



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:11 PM BST

PDB ID : 4BKK
EMDB ID: : EMD-2369
Title : The Respiratory Syncytial Virus nucleoprotein-RNA complex forms a left-handed helical nucleocapsid.
Authors : Bakker, S.E.; Duquerroy, S.; Galloux, M.; Loney, C.; Conner, E.; Eleouet, J.F.; Rey, F.A.; Bhella, D.
Deposited on : 2013-04-26
Resolution : unknown (reported)
Based on PDB ID : 2WJ8

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>

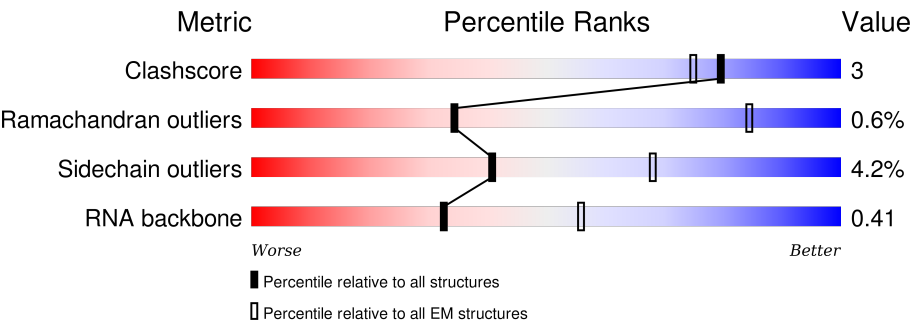
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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	161	<div><div>86%14%</div></div>
2	B	391	<div><div>86%8%5%</div></div>
2	C	391	<div><div>85%9%5%</div></div>
2	D	391	<div><div>85%9%5%</div></div>
2	E	391	<div><div>85%9%5%</div></div>
2	F	391	<div><div>85%9%5%</div></div>
2	G	391	<div><div>85%9%5%</div></div>
2	H	391	<div><div>85%9%5%</div></div>

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Mol	Chain	Length	Quality of chain
2	I	391	 85% 9% • 5%
2	J	391	 85% 9% • 5%
2	K	391	 85% 9% • 5%
2	L	391	 83% 10% • 5%
2	M	391	 83% 10% • 5%
2	N	391	 83% 10% • 5%
2	O	391	 84% 9% • 5%
2	P	391	 84% 9% • 5%
2	Q	391	 84% 9% • 5%
2	R	391	 84% 9% • 5%
2	S	391	 85% 9% • 5%
2	T	391	 84% 9% • 5%
2	U	391	 84% 9% • 5%
2	V	391	 85% 8% • 5%
2	W	391	 85% 9% • 5%
2	X	391	 85% 9% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 69483 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 RNA chain called RNA (161-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	161	Total	C	N	O	P	0	0
			3220	1449	483	1127	161		

- Molecule 2 is a protein called NUCLEOPROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	C	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	D	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	E	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	F	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	G	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	H	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	I	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	J	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	K	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	L	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	M	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	N	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	O	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		

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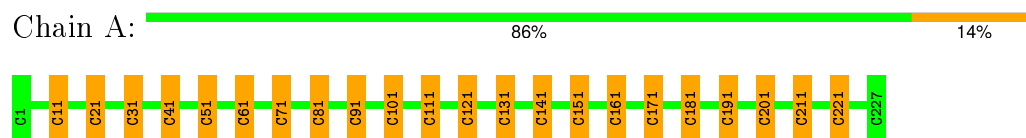
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	Q	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	R	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	S	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	T	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	U	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	V	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	W	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	X	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		

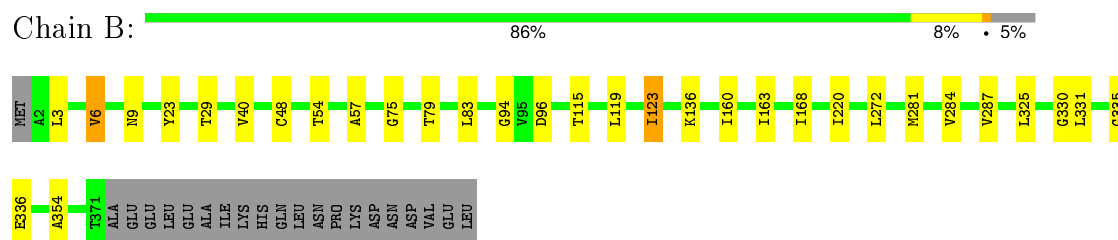
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

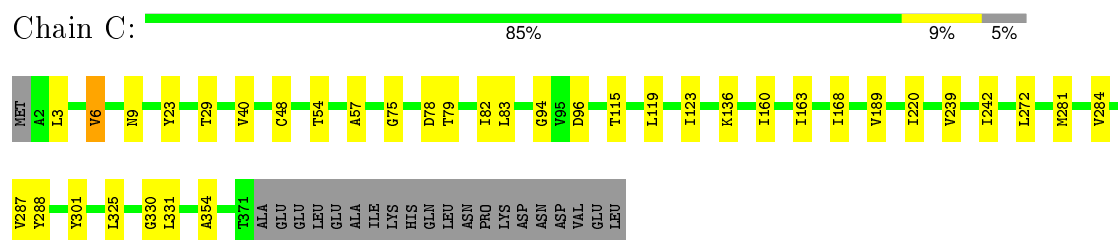
- Molecule 1: RNA (161-MER)



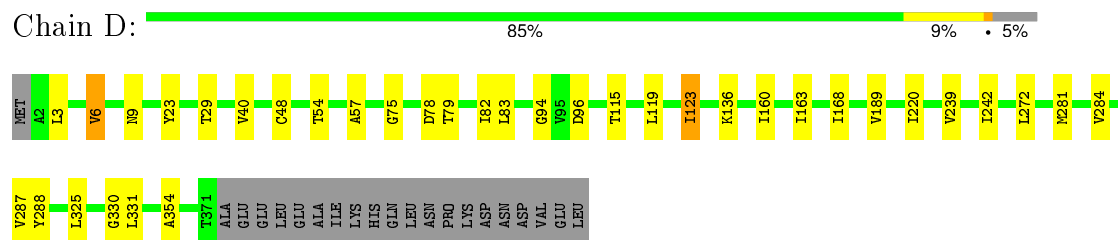
- Molecule 2: NUCLEOPROTEIN



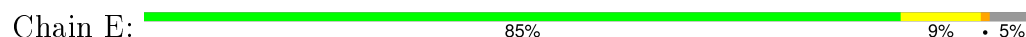
- Molecule 2: NUCLEOPROTEIN

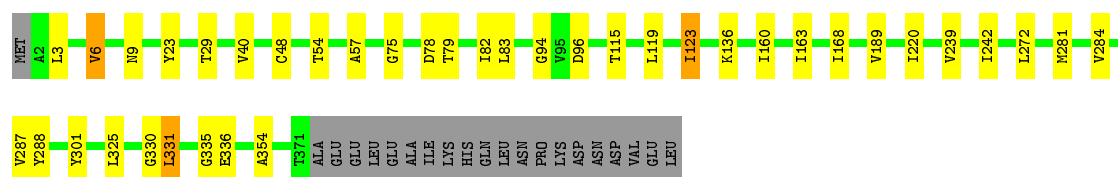


- Molecule 2: NUCLEOPROTEIN



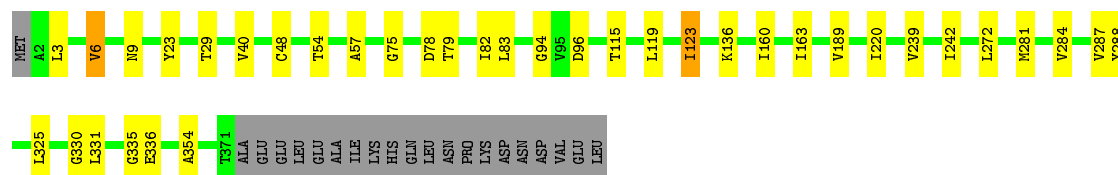
- Molecule 2: NUCLEOPROTEIN





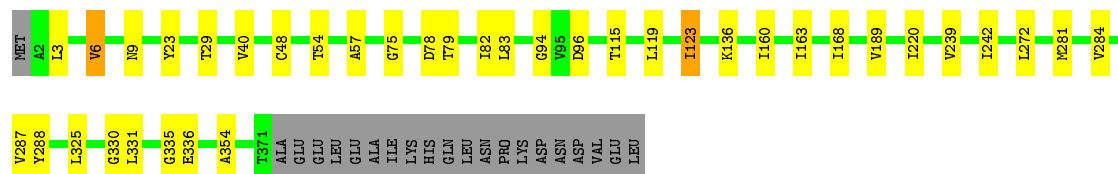
- Molecule 2: NUCLEOPROTEIN

Chain F: 85% 9% • 5%



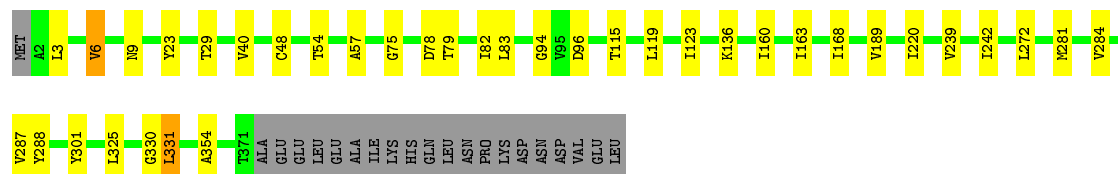
- Molecule 2: NUCLEOPROTEIN

Chain G: 85% 9% • 5%



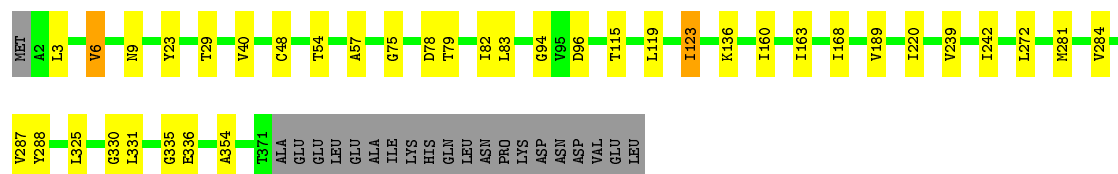
- Molecule 2: NUCLEOPROTEIN

Chain H: 85% 9% • 5%



- Molecule 2: NUCLEOPROTEIN

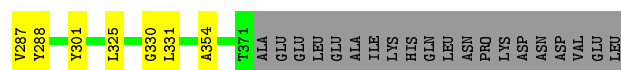
Chain I: 85% 9% • 5%



- Molecule 2: NUCLEOPROTEIN

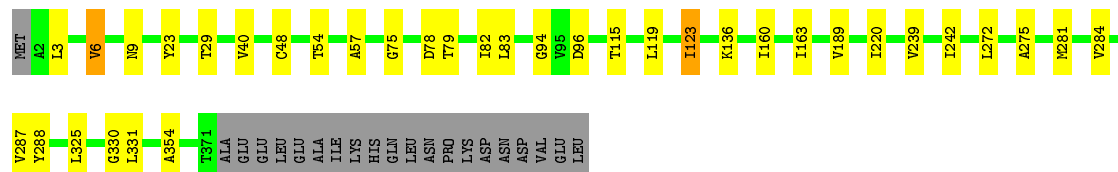
Chain J: 85% 9% • 5%





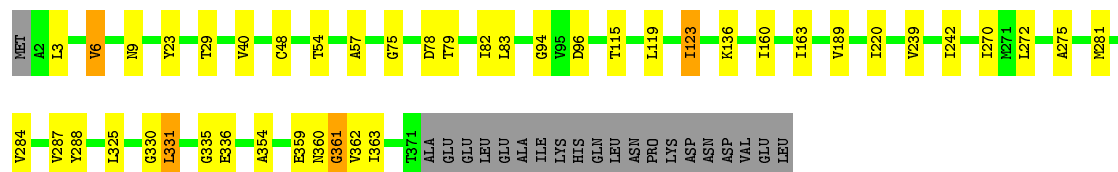
• Molecule 2: NUCLEOPROTEIN

Chain K: 85% 9% • 5%



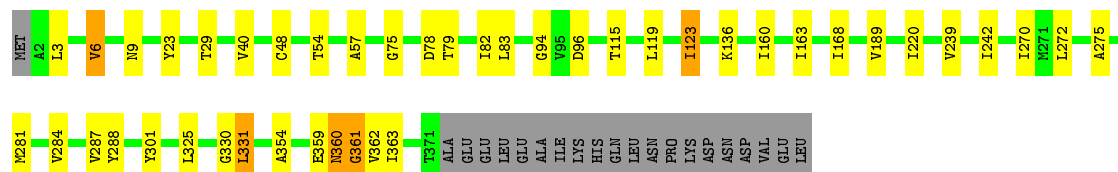
• Molecule 2: NUCLEOPROTEIN

Chain L: 83% 10% • 5%



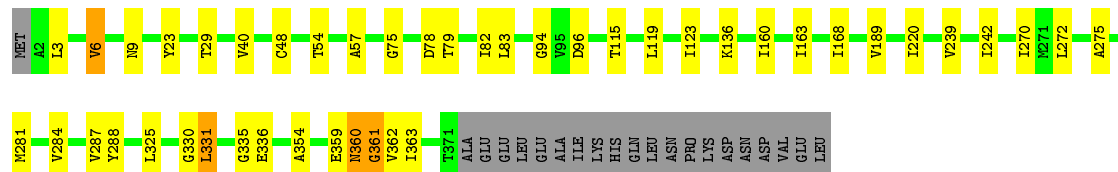
• Molecule 2: NUCLEOPROTEIN

Chain M: 83% 10% • 5%



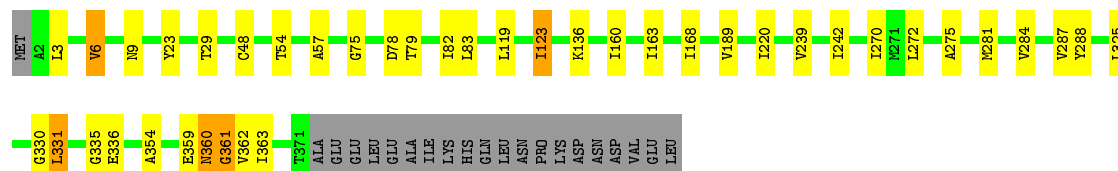
• Molecule 2: NUCLEOPROTEIN

Chain N: 83% 10% • 5%




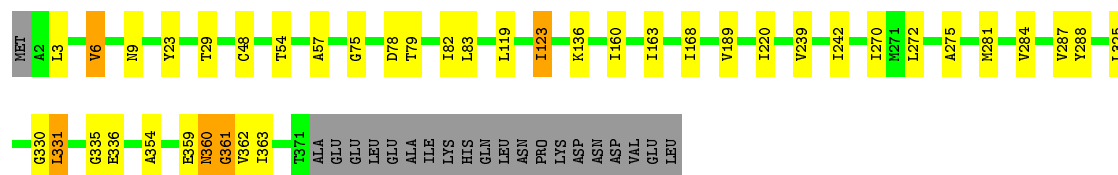
• Molecule 2: NUCLEOPROTEIN

Chain O: 84% 9% • 5%




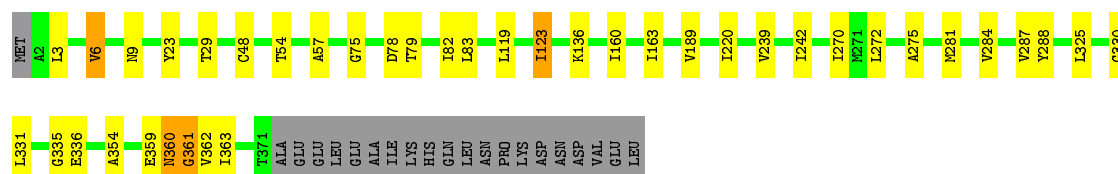
- Molecule 2: NUCLEOPROTEIN

Chain P: 




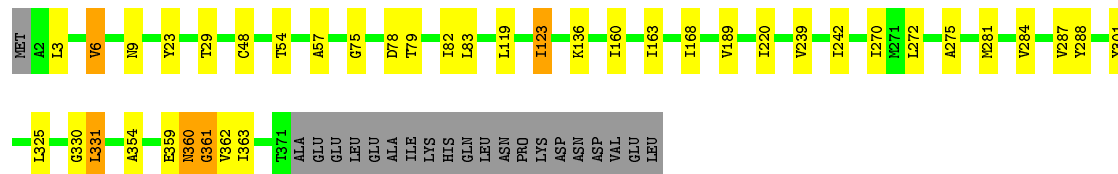
- Molecule 2: NUCLEOPROTEIN

Chain Q: 




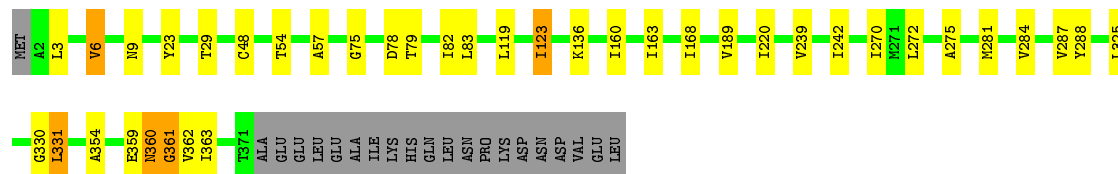
- Molecule 2: NUCLEOPROTEIN

Chain R: 




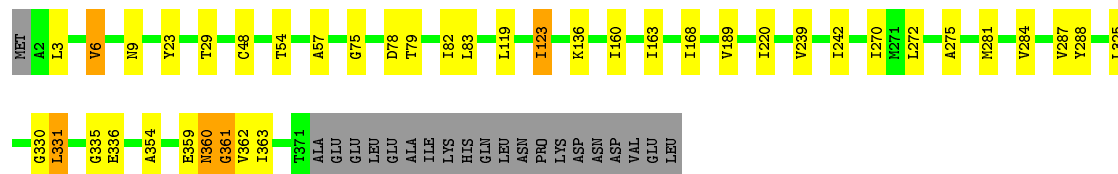
- Molecule 2: NUCLEOPROTEIN

Chain S: 



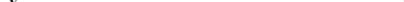
- Molecule 2: NUCLEOPROTEIN

Chain T: 



- Molecule 2: NUCLEOPROTEIN

[illegible]

Chain V:  85% 8% • 5%

L331	L332	A354	E359	I360	G361	V362	I363	T371	ALA	GLU	GLU	LEU	LEU	ALA	ALA	ILE	LYS	HIS	GLN	GLU	LEU	ASN	PRO	L32	L33	L119	L123	K136	I160	I163	V189	I220	V239	I242	I270	L271	L272	A275	M281	V284	V287	V288	L325	C330
MET	A2	L3	V6	I9	Y23	Y29	C48	T54	A57	G75	D78	T79	I82	L83	L119	I123	K136	I160	I163	V189	I220	V239	I242	I270	L271	L272	A275	M281	V284	V287	V288	L325	C330											

Chain W:  85% 9% 5%

	G330	L331	A354	E359	N360	G361	V362	I363	T371	ALA	GLU	GLU	LEU	GLU	ALA	ILE	LVS	HIS	GLN	LEU	ASN	ASP	VAL	GLU	LEU	MET	L2	V6	N9	Y23	T29	C48	T54	A57	G75	D78	T79	I82	I83	L119	I123	K136	I160	I163	I168	V189	I220	V239	I242	I270	L271	L272	M281	V284	V287	Y288	Y301	I325
--	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

Chain X: 85% 9% • 5%

A354	E359	I360	G361	I363	T371	ALA	GLU	LEU	GLU	GLU	ALA	ILE	LYS	HIS	GLN	LEU	ASP	PRO	ASP	ASP	VAL	GLU	LEU	MET	A3	V6	N9	T29	C48	T54	A57	G75	D78	T79	I82	L83	L119	I123	K136	I160	I163	I168	V189	I220	V239	I242	L272	M281	V284	V287	Y288	L325	G330	I331	G335	P346
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4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	131	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	40000	Depositor
Image detector	GATAN ULTRASCAN 4000	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	0.22	0/3541	0.73	0/5470
2	B	0.27	0/2929	0.42	0/3946
2	C	0.27	0/2929	0.42	0/3946
2	D	0.27	0/2929	0.42	0/3946
2	E	0.27	0/2929	0.42	0/3946
2	F	0.27	0/2929	0.42	0/3946
2	G	0.27	0/2929	0.42	0/3946
2	H	0.27	0/2929	0.42	0/3946
2	I	0.27	0/2929	0.42	0/3946
2	J	0.27	0/2929	0.42	0/3946
2	K	0.27	0/2929	0.42	0/3946
2	L	0.27	0/2929	0.42	0/3946
2	M	0.27	0/2929	0.43	0/3946
2	N	0.27	0/2929	0.43	0/3946
2	O	0.27	0/2929	0.42	0/3946
2	P	0.27	0/2929	0.42	0/3946
2	Q	0.27	0/2929	0.42	0/3946
2	R	0.27	0/2929	0.42	0/3946
2	S	0.27	0/2929	0.42	0/3946
2	T	0.27	0/2929	0.42	0/3946
2	U	0.27	0/2929	0.42	0/3946
2	V	0.27	0/2929	0.42	0/3946
2	W	0.27	0/2929	0.42	0/3946
2	X	0.27	0/2929	0.42	0/3946
All	All	0.27	0/70908	0.45	0/96228

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	3220	0	1772	76	0
2	B	2881	0	2915	17	0
2	C	2881	0	2915	24	0
2	D	2881	0	2915	22	0
2	E	2881	0	2915	24	0
2	F	2881	0	2915	26	0
2	G	2881	0	2915	23	0
2	H	2881	0	2915	25	0
2	I	2881	0	2915	23	0
2	J	2881	0	2915	23	0
2	K	2881	0	2915	25	0
2	L	2881	0	2915	36	0
2	M	2881	0	2915	36	0
2	N	2881	0	2915	37	0
2	O	2881	0	2915	28	0
2	P	2881	0	2915	30	0
2	Q	2881	0	2915	28	0
2	R	2881	0	2915	28	0
2	S	2881	0	2915	29	0
2	T	2881	0	2915	27	0
2	U	2881	0	2915	30	0
2	V	2881	0	2915	28	0
2	W	2881	0	2915	26	0
2	X	2881	0	2915	25	0
All	All	69483	0	68817	472	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 3.

The worst 5 of 472 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:A:221:C:H5"	2:C:189:VAL:HG22	1.77	0.66
1:A:211:C:H5"	2:D:189:VAL:HG22	1.77	0.66
1:A:101:C:H5"	2:O:189:VAL:HG22	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:C:H5"	2:X:189:VAL:HG22	1.78	0.66
1:A:91:C:H5"	2:P:189:VAL:HG22	1.78	0.66

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	
2	B	368/391 (94%)	354 (96%)	13 (4%)	1 (0%)	46	46
2	C	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	46	46
2	D	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	46	46
2	E	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	46	46
2	F	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	46	46
2	G	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	46	46
2	H	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	46	46
2	I	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	46	46
2	J	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	46	46
2	K	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	46	46
2	L	368/391 (94%)	353 (96%)	13 (4%)	2 (0%)	34	34
2	M	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	24	24
2	N	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	24	24
2	O	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	24	24
2	P	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	24	24
2	Q	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	24	24
2	R	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	24	24
2	S	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	24	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	T	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	24	24
2	U	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	24	24
2	V	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	24	24
2	W	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	24	24
2	X	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	24	24
All	All	8464/8993 (94%)	8109 (96%)	307 (4%)	48 (1%)	34	30

5 of 48 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	360	ASN
2	O	360	ASN
2	P	360	ASN
2	R	360	ASN
2	U	360	ASN

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	
2	B	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	C	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	D	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	E	309/328 (94%)	295 (96%)	14 (4%)	34	34
2	F	309/328 (94%)	297 (96%)	12 (4%)	39	39
2	G	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	H	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	I	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	J	309/328 (94%)	295 (96%)	14 (4%)	34	34
2	K	309/328 (94%)	297 (96%)	12 (4%)	39	39
2	L	309/328 (94%)	297 (96%)	12 (4%)	39	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	309/328 (94%)	295 (96%)	14 (4%)	34	34
2	N	309/328 (94%)	297 (96%)	12 (4%)	39	39
2	O	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	P	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	Q	309/328 (94%)	297 (96%)	12 (4%)	39	39
2	R	309/328 (94%)	295 (96%)	14 (4%)	34	34
2	S	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	T	309/328 (94%)	296 (96%)	13 (4%)	36	36
2	U	309/328 (94%)	295 (96%)	14 (4%)	34	34
2	V	309/328 (94%)	297 (96%)	12 (4%)	39	39
2	W	309/328 (94%)	295 (96%)	14 (4%)	34	34
2	X	309/328 (94%)	296 (96%)	13 (4%)	36	36
All	All	7107/7544 (94%)	6808 (96%)	299 (4%)	41	36

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	136	LYS
2	N	331	LEU
2	W	123	ILE
2	L	287	VAL
2	M	272	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	26	GLN
2	N	274	HIS
2	W	26	GLN
2	L	59	HIS
2	M	59	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	160/161 (99%)	22 (13%)	0

5 of 22 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	C
1	A	21	C
1	A	31	C
1	A	41	C
1	A	51	C

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.