Full wwPDB EM Validation Report ⓘ

Apr 29, 2024 – 09:05 am 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	:	Not provided
Based on initial model	:	2WJ8

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *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.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

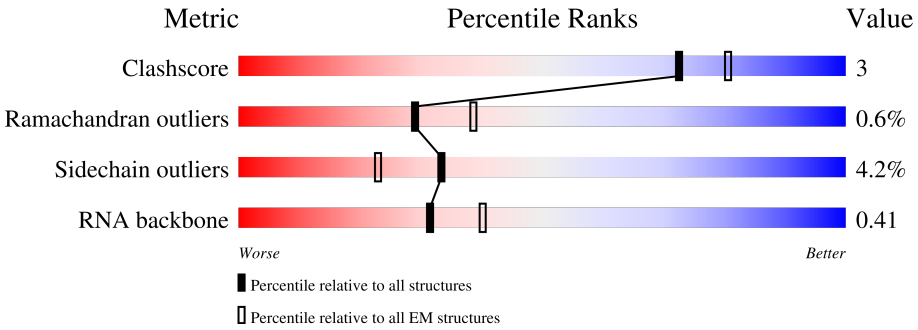
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	161	86% 14%
2	B	391	86% 8% • 5%
2	C	391	85% 9% 5%
2	D	391	85% 9% • 5%
2	E	391	85% 9% • 5%
2	F	391	85% 9% • 5%
2	G	391	85% 9% • 5%

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Mol	Chain	Length	Quality of chain
2	H	391	85% 9% • 5%
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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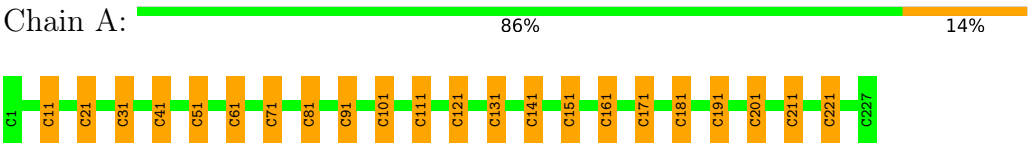
Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	Q	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	R	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	S	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
2	T	370	Total	C	N	O	S	0	0
			2881	1824	501	540	16		
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, DNA and oligosaccharide 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.

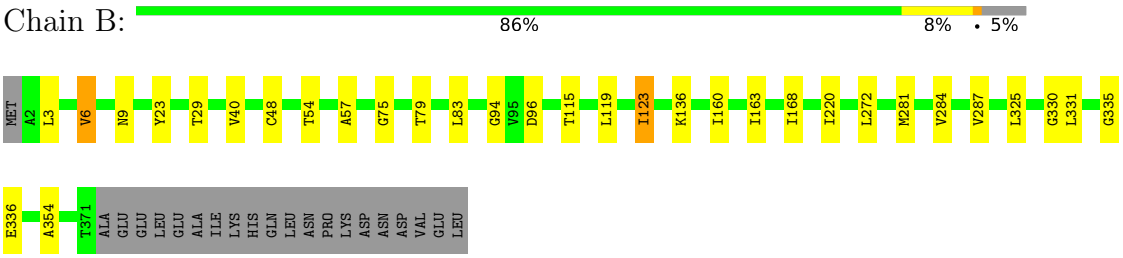
• Molecule 1: RNA (161-MER)

Chain A:



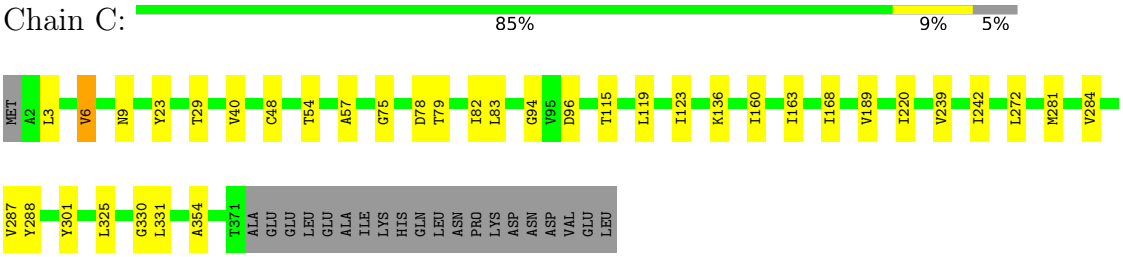
• Molecule 2: NUCLEOPROTEIN

Chain B:



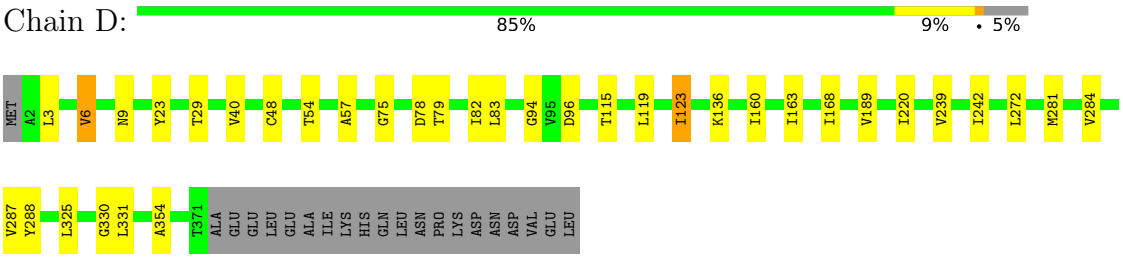
• Molecule 2: NUCLEOPROTEIN

Chain C:



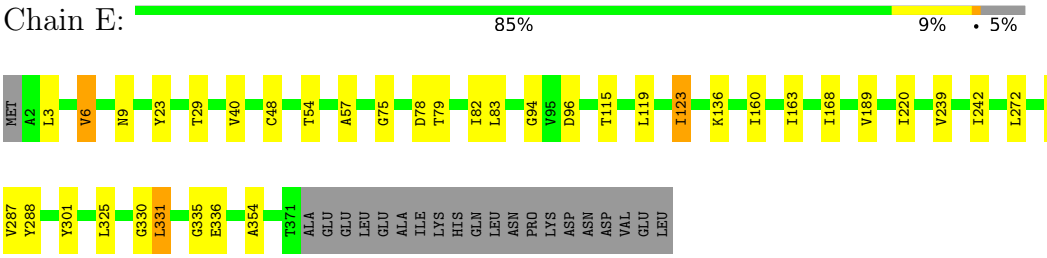
• Molecule 2: NUCLEOPROTEIN

Chain D:



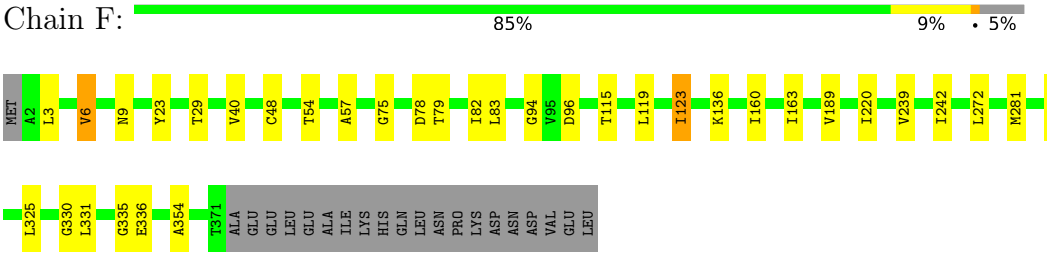
• Molecule 2: NUCLEOPROTEIN

Chain E:



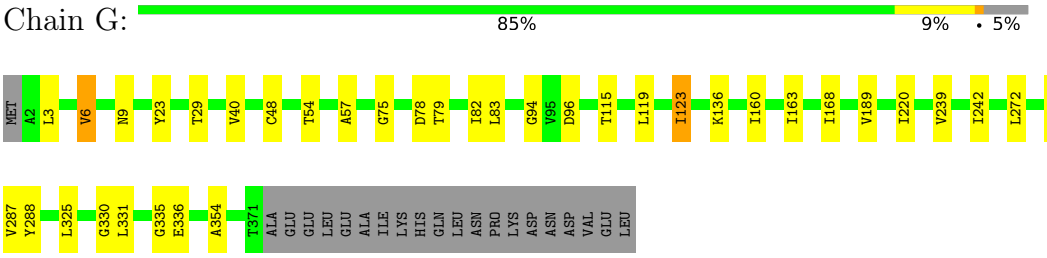
• Molecule 2: NUCLEOPROTEIN

Chain F:



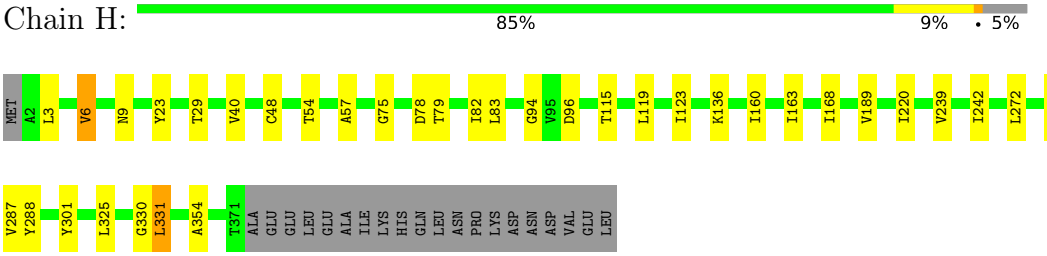
• Molecule 2: NUCLEOPROTEIN

Chain G:



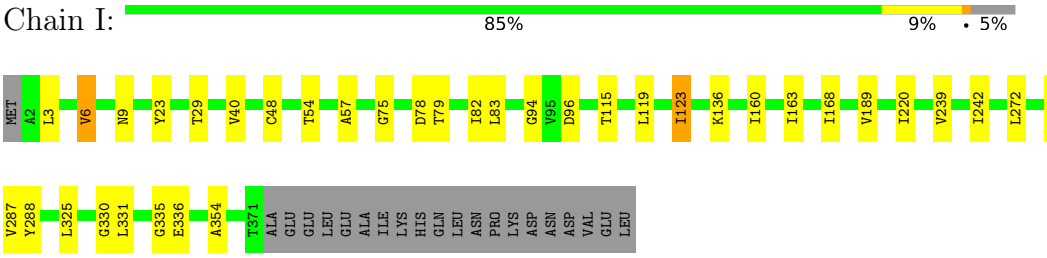
• Molecule 2: NUCLEOPROTEIN

Chain H:



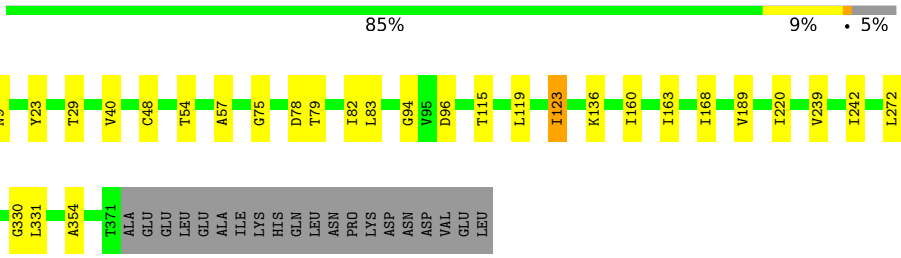
• Molecule 2: NUCLEOPROTEIN

Chain I:



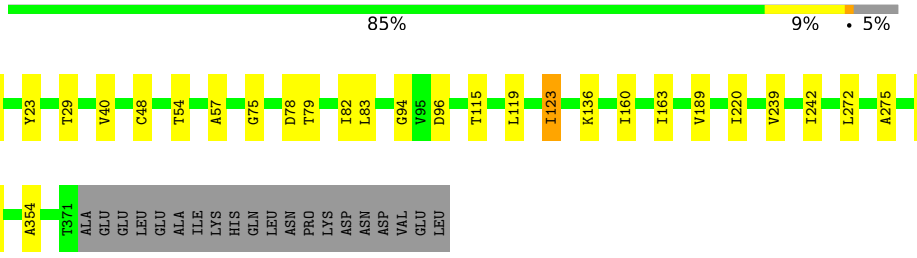
• Molecule 2: NUCLEOPROTEIN

Chain J:



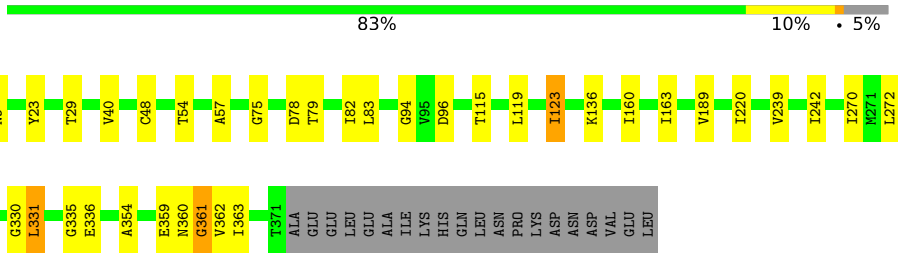
• Molecule 2: NUCLEOPROTEIN

Chain K:



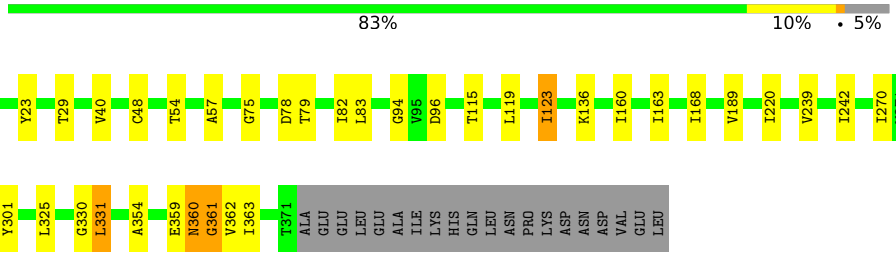
• Molecule 2: NUCLEOPROTEIN

Chain L:



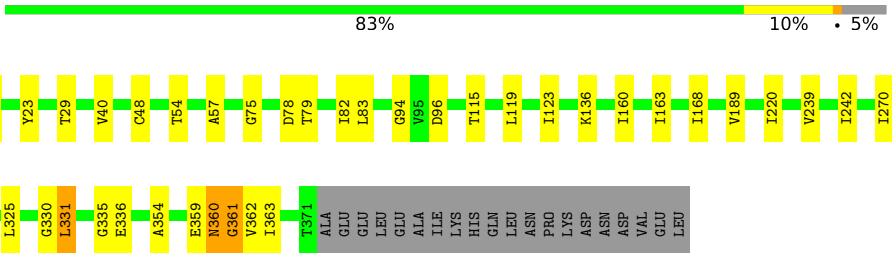
• Molecule 2: NUCLEOPROTEIN

Chain M:



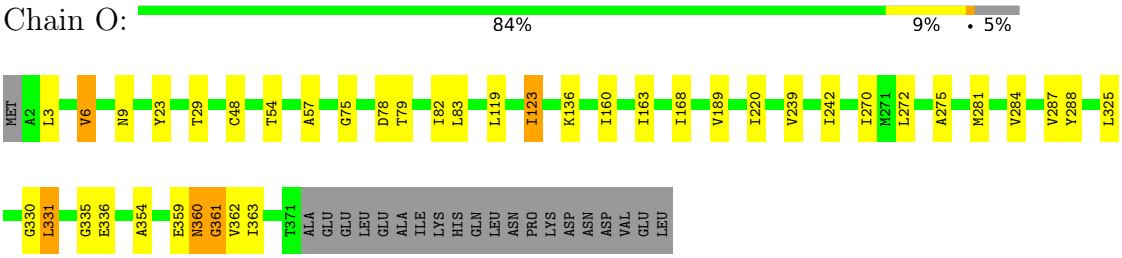
• Molecule 2: NUCLEOPROTEIN

Chain N:



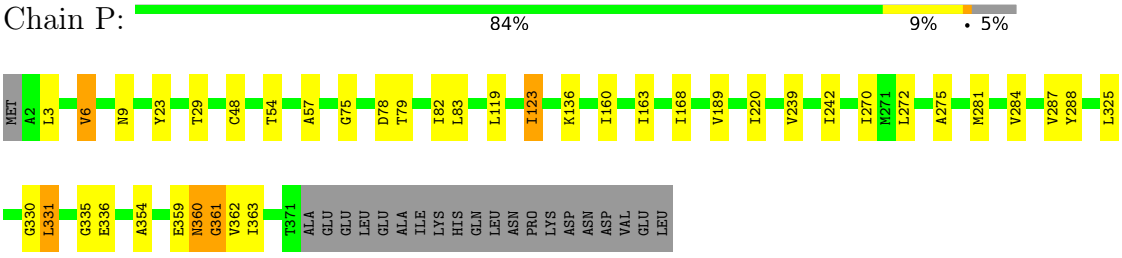
• Molecule 2: NUCLEOPROTEIN

Chain O:



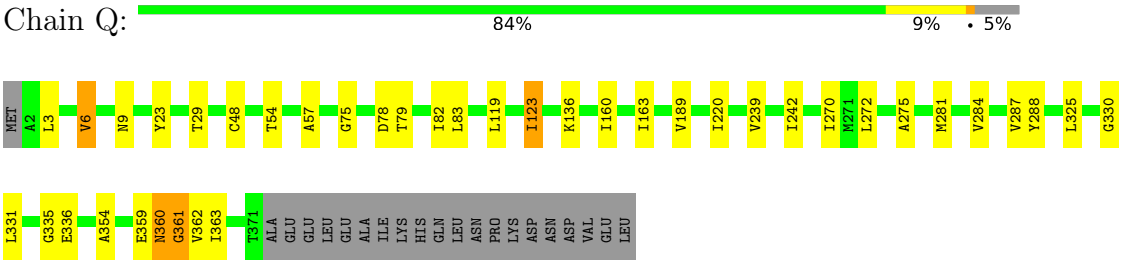
• Molecule 2: NUCLEOPROTEIN

Chain P:



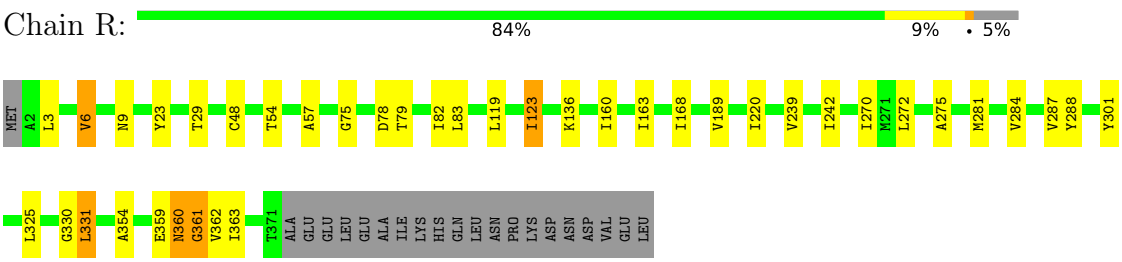
• Molecule 2: NUCLEOPROTEIN

Chain Q:



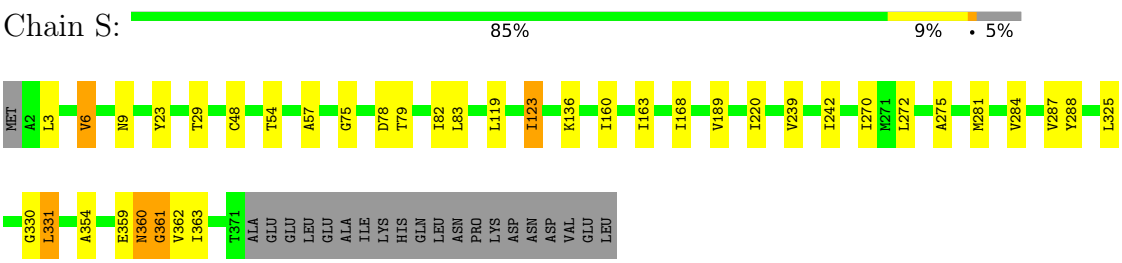
• Molecule 2: NUCLEOPROTEIN

Chain R:



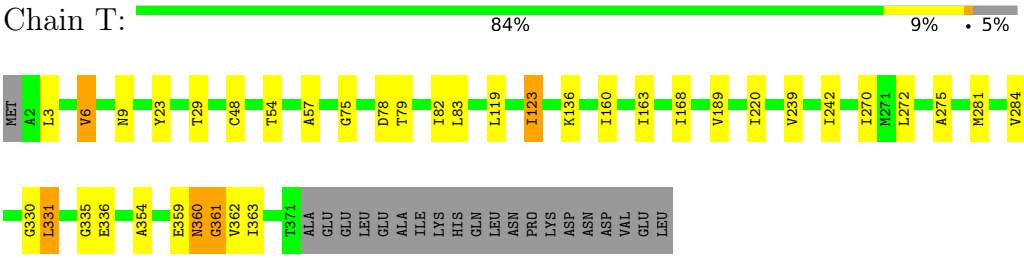
• Molecule 2: NUCLEOPROTEIN

Chain S:



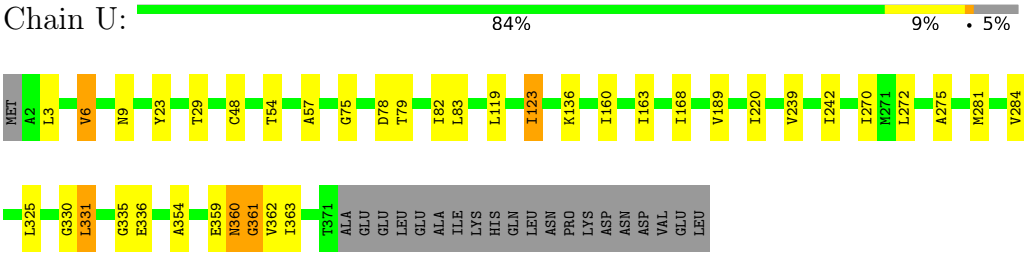
• Molecule 2: NUCLEOPROTEIN

Chain T:



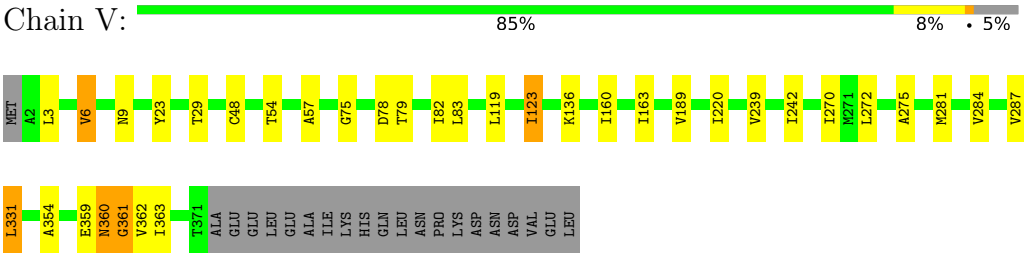
• Molecule 2: NUCLEOPROTEIN

Chain U:



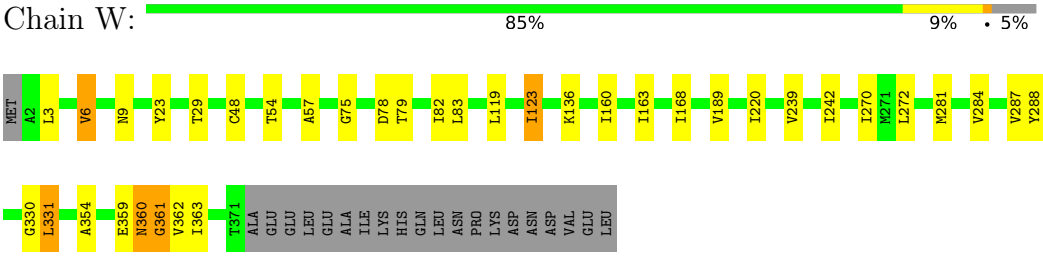
• Molecule 2: NUCLEOPROTEIN

Chain V:



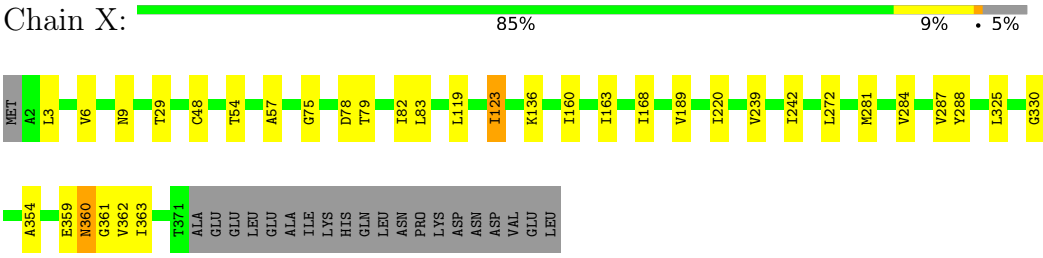
• Molecule 2: NUCLEOPROTEIN

Chain W:



• Molecule 2: NUCLEOPROTEIN

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of tilted images used	911	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	JEOL 2200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	131	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	40000	Depositor
Image detector	GATAN ULTRASCAN 4000 (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	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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.

All (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
1:A:121:C:H5”	2:M:189:VAL:HG22	1.78	0.65
1:A:81:C:H5”	2:Q:189:VAL:HG22	1.78	0.65
1:A:161:C:H5”	2:I:189:VAL:HG22	1.77	0.65
1:A:131:C:H5”	2:L:189:VAL:HG22	1.78	0.65
1:A:181:C:H5”	2:G:189:VAL:HG22	1.78	0.65
1:A:191:C:H5”	2:F:189:VAL:HG22	1.78	0.65
1:A:141:C:H5”	2:K:189:VAL:HG22	1.78	0.65
1:A:21:C:H5”	2:W:189:VAL:HG22	1.78	0.65
1:A:61:C:H5”	2:S:189:VAL:HG22	1.78	0.65
1:A:71:C:H5”	2:R:189:VAL:HG22	1.78	0.64
1:A:111:C:H5”	2:N:189:VAL:HG22	1.78	0.64
1:A:151:C:H5”	2:J:189:VAL:HG22	1.78	0.64
1:A:171:C:H5”	2:H:189:VAL:HG22	1.77	0.64
1:A:201:C:H5”	2:E:189:VAL:HG22	1.78	0.64
1:A:31:C:H5”	2:V:189:VAL:HG22	1.78	0.64
1:A:51:C:H5”	2:T:189:VAL:HG22	1.78	0.64
1:A:41:C:H5”	2:U:189:VAL:HG22	1.78	0.63
1:A:161:C:C5’	2:I:189:VAL:HG22	2.30	0.61
1:A:31:C:C5’	2:V:189:VAL:HG22	2.31	0.61
1:A:151:C:C5’	2:J:189:VAL:HG22	2.31	0.61
1:A:81:C:C5’	2:Q:189:VAL:HG22	2.31	0.61
1:A:101:C:C5’	2:O:189:VAL:HG22	2.31	0.61
1:A:131:C:C5’	2:L:189:VAL:HG22	2.31	0.61
1:A:201:C:C5’	2:E:189:VAL:HG22	2.31	0.61
1:A:181:C:C5’	2:G:189:VAL:HG22	2.31	0.61
1:A:211:C:C5’	2:D:189:VAL:HG22	2.30	0.61
1:A:91:C:C5’	2:P:189:VAL:HG22	2.31	0.60
1:A:191:C:C5’	2:F:189:VAL:HG22	2.31	0.60
1:A:51:C:C5’	2:T:189:VAL:HG22	2.31	0.60
1:A:171:C:C5’	2:H:189:VAL:HG22	2.31	0.60
1:A:141:C:C5’	2:K:189:VAL:HG22	2.31	0.60
1:A:21:C:C5’	2:W:189:VAL:HG22	2.31	0.60
1:A:221:C:C5’	2:C:189:VAL:HG22	2.31	0.60
1:A:61:C:C5’	2:S:189:VAL:HG22	2.31	0.60
1:A:11:C:C5’	2:X:189:VAL:HG22	2.31	0.60
1:A:41:C:C5’	2:U:189:VAL:HG22	2.31	0.60
1:A:71:C:C5’	2:R:189:VAL:HG22	2.31	0.59
1:A:121:C:C5’	2:M:189:VAL:HG22	2.31	0.59
1:A:111:C:C5’	2:N:189:VAL:HG22	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:119:LEU:HD11	2:X:123:ILE:HD11	1.86	0.57
2:D:40:VAL:CG2	2:D:96:ASP:HA	2.34	0.57
2:G:40:VAL:CG2	2:G:96:ASP:HA	2.34	0.57
2:L:40:VAL:CG2	2:L:96:ASP:HA	2.34	0.57
2:S:119:LEU:HD11	2:S:123:ILE:HD11	1.87	0.57
2:C:119:LEU:HD11	2:C:123:ILE:HD11	1.87	0.57
2:N:40:VAL:CG2	2:N:96:ASP:HA	2.35	0.57
2:I:40:VAL:CG2	2:I:96:ASP:HA	2.35	0.56
2:B:40:VAL:CG2	2:B:96:ASP:HA	2.35	0.56
2:J:40:VAL:CG2	2:J:96:ASP:HA	2.36	0.56
2:H:119:LEU:HD11	2:H:123:ILE:HD11	1.87	0.56
2:C:40:VAL:CG2	2:C:96:ASP:HA	2.36	0.56
2:F:40:VAL:CG2	2:F:96:ASP:HA	2.35	0.56
2:H:40:VAL:CG2	2:H:96:ASP:HA	2.36	0.56
2:P:119:LEU:HD11	2:P:123:ILE:HD11	1.88	0.56
2:K:40:VAL:CG2	2:K:96:ASP:HA	2.35	0.55
2:K:119:LEU:HD11	2:K:123:ILE:HD11	1.88	0.55
2:L:239:VAL:HA	2:L:242:ILE:HD12	1.88	0.55
2:M:40:VAL:CG2	2:M:96:ASP:HA	2.36	0.55
2:V:239:VAL:HA	2:V:242:ILE:HD12	1.88	0.55
2:E:40:VAL:CG2	2:E:96:ASP:HA	2.36	0.55
2:G:239:VAL:HA	2:G:242:ILE:HD12	1.88	0.55
2:F:119:LEU:HD11	2:F:123:ILE:HD11	1.89	0.55
2:N:119:LEU:HD11	2:N:123:ILE:HD11	1.89	0.55
2:Q:239:VAL:HA	2:Q:242:ILE:HD12	1.88	0.55
2:C:115:THR:OG1	2:M:360:ASN:OD1	2.25	0.55
2:I:239:VAL:HA	2:I:242:ILE:HD12	1.89	0.55
2:H:115:THR:OG1	2:R:360:ASN:OD1	2.25	0.55
2:W:239:VAL:HA	2:W:242:ILE:HD12	1.89	0.54
2:M:119:LEU:HD11	2:M:123:ILE:HD11	1.89	0.54
2:T:239:VAL:HA	2:T:242:ILE:HD12	1.88	0.54
2:U:119:LEU:HD11	2:U:123:ILE:HD11	1.89	0.54
2:H:239:VAL:HA	2:H:242:ILE:HD12	1.89	0.54
2:J:239:VAL:HA	2:J:242:ILE:HD12	1.89	0.54
2:M:239:VAL:HA	2:M:242:ILE:HD12	1.89	0.54
2:R:239:VAL:HA	2:R:242:ILE:HD12	1.89	0.54
2:O:239:VAL:HA	2:O:242:ILE:HD12	1.88	0.54
2:K:115:THR:OG1	2:U:360:ASN:OD1	2.26	0.54
2:I:119:LEU:HD11	2:I:123:ILE:HD11	1.90	0.54
2:K:96:ASP:OD2	2:U:360:ASN:HB3	2.09	0.53
2:Q:119:LEU:HD11	2:Q:123:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:119:LEU:HD11	2:R:123:ILE:HD11	1.91	0.53
2:D:239:VAL:HA	2:D:242:ILE:HD12	1.88	0.53
2:N:239:VAL:HA	2:N:242:ILE:HD12	1.89	0.53
2:V:119:LEU:HD11	2:V:123:ILE:HD11	1.90	0.53
2:S:239:VAL:HA	2:S:242:ILE:HD12	1.90	0.53
2:E:239:VAL:HA	2:E:242:ILE:HD12	1.89	0.53
2:X:239:VAL:HA	2:X:242:ILE:HD12	1.90	0.53
2:K:239:VAL:HA	2:K:242:ILE:HD12	1.90	0.53
2:D:119:LEU:HD11	2:D:123:ILE:HD11	1.91	0.53
2:F:239:VAL:HA	2:F:242:ILE:HD12	1.89	0.53
2:U:239:VAL:HA	2:U:242:ILE:HD12	1.91	0.52
2:C:96:ASP:OD2	2:M:360:ASN:HB3	2.09	0.52
2:P:239:VAL:HA	2:P:242:ILE:HD12	1.90	0.52
2:H:96:ASP:OD2	2:R:360:ASN:HB3	2.10	0.52
2:C:239:VAL:HA	2:C:242:ILE:HD12	1.90	0.52
2:X:48:CYS:HB3	2:X:160:ILE:HD12	1.92	0.52
2:F:96:ASP:OD2	2:P:360:ASN:HB3	2.10	0.52
2:D:48:CYS:HB3	2:D:160:ILE:HD12	1.92	0.51
2:M:96:ASP:OD2	2:W:360:ASN:HB3	2.10	0.51
2:P:48:CYS:HB3	2:P:160:ILE:HD12	1.92	0.51
2:W:119:LEU:HD11	2:W:123:ILE:HD11	1.92	0.51
2:I:48:CYS:HB3	2:I:160:ILE:HD12	1.92	0.51
2:N:48:CYS:HB3	2:N:160:ILE:HD12	1.92	0.51
2:F:48:CYS:HB3	2:F:160:ILE:HD12	1.92	0.51
2:E:48:CYS:HB3	2:E:160:ILE:HD12	1.93	0.51
2:O:48:CYS:HB3	2:O:160:ILE:HD12	1.93	0.51
2:B:48:CYS:HB3	2:B:160:ILE:HD12	1.92	0.51
2:M:48:CYS:HB3	2:M:160:ILE:HD12	1.93	0.51
2:C:48:CYS:HB3	2:C:160:ILE:HD12	1.93	0.51
2:N:96:ASP:OD2	2:X:360:ASN:HB3	2.11	0.51
2:L:48:CYS:HB3	2:L:160:ILE:HD12	1.92	0.51
2:Q:78:ASP:O	2:Q:82:ILE:HG23	2.11	0.51
2:S:48:CYS:HB3	2:S:160:ILE:HD12	1.92	0.51
2:W:48:CYS:HB3	2:W:160:ILE:HD12	1.92	0.51
2:J:78:ASP:O	2:J:82:ILE:HG23	2.11	0.50
2:L:96:ASP:OD2	2:V:360:ASN:HB3	2.11	0.50
2:N:96:ASP:HB2	2:X:360:ASN:HB3	1.93	0.50
2:J:48:CYS:HB3	2:J:160:ILE:HD12	1.93	0.50
2:D:78:ASP:O	2:D:82:ILE:HG23	2.11	0.50
2:I:78:ASP:O	2:I:82:ILE:HG23	2.12	0.50
2:K:48:CYS:HB3	2:K:160:ILE:HD12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:48:CYS:HB3	2:Q:160:ILE:HD12	1.92	0.50
2:V:48:CYS:HB3	2:V:160:ILE:HD12	1.92	0.50
2:V:78:ASP:O	2:V:82:ILE:HG23	2.12	0.50
2:E:78:ASP:O	2:E:82:ILE:HG23	2.12	0.50
2:G:78:ASP:O	2:G:82:ILE:HG23	2.11	0.50
2:J:96:ASP:OD2	2:T:360:ASN:HB3	2.12	0.50
2:F:78:ASP:O	2:F:82:ILE:HG23	2.12	0.50
2:G:48:CYS:HB3	2:G:160:ILE:HD12	1.92	0.50
2:T:48:CYS:HB3	2:T:160:ILE:HD12	1.92	0.50
2:U:78:ASP:O	2:U:82:ILE:HG23	2.12	0.50
2:C:78:ASP:O	2:C:82:ILE:HG23	2.12	0.50
2:T:78:ASP:O	2:T:82:ILE:HG23	2.12	0.50
2:D:96:ASP:HB2	2:N:360:ASN:HB3	1.94	0.50
2:G:96:ASP:OD2	2:Q:360:ASN:HB3	2.12	0.50
2:G:119:LEU:HD11	2:G:123:ILE:HD11	1.94	0.50
2:O:78:ASP:O	2:O:82:ILE:HG23	2.12	0.50
2:R:48:CYS:HB3	2:R:160:ILE:HD12	1.93	0.50
2:R:78:ASP:O	2:R:82:ILE:HG23	2.12	0.50
2:D:96:ASP:OD2	2:N:360:ASN:HB3	2.12	0.49
2:W:78:ASP:O	2:W:82:ILE:HG23	2.12	0.49
2:H:48:CYS:HB3	2:H:160:ILE:HD12	1.93	0.49
2:I:96:ASP:OD2	2:S:360:ASN:HB3	2.12	0.49
2:K:78:ASP:O	2:K:82:ILE:HG23	2.12	0.49
2:M:330:GLY:HA3	2:M:354:ALA:HB3	1.94	0.49
2:N:78:ASP:O	2:N:82:ILE:HG23	2.12	0.49
2:P:78:ASP:O	2:P:82:ILE:HG23	2.12	0.49
2:P:281:MET:HA	2:P:284:VAL:HG22	1.93	0.49
2:E:96:ASP:OD2	2:O:360:ASN:HB3	2.12	0.49
2:L:78:ASP:O	2:L:82:ILE:HG23	2.11	0.49
2:L:119:LEU:HD11	2:L:123:ILE:HD11	1.93	0.49
2:U:48:CYS:HB3	2:U:160:ILE:HD12	1.92	0.49
2:U:281:MET:HA	2:U:284:VAL:HG22	1.93	0.49
2:R:75:GLY:O	2:R:79:THR:HG22	2.13	0.49
2:E:75:GLY:O	2:E:79:THR:HG22	2.13	0.49
2:E:281:MET:HA	2:E:284:VAL:HG22	1.93	0.49
2:L:96:ASP:HB2	2:V:360:ASN:HB3	1.95	0.49
2:M:78:ASP:O	2:M:82:ILE:HG23	2.12	0.49
2:W:75:GLY:O	2:W:79:THR:HG22	2.13	0.49
2:W:330:GLY:HA3	2:W:354:ALA:HB3	1.94	0.49
2:E:115:THR:OG1	2:O:360:ASN:OD1	2.28	0.49
2:J:75:GLY:O	2:J:79:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ASP:OD2	2:L:360:ASN:HB3	2.12	0.49
2:E:119:LEU:HD11	2:E:123:ILE:HD11	1.95	0.49
2:H:78:ASP:O	2:H:82:ILE:HG23	2.12	0.49
2:J:281:MET:HA	2:J:284:VAL:HG22	1.94	0.49
2:O:330:GLY:HA3	2:O:354:ALA:HB3	1.95	0.49
2:T:281:MET:HA	2:T:284:VAL:HG22	1.94	0.49
2:F:281:MET:HA	2:F:284:VAL:HG22	1.94	0.49
2:I:96:ASP:HB2	2:S:360:ASN:HB3	1.94	0.49
2:O:281:MET:HA	2:O:284:VAL:HG22	1.94	0.49
2:R:330:GLY:HA3	2:R:354:ALA:HB3	1.94	0.49
2:B:119:LEU:HD11	2:B:123:ILE:HD11	1.94	0.48
2:S:78:ASP:O	2:S:82:ILE:HG23	2.12	0.48
2:X:78:ASP:O	2:X:82:ILE:HG23	2.12	0.48
2:C:96:ASP:HB2	2:M:360:ASN:HB3	1.95	0.48
2:M:75:GLY:O	2:M:79:THR:HG22	2.13	0.48
2:M:115:THR:OG1	2:W:360:ASN:OD1	2.25	0.48
2:J:115:THR:OG1	2:T:360:ASN:OD1	2.29	0.48
2:O:75:GLY:O	2:O:79:THR:HG22	2.14	0.48
2:O:119:LEU:HD11	2:O:123:ILE:HD11	1.95	0.48
2:T:119:LEU:HD11	2:T:123:ILE:HD11	1.95	0.48
2:H:75:GLY:O	2:H:79:THR:HG22	2.14	0.48
2:K:96:ASP:HB2	2:U:360:ASN:HB3	1.95	0.48
2:K:281:MET:HA	2:K:284:VAL:HG22	1.93	0.48
2:F:96:ASP:HB2	2:P:360:ASN:HB3	1.95	0.48
2:P:330:GLY:HA3	2:P:354:ALA:HB3	1.96	0.48
2:M:115:THR:OG1	2:W:359:GLU:HG3	2.14	0.48
2:V:281:MET:HA	2:V:284:VAL:HG22	1.96	0.48
2:E:96:ASP:HB2	2:O:360:ASN:HB3	1.96	0.48
2:M:96:ASP:HB2	2:W:360:ASN:HB3	1.96	0.48
2:D:281:MET:HA	2:D:284:VAL:HG22	1.95	0.47
2:K:115:THR:OG1	2:U:359:GLU:HG3	2.14	0.47
2:X:281:MET:HA	2:X:284:VAL:HG22	1.96	0.47
2:G:96:ASP:HB2	2:Q:360:ASN:HB3	1.95	0.47
2:J:96:ASP:HB2	2:T:360:ASN:HB3	1.96	0.47
2:T:75:GLY:O	2:T:79:THR:HG22	2.14	0.47
2:E:115:THR:OG1	2:O:359:GLU:HG3	2.14	0.47
2:H:115:THR:OG1	2:R:359:GLU:HG3	2.14	0.47
2:T:330:GLY:HA3	2:T:354:ALA:HB3	1.96	0.47
2:J:119:LEU:HD11	2:J:123:ILE:HD11	1.96	0.47
2:L:115:THR:OG1	2:V:360:ASN:OD1	2.31	0.47
2:U:75:GLY:O	2:U:79:THR:HG22	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:115:THR:OG1	2:P:360:ASN:OD1	2.27	0.47
2:B:96:ASP:HB2	2:L:360:ASN:HB3	1.97	0.47
2:C:75:GLY:O	2:C:79:THR:HG22	2.15	0.47
2:C:115:THR:OG1	2:M:359:GLU:HG3	2.15	0.47
2:J:115:THR:OG1	2:T:359:GLU:HG3	2.14	0.47
2:L:75:GLY:O	2:L:79:THR:HG22	2.15	0.47
2:B:115:THR:OG1	2:L:360:ASN:OD1	2.31	0.47
2:G:75:GLY:O	2:G:79:THR:HG22	2.14	0.47
2:I:281:MET:HA	2:I:284:VAL:HG22	1.96	0.47
2:N:281:MET:HA	2:N:284:VAL:HG22	1.96	0.47
2:B:96:ASP:CG	2:L:361:GLY:H	2.19	0.46
2:B:281:MET:HA	2:B:284:VAL:HG22	1.97	0.46
2:N:115:THR:OG1	2:X:360:ASN:OD1	2.30	0.46
2:Q:281:MET:HA	2:Q:284:VAL:HG22	1.96	0.46
2:U:330:GLY:HA3	2:U:354:ALA:HB3	1.95	0.46
2:W:281:MET:HA	2:W:284:VAL:HG22	1.98	0.46
2:B:75:GLY:O	2:B:79:THR:HG22	2.16	0.46
2:C:281:MET:HA	2:C:284:VAL:HG22	1.97	0.46
2:H:96:ASP:HB2	2:R:360:ASN:HB3	1.96	0.46
2:P:75:GLY:O	2:P:79:THR:HG22	2.16	0.46
2:D:23:TYR:CD1	2:E:82:ILE:HG22	2.51	0.46
2:D:75:GLY:O	2:D:79:THR:HG22	2.16	0.46
2:E:23:TYR:CD1	2:F:82:ILE:HG22	2.51	0.46
2:M:23:TYR:CD1	2:N:82:ILE:HG22	2.51	0.46
2:B:23:TYR:CD1	2:C:82:ILE:HG22	2.51	0.46
2:G:23:TYR:CD1	2:H:82:ILE:HG22	2.51	0.46
2:J:23:TYR:CD1	2:K:82:ILE:HG22	2.51	0.46
2:L:23:TYR:CD1	2:M:82:ILE:HG22	2.51	0.46
2:L:330:GLY:HA3	2:L:354:ALA:HB3	1.97	0.46
2:S:330:GLY:HA3	2:S:354:ALA:HB3	1.98	0.46
2:G:94:GLY:O	2:Q:360:ASN:ND2	2.49	0.46
2:I:23:TYR:CD1	2:J:82:ILE:HG22	2.51	0.46
2:C:23:TYR:CD1	2:D:82:ILE:HG22	2.51	0.46
2:H:23:TYR:CD1	2:I:82:ILE:HG22	2.51	0.46
2:Q:330:GLY:HA3	2:Q:354:ALA:HB3	1.98	0.46
2:S:281:MET:HA	2:S:284:VAL:HG22	1.97	0.46
2:X:75:GLY:O	2:X:79:THR:HG22	2.16	0.46
2:D:94:GLY:O	2:N:360:ASN:ND2	2.49	0.45
2:E:330:GLY:HA3	2:E:354:ALA:HB3	1.98	0.45
2:D:115:THR:OG1	2:N:360:ASN:OD1	2.32	0.45
2:G:115:THR:OG1	2:Q:359:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:23:TYR:CD1	2:L:82:ILE:HG22	2.51	0.45
2:L:281:MET:HA	2:L:284:VAL:HG22	1.97	0.45
2:Q:75:GLY:O	2:Q:79:THR:HG22	2.16	0.45
2:X:330:GLY:HA3	2:X:354:ALA:HB3	1.97	0.45
2:F:23:TYR:CD1	2:G:82:ILE:HG22	2.52	0.45
2:K:75:GLY:O	2:K:79:THR:HG22	2.16	0.45
2:J:330:GLY:HA3	2:J:354:ALA:HB3	1.99	0.45
2:N:23:TYR:CD1	2:O:82:ILE:HG22	2.52	0.45
2:N:75:GLY:O	2:N:79:THR:HG22	2.17	0.45
2:O:23:TYR:CD1	2:P:82:ILE:HG22	2.51	0.45
2:F:335:GLY:HA2	2:F:336:GLU:HA	1.82	0.45
2:M:281:MET:HA	2:M:284:VAL:HG22	1.98	0.45
2:Q:23:TYR:CD1	2:R:82:ILE:HG22	2.52	0.45
2:R:23:TYR:CD1	2:S:82:ILE:HG22	2.51	0.45
2:R:281:MET:HA	2:R:284:VAL:HG22	1.98	0.45
2:G:281:MET:HA	2:G:284:VAL:HG22	1.97	0.45
2:H:281:MET:HA	2:H:284:VAL:HG22	1.98	0.45
2:P:23:TYR:CD1	2:Q:82:ILE:HG22	2.52	0.45
2:S:75:GLY:O	2:S:79:THR:HG22	2.17	0.45
2:V:75:GLY:O	2:V:79:THR:HG22	2.17	0.45
2:B:115:THR:OG1	2:L:359:GLU:HG3	2.16	0.45
2:F:75:GLY:O	2:F:79:THR:HG22	2.17	0.45
2:L:94:GLY:O	2:V:360:ASN:ND2	2.49	0.45
2:M:94:GLY:O	2:W:360:ASN:ND2	2.50	0.45
2:N:115:THR:OG1	2:X:359:GLU:HG3	2.17	0.45
2:B:94:GLY:O	2:L:360:ASN:ND2	2.50	0.45
2:F:115:THR:OG1	2:P:359:GLU:HG3	2.16	0.45
2:G:115:THR:OG1	2:Q:360:ASN:OD1	2.30	0.45
2:I:75:GLY:O	2:I:79:THR:HG22	2.17	0.45
2:S:23:TYR:CD1	2:T:82:ILE:HG22	2.52	0.45
2:C:330:GLY:HA3	2:C:354:ALA:HB3	1.99	0.45
2:E:94:GLY:O	2:O:360:ASN:ND2	2.50	0.45
2:H:330:GLY:HA3	2:H:354:ALA:HB3	1.98	0.45
2:I:94:GLY:O	2:S:360:ASN:ND2	2.50	0.45
2:N:94:GLY:O	2:X:360:ASN:ND2	2.50	0.45
2:B:330:GLY:HA3	2:B:354:ALA:HB3	2.00	0.44
2:D:115:THR:OG1	2:N:359:GLU:HG3	2.17	0.44
2:N:335:GLY:HA2	2:N:336:GLU:HA	1.82	0.44
2:T:23:TYR:CD1	2:U:82:ILE:HG22	2.51	0.44
2:H:94:GLY:O	2:R:360:ASN:ND2	2.50	0.44
2:W:23:TYR:CD1	2:X:82:ILE:HG22	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:94:GLY:O	2:T:360:ASN:ND2	2.50	0.44
2:N:362:VAL:HG12	2:N:363:ILE:N	2.33	0.44
2:H:96:ASP:N	2:R:360:ASN:OD1	2.49	0.44
2:V:23:TYR:CD1	2:W:82:ILE:HG22	2.52	0.44
2:V:330:GLY:HA3	2:V:354:ALA:HB3	1.98	0.44
2:X:335:GLY:HA2	2:X:336:GLU:HA	1.82	0.44
1:A:21:C:C4	2:W:242:ILE:HG12	2.53	0.44
2:F:94:GLY:O	2:P:360:ASN:ND2	2.51	0.44
2:I:115:THR:OG1	2:S:359:GLU:HG3	2.17	0.44
2:N:330:GLY:HA3	2:N:354:ALA:HB3	1.98	0.44
1:A:181:C:C4	2:G:242:ILE:HG12	2.53	0.44
2:U:23:TYR:CD1	2:V:82:ILE:HG22	2.52	0.44
2:X:119:LEU:CD1	2:X:123:ILE:HD11	2.48	0.44
2:L:115:THR:OG1	2:V:359:GLU:HG3	2.17	0.44
1:A:71:C:C4	2:R:242:ILE:HG12	2.53	0.43
1:A:91:C:C4	2:P:242:ILE:HG12	2.53	0.43
1:A:131:C:C4	2:L:242:ILE:HG12	2.53	0.43
2:C:94:GLY:O	2:M:360:ASN:ND2	2.51	0.43
2:K:94:GLY:O	2:U:360:ASN:ND2	2.51	0.43
2:M:331:LEU:HD13	2:M:354:ALA:HB1	2.00	0.43
2:C:119:LEU:CD1	2:C:123:ILE:HD11	2.48	0.43
1:A:41:C:C4	2:U:242:ILE:HG12	2.53	0.43
2:Q:275:ALA:HB3	2:R:361:GLY:HA2	1.99	0.43
2:V:362:VAL:HG12	2:V:363:ILE:N	2.34	0.43
1:A:221:C:C4	2:C:242:ILE:HG12	2.54	0.43
2:L:335:GLY:HA2	2:L:336:GLU:HA	1.82	0.43
2:W:331:LEU:HD13	2:W:354:ALA:HB1	2.00	0.43
1:A:121:C:C4	2:M:242:ILE:HG12	2.53	0.43
1:A:101:C:C4	2:O:242:ILE:HG12	2.54	0.43
1:A:201:C:C4	2:E:242:ILE:HG12	2.54	0.43
2:G:335:GLY:HA2	2:G:336:GLU:HA	1.82	0.43
2:S:119:LEU:CD1	2:S:123:ILE:HD11	2.49	0.43
2:X:362:VAL:HG12	2:X:363:ILE:N	2.34	0.43
1:A:191:C:C4	2:F:242:ILE:HG12	2.53	0.43
2:L:275:ALA:HB3	2:M:361:GLY:HA2	2.00	0.43
2:T:362:VAL:HG12	2:T:363:ILE:N	2.34	0.43
2:V:275:ALA:HB3	2:W:361:GLY:HA2	2.00	0.43
1:A:11:C:C4	2:X:242:ILE:HG12	2.54	0.42
1:A:31:C:C4	2:V:242:ILE:HG12	2.53	0.42
1:A:151:C:C4	2:J:242:ILE:HG12	2.54	0.42
2:T:275:ALA:HB3	2:U:361:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:335:GLY:HA2	2:U:336:GLU:HA	1.82	0.42
1:A:61:C:C4	2:S:242:ILE:HG12	2.54	0.42
1:A:141:C:C4	2:K:242:ILE:HG12	2.53	0.42
1:A:171:C:C4	2:H:242:ILE:HG12	2.54	0.42
1:A:211:C:C4	2:D:242:ILE:HG12	2.55	0.42
1:A:51:C:C4	2:T:242:ILE:HG12	2.54	0.42
1:A:161:C:C4	2:I:242:ILE:HG12	2.55	0.42
2:I:335:GLY:HA2	2:I:336:GLU:HA	1.82	0.42
2:M:96:ASP:N	2:W:360:ASN:OD1	2.49	0.42
2:R:331:LEU:HD13	2:R:354:ALA:HB1	2.01	0.42
2:S:6:VAL:HG23	2:T:288:TYR:CE2	2.55	0.42
2:S:275:ALA:HB3	2:T:361:GLY:HA2	2.01	0.42
2:L:270:ILE:HG23	2:M:363:ILE:HG21	2.02	0.42
2:O:335:GLY:HA2	2:O:336:GLU:HA	1.82	0.42
2:S:362:VAL:HG12	2:S:363:ILE:N	2.34	0.42
1:A:81:C:C4	2:Q:242:ILE:HG12	2.53	0.42
1:A:111:C:C4	2:N:242:ILE:HG12	2.55	0.42
2:K:330:GLY:HA3	2:K:354:ALA:HB3	2.01	0.42
2:N:275:ALA:HB3	2:O:361:GLY:HA2	2.01	0.42
2:O:331:LEU:HD13	2:O:354:ALA:HB1	2.02	0.42
2:O:362:VAL:HG12	2:O:363:ILE:N	2.34	0.42
2:Q:335:GLY:HA2	2:Q:336:GLU:HA	1.82	0.42
2:C:6:VAL:HG23	2:D:288:TYR:CE2	2.55	0.42
2:N:6:VAL:HG23	2:O:288:TYR:CE2	2.55	0.42
2:O:275:ALA:HB3	2:P:361:GLY:HA2	2.02	0.42
2:H:119:LEU:CD1	2:H:123:ILE:HD11	2.49	0.42
2:I:6:VAL:HG23	2:J:288:TYR:CE2	2.55	0.42
2:K:275:ALA:HB3	2:L:361:GLY:HA2	2.02	0.42
2:L:362:VAL:HG12	2:L:363:ILE:N	2.35	0.42
2:S:270:ILE:HG23	2:T:363:ILE:HG21	2.02	0.42
2:H:54:THR:HB	2:H:57:ALA:HB2	2.02	0.42
2:O:270:ILE:HG23	2:P:363:ILE:HG21	2.02	0.42
2:Q:270:ILE:HG23	2:R:363:ILE:HG21	2.02	0.42
2:F:330:GLY:HA3	2:F:354:ALA:HB3	2.02	0.42
2:G:330:GLY:HA3	2:G:354:ALA:HB3	2.01	0.42
2:H:6:VAL:HG23	2:I:288:TYR:CE2	2.55	0.42
2:I:330:GLY:HA3	2:I:354:ALA:HB3	2.02	0.42
2:K:119:LEU:CD1	2:K:123:ILE:HD11	2.50	0.42
2:X:331:LEU:HD13	2:X:354:ALA:HB1	2.02	0.42
2:D:96:ASP:CB	2:N:360:ASN:HB3	2.50	0.41
2:F:6:VAL:HG23	2:G:288:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:96:ASP:CB	2:X:360:ASN:HB3	2.50	0.41
2:R:54:THR:HB	2:R:57:ALA:HB2	2.02	0.41
2:I:96:ASP:CB	2:S:360:ASN:HB3	2.50	0.41
2:P:6:VAL:HG23	2:Q:288:TYR:CE2	2.55	0.41
2:U:270:ILE:HD13	2:U:270:ILE:HA	1.97	0.41
2:V:270:ILE:HG23	2:W:363:ILE:HG21	2.02	0.41
2:M:54:THR:HB	2:M:57:ALA:HB2	2.02	0.41
2:P:54:THR:HB	2:P:57:ALA:HB2	2.03	0.41
2:S:54:THR:HB	2:S:57:ALA:HB2	2.03	0.41
2:U:331:LEU:HD13	2:U:354:ALA:HB1	2.01	0.41
2:I:115:THR:OG1	2:S:360:ASN:OD1	2.31	0.41
2:P:331:LEU:HD13	2:P:354:ALA:HB1	2.02	0.41
2:T:335:GLY:HA2	2:T:336:GLU:HA	1.82	0.41
2:W:362:VAL:HG12	2:W:363:ILE:N	2.35	0.41
2:X:54:THR:HB	2:X:57:ALA:HB2	2.02	0.41
2:C:54:THR:HB	2:C:57:ALA:HB2	2.02	0.41
2:F:54:THR:HB	2:F:57:ALA:HB2	2.03	0.41
2:K:54:THR:HB	2:K:57:ALA:HB2	2.03	0.41
2:M:119:LEU:CD1	2:M:123:ILE:HD11	2.51	0.41
2:M:362:VAL:HG12	2:M:363:ILE:N	2.36	0.41
2:P:335:GLY:HA2	2:P:336:GLU:HA	1.82	0.41
2:Q:6:VAL:HG23	2:R:288:TYR:CE2	2.56	0.41
2:U:54:THR:HB	2:U:57:ALA:HB2	2.03	0.41
2:U:275:ALA:HB3	2:V:361:GLY:HA2	2.02	0.41
2:B:335:GLY:HA2	2:B:336:GLU:HA	1.82	0.41
2:C:96:ASP:N	2:M:360:ASN:OD1	2.49	0.41
2:L:331:LEU:HD13	2:L:354:ALA:HB1	2.02	0.41
2:N:119:LEU:CD1	2:N:123:ILE:HD11	2.50	0.41
2:N:331:LEU:HD13	2:N:354:ALA:HB1	2.03	0.41
2:S:270:ILE:HD13	2:S:270:ILE:HA	1.97	0.41
2:T:270:ILE:HG23	2:U:363:ILE:HG21	2.03	0.41
2:U:362:VAL:HG12	2:U:363:ILE:N	2.35	0.41
2:B:96:ASP:OD2	2:L:361:GLY:N	2.41	0.41
2:E:23:TYR:CG	2:F:82:ILE:HG22	2.56	0.41
2:J:23:TYR:CG	2:K:82:ILE:HG22	2.56	0.41
2:N:270:ILE:HG23	2:O:363:ILE:HG21	2.03	0.41
2:R:362:VAL:HG12	2:R:363:ILE:N	2.36	0.41
2:T:6:VAL:HG23	2:U:288:TYR:CE2	2.56	0.41
2:V:6:VAL:HG23	2:W:288:TYR:CE2	2.55	0.41
2:D:6:VAL:HG23	2:E:288:TYR:CE2	2.55	0.41
2:M:275:ALA:HB3	2:N:361:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:362:VAL:HG12	2:P:363:ILE:N	2.35	0.41
2:Q:54:THR:HB	2:Q:57:ALA:HB2	2.03	0.41
2:Q:270:ILE:HD13	2:Q:270:ILE:HA	1.96	0.41
2:R:6:VAL:HG23	2:S:288:TYR:CE2	2.56	0.41
2:E:54:THR:HB	2:E:57:ALA:HB2	2.03	0.41
2:E:335:GLY:HA2	2:E:336:GLU:HA	1.82	0.41
2:G:6:VAL:HG23	2:H:288:TYR:CE2	2.56	0.41
2:J:6:VAL:HG23	2:K:288:TYR:CE2	2.56	0.41
2:K:6:VAL:HG23	2:L:288:TYR:CE2	2.55	0.41
2:L:96:ASP:CB	2:V:360:ASN:HB3	2.51	0.41
2:M:6:VAL:HG23	2:N:288:TYR:CE2	2.55	0.41
2:P:119:LEU:CD1	2:P:123:ILE:HD11	2.50	0.41
2:T:331:LEU:HD13	2:T:354:ALA:HB1	2.02	0.41
2:W:54:THR:HB	2:W:57:ALA:HB2	2.03	0.41
2:D:330:GLY:HA3	2:D:354:ALA:HB3	2.02	0.41
2:E:6:VAL:HG23	2:F:288:TYR:CE2	2.56	0.41
2:G:54:THR:HB	2:G:57:ALA:HB2	2.03	0.41
2:H:331:LEU:HD13	2:H:354:ALA:HB1	2.03	0.41
2:I:54:THR:HB	2:I:57:ALA:HB2	2.03	0.41
2:S:331:LEU:HD13	2:S:354:ALA:HB1	2.02	0.41
2:T:54:THR:HB	2:T:57:ALA:HB2	2.03	0.41
2:U:6:VAL:HG23	2:V:288:TYR:CE2	2.56	0.41
2:U:119:LEU:CD1	2:U:123:ILE:HD11	2.51	0.41
2:W:6:VAL:HG23	2:X:288:TYR:CE2	2.56	0.41
1:A:221:C:C2	2:C:242:ILE:HA	2.56	0.40
2:J:54:THR:HB	2:J:57:ALA:HB2	2.03	0.40
2:U:270:ILE:HG23	2:V:363:ILE:HG21	2.03	0.40
1:A:11:C:C2	2:X:242:ILE:HA	2.57	0.40
1:A:191:C:C2	2:F:242:ILE:HA	2.57	0.40
2:B:54:THR:HB	2:B:57:ALA:HB2	2.03	0.40
2:F:96:ASP:CB	2:P:360:ASN:HB3	2.50	0.40
2:F:119:LEU:CD1	2:F:123:ILE:HD11	2.50	0.40
2:G:96:ASP:CB	2:Q:360:ASN:HB3	2.52	0.40
2:L:54:THR:HB	2:L:57:ALA:HB2	2.03	0.40
2:M:23:TYR:CG	2:N:82:ILE:HG22	2.56	0.40
2:N:54:THR:HB	2:N:57:ALA:HB2	2.03	0.40
2:P:270:ILE:HG23	2:Q:363:ILE:HG21	2.03	0.40
2:P:275:ALA:HB3	2:Q:361:GLY:HA2	2.02	0.40
2:R:275:ALA:HB3	2:S:361:GLY:HA2	2.02	0.40
2:V:331:LEU:HD13	2:V:354:ALA:HB1	2.03	0.40
2:W:270:ILE:HG23	2:X:363:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:C:C2	2:P:242:ILE:HA	2.57	0.40
1:A:171:C:C2	2:H:242:ILE:HA	2.57	0.40
2:B:6:VAL:HG23	2:C:288:TYR:CE2	2.56	0.40
2:O:6:VAL:HG23	2:P:288:TYR:CE2	2.56	0.40
2:V:54:THR:HB	2:V:57:ALA:HB2	2.03	0.40
1:A:71:C:C2	2:R:242:ILE:HA	2.57	0.40
1:A:101:C:C2	2:O:242:ILE:HA	2.57	0.40
1:A:131:C:C2	2:L:242:ILE:HA	2.57	0.40
2:D:54:THR:HB	2:D:57:ALA:HB2	2.03	0.40
2:E:331:LEU:HD13	2:E:354:ALA:HB1	2.03	0.40
2:K:96:ASP:CB	2:U:360:ASN:HB3	2.51	0.40
2:M:270:ILE:HG23	2:N:363:ILE:HG21	2.03	0.40
2:O:54:THR:HB	2:O:57:ALA:HB2	2.03	0.40
2:R:270:ILE:HG23	2:S:363:ILE:HG21	2.03	0.40
1:A:31:C:C2	2:V:242:ILE:HA	2.57	0.40
1:A:151:C:C2	2:J:242:ILE:HA	2.57	0.40
2:L:6:VAL:HG23	2:M:288:TYR:CE2	2.56	0.40
2:Q:362:VAL:HG12	2:Q:363:ILE:N	2.35	0.40

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%)	41	41
2	C	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	41	41
2	D	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	41	41
2	E	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	41	41
2	F	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	41	41
2	G	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	41	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	41	41
2	I	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	41	41
2	J	368/391 (94%)	353 (96%)	14 (4%)	1 (0%)	41	41
2	K	368/391 (94%)	352 (96%)	15 (4%)	1 (0%)	41	41
2	L	368/391 (94%)	353 (96%)	13 (4%)	2 (0%)	29	29
2	M	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	19	19
2	N	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	19	19
2	O	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	19	19
2	P	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	19	19
2	Q	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	19	19
2	R	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	19	19
2	S	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	19	19
2	T	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	19	19
2	U	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	19	19
2	V	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	19	19
2	W	368/391 (94%)	353 (96%)	12 (3%)	3 (1%)	19	19
2	X	368/391 (94%)	352 (96%)	13 (4%)	3 (1%)	19	19
All	All	8464/8993 (94%)	8109 (96%)	307 (4%)	48 (1%)	29	25

All (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
2	W	360	ASN
2	X	360	ASN
2	M	361	GLY
2	O	361	GLY
2	P	361	GLY
2	R	361	GLY
2	S	360	ASN
2	S	361	GLY
2	T	360	ASN

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Mol	Chain	Res	Type
2	W	361	GLY
2	X	361	GLY
2	N	360	ASN
2	N	361	GLY
2	Q	360	ASN
2	Q	361	GLY
2	T	361	GLY
2	U	361	GLY
2	V	360	ASN
2	V	361	GLY
2	L	361	GLY
2	C	6	VAL
2	D	6	VAL
2	E	6	VAL
2	H	6	VAL
2	I	6	VAL
2	J	6	VAL
2	M	6	VAL
2	N	6	VAL
2	O	6	VAL
2	S	6	VAL
2	T	6	VAL
2	W	6	VAL
2	X	6	VAL
2	B	6	VAL
2	F	6	VAL
2	G	6	VAL
2	K	6	VAL
2	L	6	VAL
2	P	6	VAL
2	Q	6	VAL
2	R	6	VAL
2	U	6	VAL
2	V	6	VAL

5.3.2 Protein sidechains (i)

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%)	30	30
2	C	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	D	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	E	309/328 (94%)	295 (96%)	14 (4%)	27	27
2	F	309/328 (94%)	297 (96%)	12 (4%)	32	32
2	G	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	H	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	I	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	J	309/328 (94%)	295 (96%)	14 (4%)	27	27
2	K	309/328 (94%)	297 (96%)	12 (4%)	32	32
2	L	309/328 (94%)	297 (96%)	12 (4%)	32	32
2	M	309/328 (94%)	295 (96%)	14 (4%)	27	27
2	N	309/328 (94%)	297 (96%)	12 (4%)	32	32
2	O	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	P	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	Q	309/328 (94%)	297 (96%)	12 (4%)	32	32
2	R	309/328 (94%)	295 (96%)	14 (4%)	27	27
2	S	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	T	309/328 (94%)	296 (96%)	13 (4%)	30	30
2	U	309/328 (94%)	295 (96%)	14 (4%)	27	27
2	V	309/328 (94%)	297 (96%)	12 (4%)	32	32
2	W	309/328 (94%)	295 (96%)	14 (4%)	27	27
2	X	309/328 (94%)	296 (96%)	13 (4%)	30	30
All	All	7107/7544 (94%)	6808 (96%)	299 (4%)	33	30

All (299) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3	LEU
2	B	9	ASN
2	B	29	THR
2	B	83	LEU
2	B	123	ILE
2	B	136	LYS
2	B	163	ILE

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Mol	Chain	Res	Type
2	B	168	ILE
2	B	220	ILE
2	B	272	LEU
2	B	287	VAL
2	B	325	LEU
2	B	331	LEU
2	C	3	LEU
2	C	9	ASN
2	C	29	THR
2	C	83	LEU
2	C	136	LYS
2	C	163	ILE
2	C	168	ILE
2	C	220	ILE
2	C	272	LEU
2	C	287	VAL
2	C	301	TYR
2	C	325	LEU
2	C	331	LEU
2	D	3	LEU
2	D	9	ASN
2	D	29	THR
2	D	83	LEU
2	D	123	ILE
2	D	136	LYS
2	D	163	ILE
2	D	168	ILE
2	D	220	ILE
2	D	272	LEU
2	D	287	VAL
2	D	325	LEU
2	D	331	LEU
2	E	3	LEU
2	E	9	ASN
2	E	29	THR
2	E	83	LEU
2	E	123	ILE
2	E	136	LYS
2	E	163	ILE
2	E	168	ILE
2	E	220	ILE
2	E	272	LEU

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Mol	Chain	Res	Type
2	E	287	VAL
2	E	301	TYR
2	E	325	LEU
2	E	331	LEU
2	F	3	LEU
2	F	9	ASN
2	F	29	THR
2	F	83	LEU
2	F	123	ILE
2	F	136	LYS
2	F	163	ILE
2	F	220	ILE
2	F	272	LEU
2	F	287	VAL
2	F	325	LEU
2	F	331	LEU
2	G	3	LEU
2	G	9	ASN
2	G	29	THR
2	G	83	LEU
2	G	123	ILE
2	G	136	LYS
2	G	163	ILE
2	G	168	ILE
2	G	220	ILE
2	G	272	LEU
2	G	287	VAL
2	G	325	LEU
2	G	331	LEU
2	H	3	LEU
2	H	9	ASN
2	H	29	THR
2	H	83	LEU
2	H	136	LYS
2	H	163	ILE
2	H	168	ILE
2	H	220	ILE
2	H	272	LEU
2	H	287	VAL
2	H	301	TYR
2	H	325	LEU
2	H	331	LEU

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Mol	Chain	Res	Type
2	I	3	LEU
2	I	9	ASN
2	I	29	THR
2	I	83	LEU
2	I	123	ILE
2	I	136	LYS
2	I	163	ILE
2	I	168	ILE
2	I	220	ILE
2	I	272	LEU
2	I	287	VAL
2	I	325	LEU
2	I	331	LEU
2	J	3	LEU
2	J	9	ASN
2	J	29	THR
2	J	83	LEU
2	J	123	ILE
2	J	136	LYS
2	J	163	ILE
2	J	168	ILE
2	J	220	ILE
2	J	272	LEU
2	J	287	VAL
2	J	301	TYR
2	J	325	LEU
2	J	331	LEU
2	K	3	LEU
2	K	9	ASN
2	K	29	THR
2	K	83	LEU
2	K	123	ILE
2	K	136	LYS
2	K	163	ILE
2	K	220	ILE
2	K	272	LEU
2	K	287	VAL
2	K	325	LEU
2	K	331	LEU
2	L	3	LEU
2	L	9	ASN
2	L	29	THR

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Mol	Chain	Res	Type
2	L	83	LEU
2	L	123	ILE
2	L	136	LYS
2	L	163	ILE
2	L	220	ILE
2	L	272	LEU
2	L	287	VAL
2	L	325	LEU
2	L	331	LEU
2	M	3	LEU
2	M	9	ASN
2	M	29	THR
2	M	83	LEU
2	M	123	ILE
2	M	136	LYS
2	M	163	ILE
2	M	168	ILE
2	M	220	ILE
2	M	272	LEU
2	M	287	VAL
2	M	301	TYR
2	M	325	LEU
2	M	331	LEU
2	N	3	LEU
2	N	9	ASN
2	N	29	THR
2	N	83	LEU
2	N	136	LYS
2	N	163	ILE
2	N	168	ILE
2	N	220	ILE
2	N	272	LEU
2	N	287	VAL
2	N	325	LEU
2	N	331	LEU
2	O	3	LEU
2	O	9	ASN
2	O	29	THR
2	O	83	LEU
2	O	123	ILE
2	O	136	LYS
2	O	163	ILE

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Mol	Chain	Res	Type
2	O	168	ILE
2	O	220	ILE
2	O	272	LEU
2	O	287	VAL
2	O	325	LEU
2	O	331	LEU
2	P	3	LEU
2	P	9	ASN
2	P	29	THR
2	P	83	LEU
2	P	123	ILE
2	P	136	LYS
2	P	163	ILE
2	P	168	ILE
2	P	220	ILE
2	P	272	LEU
2	P	287	VAL
2	P	325	LEU
2	P	331	LEU
2	Q	3	LEU
2	Q	9	ASN
2	Q	29	THR
2	Q	83	LEU
2	Q	123	ILE
2	Q	136	LYS
2	Q	163	ILE
2	Q	220	ILE
2	Q	272	LEU
2	Q	287	VAL
2	Q	325	LEU
2	Q	331	LEU
2	R	3	LEU
2	R	9	ASN
2	R	29	THR
2	R	83	LEU
2	R	123	ILE
2	R	136	LYS
2	R	163	ILE
2	R	168	ILE
2	R	220	ILE
2	R	272	LEU
2	R	287	VAL

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Mol	Chain	Res	Type
2	R	301	TYR
2	R	325	LEU
2	R	331	LEU
2	S	3	LEU
2	S	9	ASN
2	S	29	THR
2	S	83	LEU
2	S	123	ILE
2	S	136	LYS
2	S	163	ILE
2	S	168	ILE
2	S	220	ILE
2	S	272	LEU
2	S	287	VAL
2	S	325	LEU
2	S	331	LEU
2	T	3	LEU
2	T	9	ASN
2	T	29	THR
2	T	83	LEU
2	T	123	ILE
2	T	136	LYS
2	T	163	ILE
2	T	168	ILE
2	T	220	ILE
2	T	272	LEU
2	T	287	VAL
2	T	325	LEU
2	T	331	LEU
2	U	3	LEU
2	U	9	ASN
2	U	29	THR
2	U	83	LEU
2	U	123	ILE
2	U	136	LYS
2	U	163	ILE
2	U	168	ILE
2	U	220	ILE
2	U	272	LEU
2	U	287	VAL
2	U	301	TYR
2	U	325	LEU

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Mol	Chain	Res	Type
2	U	331	LEU
2	V	3	LEU
2	V	9	ASN
2	V	29	THR
2	V	83	LEU
2	V	123	ILE
2	V	136	LYS
2	V	163	ILE
2	V	220	ILE
2	V	272	LEU
2	V	287	VAL
2	V	325	LEU
2	V	331	LEU
2	W	3	LEU
2	W	9	ASN
2	W	29	THR
2	W	83	LEU
2	W	123	ILE
2	W	136	LYS
2	W	163	ILE
2	W	168	ILE
2	W	220	ILE
2	W	272	LEU
2	W	287	VAL
2	W	301	TYR
2	W	325	LEU
2	W	331	LEU
2	X	3	LEU
2	X	9	ASN
2	X	29	THR
2	X	83	LEU
2	X	123	ILE
2	X	136	LYS
2	X	163	ILE
2	X	168	ILE
2	X	220	ILE
2	X	272	LEU
2	X	287	VAL
2	X	325	LEU
2	X	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	GLN
2	B	59	HIS
2	B	187	ASN
2	B	274	HIS
2	B	327	ASN
2	C	26	GLN
2	C	59	HIS
2	C	274	HIS
2	C	327	ASN
2	D	26	GLN
2	D	59	HIS
2	D	274	HIS
2	D	327	ASN
2	E	26	GLN
2	E	59	HIS
2	E	274	HIS
2	E	327	ASN
2	F	26	GLN
2	F	59	HIS
2	F	274	HIS
2	F	327	ASN
2	G	26	GLN
2	G	59	HIS
2	G	274	HIS
2	G	327	ASN
2	H	26	GLN
2	H	59	HIS
2	H	274	HIS
2	H	327	ASN
2	I	26	GLN
2	I	59	HIS
2	I	274	HIS
2	I	327	ASN
2	J	26	GLN
2	J	59	HIS
2	J	274	HIS
2	J	327	ASN
2	K	26	GLN
2	K	59	HIS
2	K	274	HIS
2	K	327	ASN
2	L	26	GLN
2	L	59	HIS

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Mol	Chain	Res	Type
2	L	274	HIS
2	L	327	ASN
2	M	26	GLN
2	M	59	HIS
2	M	274	HIS
2	M	327	ASN
2	N	26	GLN
2	N	59	HIS
2	N	274	HIS
2	N	327	ASN
2	O	26	GLN
2	O	59	HIS
2	O	274	HIS
2	O	327	ASN
2	P	26	GLN
2	P	59	HIS
2	P	274	HIS
2	P	327	ASN
2	Q	26	GLN
2	Q	59	HIS
2	Q	274	HIS
2	Q	327	ASN
2	R	26	GLN
2	R	59	HIS
2	R	274	HIS
2	R	327	ASN
2	S	26	GLN
2	S	59	HIS
2	S	274	HIS
2	S	327	ASN
2	T	26	GLN
2	T	59	HIS
2	T	274	HIS
2	T	327	ASN
2	U	26	GLN
2	U	59	HIS
2	U	274	HIS
2	U	327	ASN
2	V	26	GLN
2	V	59	HIS
2	V	274	HIS
2	V	327	ASN

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Mol	Chain	Res	Type
2	W	26	GLN
2	W	59	HIS
2	W	274	HIS
2	W	327	ASN
2	X	59	HIS
2	X	274	HIS
2	X	327	ASN

5.3.3 RNA

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

All (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
1	A	61	C
1	A	71	C
1	A	81	C
1	A	91	C
1	A	101	C
1	A	111	C
1	A	121	C
1	A	131	C
1	A	141	C
1	A	151	C
1	A	161	C
1	A	171	C
1	A	181	C
1	A	191	C
1	A	201	C
1	A	211	C
1	A	221	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 monosaccharides 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.

6 Tomogram visualisation

This section contains visualisations of the EMDB entry EMD-2369. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Tomogram analysis (i)

This section contains the results of statistical analysis of the tomogram.

7.1 Map-value distribution (i)

This section was not generated.

8 Map-model fit

This section was not generated.