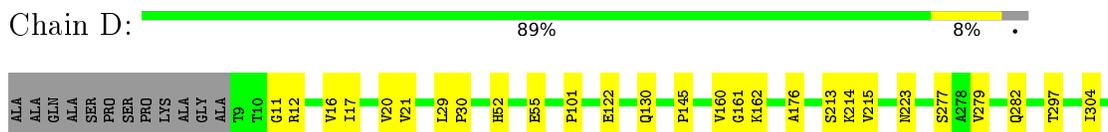
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



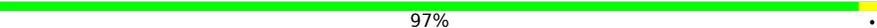
- Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



- Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





Chain J:  97%



- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain K:  99%



- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain M:  97%



- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain O:  99%

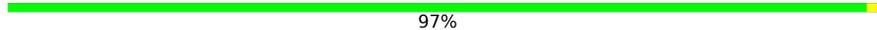


- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain P:  99%

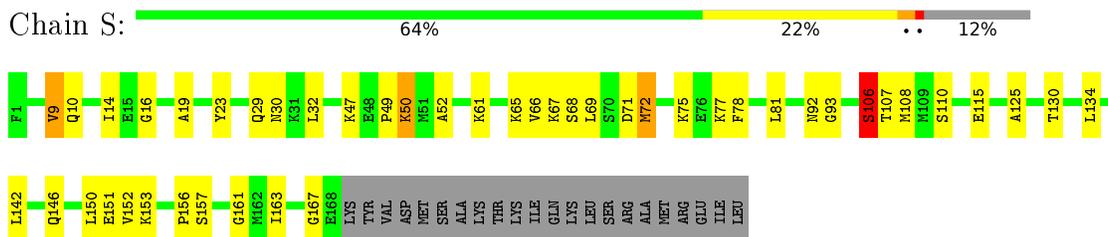


- Molecule 6: ATP SYNTHASE F(0) COMPLEX SUBUNIT C1, MITOCHONDRIAL

Chain Q:  97%



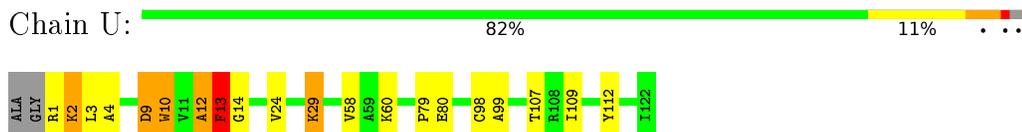
- Molecule 7: ATP SYNTHASE SUBUNIT O, MITOCHONDRIAL



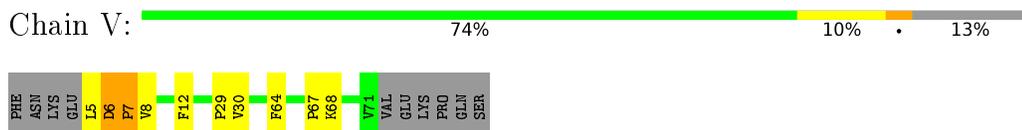
- Molecule 8: ATP SYNTHASE F(0) COMPLEX SUBUNIT B1, MITOCHONDRIAL



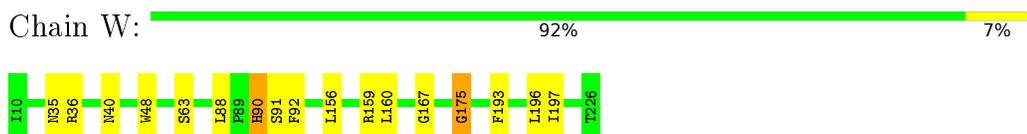
- Molecule 9: ATP SYNTHASE SUBUNIT D, MITOCHONDRIAL



- Molecule 10: ATP SYNTHASE-COUPLING FACTOR 6, MITOCHONDRIAL



- Molecule 11: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	24140	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4100	Depositor
Magnification	30487	Depositor
Image detector	GATAN K2 (4K X 4K)	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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  >2	RMSZ	# Z  >2
1	A	1.79	2/2034 (0.1%)	1.43	19/2541 (0.7%)
1	B	1.80	1/1916 (0.1%)	1.42	19/2392 (0.8%)
1	C	1.84	7/1946 (0.4%)	1.39	14/2431 (0.6%)
10	V	0.81	1/264 (0.4%)	1.43	5/329 (1.5%)
11	W	0.86	4/868 (0.5%)	0.98	2/1082 (0.2%)
2	D	1.78	3/1866 (0.2%)	1.39	12/2331 (0.5%)
2	E	1.81	1/1862 (0.1%)	1.49	21/2326 (0.9%)
2	F	1.84	4/1862 (0.2%)	1.50	24/2326 (1.0%)
3	G	2.04	5/1050 (0.5%)	1.56	16/1308 (1.2%)
4	H	2.18	7/522 (1.3%)	1.79	14/651 (2.2%)
5	I	1.96	1/186 (0.5%)	1.28	1/231 (0.4%)
6	J	0.30	0/287	0.41	0/357
6	K	0.30	0/287	0.42	0/357
6	L	0.31	0/287	0.45	0/357
6	M	0.29	0/287	0.44	0/357
6	N	0.28	0/287	0.40	0/357
6	O	0.31	0/287	0.41	0/357
6	P	0.29	0/287	0.43	0/357
6	Q	0.30	0/287	0.44	0/357
7	S	1.69	0/668	1.78	12/834 (1.4%)
8	T	1.10	4/696 (0.6%)	1.54	17/867 (2.0%)
9	U	0.99	3/484 (0.6%)	1.39	10/604 (1.7%)
All	All	1.63	43/18520 (0.2%)	1.37	186/23109 (0.8%)

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
1	A	0	4
1	B	0	2
1	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	V	0	6
11	W	0	10
2	D	0	6
2	E	0	2
2	F	0	2
3	G	0	4
4	H	0	2
7	S	0	5
8	T	0	21
9	U	0	14
All	All	0	79

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	U	10	TRP	N-CA	8.48	1.63	1.46
8	T	28	ILE	CA-C	8.06	1.74	1.52
8	T	161	ILE	C-O	-7.20	1.09	1.23
3	G	261	GLU	CA-C	-7.02	1.34	1.52
3	G	139	GLY	CA-C	-6.24	1.41	1.51

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	110	SER	C-N-CA	15.61	160.72	121.70
8	T	161	ILE	CA-C-O	-15.32	87.94	120.10
8	T	158	LYS	O-C-N	11.98	141.86	122.70
10	V	6	ASP	O-C-N	-11.58	99.10	121.10
8	T	162	ALA	N-CA-C	11.23	141.33	111.00

There are no chirality outliers.

5 of 79 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	THR	Mainchain,Peptide
1	A	287	ARG	Peptide
1	A	336	ALA	Peptide
1	B	371	VAL	Peptide
1	B	379	GLN	Peptide

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2035	0	589	4	0
1	B	1918	0	553	8	0
1	C	1947	0	562	6	0
2	D	1867	0	533	3	0
2	E	1863	0	532	1	0
2	F	1863	0	532	7	0
3	G	1053	0	283	6	0
4	H	523	0	140	1	0
5	I	187	0	53	2	0
6	J	288	0	92	0	0
6	K	288	0	92	0	0
6	L	288	0	92	0	0
6	M	288	0	92	0	0
6	N	288	0	92	0	0
6	O	288	0	92	0	0
6	P	288	0	92	0	0
6	Q	288	0	92	0	0
7	S	669	0	178	9	0
8	T	697	0	182	7	0
9	U	485	0	121	0	0
10	V	265	0	68	0	0
11	W	869	0	226	3	0
All	All	18545	0	5288	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 50 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:ILE:H	2:F:114:ALA:H	1.24	0.83
1:B:49:ALA:H	2:F:69:LEU:H	1.31	0.79
7:S:163:ILE:O	7:S:167:GLY:O	2.16	0.63
8:T:19:VAL:O	11:W:91:SER:N	2.32	0.62
1:C:149:GLY:HA3	1:C:436:MET:H	1.66	0.60

There are no symmetry-related clashes.

## 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	507/510 (99%)	452 (89%)	30 (6%)	25 (5%)	3	31
1	B	476/510 (93%)	419 (88%)	38 (8%)	19 (4%)	4	35
1	C	485/510 (95%)	443 (91%)	26 (5%)	16 (3%)	5	40
2	D	465/482 (96%)	418 (90%)	33 (7%)	14 (3%)	5	42
2	E	464/482 (96%)	409 (88%)	35 (8%)	20 (4%)	3	34
2	F	464/482 (96%)	417 (90%)	27 (6%)	20 (4%)	3	34
3	G	258/273 (94%)	199 (77%)	34 (13%)	25 (10%)	1	14
4	H	129/146 (88%)	114 (88%)	8 (6%)	7 (5%)	2	29
5	I	45/50 (90%)	38 (84%)	6 (13%)	1 (2%)	8	49
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	6	43
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14	58
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100	100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	6	43
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100	100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14	58
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	14	58
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	6	43
7	S	166/190 (87%)	117 (70%)	27 (16%)	22 (13%)	0	7
8	T	172/174 (99%)	157 (91%)	10 (6%)	5 (3%)	6	43
9	U	120/124 (97%)	102 (85%)	11 (9%)	7 (6%)	2	27
10	V	65/77 (84%)	53 (82%)	8 (12%)	4 (6%)	2	25
11	W	215/217 (99%)	191 (89%)	21 (10%)	3 (1%)	14	58
All	All	4591/4803 (96%)	4026 (88%)	368 (8%)	197 (4%)	6	34

5 of 197 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	14	GLU
1	A	45	ARG
1	A	48	GLN
1	A	171	ARG

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA [i](#)

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 carbohydrates 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.