



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 30, 2017 – 08:39 PM EDT

PDB ID : 5ODV
EMDB ID: : EMD-3785
Title : Structure of Watermelon mosaic virus potyvirus.
Authors : Zamora, M.; Mendez-Lopez, E.; Agirrezabala, X.; Cuesta, R.; Lavin, J.L.;
Sanchez-Pina, M.A.; Aranda, M.; Valle, M.
Deposited on : unknown
Resolution : 4.00 Å(reported)

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

We welcome your comments at 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-20030345

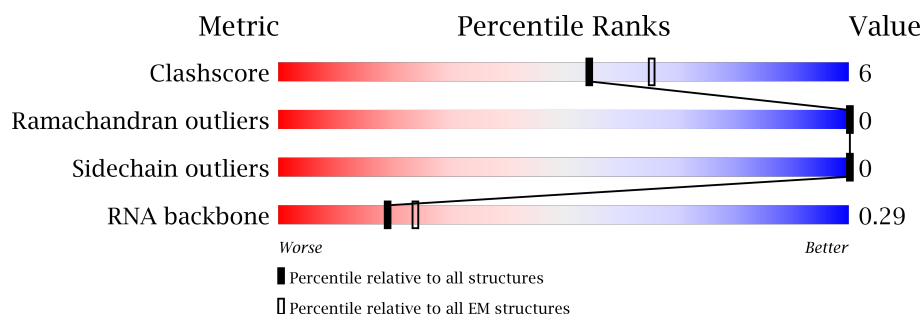
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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.
















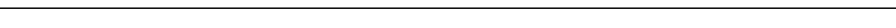



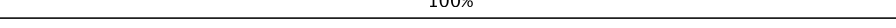
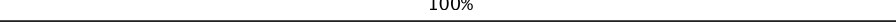
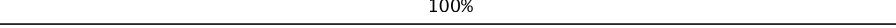
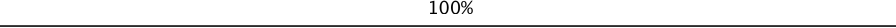
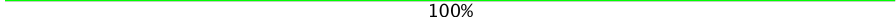
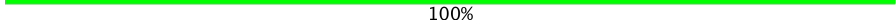
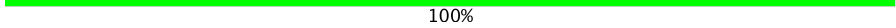
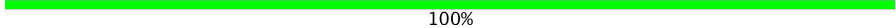
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	281	68% 6% 26%
1	B	281	65% 9% 26%
1	C	281	65% 9% 26%
1	D	281	65% 9% 26%
1	E	281	65% 8% 26%
1	F	281	64% 10% 26%
1	G	281	65% 9% 26%
1	H	281	66% 8% 26%

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Mol	Chain	Length	Quality of chain
1	I	281	
1	J	281	
1	K	281	
1	L	281	
1	M	281	
1	N	281	
1	O	281	
1	P	281	
1	Q	281	
1	R	281	
1	S	281	
1	T	281	
1	U	281	
1	V	281	
1	W	281	
1	X	281	
2	a	5	
2	b	5	
2	c	5	
2	d	5	
2	e	5	
2	f	5	
2	g	5	
2	h	5	
2	i	5	

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Mol	Chain	Length	Quality of chain
2	j	5	 100%
2	k	5	 100%
2	l	5	 100%
2	m	5	 100%
2	n	5	 100%
2	o	5	 100%
2	p	5	 100%
2	q	5	 100%
2	r	5	 100%
2	s	5	 100%
2	t	5	 100%
2	u	5	 100%
2	v	5	 100%
2	w	5	 100%
2	x	5	 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 82656 atoms, of which 40368 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	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	B	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	C	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	D	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	E	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	F	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	G	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	H	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	I	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	J	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	K	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	L	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	M	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	N	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	O	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	P	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0
1	Q	207	Total 3293	C 1046	H 1631	N 290	O 315	S 11	0	0

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	207	Total	C	H	N	O	S	0	0
			3293	1046	1631	290	315	11		
1	S	207	Total	C	H	N	O	S	0	0
			3293	1046	1631	290	315	11		
1	T	207	Total	C	H	N	O	S	0	0
			3293	1046	1631	290	315	11		
1	U	207	Total	C	H	N	O	S	0	0
			3293	1046	1631	290	315	11		
1	V	207	Total	C	H	N	O	S	0	0
			3293	1046	1631	290	315	11		
1	W	207	Total	C	H	N	O	S	0	0
			3293	1046	1631	290	315	11		
1	X	207	Total	C	H	N	O	S	0	0
			3293	1046	1631	290	315	11		

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						AltConf	Trace
2	a	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	b	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	c	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	d	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	e	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	f	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	g	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	h	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	i	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	j	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	k	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		
2	l	5	Total	C	H	N	O	P	0	0
			151	45	51	10	40	5		

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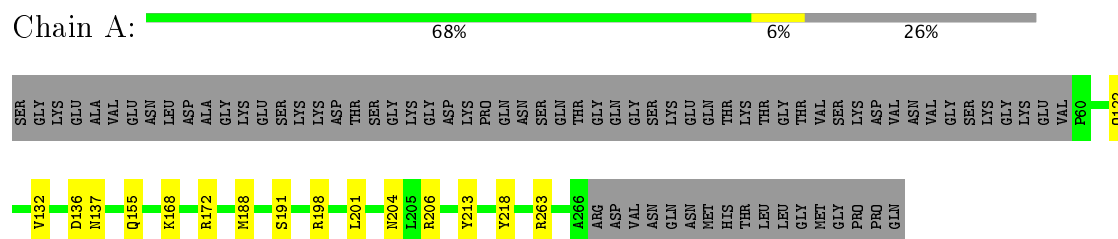
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Mol	Chain	Residues	Atoms						AltConf	Trace
2	m	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	n	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	o	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	p	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	q	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	r	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	s	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	t	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	u	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	v	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	w	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0
2	x	5	Total 151	C 45	H 51	N 10	O 40	P 5	0	0

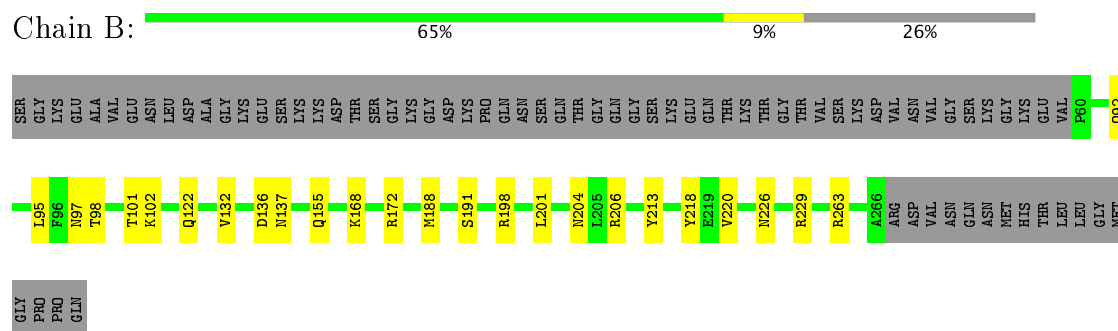
3 Residue-property plots

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.

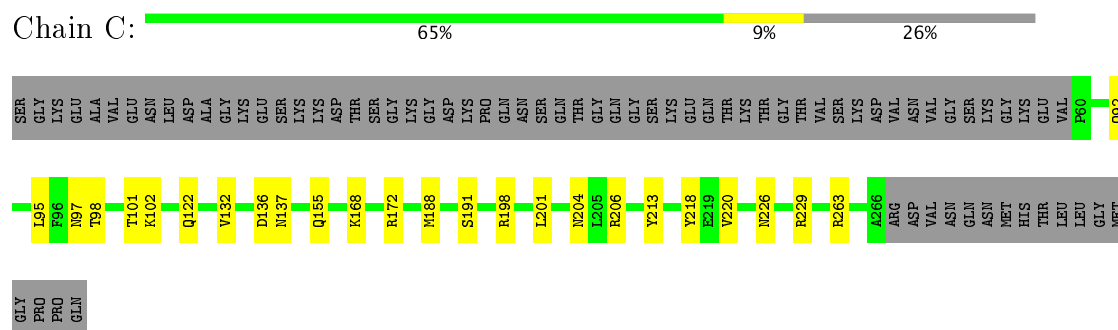
- Molecule 1: coat protein



- Molecule 1: coat protein



- Molecule 1: coat protein



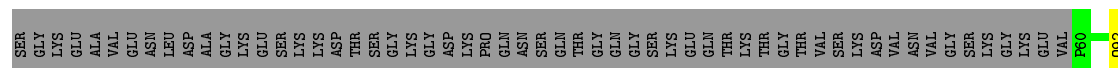
- Molecule 1: coat protein





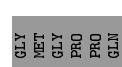
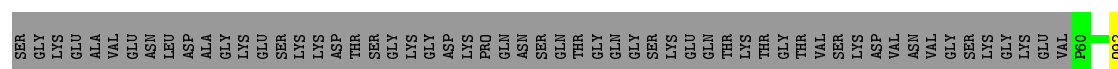
- Molecule 1: coat protein

Chain I: 64% 10% 26%



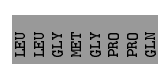
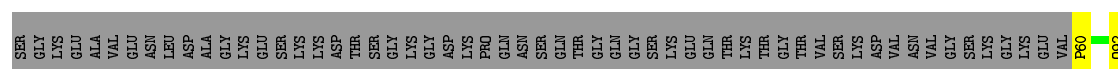
- Molecule 1: coat protein

Chain J: 64% 10% 26%



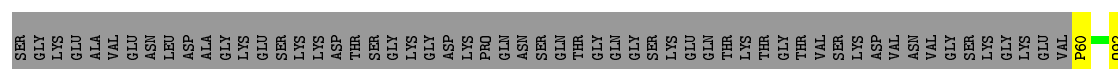
- Molecule 1: coat protein

Chain K: 63% 10% 26%



- Molecule 1: coat protein

Chain L: 64% 10% 26%



MET
GLY
PRO
PRO
GLN

- Molecule 1: coat protein

Chain M:  64% 10% 26%

SER GLY LYS GLU VAL ASN LEU ASP GLY LYS GLU VAL P60 Q92
L95 F96 N97 T98 T101 K102 Q122 V132 D136 N137 Q155 Q168 R172 M188 S191 E192 S193 P194 R198 L201 N204 L205 R206 Y213 Y218 E219 V220 N226 R229 A266 ARG ASP VAL GLY SER ASN GLN MET HIS THR LEU LEU GLY

MET
GLY
PRO
PRO
GLN

- Molecule 1: coat protein

Chain N:  64% 10% 26%

SER GLY LYS GLU VAL ASN LEU ASP GLY LYS GLU VAL P60 Q92
L95 F96 N97 T98 T101 K102 Q122 V132 D136 N137 Q155 Q168 R172 M188 S191 E192 S193 P194 R198 L201 N204 L205 R206 Y213 Y218 E219 V220 N226 R229 A266 ARG ASP VAL GLY SER ASN GLN MET HIS THR LEU LEU GLY

MET
GLY
PRO
PRO
GLN

- Molecule 1: coat protein

Chain O:  64% 9% 26%

SER GLY LYS GLU VAL ASN LEU ASP GLY LYS GLU VAL P60 Q92
L95 F96 N97 T98 T101 K102 Q122 V132 D136 N137 Q155 Q168 R172 M188 S191 E192 S193 P194 R198 L201 N204 L205 R206 Y213 Y218 E219 V220 N226 R229 A266 ARG ASP VAL GLY SER ASN GLN MET HIS THR LEU LEU GLY

PRO
PRO
GLN

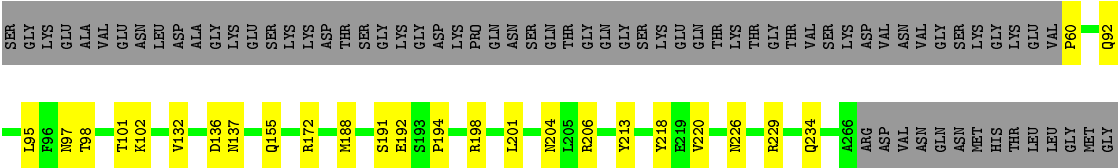
- Molecule 1: coat protein

Chain P:  64% 9% 26%

SER GLY LYS GLU VAL ASN LEU ASP GLY LYS GLU VAL P60 Q92
L95 F96 N97 T98 T101 K102 Q122 V132 D136 N137 Q155 Q168 R172 M188 S191 E192 S193 P194 R198 L201 N204 L205 R206 Y220 N226 R229 N260 T261 A266 ARG ASP VAL GLY SER ASN GLN MET HIS THR LEU LEU GLY MET MET PRO

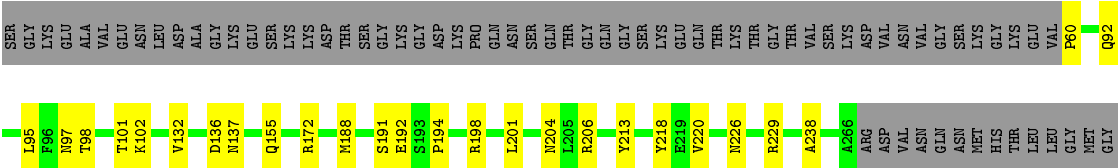
PRO
GLN

- Molecule 1: coat protein



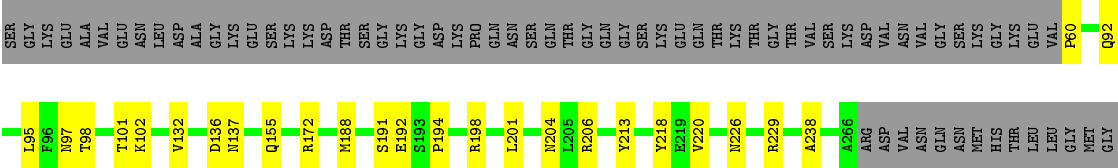
PRO
PRO
GLN

- Molecule 1: coat protein



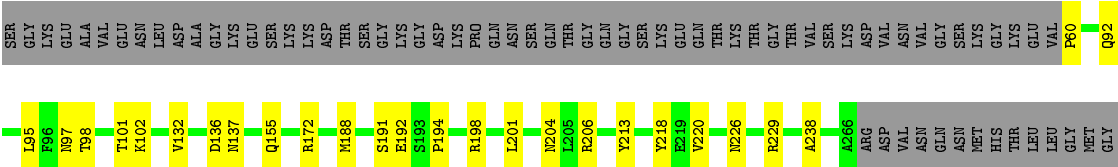
PRO
PRO
GLN

- Molecule 1: coat protein



PRO
PRO
GLN

- Molecule 1: coat protein



WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain b:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain e:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain g:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain h:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain i:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain j:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain k:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain l:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain m:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain n:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain o:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain p:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain s:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain t:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain u:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain v:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain w:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*U)-3')

Chain x:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-40.87°, rise=3.99 Å, axial sym=C1	Depositor
Number of segments used	50045	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 ($e^-/\text{Å}^2$)	1	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (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	0.38	0/1697	0.60	1/2295 (0.0%)
1	B	0.38	0/1697	0.60	1/2295 (0.0%)
1	C	0.38	0/1697	0.60	1/2295 (0.0%)
1	D	0.38	0/1697	0.60	1/2295 (0.0%)
1	E	0.38	0/1697	0.60	1/2295 (0.0%)
1	F	0.38	0/1697	0.60	1/2295 (0.0%)
1	G	0.38	0/1697	0.60	1/2295 (0.0%)
1	H	0.38	0/1697	0.60	1/2295 (0.0%)
1	I	0.38	0/1697	0.60	0/2295
1	J	0.38	0/1697	0.60	2/2295 (0.1%)
1	K	0.38	0/1697	0.60	1/2295 (0.0%)
1	L	0.38	0/1697	0.60	1/2295 (0.0%)
1	M	0.38	0/1697	0.60	1/2295 (0.0%)
1	N	0.38	0/1697	0.60	1/2295 (0.0%)
1	O	0.38	0/1697	0.60	1/2295 (0.0%)
1	P	0.38	0/1697	0.60	1/2295 (0.0%)
1	Q	0.38	0/1697	0.60	1/2295 (0.0%)
1	R	0.38	0/1697	0.60	1/2295 (0.0%)
1	S	0.38	0/1697	0.60	1/2295 (0.0%)
1	T	0.38	0/1697	0.60	1/2295 (0.0%)
1	U	0.38	0/1697	0.60	1/2295 (0.0%)
1	V	0.38	0/1697	0.60	1/2295 (0.0%)
1	W	0.38	0/1697	0.60	1/2295 (0.0%)
1	X	0.38	0/1697	0.60	1/2295 (0.0%)
2	a	0.40	0/109	0.97	0/166
2	b	0.39	0/109	0.96	0/166
2	c	0.39	0/109	0.96	0/166
2	d	0.39	0/109	0.96	0/166
2	e	0.39	0/109	0.97	0/166
2	f	0.39	0/109	0.97	0/166
2	g	0.39	0/109	0.96	0/166
2	h	0.40	0/109	0.96	0/166
2	i	0.39	0/109	0.96	0/166
2	j	0.38	0/109	0.96	0/166

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
2	k	0.39	0/109	0.97	0/166
2	l	0.39	0/109	0.96	0/166
2	m	0.38	0/109	0.96	0/166
2	n	0.39	0/109	0.96	0/166
2	o	0.39	0/109	0.96	0/166
2	p	0.39	0/109	0.96	0/166
2	q	0.39	0/109	0.96	0/166
2	r	0.40	0/109	0.96	0/166
2	s	0.38	0/109	0.96	0/166
2	t	0.40	0/109	0.96	0/166
2	u	0.40	0/109	0.96	0/166
2	v	0.39	0/109	0.97	0/166
2	w	0.39	0/109	0.96	0/166
2	x	0.39	0/109	0.96	0/166
All	All	0.38	0/43344	0.63	24/59064 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	172	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	J	172	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	M	172	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	P	172	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	R	172	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	K	172	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	172	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	N	172	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	W	172	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	H	172	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	T	172	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	V	172	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	U	172	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	O	172	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	F	172	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	S	172	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	X	172	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	E	172	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	172	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	L	172	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	172	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	172	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	J	212	ARG	NE-CZ-NH1	5.01	122.81	120.30

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	1662	1631	1633	17	0
1	B	1662	1631	1633	28	0
1	C	1662	1631	1633	29	0
1	D	1662	1631	1633	29	0
1	E	1662	1631	1633	28	0
1	F	1662	1631	1633	29	0
1	G	1662	1631	1633	27	0
1	H	1662	1631	1633	25	0
1	I	1662	1631	1633	31	0
1	J	1662	1631	1633	30	0
1	K	1662	1631	1633	32	0
1	L	1662	1631	1633	31	0
1	M	1662	1631	1633	31	0
1	N	1662	1631	1633	31	0
1	O	1662	1631	1633	31	0
1	P	1662	1631	1633	31	0
1	Q	1662	1631	1633	29	0
1	R	1662	1631	1633	29	0
1	S	1662	1631	1633	29	0
1	T	1662	1631	1633	29	0
1	U	1662	1631	1633	28	0
1	V	1662	1631	1633	30	0
1	W	1662	1631	1633	30	0
1	X	1662	1631	1633	18	0
2	a	100	51	51	0	0
2	b	100	51	51	0	0
2	c	100	51	51	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	100	51	51	0	0
2	e	100	51	51	0	0
2	f	100	51	51	0	0
2	g	100	51	51	0	0
2	h	100	51	51	0	0
2	i	100	51	51	0	0
2	j	100	51	51	0	0
2	k	100	51	51	0	0
2	l	100	51	51	0	0
2	m	100	51	51	0	0
2	n	100	51	51	0	0
2	o	100	51	51	0	0
2	p	100	51	51	0	0
2	q	100	51	51	0	0
2	r	100	51	51	0	0
2	s	100	51	51	0	0
2	t	100	51	51	0	0
2	u	100	51	51	0	0
2	v	100	51	51	0	0
2	w	100	51	51	0	0
2	x	100	51	51	0	0
All	All	42288	40368	40416	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 6.

All (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:J:136:ASP:OD2	1:K:92:GLN:NE2	2.11	0.84
1:F:136:ASP:OD2	1:G:92:GLN:NE2	2.11	0.84
1:R:136:ASP:OD2	1:S:92:GLN:NE2	2.11	0.84
1:B:136:ASP:OD2	1:C:92:GLN:NE2	2.11	0.84
1:E:136:ASP:OD2	1:F:92:GLN:NE2	2.11	0.84
1:L:136:ASP:OD2	1:M:92:GLN:NE2	2.11	0.84
1:M:136:ASP:OD2	1:N:92:GLN:NE2	2.11	0.84
1:N:136:ASP:OD2	1:O:92:GLN:NE2	2.11	0.83
1:W:136:ASP:OD2	1:X:92:GLN:NE2	2.11	0.83
1:C:136:ASP:OD2	1:D:92:GLN:NE2	2.11	0.83
1:D:136:ASP:OD2	1:E:92:GLN:NE2	2.11	0.83
1:P:136:ASP:OD2	1:Q:92:GLN:NE2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:136:ASP:OD2	1:U:92:GLN:NE2	2.11	0.83
1:U:136:ASP:OD2	1:V:92:GLN:NE2	2.11	0.83
1:H:136:ASP:OD2	1:I:92:GLN:NE2	2.11	0.83
1:K:136:ASP:OD2	1:L:92:GLN:NE2	2.11	0.83
1:V:136:ASP:OD2	1:W:92:GLN:NE2	2.11	0.83
1:O:136:ASP:OD2	1:P:92:GLN:NE2	2.11	0.83
1:I:136:ASP:OD2	1:J:92:GLN:NE2	2.11	0.83
1:Q:136:ASP:OD2	1:R:92:GLN:NE2	2.11	0.83
1:G:136:ASP:OD2	1:H:92:GLN:NE2	2.11	0.83
1:S:136:ASP:OD2	1:T:92:GLN:NE2	2.11	0.83
1:A:136:ASP:OD2	1:B:92:GLN:NE2	2.11	0.82
1:G:155:GLN:OE1	1:H:102:LYS:N	2.17	0.78
1:H:155:GLN:OE1	1:I:102:LYS:N	2.17	0.78
1:F:155:GLN:OE1	1:G:102:LYS:N	2.17	0.77
1:K:155:GLN:OE1	1:L:102:LYS:N	2.17	0.77
1:Q:155:GLN:OE1	1:R:102:LYS:N	2.17	0.77
1:U:155:GLN:OE1	1:V:102:LYS:N	2.17	0.77
1:W:155:GLN:OE1	1:X:102:LYS:N	2.17	0.77
1:C:155:GLN:OE1	1:D:102:LYS:N	2.17	0.77
1:R:155:GLN:OE1	1:S:102:LYS:N	2.17	0.77
1:D:155:GLN:OE1	1:E:102:LYS:N	2.17	0.77
1:M:155:GLN:OE1	1:N:102:LYS:N	2.17	0.77
1:T:155:GLN:OE1	1:U:102:LYS:N	2.17	0.77
1:B:155:GLN:OE1	1:C:102:LYS:N	2.17	0.76
1:P:155:GLN:OE1	1:Q:102:LYS:N	2.17	0.76
1:S:155:GLN:OE1	1:T:102:LYS:N	2.17	0.76
1:E:155:GLN:OE1	1:F:102:LYS:N	2.17	0.76
1:A:155:GLN:OE1	1:B:102:LYS:N	2.17	0.76
1:L:155:GLN:OE1	1:M:102:LYS:N	2.17	0.76
1:V:155:GLN:OE1	1:W:102:LYS:N	2.17	0.76
1:J:155:GLN:OE1	1:K:102:LYS:N	2.17	0.75
1:O:155:GLN:OE1	1:P:102:LYS:N	2.17	0.75
1:I:155:GLN:OE1	1:J:102:LYS:N	2.17	0.75
1:N:155:GLN:OE1	1:O:102:LYS:N	2.17	0.75
1:I:168:LYS:HD3	1:Q:192:GLU:O	2.04	0.58
1:N:168:LYS:HD3	1:V:192:GLU:O	2.04	0.58
1:M:168:LYS:HD3	1:U:192:GLU:O	2.04	0.58
1:E:168:LYS:HD3	1:M:192:GLU:O	2.04	0.58
1:A:168:LYS:HD3	1:I:192:GLU:O	2.04	0.58
1:H:168:LYS:HD3	1:P:192:GLU:O	2.04	0.57
1:F:168:LYS:HD3	1:N:192:GLU:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:168:LYS:HD3	1:T:192:GLU:O	2.04	0.57
1:C:168:LYS:HD3	1:K:192:GLU:O	2.04	0.57
1:P:168:LYS:HD3	1:X:192:GLU:O	2.04	0.57
1:O:168:LYS:HD3	1:W:192:GLU:O	2.04	0.57
1:B:168:LYS:HD3	1:J:192:GLU:O	2.04	0.57
1:J:168:LYS:HD3	1:R:192:GLU:O	2.04	0.57
1:G:168:LYS:HD3	1:O:192:GLU:O	2.04	0.57
1:D:168:LYS:HD3	1:L:192:GLU:O	2.04	0.56
1:B:122:GLN:OE1	1:L:60:PRO:HB3	2.06	0.56
1:M:122:GLN:OE1	1:W:60:PRO:HB3	2.06	0.56
1:H:122:GLN:OE1	1:R:60:PRO:HB3	2.06	0.56
1:L:122:GLN:OE1	1:V:60:PRO:HB3	2.06	0.56
1:A:122:GLN:OE1	1:K:60:PRO:HB3	2.06	0.56
1:D:122:GLN:OE1	1:N:60:PRO:HB3	2.06	0.56
1:K:168:LYS:HD3	1:S:192:GLU:O	2.04	0.56
1:G:122:GLN:OE1	1:Q:60:PRO:HB3	2.06	0.55
1:C:122:GLN:OE1	1:M:60:PRO:HB3	2.06	0.55
1:E:122:GLN:OE1	1:O:60:PRO:HB3	2.06	0.55
1:I:122:GLN:OE1	1:S:60:PRO:HB3	2.06	0.55
1:K:122:GLN:OE1	1:U:60:PRO:HB3	2.06	0.55
1:N:122:GLN:OE1	1:X:60:PRO:HB3	2.06	0.55
1:F:122:GLN:OE1	1:P:60:PRO:HB3	2.06	0.55
1:J:122:GLN:OE1	1:T:60:PRO:HB3	2.06	0.55
1:A:155:GLN:HE22	1:B:101:THR:HA	1.74	0.53
1:M:155:GLN:HE22	1:N:101:THR:HA	1.74	0.53
1:P:155:GLN:HE22	1:Q:101:THR:HA	1.74	0.53
1:F:155:GLN:HE22	1:G:101:THR:HA	1.74	0.53
1:G:155:GLN:HE22	1:H:101:THR:HA	1.74	0.53
1:H:155:GLN:HE22	1:I:101:THR:HA	1.74	0.53
1:I:155:GLN:HE22	1:J:101:THR:HA	1.74	0.53
1:N:155:GLN:HE22	1:O:101:THR:HA	1.73	0.53
1:B:155:GLN:HE22	1:C:101:THR:HA	1.74	0.53
1:E:155:GLN:HE22	1:F:101:THR:HA	1.73	0.53
1:S:155:GLN:HE22	1:T:101:THR:HA	1.74	0.53
1:T:155:GLN:HE22	1:U:101:THR:HA	1.74	0.53
1:L:155:GLN:HE22	1:M:101:THR:HA	1.73	0.53
1:R:155:GLN:HE22	1:S:101:THR:HA	1.73	0.53
1:U:155:GLN:HE22	1:V:101:THR:HA	1.74	0.52
1:W:155:GLN:HE22	1:X:101:THR:HA	1.74	0.52
1:O:155:GLN:HE22	1:P:101:THR:HA	1.74	0.52
1:D:168:LYS:HA	1:L:194:PRO:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:155:GLN:HE22	1:K:101:THR:HA	1.74	0.52
1:C:155:GLN:HE22	1:D:101:THR:HA	1.74	0.52
1:M:168:LYS:HA	1:U:194:PRO:HD3	1.92	0.52
1:E:168:LYS:HA	1:M:194:PRO:HD3	1.92	0.52
1:N:168:LYS:HA	1:V:194:PRO:HD3	1.92	0.52
1:L:168:LYS:HA	1:T:194:PRO:HD3	1.92	0.52
1:C:168:LYS:HA	1:K:194:PRO:HD3	1.92	0.52
1:F:168:LYS:HA	1:N:194:PRO:HD3	1.92	0.52
1:O:168:LYS:HA	1:W:194:PRO:HD3	1.92	0.52
1:B:168:LYS:HA	1:J:194:PRO:HD3	1.92	0.52
1:Q:155:GLN:HE22	1:R:101:THR:HA	1.74	0.52
1:D:155:GLN:HE22	1:E:101:THR:HA	1.74	0.51
1:G:168:LYS:HA	1:O:194:PRO:HD3	1.92	0.51
1:K:168:LYS:HA	1:S:194:PRO:HD3	1.92	0.51
1:K:155:GLN:HE22	1:L:101:THR:HA	1.74	0.51
1:J:168:LYS:HA	1:R:194:PRO:HD3	1.92	0.51
1:F:204:ASN:OD1	1:G:229:ARG:HG2	2.11	0.51
1:I:204:ASN:OD1	1:J:229:ARG:HG2	2.11	0.51
1:V:155:GLN:HE22	1:W:101:THR:HA	1.74	0.51
1:W:204:ASN:OD1	1:X:229:ARG:HG2	2.11	0.51
1:E:204:ASN:OD1	1:F:229:ARG:HG2	2.11	0.51
1:G:204:ASN:OD1	1:H:229:ARG:HG2	2.11	0.51
1:P:168:LYS:HA	1:X:194:PRO:HD3	1.92	0.51
1:H:168:LYS:HA	1:P:194:PRO:HD3	1.92	0.51
1:J:204:ASN:OD1	1:K:229:ARG:HG2	2.11	0.51
1:V:204:ASN:OD1	1:W:229:ARG:HG2	2.11	0.51
1:C:204:ASN:OD1	1:D:229:ARG:HG2	2.11	0.51
1:H:204:ASN:OD1	1:I:229:ARG:HG2	2.11	0.51
1:M:204:ASN:OD1	1:N:229:ARG:HG2	2.11	0.51
1:T:204:ASN:OD1	1:U:229:ARG:HG2	2.11	0.51
1:U:204:ASN:OD1	1:V:229:ARG:HG2	2.11	0.51
1:B:204:ASN:OD1	1:C:229:ARG:HG2	2.11	0.51
1:K:204:ASN:OD1	1:L:229:ARG:HG2	2.11	0.51
1:A:168:LYS:HA	1:I:194:PRO:HD3	1.92	0.51
1:A:204:ASN:OD1	1:B:229:ARG:HG2	2.11	0.50
1:L:204:ASN:OD1	1:M:229:ARG:HG2	2.11	0.50
1:I:168:LYS:HA	1:Q:194:PRO:HD3	1.92	0.50
1:D:204:ASN:OD1	1:E:229:ARG:HG2	2.11	0.50
1:B:213:TYR:HE1	1:B:218:TYR:HH	1.58	0.50
1:R:204:ASN:OD1	1:S:229:ARG:HG2	2.11	0.50
1:S:204:ASN:OD1	1:T:229:ARG:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:204:ASN:OD1	1:O:229:ARG:HG2	2.11	0.50
1:Q:204:ASN:OD1	1:R:229:ARG:HG2	2.11	0.50
1:I:188:MET:O	1:I:191:SER:OG	2.13	0.50
1:O:204:ASN:OD1	1:P:229:ARG:HG2	2.11	0.49
1:P:204:ASN:OD1	1:Q:229:ARG:HG2	2.11	0.49
1:R:188:MET:O	1:R:191:SER:OG	2.13	0.49
1:I:213:TYR:HE1	1:I:218:TYR:HH	1.59	0.49
1:K:213:TYR:HE1	1:K:218:TYR:HH	1.59	0.48
1:D:213:TYR:HE1	1:D:218:TYR:HH	1.61	0.48
1:F:155:GLN:OE1	1:G:102:LYS:HG2	2.14	0.48
1:J:155:GLN:OE1	1:K:102:LYS:HG2	2.14	0.48
1:K:155:GLN:OE1	1:L:102:LYS:HG2	2.14	0.48
1:Q:155:GLN:OE1	1:R:102:LYS:HG2	2.14	0.48
1:W:155:GLN:OE1	1:X:102:LYS:HG2	2.14	0.48
1:E:155:GLN:OE1	1:F:102:LYS:HG2	2.14	0.48
1:C:155:GLN:OE1	1:D:102:LYS:HG2	2.14	0.48
1:D:155:GLN:OE1	1:E:102:LYS:HG2	2.14	0.48
1:H:155:GLN:OE1	1:I:102:LYS:HG2	2.14	0.48
1:P:155:GLN:OE1	1:Q:102:LYS:HG2	2.14	0.48
1:R:155:GLN:OE1	1:S:102:LYS:HG2	2.14	0.48
1:I:155:GLN:OE1	1:J:102:LYS:HG2	2.14	0.48
1:V:155:GLN:OE1	1:W:102:LYS:HG2	2.14	0.48
1:G:155:GLN:OE1	1:H:102:LYS:HG2	2.14	0.48
1:L:155:GLN:OE1	1:M:102:LYS:HG2	2.14	0.48
1:B:155:GLN:OE1	1:C:102:LYS:HG2	2.14	0.47
1:O:155:GLN:OE1	1:P:102:LYS:HG2	2.14	0.47
1:S:155:GLN:OE1	1:T:102:LYS:HG2	2.14	0.47
1:U:155:GLN:OE1	1:V:102:LYS:HG2	2.14	0.47
1:M:155:GLN:OE1	1:N:102:LYS:HG2	2.14	0.47
1:T:188:MET:O	1:T:191:SER:OG	2.13	0.47
1:D:188:MET:O	1:D:191:SER:OG	2.13	0.47
1:T:155:GLN:OE1	1:U:102:LYS:HG2	2.14	0.47
1:J:188:MET:O	1:J:191:SER:OG	2.13	0.47
1:P:137:ASN:ND2	1:Q:97:ASN:HB2	2.30	0.47
1:A:155:GLN:OE1	1:B:102:LYS:HG2	2.14	0.47
1:I:137:ASN:ND2	1:J:97:ASN:HB2	2.30	0.47
1:N:155:GLN:OE1	1:O:102:LYS:HG2	2.14	0.47
1:Q:137:ASN:ND2	1:R:97:ASN:HB2	2.30	0.47
1:Q:188:MET:O	1:Q:191:SER:OG	2.13	0.47
1:C:188:MET:O	1:C:191:SER:OG	2.13	0.47
1:D:137:ASN:ND2	1:E:97:ASN:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:137:ASN:ND2	1:P:97:ASN:HB2	2.30	0.47
1:H:137:ASN:ND2	1:I:97:ASN:HB2	2.30	0.47
1:H:188:MET:O	1:H:191:SER:OG	2.13	0.47
1:T:137:ASN:ND2	1:U:97:ASN:HB2	2.30	0.47
1:U:137:ASN:ND2	1:V:97:ASN:HB2	2.30	0.47
1:J:213:TYR:HE1	1:J:218:TYR:HH	1.62	0.47
1:K:137:ASN:ND2	1:L:97:ASN:HB2	2.30	0.47
1:W:137:ASN:ND2	1:X:97:ASN:HB2	2.30	0.47
1:M:188:MET:O	1:M:191:SER:OG	2.13	0.46
1:C:137:ASN:ND2	1:D:97:ASN:HB2	2.30	0.46
1:J:137:ASN:ND2	1:K:97:ASN:HB2	2.30	0.46
1:V:137:ASN:ND2	1:W:97:ASN:HB2	2.30	0.46
1:E:137:ASN:ND2	1:F:97:ASN:HB2	2.30	0.46
1:Q:213:TYR:HE1	1:Q:218:TYR:HH	1.61	0.46
1:A:263:ARG:HD2	1:R:238:ALA:HB2	1.98	0.46
1:R:137:ASN:ND2	1:S:97:ASN:HB2	2.30	0.46
1:G:137:ASN:ND2	1:H:97:ASN:HB2	2.30	0.46
1:L:137:ASN:ND2	1:M:97:ASN:HB2	2.30	0.46
1:N:137:ASN:ND2	1:O:97:ASN:HB2	2.30	0.46
1:S:137:ASN:ND2	1:T:97:ASN:HB2	2.30	0.46
1:F:137:ASN:ND2	1:G:97:ASN:HB2	2.30	0.46
1:M:137:ASN:ND2	1:N:97:ASN:HB2	2.30	0.46
1:B:137:ASN:ND2	1:C:97:ASN:HB2	2.30	0.46
1:B:263:ARG:HD2	1:S:238:ALA:HB2	1.98	0.45
1:V:188:MET:O	1:V:191:SER:OG	2.13	0.45
1:A:137:ASN:ND2	1:B:97:ASN:HB2	2.30	0.45
1:E:263:ARG:HD2	1:V:238:ALA:HB2	1.98	0.45
1:R:213:TYR:HE1	1:R:218:TYR:HH	1.64	0.45
1:F:263:ARG:HD2	1:W:238:ALA:HB2	1.98	0.45
1:K:188:MET:O	1:K:191:SER:OG	2.13	0.45
1:T:213:TYR:HE1	1:T:218:TYR:HH	1.64	0.45
1:D:263:ARG:HD2	1:U:238:ALA:HB2	1.98	0.45
1:W:213:TYR:HE1	1:W:218:TYR:HH	1.65	0.45
1:G:263:ARG:HD2	1:X:238:ALA:HB2	1.98	0.45
1:A:188:MET:O	1:A:191:SER:OG	2.13	0.44
1:C:263:ARG:HD2	1:T:238:ALA:HB2	1.98	0.44
1:L:213:TYR:HE1	1:L:218:TYR:HH	1.65	0.44
1:S:213:TYR:HE1	1:S:218:TYR:HH	1.62	0.44
1:U:188:MET:O	1:U:191:SER:OG	2.13	0.44
1:E:188:MET:O	1:E:191:SER:OG	2.13	0.44
1:P:188:MET:O	1:P:191:SER:OG	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:213:TYR:HE1	1:O:218:TYR:HH	1.66	0.43
1:D:168:LYS:HB3	1:L:192:GLU:O	2.19	0.43
1:G:188:MET:O	1:G:191:SER:OG	2.13	0.43
1:I:260:ASN:O	1:I:261:THR:OG1	2.33	0.43
1:J:168:LYS:HB3	1:R:192:GLU:O	2.19	0.43
1:G:213:TYR:HE1	1:G:218:TYR:HH	1.66	0.43
1:A:168:LYS:HB3	1:I:192:GLU:O	2.19	0.43
1:C:168:LYS:HB3	1:K:192:GLU:O	2.19	0.43
1:N:188:MET:O	1:N:191:SER:OG	2.13	0.43
1:I:168:LYS:HB3	1:Q:192:GLU:O	2.19	0.43
1:N:168:LYS:HB3	1:V:192:GLU:O	2.19	0.43
1:B:168:LYS:HB3	1:J:192:GLU:O	2.19	0.43
1:F:168:LYS:HB3	1:N:192:GLU:O	2.19	0.43
1:X:213:TYR:HE1	1:X:218:TYR:HH	1.63	0.43
1:K:201:LEU:HD13	1:L:220:VAL:HG12	2.01	0.43
1:K:168:LYS:HB3	1:S:192:GLU:O	2.19	0.43
1:M:168:LYS:HB3	1:U:192:GLU:O	2.19	0.43
1:L:201:LEU:HD13	1:M:220:VAL:HG12	2.01	0.43
1:W:188:MET:O	1:W:191:SER:OG	2.13	0.43
1:E:168:LYS:HB3	1:M:192:GLU:O	2.19	0.43
1:J:201:LEU:HD13	1:K:220:VAL:HG12	2.01	0.43
1:U:201:LEU:HD13	1:V:220:VAL:HG12	2.01	0.43
1:V:201:LEU:HD13	1:W:220:VAL:HG12	2.01	0.43
1:O:168:LYS:HB3	1:W:192:GLU:O	2.19	0.42
1:H:132:VAL:HG12	1:I:95:LEU:HD21	2.01	0.42
1:G:168:LYS:HB3	1:O:192:GLU:O	2.19	0.42
1:O:188:MET:O	1:O:191:SER:OG	2.13	0.42
1:T:201:LEU:HD13	1:U:220:VAL:HG12	2.01	0.42
1:B:188:MET:O	1:B:191:SER:OG	2.13	0.42
1:A:201:LEU:HD13	1:B:220:VAL:HG12	2.01	0.42
1:C:132:VAL:HG12	1:D:95:LEU:HD21	2.01	0.42
1:D:201:LEU:HD13	1:E:220:VAL:HG12	2.01	0.42
1:E:201:LEU:HD13	1:F:220:VAL:HG12	2.01	0.42
1:G:132:VAL:HG12	1:H:95:LEU:HD21	2.01	0.42
1:P:132:VAL:HG12	1:Q:95:LEU:HD21	2.01	0.42
1:Q:132:VAL:HG12	1:R:95:LEU:HD21	2.01	0.42
1:L:168:LYS:HB3	1:T:192:GLU:O	2.19	0.42
1:X:188:MET:O	1:X:191:SER:OG	2.13	0.42
1:P:168:LYS:HB3	1:X:192:GLU:O	2.19	0.42
1:F:188:MET:O	1:F:191:SER:OG	2.13	0.42
1:I:201:LEU:HD13	1:J:220:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:ARG:CD	1:I:226:ASN:HB3	2.50	0.42
1:M:201:LEU:HD13	1:N:220:VAL:HG12	2.01	0.42
1:U:132:VAL:HG12	1:V:95:LEU:HD21	2.01	0.42
1:A:213:TYR:HE1	1:A:218:TYR:HH	1.66	0.42
1:H:168:LYS:HB3	1:P:192:GLU:O	2.19	0.42
1:B:201:LEU:HD13	1:C:220:VAL:HG12	2.01	0.42
1:C:201:LEU:HD13	1:D:220:VAL:HG12	2.01	0.42
1:K:132:VAL:HG12	1:L:95:LEU:HD21	2.01	0.42
1:L:206:ARG:CD	1:M:226:ASN:HB3	2.50	0.42
1:M:132:VAL:HG12	1:N:95:LEU:HD21	2.01	0.42
1:P:201:LEU:HD13	1:Q:220:VAL:HG12	2.01	0.42
1:U:206:ARG:CD	1:V:226:ASN:HB3	2.50	0.42
1:W:201:LEU:HD13	1:X:220:VAL:HG12	2.01	0.42
1:A:206:ARG:CD	1:B:226:ASN:HB3	2.50	0.42
1:A:198:ARG:NH2	1:B:98:THR:HG21	2.35	0.42
1:C:198:ARG:NH2	1:D:98:THR:HG21	2.35	0.42
1:F:132:VAL:HG12	1:G:95:LEU:HD21	2.01	0.42
1:G:201:LEU:HD13	1:H:220:VAL:HG12	2.01	0.42
1:I:132:VAL:HG12	1:J:95:LEU:HD21	2.01	0.42
1:I:206:ARG:CD	1:J:226:ASN:HB3	2.50	0.42
1:L:188:MET:O	1:L:191:SER:OG	2.13	0.42
1:O:206:ARG:CD	1:P:226:ASN:HB3	2.50	0.42
1:N:198:ARG:NH2	1:O:98:THR:HG21	2.35	0.42
1:O:155:GLN:NE2	1:P:101:THR:HA	2.35	0.42
1:R:206:ARG:CD	1:S:226:ASN:HB3	2.50	0.42
1:Q:201:LEU:HD13	1:R:220:VAL:HG12	2.01	0.42
1:S:188:MET:O	1:S:191:SER:OG	2.13	0.42
1:U:198:ARG:NH2	1:V:98:THR:HG21	2.35	0.42
1:B:198:ARG:NH2	1:C:98:THR:HG21	2.35	0.42
1:C:206:ARG:CD	1:D:226:ASN:HB3	2.50	0.42
1:D:132:VAL:HG12	1:E:95:LEU:HD21	2.01	0.42
1:G:198:ARG:NH2	1:H:98:THR:HG21	2.35	0.42
1:I:198:ARG:NH2	1:J:98:THR:HG21	2.35	0.42
1:P:155:GLN:NE2	1:Q:101:THR:HA	2.35	0.42
1:Q:206:ARG:CD	1:R:226:ASN:HB3	2.50	0.42
1:S:206:ARG:CD	1:T:226:ASN:HB3	2.50	0.42
1:R:201:LEU:HD13	1:S:220:VAL:HG12	2.01	0.42
1:R:132:VAL:HG12	1:S:95:LEU:HD21	2.01	0.42
1:D:206:ARG:CD	1:E:226:ASN:HB3	2.50	0.41
1:N:155:GLN:NE2	1:O:101:THR:HA	2.35	0.41
1:P:206:ARG:CD	1:Q:226:ASN:HB3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:198:ARG:NH2	1:U:98:THR:HG21	2.35	0.41
1:F:201:LEU:HD13	1:G:220:VAL:HG12	2.01	0.41
1:G:206:ARG:CD	1:H:226:ASN:HB3	2.50	0.41
1:H:201:LEU:HD13	1:I:220:VAL:HG12	2.01	0.41
1:M:198:ARG:NH2	1:N:98:THR:HG21	2.35	0.41
1:O:201:LEU:HD13	1:P:220:VAL:HG12	2.01	0.41
1:O:132:VAL:HG12	1:P:95:LEU:HD21	2.01	0.41
1:O:198:ARG:NH2	1:P:98:THR:HG21	2.35	0.41
1:Q:155:GLN:NE2	1:R:101:THR:HA	2.35	0.41
1:R:198:ARG:NH2	1:S:98:THR:HG21	2.35	0.41
1:S:201:LEU:HD13	1:T:220:VAL:HG12	2.01	0.41
1:V:132:VAL:HG12	1:W:95:LEU:HD21	2.01	0.41
1:W:206:ARG:CD	1:X:226:ASN:HB3	2.50	0.41
1:B:206:ARG:CD	1:C:226:ASN:HB3	2.50	0.41
1:F:198:ARG:NH2	1:G:98:THR:HG21	2.35	0.41
1:N:213:TYR:HE1	1:N:218:TYR:HH	1.68	0.41
1:N:206:ARG:CD	1:O:226:ASN:HB3	2.50	0.41
1:Q:198:ARG:NH2	1:R:98:THR:HG21	2.35	0.41
1:S:132:VAL:HG12	1:T:95:LEU:HD21	2.01	0.41
1:A:132:VAL:HG12	1:B:95:LEU:HD21	2.01	0.41
1:E:132:VAL:HG12	1:F:95:LEU:HD21	2.01	0.41
1:H:198:ARG:NH2	1:I:98:THR:HG21	2.35	0.41
1:L:132:VAL:HG12	1:M:95:LEU:HD21	2.01	0.41
1:V:198:ARG:NH2	1:W:98:THR:HG21	2.35	0.41
1:V:213:TYR:HE1	1:V:218:TYR:HH	1.68	0.41
1:E:206:ARG:CD	1:F:226:ASN:HB3	2.50	0.41
1:J:198:ARG:NH2	1:K:98:THR:HG21	2.35	0.41
1:C:213:TYR:HE1	1:C:218:TYR:HH	1.66	0.41
1:D:198:ARG:NH2	1:E:98:THR:HG21	2.35	0.41
1:K:206:ARG:CD	1:L:226:ASN:HB3	2.50	0.41
1:N:132:VAL:HG12	1:O:95:LEU:HD21	2.01	0.41
1:M:206:ARG:CD	1:N:226:ASN:HB3	2.50	0.41
1:J:132:VAL:HG12	1:K:95:LEU:HD21	2.01	0.41
1:M:213:TYR:HE1	1:M:218:TYR:HH	1.65	0.41
1:S:198:ARG:NH2	1:T:98:THR:HG21	2.35	0.41
1:T:206:ARG:CD	1:U:226:ASN:HB3	2.50	0.41
1:V:155:GLN:NE2	1:W:101:THR:HA	2.35	0.41
1:V:206:ARG:CD	1:W:226:ASN:HB3	2.50	0.41
1:W:155:GLN:NE2	1:X:101:THR:HA	2.35	0.41
1:F:206:ARG:CD	1:G:226:ASN:HB3	2.50	0.41
1:K:198:ARG:NH2	1:L:98:THR:HG21	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:198:ARG:NH2	1:Q:98:THR:HG21	2.35	0.41
1:T:132:VAL:HG12	1:U:95:LEU:HD21	2.01	0.41
1:P:260:ASN:O	1:P:261:THR:OG1	2.33	0.41
1:F:213:TYR:HE1	1:F:218:TYR:HH	1.67	0.41
1:J:155:GLN:NE2	1:K:101:THR:HA	2.35	0.41
1:N:201:LEU:HD13	1:O:220:VAL:HG12	2.01	0.41
1:T:155:GLN:NE2	1:U:101:THR:HA	2.35	0.41
1:B:132:VAL:HG12	1:C:95:LEU:HD21	2.01	0.41
1:D:155:GLN:NE2	1:E:101:THR:HA	2.35	0.41
1:F:260:ASN:O	1:F:261:THR:OG1	2.33	0.41
1:J:206:ARG:CD	1:K:226:ASN:HB3	2.50	0.41
1:L:198:ARG:NH2	1:M:98:THR:HG21	2.35	0.41
1:U:155:GLN:NE2	1:V:101:THR:HA	2.35	0.41
1:W:132:VAL:HG12	1:X:95:LEU:HD21	2.01	0.41
1:C:155:GLN:NE2	1:D:101:THR:HA	2.35	0.40
1:E:198:ARG:NH2	1:F:98:THR:HG21	2.35	0.40
1:E:155:GLN:NE2	1:F:101:THR:HA	2.35	0.40
1:R:155:GLN:NE2	1:S:101:THR:HA	2.35	0.40
1:B:155:GLN:NE2	1:C:101:THR:HA	2.35	0.40
1:L:155:GLN:NE2	1:M:101:THR:HA	2.35	0.40
1:W:198:ARG:NH2	1:X:98:THR:HG21	2.35	0.40
1:K:260:ASN:O	1:K:261:THR:OG1	2.33	0.40
1:S:155:GLN:NE2	1:T:101:THR:HA	2.35	0.40
1:I:248:PHE:CZ	1:Q:234:GLN:HB2	2.57	0.40
1:V:189:ARG:HH22	1:W:89:LYS:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	205/281 (73%)	178 (87%)	27 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	C	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	D	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	E	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	F	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	G	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	H	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	I	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	J	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	K	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	L	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	M	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	N	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	O	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	P	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	Q	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	R	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	S	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	T	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	U	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	V	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	W	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
1	X	205/281 (73%)	178 (87%)	27 (13%)	0	100	100
All	All	4920/6744 (73%)	4272 (87%)	648 (13%)	0	100	100

There are no Ramachandran outliers to report.

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	180/241 (75%)	180 (100%)	0	100	100
1	B	180/241 (75%)	180 (100%)	0	100	100
1	C	180/241 (75%)	180 (100%)	0	100	100
1	D	180/241 (75%)	180 (100%)	0	100	100
1	E	180/241 (75%)	180 (100%)	0	100	100
1	F	180/241 (75%)	180 (100%)	0	100	100
1	G	180/241 (75%)	180 (100%)	0	100	100
1	H	180/241 (75%)	180 (100%)	0	100	100
1	I	180/241 (75%)	180 (100%)	0	100	100
1	J	180/241 (75%)	180 (100%)	0	100	100
1	K	180/241 (75%)	180 (100%)	0	100	100
1	L	180/241 (75%)	180 (100%)	0	100	100
1	M	180/241 (75%)	180 (100%)	0	100	100
1	N	180/241 (75%)	180 (100%)	0	100	100
1	O	180/241 (75%)	180 (100%)	0	100	100
1	P	180/241 (75%)	180 (100%)	0	100	100
1	Q	180/241 (75%)	180 (100%)	0	100	100
1	R	180/241 (75%)	180 (100%)	0	100	100
1	S	180/241 (75%)	180 (100%)	0	100	100
1	T	180/241 (75%)	180 (100%)	0	100	100
1	U	180/241 (75%)	180 (100%)	0	100	100
1	V	180/241 (75%)	180 (100%)	0	100	100
1	W	180/241 (75%)	180 (100%)	0	100	100
1	X	180/241 (75%)	180 (100%)	0	100	100
All	All	4320/5784 (75%)	4320 (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. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	B	137	ASN
1	C	137	ASN

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Mol	Chain	Res	Type
1	D	137	ASN
1	E	137	ASN
1	F	137	ASN
1	G	137	ASN
1	H	137	ASN
1	I	137	ASN
1	J	137	ASN
1	K	137	ASN
1	L	137	ASN
1	M	137	ASN
1	N	137	ASN
1	O	137	ASN
1	P	137	ASN
1	Q	137	ASN
1	R	137	ASN
1	S	137	ASN
1	T	137	ASN
1	U	137	ASN
1	V	137	ASN
1	W	137	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	a	4/5 (80%)	0	0
2	b	4/5 (80%)	0	0
2	c	4/5 (80%)	0	0
2	d	4/5 (80%)	0	0
2	e	4/5 (80%)	0	0
2	f	4/5 (80%)	0	0
2	g	4/5 (80%)	0	0
2	h	4/5 (80%)	0	0
2	i	4/5 (80%)	0	0
2	j	4/5 (80%)	0	0
2	k	4/5 (80%)	0	0
2	l	4/5 (80%)	0	0
2	m	4/5 (80%)	0	0
2	n	4/5 (80%)	0	0
2	o	4/5 (80%)	0	0
2	p	4/5 (80%)	0	0
2	q	4/5 (80%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	r	4/5 (80%)	0	0
2	s	4/5 (80%)	0	0
2	t	4/5 (80%)	0	0
2	u	4/5 (80%)	0	0
2	v	4/5 (80%)	0	0
2	w	4/5 (80%)	0	0
2	x	4/5 (80%)	0	0
All	All	96/120 (80%)	0	0

There are no RNA backbone outliers to report.

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.