



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

Sep 4, 2018 – 04:38 PM EDT

PDB ID : 6D5F  
EMDB ID: : EMD-7797  
Title : Cryo-EM reconstruction of membrane-enveloped filamentous virus SFV1 (Sulfolobus filamentous virus 1)  
Authors : Wang, F.; Osinski, T.; Liu, Y.; Krupovic, M.; Prangishvili, D.; Egelman, E.H.  
Deposited on : 2018-04-19  
Resolution : 3.70 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

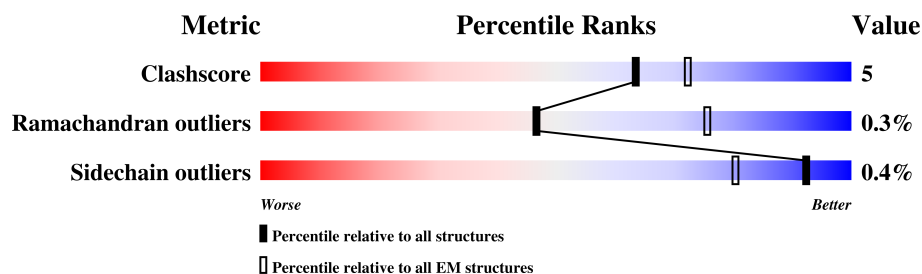
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.70 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.




















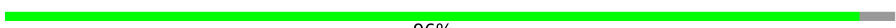
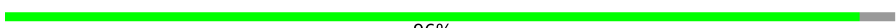
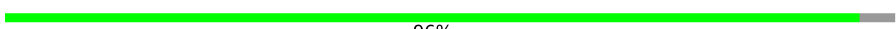
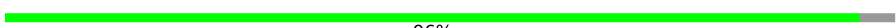

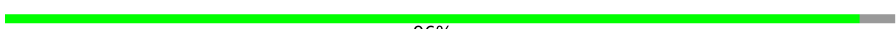


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	199	90% 7% .
1	B	199	89% 8% .
1	C	199	89% 9% .
1	D	199	90% 8% .
1	E	199	89% 8% .
1	F	199	89% 8% .
1	G	199	88% 10% .
1	H	199	90% 7% .
1	I	199	88% 10% .

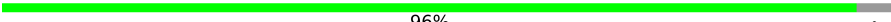
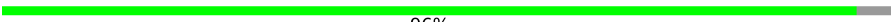
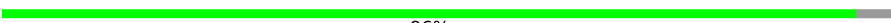












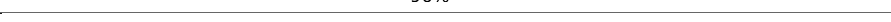
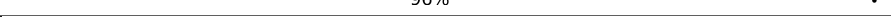
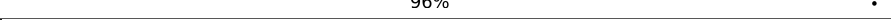
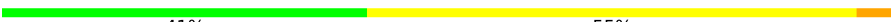

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Mol	Chain	Length	Quality of chain
1	J	199	 90% 7% .
1	K	199	 89% 9% .
1	L	199	 89% 8% .
1	M	199	 88% 9% .
1	N	199	 88% 9% .
1	O	199	 90% 8% .
1	P	199	 88% 9% .
1	Q	199	 88% 9% .
1	R	199	 88% 10% .
1	S	199	 88% 9% .
1	T	199	 87% 10% .
1	U	199	 87% 10% .
1	V	199	 88% 10% .
1	W	199	 89% 8% .
1	X	199	 88% 9% .
1	Y	199	 89% 8% .
1	Z	199	 88% 10% .
2	a	137	 96% .
2	b	137	 96% .
2	c	137	 96% .
2	d	137	 96% .
2	e	137	 96% .
2	f	137	 96% .
2	g	137	 96% .
2	h	137	 96% .

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Mol	Chain	Length	Quality of chain
2	i	137	 96% .
2	j	137	 96% .
2	k	137	 96% .
2	l	137	 96% .
2	m	137	 96% .
2	n	137	 96% .
2	o	137	 96% .
2	p	137	 96% .
2	q	137	 96% .
2	r	137	 96% .
2	s	137	 96% .
2	t	137	 96% .
2	u	137	 96% .
2	v	137	 96% .
2	w	137	 96% .
2	x	137	 96% .
2	y	137	 96% .
2	z	137	 96% .
3	1	336	 41% 55% .
3	2	336	 53% 42% 5% .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 79946 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 Fimbrial protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	B	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	C	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	D	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	E	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	F	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	G	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	H	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	I	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	J	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	K	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	L	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	M	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	N	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	O	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	P	194	Total 1486	C 949	N 241	O 289	S 7	0	0
1	Q	194	Total 1486	C 949	N 241	O 289	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	S	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	T	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	U	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	V	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	W	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	X	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	Y	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		
1	Z	194	Total	C	N	O	S	0	0
			1486	949	241	289	7		

- Molecule 2 is a protein called Fimbrial protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	b	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	c	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	d	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	e	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	f	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	g	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	h	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	i	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	j	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	k	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	l	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	m	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	n	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	o	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	p	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	q	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	r	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	s	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	t	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	u	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	v	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	w	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	x	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	y	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		
2	z	131	Total	C	N	O	S	0	0
			1059	675	183	196	5		


- Molecule 3 is a DNA chain called DNA (336-MER).

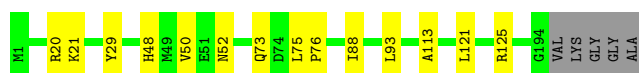
Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	336	Total	C	N	O	P	0	0
			6888	3360	1176	2016	336		
3	2	336	Total	C	N	O	P	0	0
			6888	3360	1176	2016	336		

### 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: Fimbrial protein

Chain A:  90% 7% .



- Molecule 1: Fimbrial protein

Chain B:  89% 8% .



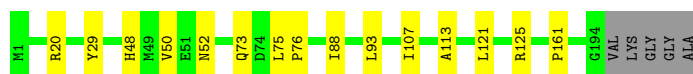
- Molecule 1: Fimbrial protein

Chain C:  89% 9% .



- Molecule 1: Fimbrial protein

Chain D:  90% 8% .




- Molecule 1: Fimbrial protein

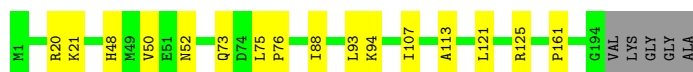
Chain E:  89% 8% .



- Molecule 1: Fimbrial protein

Chain F:  89% 8% .





- Molecule 1: Fimbrial protein

Chain G: 88% 10% .



- Molecule 1: Fimbrial protein

Chain H: 90% 7% .



- Molecule 1: Fimbrial protein

Chain I: 88% 10% .



- Molecule 1: Fimbrial protein

Chain J: 90% 7% .



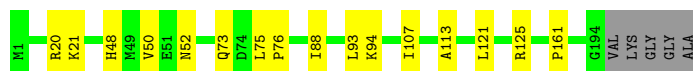
- Molecule 1: Fimbrial protein

Chain K: 89% 9% .



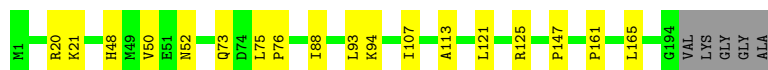
- Molecule 1: Fimbrial protein

Chain L: 89% 8% .

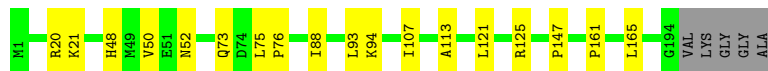


- Molecule 1: Fimbrial protein


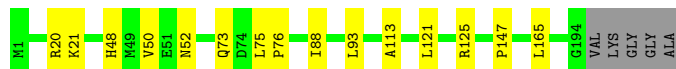
Chain M: 88% 9% .




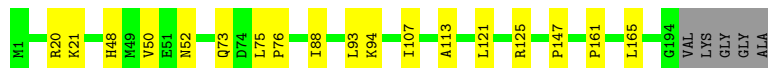
## • Molecule 1: Fimbrial protein

Chain N:  88% 9% .


## • Molecule 1: Fimbrial protein

Chain O:  90% 8% .


## • Molecule 1: Fimbrial protein

Chain P:  88% 9% .


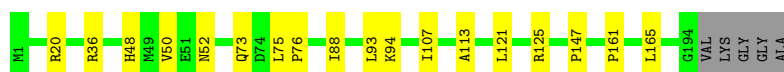
## • Molecule 1: Fimbrial protein

Chain Q:  88% 9% .


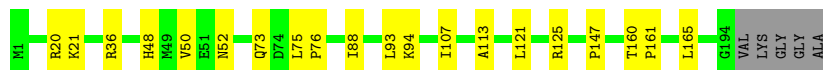
## • Molecule 1: Fimbrial protein

Chain R:  88% 10% .


## • Molecule 1: Fimbrial protein

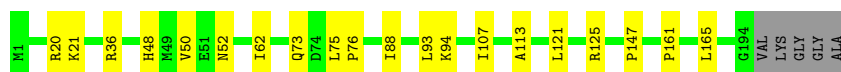
Chain S:  88% 9% .

## • Molecule 1: Fimbrial protein


Chain T:  87% 10% .

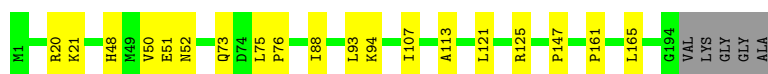
## • Molecule 1: Fimbrial protein

Chain U:  87% 10%



- Molecule 1: Fimbrial protein

Chain V:  88% 10%




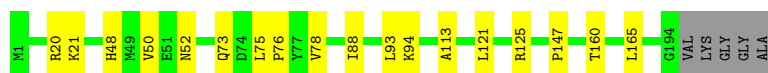
- Molecule 1: Fimbrial protein

Chain W:  89% 8%




- Molecule 1: Fimbrial protein

Chain X:  88% 9%




- Molecule 1: Fimbrial protein

Chain Y:  89% 8%



- Molecule 1: Fimbrial protein

Chain Z:  88% 10%



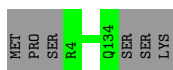
- Molecule 2: Fimbrial protein

Chain a:  96%



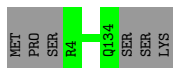
- Molecule 2: Fimbrial protein

Chain b:  96%



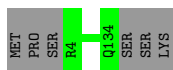
- Molecule 2: Fimbrial protein

Chain c:  96% .



- Molecule 2: Fimbrial protein

Chain d:  96% .



- Molecule 2: Fimbrial protein

Chain e:  96% .



- Molecule 2: Fimbrial protein

Chain f:  96% .



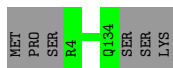
- Molecule 2: Fimbrial protein

Chain g:  96% .



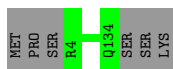
- Molecule 2: Fimbrial protein

Chain h:  96% .



- Molecule 2: Fimbrial protein

Chain i:  96% .



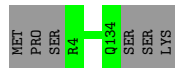
- Molecule 2: Fimbrial protein

Chain j:  96% .



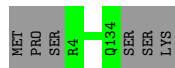
- Molecule 2: Fimbrial protein

Chain k:  96% .



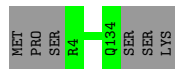
- Molecule 2: Fimbrial protein

Chain l:  96% .



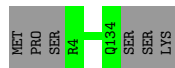
- Molecule 2: Fimbrial protein

Chain m:  96% .



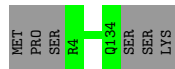
- Molecule 2: Fimbrial protein

Chain n:  96% .



- Molecule 2: Fimbrial protein

Chain o:  96% .



- Molecule 2: Fimbrial protein

Chain p:  96% .



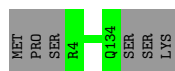
- Molecule 2: Fimbrial protein

Chain q:  96% .



• Molecule 2: Fimbrial protein

Chain r:  96% .



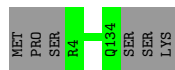
• Molecule 2: Fimbrial protein

Chain s:  96% .



• Molecule 2: Fimbrial protein

Chain t:  96% .



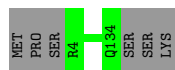
• Molecule 2: Fimbrial protein

Chain u:  96% .



• Molecule 2: Fimbrial protein

Chain v:  96% .



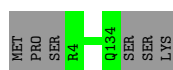
• Molecule 2: Fimbrial protein

Chain w:  96% .



• Molecule 2: Fimbrial protein

Chain x:  96% .



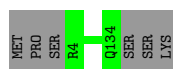
- Molecule 2: Fimbrial protein

Chain y: 96%



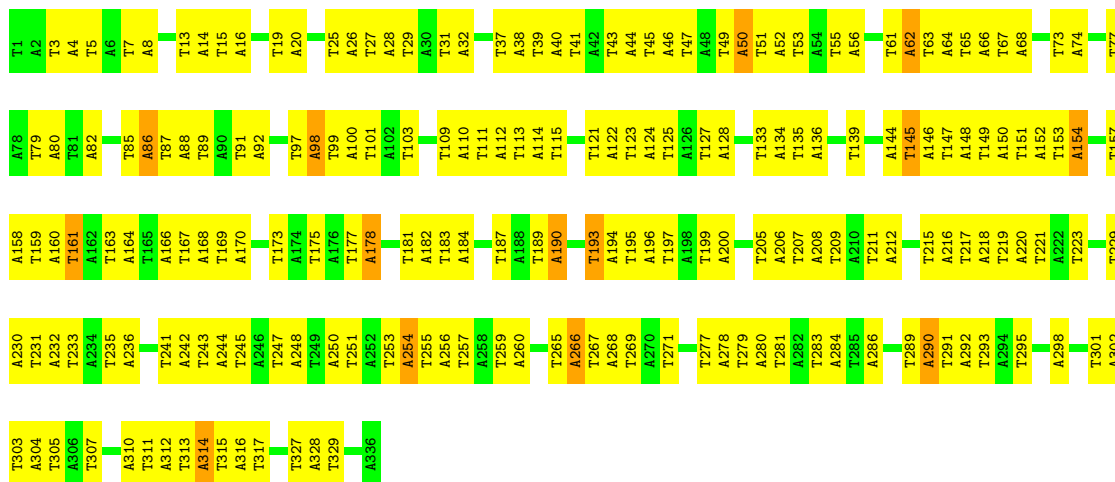
- Molecule 2: Fimbrial protein

Chain z: 96%



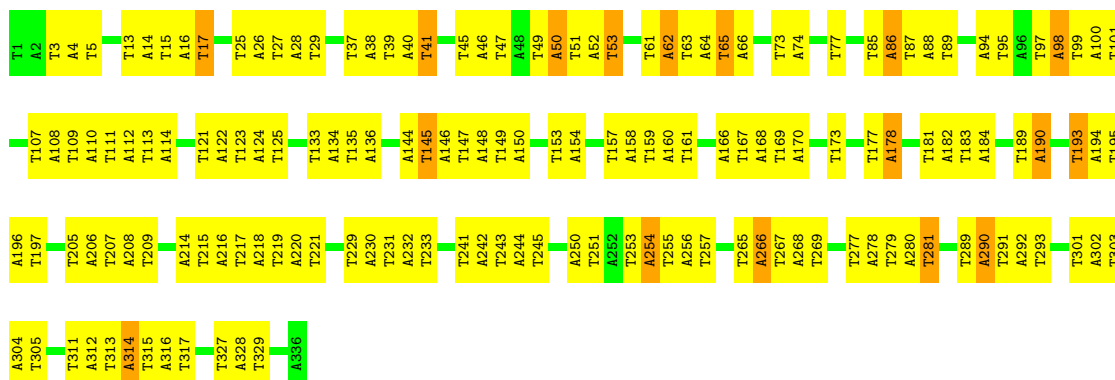
- Molecule 3: DNA (336-MER)

Chain 1: 41% 55%



- Molecule 3: DNA (336-MER)

Chain 2: 53% 42% 5%



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=21.02572°, rise=2.76412 Å, axial sym=C1	Depositor
Number of segments used	87803	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{Å}^2$ )	48	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.41	0/1517	0.59	1/2063 (0.0%)
1	B	0.41	0/1517	0.59	1/2063 (0.0%)
1	C	0.41	0/1517	0.59	1/2063 (0.0%)
1	D	0.41	0/1517	0.59	1/2063 (0.0%)
1	E	0.41	0/1517	0.59	1/2063 (0.0%)
1	F	0.41	0/1517	0.59	1/2063 (0.0%)
1	G	0.41	0/1517	0.59	1/2063 (0.0%)
1	H	0.41	0/1517	0.59	1/2063 (0.0%)
1	I	0.41	0/1517	0.59	1/2063 (0.0%)
1	J	0.41	0/1517	0.59	1/2063 (0.0%)
1	K	0.41	0/1517	0.59	1/2063 (0.0%)
1	L	0.41	0/1517	0.59	1/2063 (0.0%)
1	M	0.41	0/1517	0.59	1/2063 (0.0%)
1	N	0.41	0/1517	0.59	1/2063 (0.0%)
1	O	0.41	0/1517	0.59	1/2063 (0.0%)
1	P	0.41	0/1517	0.59	1/2063 (0.0%)
1	Q	0.41	0/1517	0.59	1/2063 (0.0%)
1	R	0.41	0/1517	0.59	1/2063 (0.0%)
1	S	0.41	0/1517	0.59	1/2063 (0.0%)
1	T	0.41	0/1517	0.59	1/2063 (0.0%)
1	U	0.41	0/1517	0.59	1/2063 (0.0%)
1	V	0.41	0/1517	0.59	1/2063 (0.0%)
1	W	0.41	0/1517	0.59	1/2063 (0.0%)
1	X	0.41	0/1517	0.59	1/2063 (0.0%)
1	Y	0.41	0/1517	0.59	1/2063 (0.0%)
1	Z	0.41	0/1517	0.59	1/2063 (0.0%)
2	a	0.46	0/1076	0.62	0/1453
2	b	0.46	0/1076	0.62	0/1453
2	c	0.46	0/1076	0.62	0/1453
2	d	0.46	0/1076	0.62	0/1453
2	e	0.46	0/1076	0.62	0/1453
2	f	0.46	0/1076	0.62	0/1453
2	g	0.46	0/1076	0.62	0/1453
2	h	0.46	0/1076	0.62	0/1453

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
2	i	0.46	0/1076	0.62	0/1453
2	j	0.46	0/1076	0.62	0/1453
2	k	0.46	0/1076	0.62	0/1453
2	l	0.46	0/1076	0.62	0/1453
2	m	0.46	0/1076	0.62	0/1453
2	n	0.46	0/1076	0.62	0/1453
2	o	0.46	0/1076	0.62	0/1453
2	p	0.46	0/1076	0.62	0/1453
2	q	0.46	0/1076	0.62	0/1453
2	r	0.46	0/1076	0.62	0/1453
2	s	0.46	0/1076	0.62	0/1453
2	t	0.46	0/1076	0.62	0/1453
2	u	0.46	0/1076	0.62	0/1453
2	v	0.46	0/1076	0.62	0/1453
2	w	0.46	0/1076	0.62	0/1453
2	x	0.46	0/1076	0.62	0/1453
2	y	0.46	0/1076	0.62	0/1453
2	z	0.46	0/1076	0.62	0/1453
3	1	1.30	8/7727 (0.1%)	1.15	33/11924 (0.3%)
3	2	1.30	7/7727 (0.1%)	1.15	34/11924 (0.3%)
All	All	0.68	15/82872 (0.0%)	0.75	93/115264 (0.1%)

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	1	66	DA	C3'-O3'	-6.97	1.34	1.44
3	2	66	DA	C3'-O3'	-6.93	1.34	1.44
3	1	144	DA	N9-C4	-6.17	1.34	1.37
3	2	144	DA	N9-C4	-6.04	1.34	1.37
3	2	178	DA	C3'-O3'	-5.87	1.36	1.44

The worst 5 of 93 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2	314	DA	O4'-C4'-C3'	-6.35	101.96	104.50
3	1	314	DA	O4'-C4'-C3'	-6.26	101.99	104.50
3	1	197	DT	O4'-C4'-C3'	-6.11	102.06	104.50
3	2	197	DT	O4'-C4'-C3'	-6.04	102.08	104.50
3	1	101	DT	O4'-C4'-C3'	-6.02	102.09	104.50

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	1486	0	1450	7	0
1	B	1486	0	1450	8	0
1	C	1486	0	1450	8	0
1	D	1486	0	1450	7	0
1	E	1486	0	1450	9	0
1	F	1486	0	1450	8	0
1	G	1486	0	1450	11	0
1	H	1486	0	1450	6	0
1	I	1486	0	1450	10	0
1	J	1486	0	1450	6	0
1	K	1486	0	1450	9	0
1	L	1486	0	1450	9	0
1	M	1486	0	1450	9	0
1	N	1486	0	1450	10	0
1	O	1486	0	1450	7	0
1	P	1486	0	1450	10	0
1	Q	1486	0	1450	11	0
1	R	1486	0	1450	11	0
1	S	1486	0	1450	9	0
1	T	1486	0	1450	12	0
1	U	1486	0	1450	12	0
1	V	1486	0	1450	12	0
1	W	1486	0	1450	8	0
1	X	1486	0	1450	10	0
1	Y	1486	0	1450	8	0
1	Z	1486	0	1450	11	0
2	a	1059	0	1076	0	0
2	b	1059	0	1076	0	0
2	c	1059	0	1076	0	0
2	d	1059	0	1076	0	0
2	e	1059	0	1076	0	0
2	f	1059	0	1076	0	0
2	g	1059	0	1076	0	0
2	h	1059	0	1076	0	0
2	i	1059	0	1076	0	0
2	j	1059	0	1076	0	0
2	k	1059	0	1076	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	l	1059	0	1076	0	0
2	m	1059	0	1076	0	0
2	n	1059	0	1076	0	0
2	o	1059	0	1076	0	0
2	p	1059	0	1076	0	0
2	q	1059	0	1076	0	0
2	r	1059	0	1076	0	0
2	s	1059	0	1076	0	0
2	t	1059	0	1076	0	0
2	u	1059	0	1076	0	0
2	v	1059	0	1076	0	0
2	w	1059	0	1076	0	0
2	x	1059	0	1076	0	0
2	y	1059	0	1076	0	0
2	z	1059	0	1076	0	0
3	1	6888	0	3865	122	0
3	2	6888	0	3865	93	0
All	All	79946	0	73406	365	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 5.

The worst 5 of 365 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:P:20:ARG:NH2	3:1:67:DT:OP1	2.30	0.65
1:S:20:ARG:NH2	3:1:271:DT:OP1	2.31	0.64
1:H:20:ARG:NH2	3:1:115:DT:OP1	2.31	0.64
1:I:20:ARG:NH2	3:1:211:DT:OP1	2.30	0.63
1:U:20:ARG:NH2	3:1:283:DT:OP1	2.31	0.63

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	192/199 (96%)	172 (90%)	19 (10%)	1 (0%)	31	71
1	B	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	C	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	D	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	E	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	F	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	G	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	H	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	I	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	J	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	K	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	L	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	M	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	N	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	O	192/199 (96%)	172 (90%)	19 (10%)	1 (0%)	31	71
1	P	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	Q	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	R	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	S	192/199 (96%)	172 (90%)	19 (10%)	1 (0%)	31	71
1	T	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	U	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	V	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	W	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	X	192/199 (96%)	172 (90%)	19 (10%)	1 (0%)	31	71
1	Y	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
1	Z	192/199 (96%)	171 (89%)	20 (10%)	1 (0%)	31	71
2	a	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	b	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	c	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	d	129/137 (94%)	122 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	f	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	g	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	h	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	i	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	j	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	k	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	l	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	m	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	n	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	o	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	p	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	q	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	r	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	s	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	t	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	u	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	v	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	w	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	x	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	y	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
2	z	129/137 (94%)	122 (95%)	7 (5%)	0	100	100
All	All	8346/8736 (96%)	7622 (91%)	698 (8%)	26 (0%)	47	78

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	PRO
1	B	76	PRO
1	C	76	PRO
1	D	76	PRO
1	E	76	PRO

### 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	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	B	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	C	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	D	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	E	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	F	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	G	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	H	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	I	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	J	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	K	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	L	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	M	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	N	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	O	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	P	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	Q	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	R	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	S	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	T	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	U	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	V	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	W	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	X	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	Y	158/168 (94%)	157 (99%)	1 (1%)	87	94
1	Z	158/168 (94%)	157 (99%)	1 (1%)	87	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	114/121 (94%)	114 (100%)	0	100	100
2	b	114/121 (94%)	114 (100%)	0	100	100
2	c	114/121 (94%)	114 (100%)	0	100	100
2	d	114/121 (94%)	114 (100%)	0	100	100
2	e	114/121 (94%)	114 (100%)	0	100	100
2	f	114/121 (94%)	114 (100%)	0	100	100
2	g	114/121 (94%)	114 (100%)	0	100	100
2	h	114/121 (94%)	114 (100%)	0	100	100
2	i	114/121 (94%)	114 (100%)	0	100	100
2	j	114/121 (94%)	114 (100%)	0	100	100
2	k	114/121 (94%)	114 (100%)	0	100	100
2	l	114/121 (94%)	114 (100%)	0	100	100
2	m	114/121 (94%)	114 (100%)	0	100	100
2	n	114/121 (94%)	114 (100%)	0	100	100
2	o	114/121 (94%)	114 (100%)	0	100	100
2	p	114/121 (94%)	114 (100%)	0	100	100
2	q	114/121 (94%)	114 (100%)	0	100	100
2	r	114/121 (94%)	114 (100%)	0	100	100
2	s	114/121 (94%)	114 (100%)	0	100	100
2	t	114/121 (94%)	114 (100%)	0	100	100
2	u	114/121 (94%)	114 (100%)	0	100	100
2	v	114/121 (94%)	114 (100%)	0	100	100
2	w	114/121 (94%)	114 (100%)	0	100	100
2	x	114/121 (94%)	114 (100%)	0	100	100
2	y	114/121 (94%)	114 (100%)	0	100	100
2	z	114/121 (94%)	114 (100%)	0	100	100
All	All	7072/7514 (94%)	7046 (100%)	26 (0%)	92	97

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	75	LEU
1	O	75	LEU

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Mol	Chain	Res	Type
1	Y	75	LEU
1	M	75	LEU
1	N	75	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	52	ASN
2	d	41	ASN
2	w	41	ASN
1	X	120	ASN
2	a	44	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.