



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:32 PM BST

PDB ID : 5A2T
EMDB ID: : EMD-3020
Title : The Molecular Basis for Flexibility in the Flexible Filamentous Plant Viruses
Authors : DiMaio, F.; Chen, C.C.; Yu, X.; Frenz, B.; Hsu, Y.H.; Lin, N.S.; Egelman, E.H.
Deposited on : 2015-05-23
Resolution : 5.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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) : trunk27241

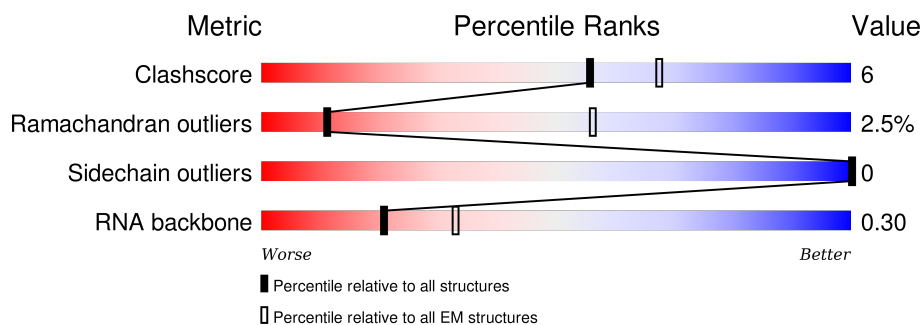
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.60 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.













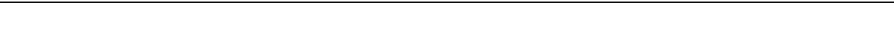

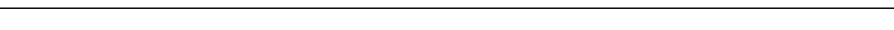
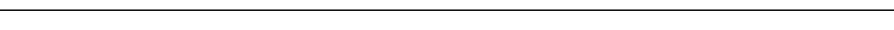
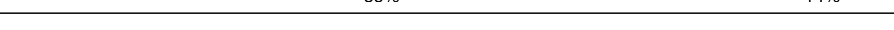



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 ≥ 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	204	82% 17% .
1	B	204	84% 15% .
1	C	204	84% 15% .
1	D	204	81% 18% .
1	E	204	83% 16% .
1	F	204	84% 15% .
1	G	204	84% 15% .
1	H	204	83% 16% .

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Mol	Chain	Length	Quality of chain
1	I	204	 85% 14% .
1	J	204	 85% 14% .
1	K	204	 83% 16% .
1	L	204	 83% 16% .
1	M	204	 84% 15% .
1	N	204	 84% 15% .
1	O	204	 83% 16% .
1	P	204	 85% 14% .
1	Q	204	 83% 16% .
1	R	204	 84% 15% .
1	S	204	 84% 15% .
1	T	204	 83% 16% .
1	U	204	 84% 15% .
1	V	204	 85% 14% .
1	W	204	 83% 16% .
1	X	204	 84% 15% .
1	Y	204	 82% 17% .
2	Z	125	 60% 40%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41925 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 COAT PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	B	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	C	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	D	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	E	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	F	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	G	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	H	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	I	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	J	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	K	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	L	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	M	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	N	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	O	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	P	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	Q	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	S	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	T	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	U	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	V	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	W	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	X	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		
1	Y	204	Total	C	N	O	S	0	0
			1577	1008	264	300	5		

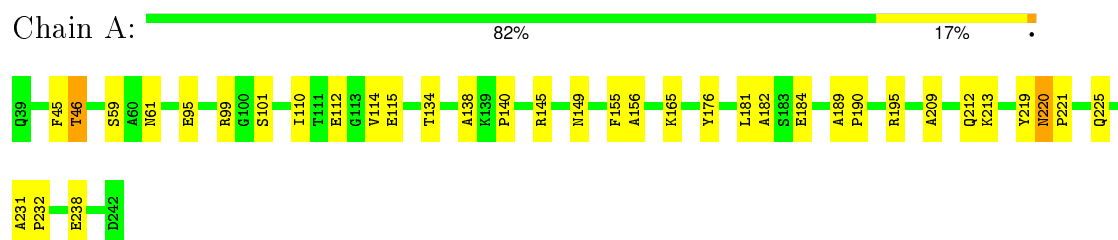
- Molecule 2 is a RNA chain called BAMBOO MOSAIC VIRUS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	125	Total	C	N	O	P	0	0
			2500	1125	250	1000	125		

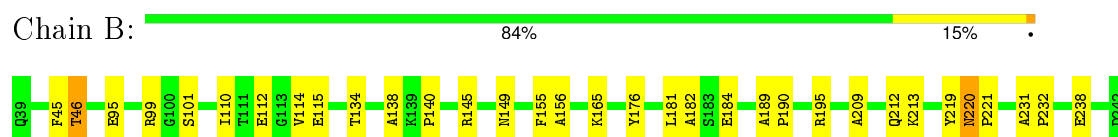
3 Residue-property plots

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

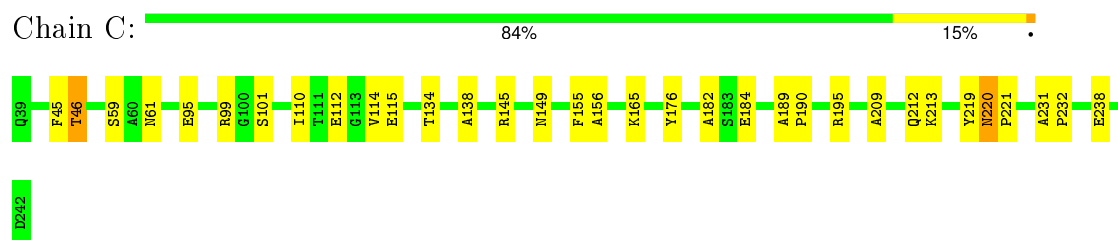
- Molecule 1: COAT PROTEIN



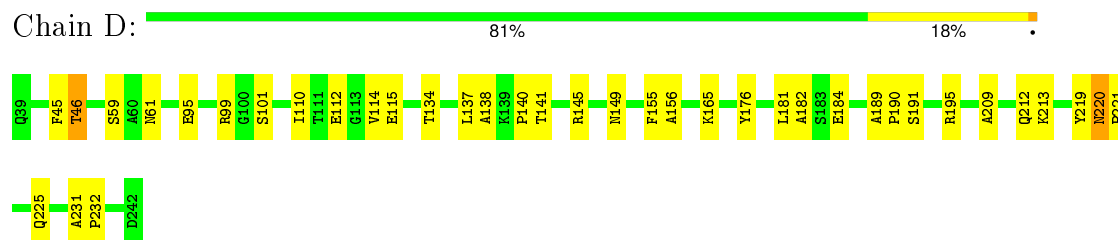
- Molecule 1: COAT PROTEIN



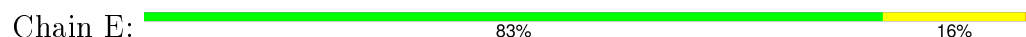
- Molecule 1: COAT PROTEIN

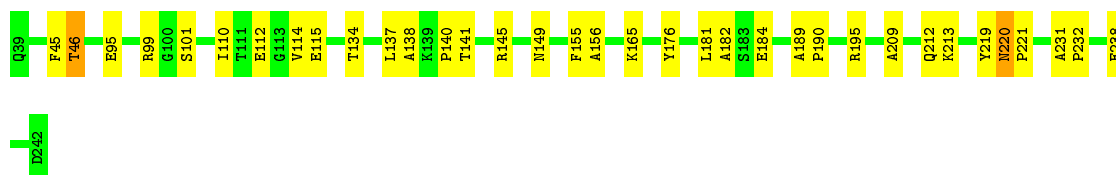


- Molecule 1: COAT PROTEIN



- Molecule 1: COAT PROTEIN





- Molecule 1: COAT PROTEIN

Chain F: 84% 15% .



- Molecule 1: COAT PROTEIN

Chain G: 84% 15% .



- Molecule 1: COAT PROTEIN

Chain H: 83% 16% .



- Molecule 1: COAT PROTEIN

Chain I: 85% 14% .



- Molecule 1: COAT PROTEIN

Chain J: 85% 14% .



- Molecule 1: COAT PROTEIN

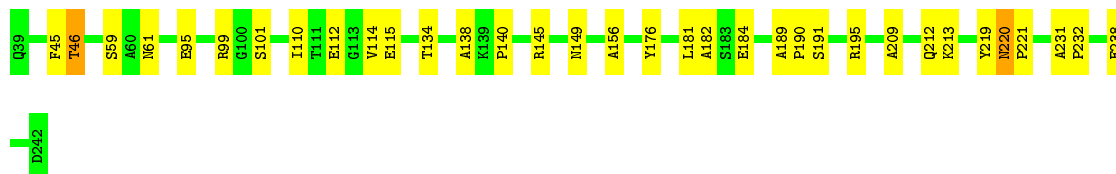
Chain K: 83% 16% .





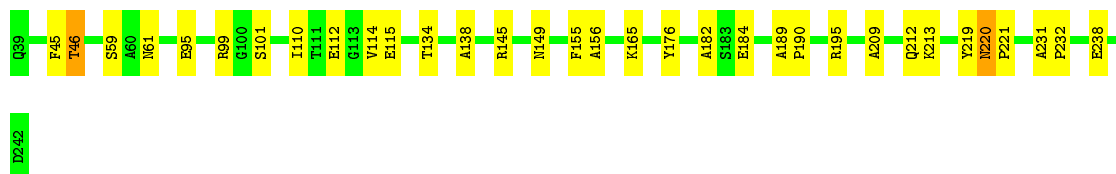
• Molecule 1: COAT PROTEIN

Chain L: 83% 16%



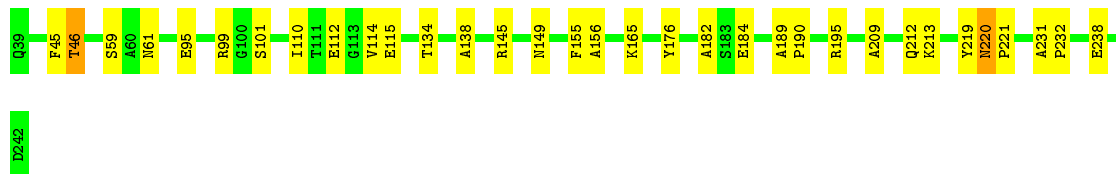
• Molecule 1: COAT PROTEIN

Chain M: 84% 15%



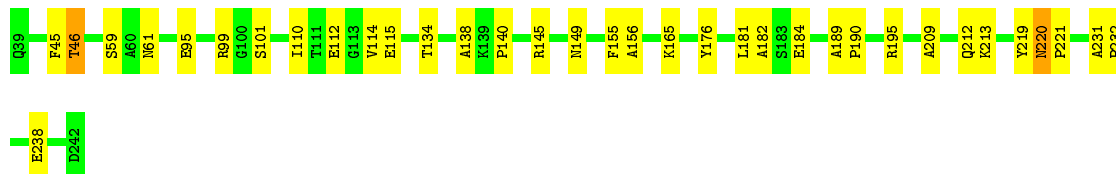
• Molecule 1: COAT PROTEIN

Chain N: 84% 15%



• Molecule 1: COAT PROTEIN

Chain O: 83% 16%

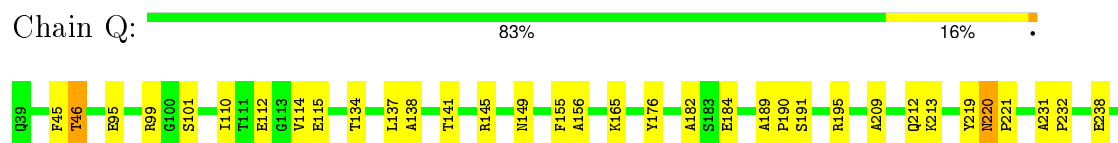


• Molecule 1: COAT PROTEIN

Chain P: 85% 14%

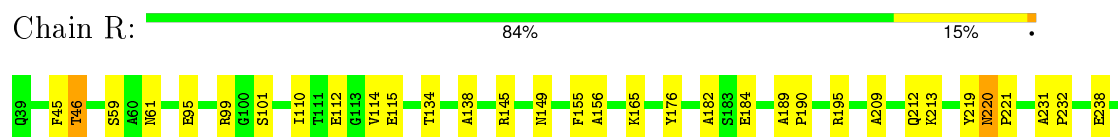


• Molecule 1: COAT PROTEIN



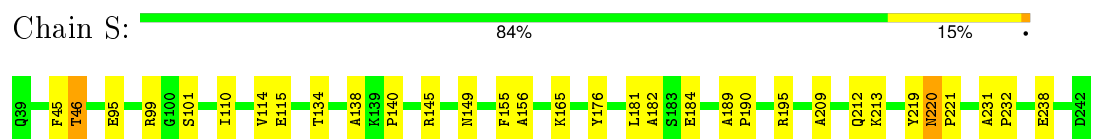
D242

- Molecule 1: COAT PROTEIN

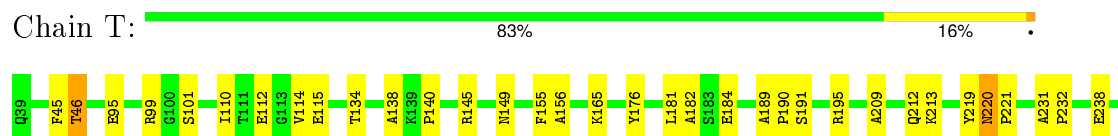


D242

- Molecule 1: COAT PROTEIN

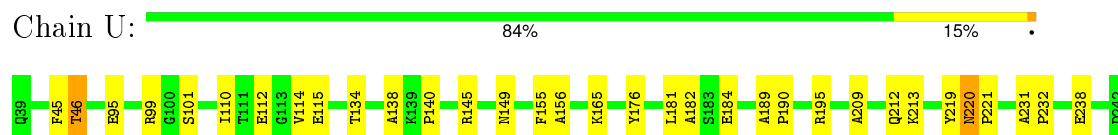


- Molecule 1: COAT PROTEIN

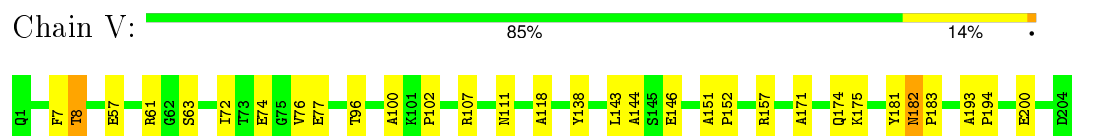


D242

- Molecule 1: COAT PROTEIN

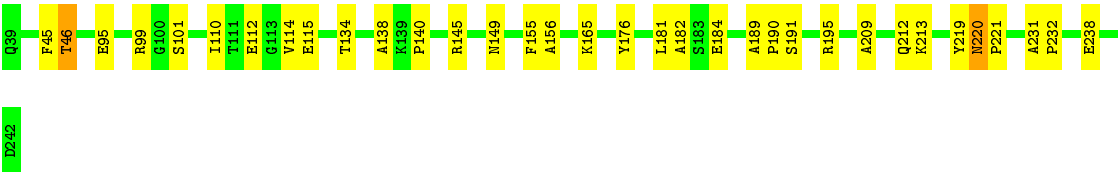


- Molecule 1: COAT PROTEIN

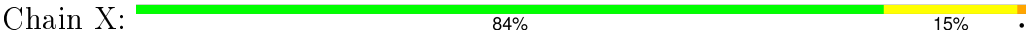


- Molecule 1: COAT PROTEIN

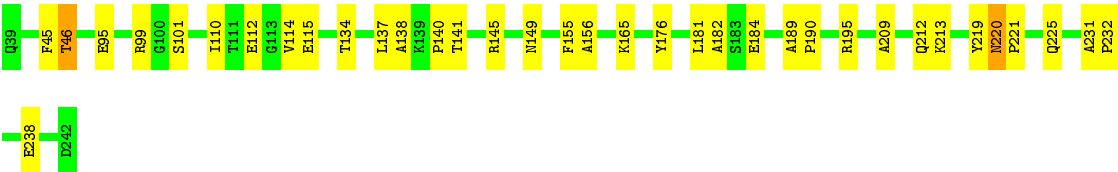
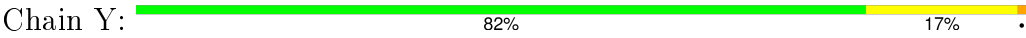




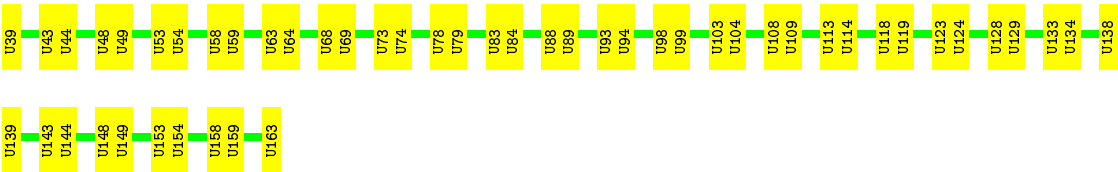
• Molecule 1: COAT PROTEIN



• Molecule 1: COAT PROTEIN



• Molecule 2: BAMBOO MOSAIC VIRUS



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	IMAGES, Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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	0.62	0/1620	0.53	0/2211
1	B	0.63	0/1620	0.53	0/2211
1	C	0.63	0/1620	0.53	0/2211
1	D	0.62	0/1620	0.53	0/2211
1	E	0.62	0/1620	0.53	0/2211
1	F	0.62	0/1620	0.53	0/2211
1	G	0.62	0/1620	0.53	0/2211
1	H	0.62	0/1620	0.53	0/2211
1	I	0.63	0/1620	0.53	0/2211
1	J	0.62	0/1620	0.53	0/2211
1	K	0.62	0/1620	0.53	0/2211
1	L	0.62	0/1620	0.53	0/2211
1	M	0.62	0/1620	0.53	0/2211
1	N	0.63	0/1620	0.53	0/2211
1	O	0.62	0/1620	0.53	0/2211
1	P	0.62	0/1620	0.53	0/2211
1	Q	0.63	0/1620	0.53	0/2211
1	R	0.62	0/1620	0.53	0/2211
1	S	0.62	0/1620	0.53	0/2211
1	T	0.62	0/1620	0.53	0/2211
1	U	0.63	0/1620	0.53	0/2211
1	V	0.62	0/1620	0.53	0/2211
1	W	0.62	0/1620	0.53	0/2211
1	X	0.63	0/1620	0.53	0/2211
1	Y	0.62	0/1620	0.53	0/2211
2	Z	0.11	0/2749	0.71	0/4246
All	All	0.60	0/43249	0.54	0/59521

There are no bond length outliers.

There are no bond angle outliers.

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	1577	0	1547	24	0
1	B	1577	0	1547	21	0
1	C	1577	0	1547	21	0
1	D	1577	0	1547	24	0
1	E	1577	0	1547	23	0
1	F	1577	0	1547	22	0
1	G	1577	0	1547	22	0
1	H	1577	0	1547	23	0
1	I	1577	0	1547	21	0
1	J	1577	0	1547	20	0
1	K	1577	0	1547	23	0
1	L	1577	0	1547	22	0
1	M	1577	0	1547	22	0
1	N	1577	0	1547	22	0
1	O	1577	0	1547	21	0
1	P	1577	0	1547	21	0
1	Q	1577	0	1547	22	0
1	R	1577	0	1547	22	0
1	S	1577	0	1547	20	0
1	T	1577	0	1547	22	0
1	U	1577	0	1547	21	0
1	V	1577	0	1550	20	0
1	W	1577	0	1547	22	0
1	X	1577	0	1547	22	0
1	Y	1577	0	1547	24	0
2	Z	2500	0	1251	25	0
All	All	41925	0	39929	523	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 6.

The worst 5 of 523 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:95:GLU:OE1	1:B:95:GLU:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:95:GLU:HA	1:Y:95:GLU:OE1	2.02	0.60
1:I:95:GLU:OE1	1:I:95:GLU:HA	2.02	0.60
1:C:95:GLU:HA	1:C:95:GLU:OE1	2.02	0.60
1:D:95:GLU:OE1	1:D:95:GLU:HA	2.02	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	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	B	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	C	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	D	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	E	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	F	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	G	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	H	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	I	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	J	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	K	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	L	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	M	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	N	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	O	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	P	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	R	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	S	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	T	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	U	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	V	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	W	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	X	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
1	Y	202/204 (99%)	186 (92%)	11 (5%)	5 (2%)	7	46
All	All	5050/5100 (99%)	4650 (92%)	275 (5%)	125 (2%)	11	46

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	SER
1	B	101	SER
1	C	101	SER
1	D	101	SER
1	E	101	SER

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	165/165 (100%)	165 (100%)	0	100	100
1	B	165/165 (100%)	165 (100%)	0	100	100
1	C	165/165 (100%)	165 (100%)	0	100	100
1	D	165/165 (100%)	165 (100%)	0	100	100
1	E	165/165 (100%)	165 (100%)	0	100	100
1	F	165/165 (100%)	165 (100%)	0	100	100
1	G	165/165 (100%)	165 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	165/165 (100%)	165 (100%)	0	100	100
1	I	165/165 (100%)	165 (100%)	0	100	100
1	J	165/165 (100%)	165 (100%)	0	100	100
1	K	165/165 (100%)	165 (100%)	0	100	100
1	L	165/165 (100%)	165 (100%)	0	100	100
1	M	165/165 (100%)	165 (100%)	0	100	100
1	N	165/165 (100%)	165 (100%)	0	100	100
1	O	165/165 (100%)	165 (100%)	0	100	100
1	P	165/165 (100%)	165 (100%)	0	100	100
1	Q	165/165 (100%)	165 (100%)	0	100	100
1	R	165/165 (100%)	165 (100%)	0	100	100
1	S	165/165 (100%)	165 (100%)	0	100	100
1	T	165/165 (100%)	165 (100%)	0	100	100
1	U	165/165 (100%)	165 (100%)	0	100	100
1	V	165/165 (100%)	165 (100%)	0	100	100
1	W	165/165 (100%)	165 (100%)	0	100	100
1	X	165/165 (100%)	165 (100%)	0	100	100
1	Y	165/165 (100%)	165 (100%)	0	100	100
All	All	4125/4125 (100%)	4125 (100%)	0	100	100

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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	146	GLN
1	N	146	GLN
1	X	146	GLN
1	M	146	GLN
1	O	146	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	Z	124/125 (99%)	25 (20%)	0

5 of 25 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Z	43	U
2	Z	48	U
2	Z	53	U
2	Z	58	U
2	Z	63	U

There are no RNA pucker outliers to report.

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.