



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

Aug 17, 2017 – 12:42 PM EDT

PDB ID : 2C9F  
EMDB ID: : EMD-1178  
Title : THE QUASI-ATOMIC MODEL OF THE ADENOVIRUS TYPE 3 PENTON  
DODECAHEDRON  
Authors : Fuschiotti, P.; Schoehn, G.; Fender, P.; Fabry, C.M.S.; Hewat, E.A.;  
Chroboczek, J.; Ruigrok, R.W.H.; Conway, J.F.  
Deposited on : unknown  
Resolution : 16.50 Å(reported)

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.

---

MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

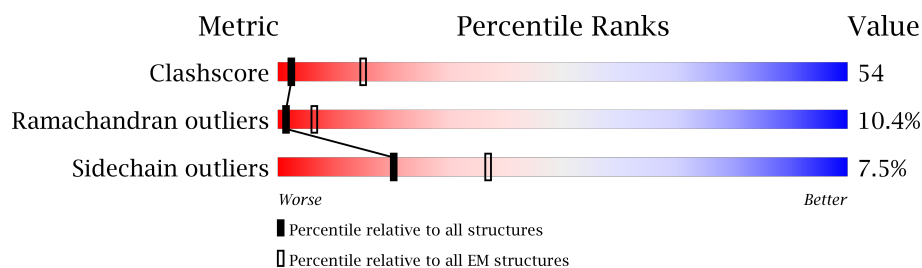
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 16.50 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	523	
1	B	523	
1	C	523	
1	D	523	
1	E	523	
2	S	19	
2	T	19	
2	U	19	
2	V	19	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	W	19	 A horizontal bar chart showing the quality of chain W. The bar is divided into four segments: green (26%), yellow (21%), orange (5%), and grey (47%).

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18025 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 PENTON PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	B	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	C	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	D	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		
1	E	440	Total	C	N	O	S	0	0
			3519	2227	608	672	12		

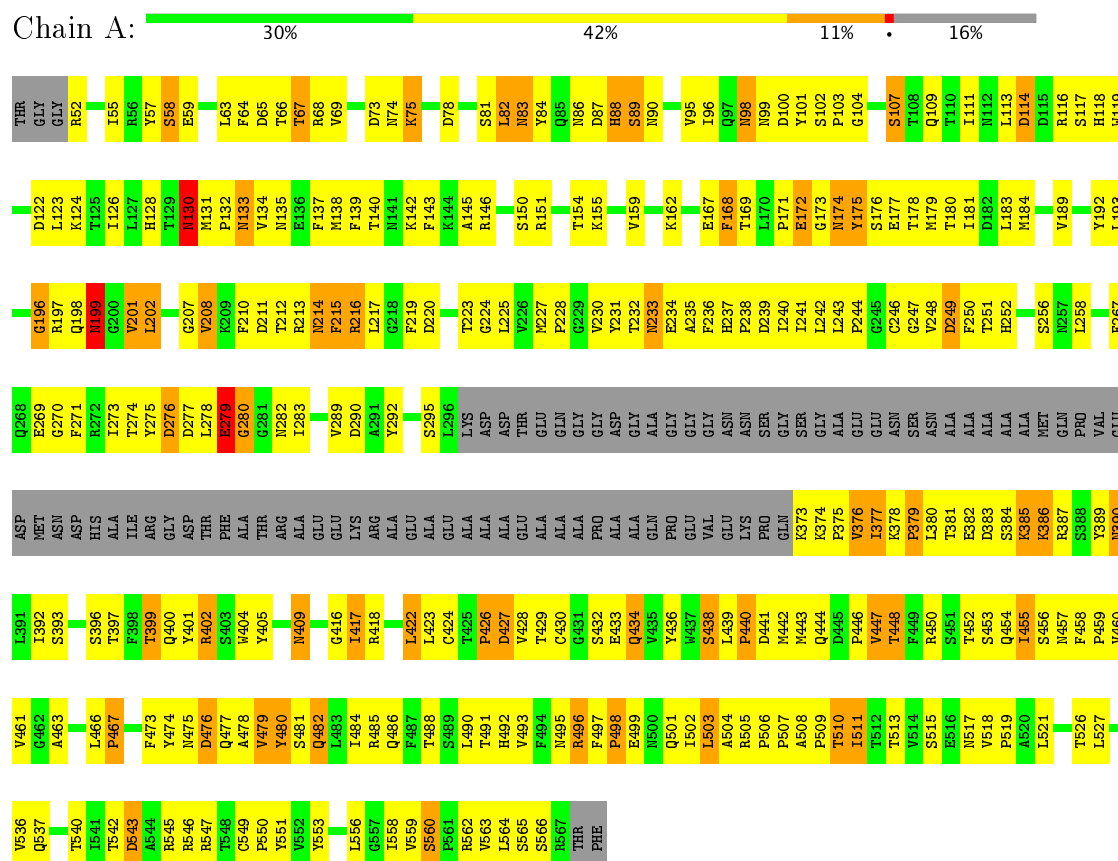
- Molecule 2 is a protein called FIBER.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	S	10	Total	C	N	O	0	0
			86	58	11	17		
2	T	10	Total	C	N	O	0	0
			86	58	11	17		
2	U	10	Total	C	N	O	0	0
			86	58	11	17		
2	V	10	Total	C	N	O	0	0
			86	58	11	17		
2	W	10	Total	C	N	O	0	0
			86	58	11	17		

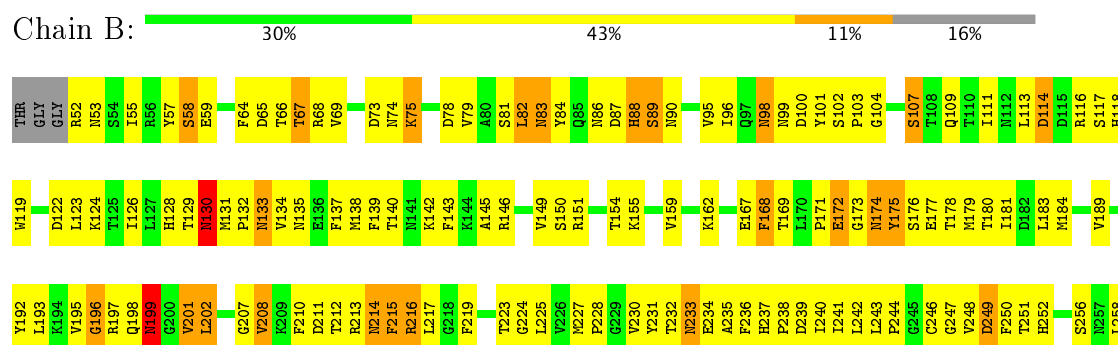
### 3 Residue-property plots

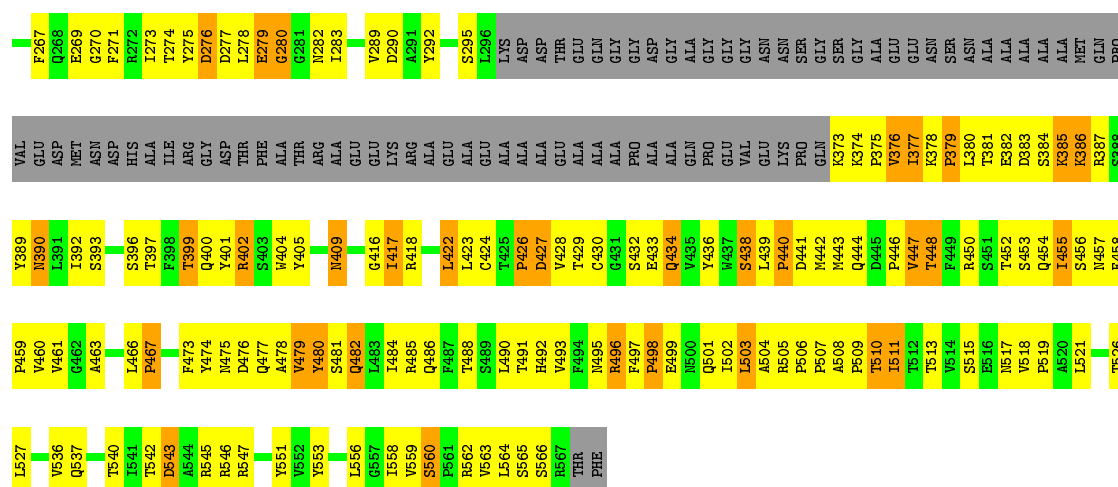
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: PENTON PROTEIN



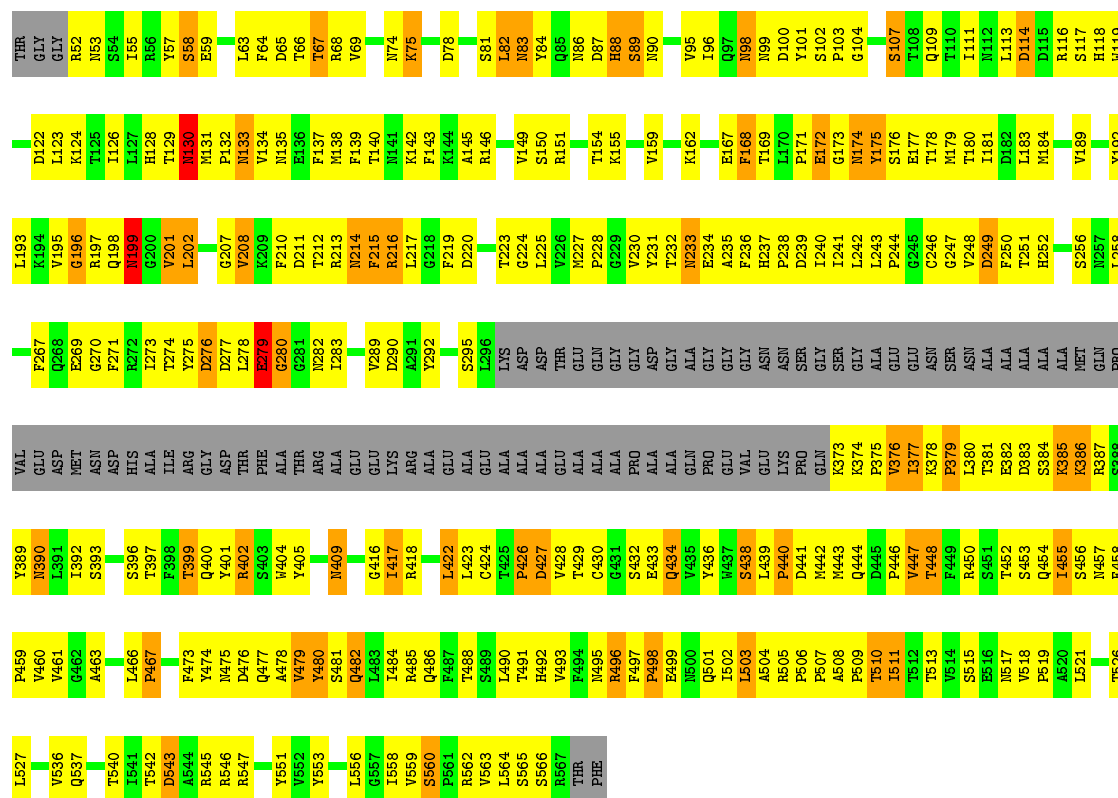
#### • Molecule 1: PENTON PROTEIN





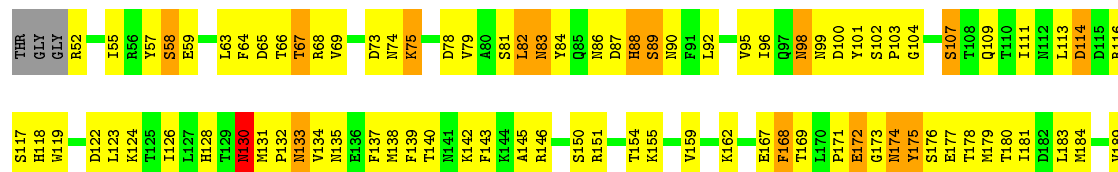
### • Molecule 1: PENTON PROTEIN

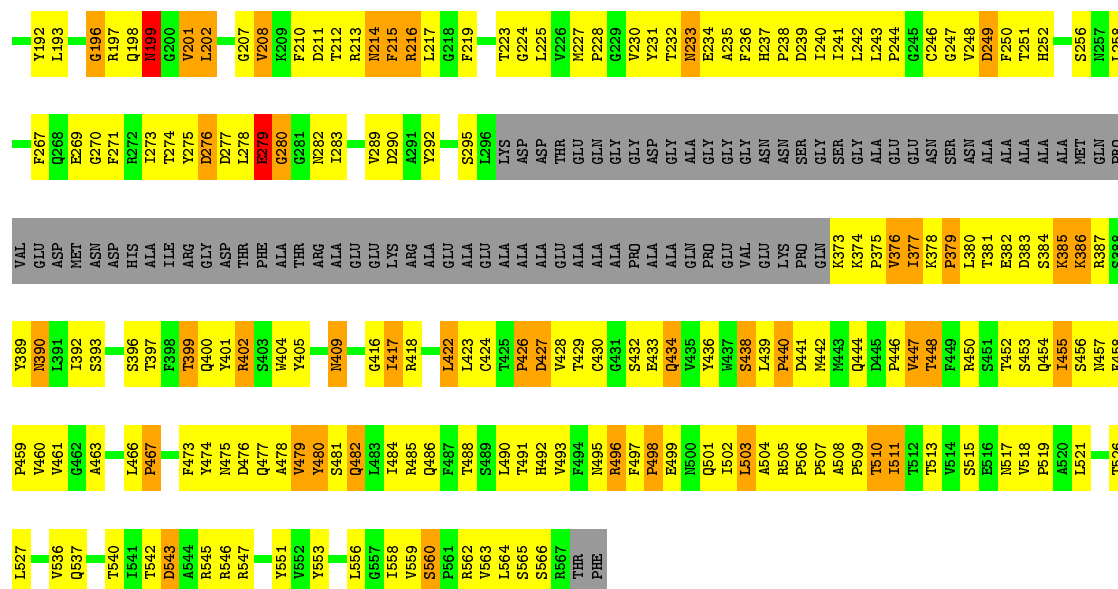
Chain C: 30% 43% 11% 16%



### • Molecule 1: PENTON PROTEIN

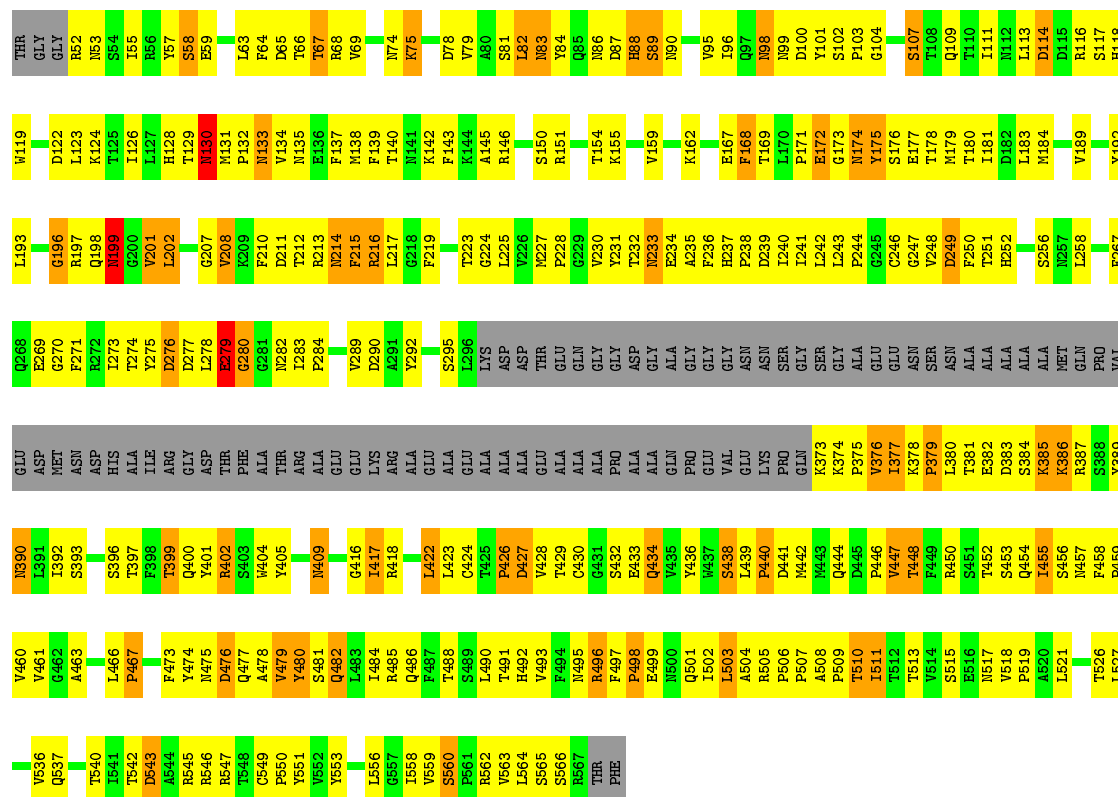
Chain D: 31% 42% 11% 16%





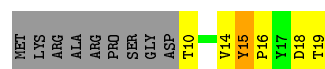
### • Molecule 1: PENTON PROTEIN

Chain E: 30% 43% 11% 16%

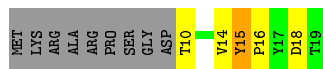


### • Molecule 2: FIBER

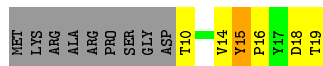
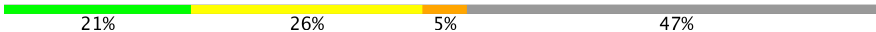
Chain S: 21% 26% 5% 47%



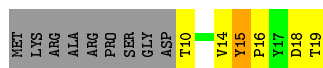
## ● Molecule 2: FIBER

Chain T: 

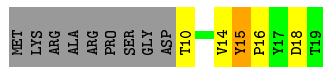
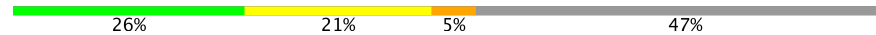
## ● Molecule 2: FIBER

Chain U: 

## ● Molecule 2: FIBER

Chain V: 

## ● Molecule 2: FIBER

Chain W: 



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	1849	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	AMPLITUDE, PHASE	Depositor
Microscope	FEI/PHILIPS CM200T	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	40930	Depositor
Image detector	KODAK SO-163 FILM	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	0.61	0/3602	0.81	1/4904 (0.0%)
1	B	0.61	0/3602	0.81	1/4904 (0.0%)
1	C	0.61	0/3602	0.81	1/4904 (0.0%)
1	D	0.61	0/3602	0.81	1/4904 (0.0%)
1	E	0.61	0/3602	0.81	1/4904 (0.0%)
2	S	0.66	0/90	0.69	0/125
2	T	0.66	0/90	0.69	0/125
2	U	0.67	0/90	0.68	0/125
2	V	0.66	0/90	0.69	0/125
2	W	0.66	0/90	0.69	0/125
All	All	0.61	0/18460	0.81	5/25145 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	480	TYR	N-CA-C	-7.27	91.37	111.00
1	A	480	TYR	N-CA-C	-7.26	91.40	111.00
1	D	480	TYR	N-CA-C	-7.26	91.40	111.00
1	B	480	TYR	N-CA-C	-7.25	91.44	111.00
1	E	480	TYR	N-CA-C	-7.24	91.46	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3519	0	3452	425	0
1	B	3519	0	3452	410	0
1	C	3519	0	3452	414	0
1	D	3519	0	3452	420	0
1	E	3519	0	3452	425	0
2	S	86	0	73	19	0
2	T	86	0	73	16	0
2	U	86	0	73	19	0
2	V	86	0	73	17	0
2	W	86	0	73	18	0
All	All	18025	0	17625	1930	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 54.

The worst 5 of 1930 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)
1:B:68:ARG:NH1	1:B:560:SER:HB3	1.68	1.09
1:D:68:ARG:NH1	1:D:560:SER:HB3	1.68	1.09
1:C:68:ARG:NH1	1:C:560:SER:HB3	1.68	1.09
1:A:68:ARG:NH1	1:A:560:SER:HB3	1.68	1.08
1:E:68:ARG:NH1	1:E:560:SER:HB3	1.68	1.08

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	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	10
1	B	436/523 (83%)	320 (73%)	70 (16%)	46 (11%)	0	10

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	10
1	D	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	10
1	E	436/523 (83%)	321 (74%)	69 (16%)	46 (11%)	0	10
2	S	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	T	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	U	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	V	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
2	W	8/19 (42%)	5 (62%)	3 (38%)	0	100	100
All	All	2220/2710 (82%)	1629 (73%)	361 (16%)	230 (10%)	1	10

5 of 230 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	A	130	ASN
1	A	172	GLU
1	A	174	ASN
1	A	201	VAL

### 5.3.2 Protein sidechains ⓘ

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	399/451 (88%)	369 (92%)	30 (8%)	16	48
1	B	399/451 (88%)	370 (93%)	29 (7%)	16	49
1	C	399/451 (88%)	369 (92%)	30 (8%)	16	48
1	D	399/451 (88%)	369 (92%)	30 (8%)	16	48
1	E	399/451 (88%)	369 (92%)	30 (8%)	16	48
2	S	10/17 (59%)	9 (90%)	1 (10%)	9	33
2	T	10/17 (59%)	9 (90%)	1 (10%)	9	33
2	U	10/17 (59%)	9 (90%)	1 (10%)	9	33

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	10/17 (59%)	9 (90%)	1 (10%)	9	33
2	W	10/17 (59%)	9 (90%)	1 (10%)	9	33
All	All	2045/2340 (87%)	1891 (92%)	154 (8%)	20	48

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	249	ASP
1	C	510	THR
1	E	448	THR
1	C	271	PHE
1	C	422	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	109	GLN
1	C	457	ASN
1	E	237	HIS
1	C	130	ASN
1	C	214	ASN

### 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.