



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 2, 2019 – 11:13 AM EST

PDB ID : 6Q1F
EMDB ID: : EMD-20557
Title : Atomic structure of the Human Herpesvirus 6B Capsid and Capsid-Associated Tegument Complexes
Authors : Zhang, Y.B.; Liu, W.; Li, Z.H.; Kumar, V.; Alvarez-Cabrera, A.L.; Leibovitch, E.; Cui, Y.X.; Mei, Y.; Bi, G.Q.; Jacobson, S.; Zhou, Z.H.
Deposited on : 2019-08-03
Resolution : 9.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

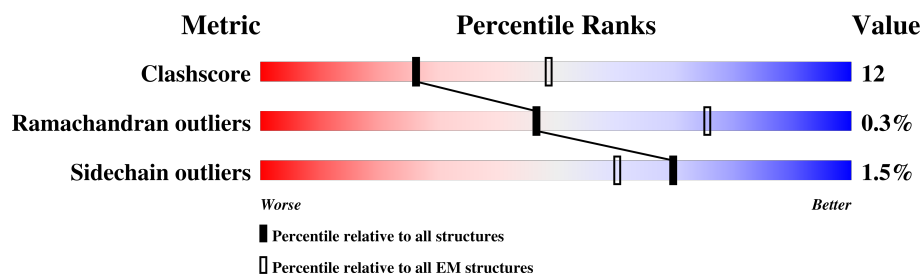
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.00 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.



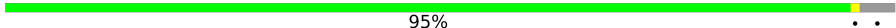
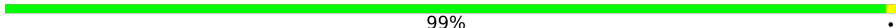

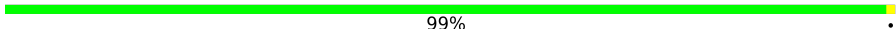
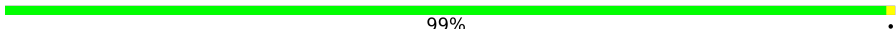
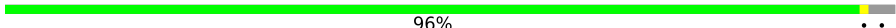













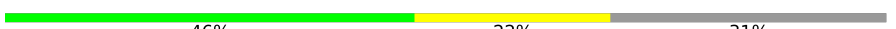
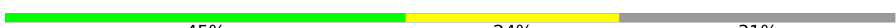

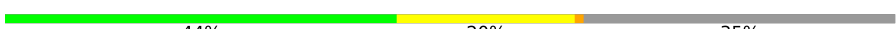


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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	1345	79% 20%
1	B	1345	78% 21%
1	C	1345	80% 18% ..
1	D	1345	79% 20% .
1	E	1345	77% 22% .
1	F	1345	78% 21% .
1	G	1345	76% 23% .
1	H	1345	80% 19% .
1	I	1345	83% 17% .


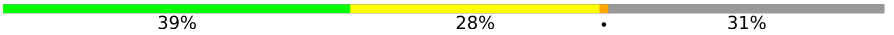

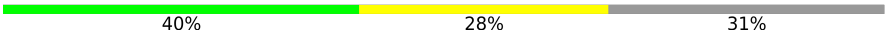
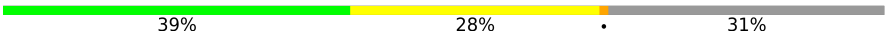
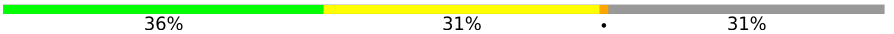
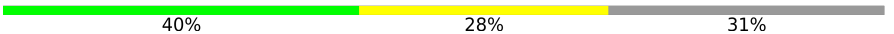














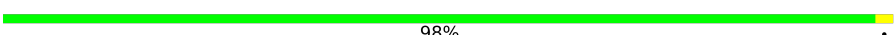
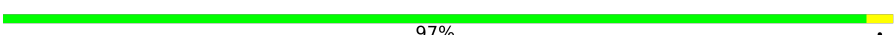
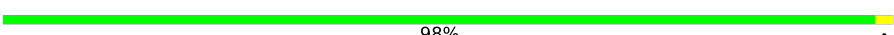
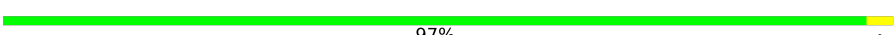
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Mol	Chain	Length	Quality of chain
1	q	1345	 95%
1	r	1345	 99%
1	s	1345	 99%
1	t	1345	 99%
1	u	1345	 99%
1	v	1345	 96%
1	w	1345	 92% 7%
2	e	858	 31% 69%
2	f	858	 31% 69%
2	g	858	 30% 69%
2	h	858	 31% 69%
2	i	858	 30% 69%
2	j	858	 30% 69%
2	k	858	 30% 69%
2	l	858	 30% 69%
2	m	858	 31% 69%
2	n	858	 30% 69%
2	o	858	 30% 69%
2	p	858	 31% 69%
3	1	89	 46% 22% 31%
3	2	89	 45% 24% 31%
3	3	89	 47% 21% 31%
3	4	89	 44% 20% 35%
3	J	89	 42% 24% 31%
3	K	89	 42% 27% 31%

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Mol	Chain	Length	Quality of chain
3	L	89	
3	M	89	
3	N	89	
3	O	89	
3	P	89	
3	Q	89	
3	R	89	
3	x	89	
3	y	89	
3	z	89	
4	5	299	
4	S	299	
4	T	299	
4	U	299	
4	V	299	
5	6	296	
5	7	296	
5	W	296	
5	X	296	
5	Y	296	
5	Z	296	
5	a	296	
5	b	296	
5	c	296	
5	d	296	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 238552 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	B	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	C	1325	Total	C	N	O	S	0	0
			10552	6709	1792	1991	60		
1	D	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	E	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	F	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	G	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	H	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	I	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	q	1296	Total	C	N	O	S	0	0
			10313	6561	1751	1942	59		
1	r	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	s	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	t	1343	Total	C	N	O	S	0	0
			10682	6792	1813	2017	60		
1	u	1344	Total	C	N	O	S	0	0
			10690	6797	1814	2018	61		
1	v	1301	Total	C	N	O	S	0	0
			10331	6564	1759	1948	60		
1	w	1248	Total	C	N	O	S	0	0
			9933	6324	1691	1860	58		

- Molecule 2 is a protein called Large structural phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	e	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	f	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	g	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	h	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	i	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	j	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	k	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	l	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	m	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	n	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	o	269	Total 2224	C 1417	N 376	O 426	S 5	0	0
2	p	269	Total 2224	C 1417	N 376	O 426	S 5	0	0

- Molecule 3 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	K	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	L	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	M	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	N	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	O	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	P	61	Total 483	C 308	N 89	O 83	S 3	0	0
3	Q	61	Total 483	C 308	N 89	O 83	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	R	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	x	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	y	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	z	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	1	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	2	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	3	61	Total	C	N	O	S	0	0
			483	308	89	83	3		
3	4	58	Total	C	N	O	S	0	0
			456	292	85	76	3		

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	251	Total	C	N	O	S	0	0
			2023	1306	327	376	14		
4	S	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	T	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	U	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		
4	V	299	Total	C	N	O	S	0	0
			2398	1542	395	446	15		

- Molecule 5 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	282	Total	C	N	O	S	0	0
			2226	1422	370	415	19		
5	W	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	X	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	Y	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		

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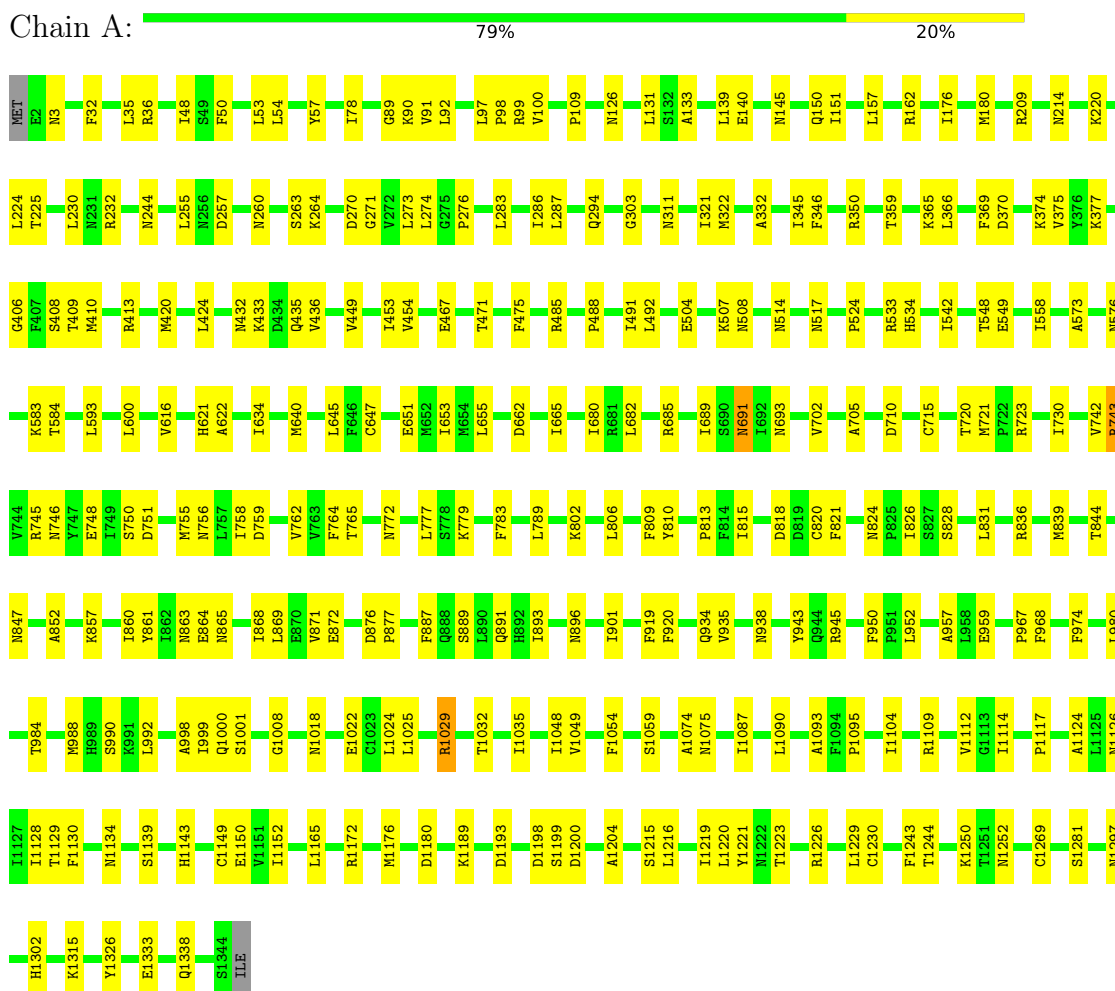
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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Z	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	7	296	Total	C	N	O	S	0	0
			2337	1486	393	437	21		
5	a	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	b	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	c	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		
5	d	295	Total	C	N	O	S	0	0
			2329	1481	392	436	20		

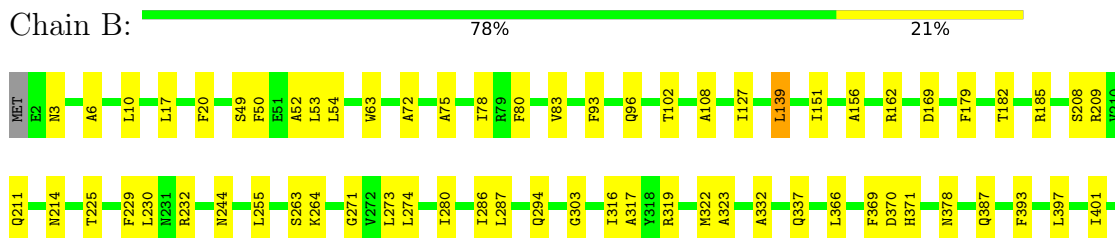
3 Residue-property plots

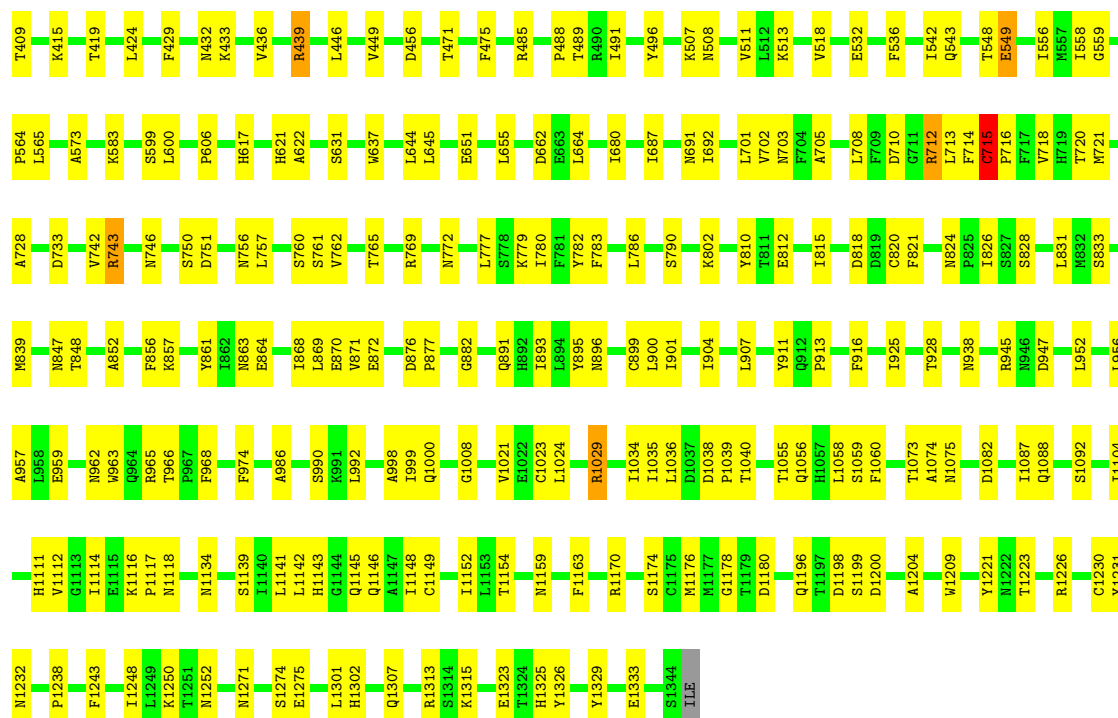
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: Major capsid protein



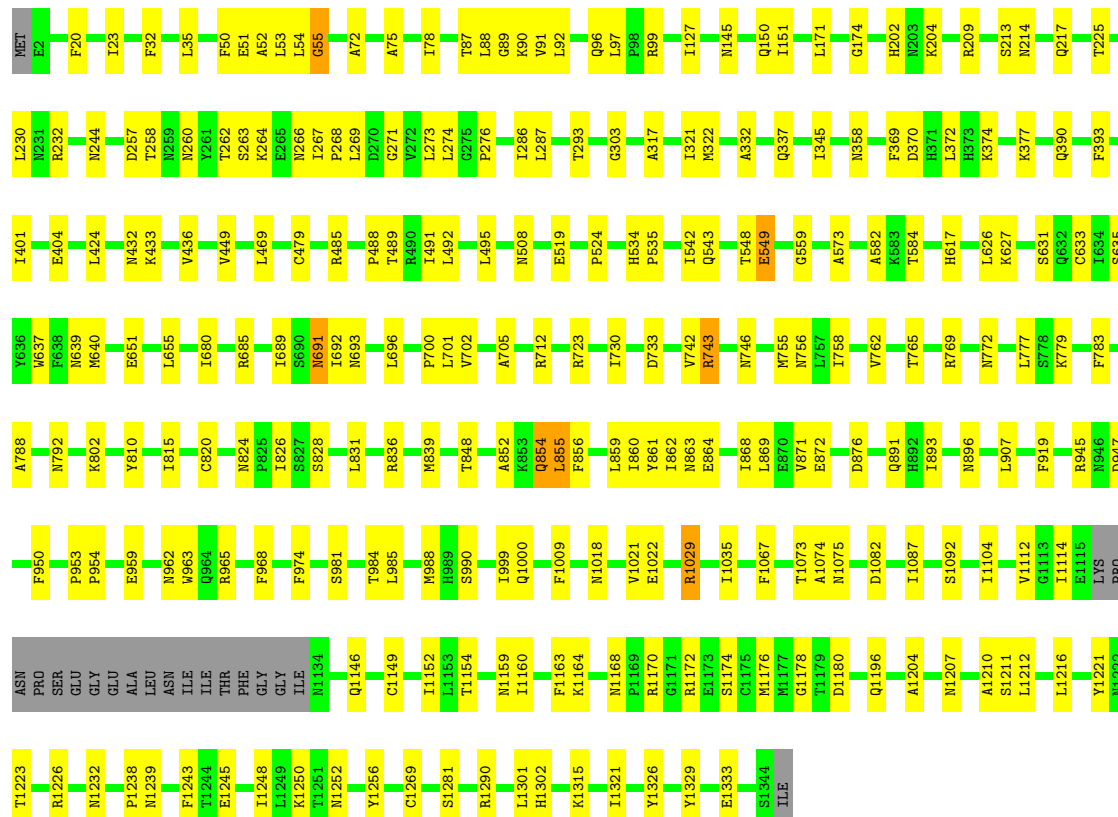
- Molecule 1: Major capsid protein






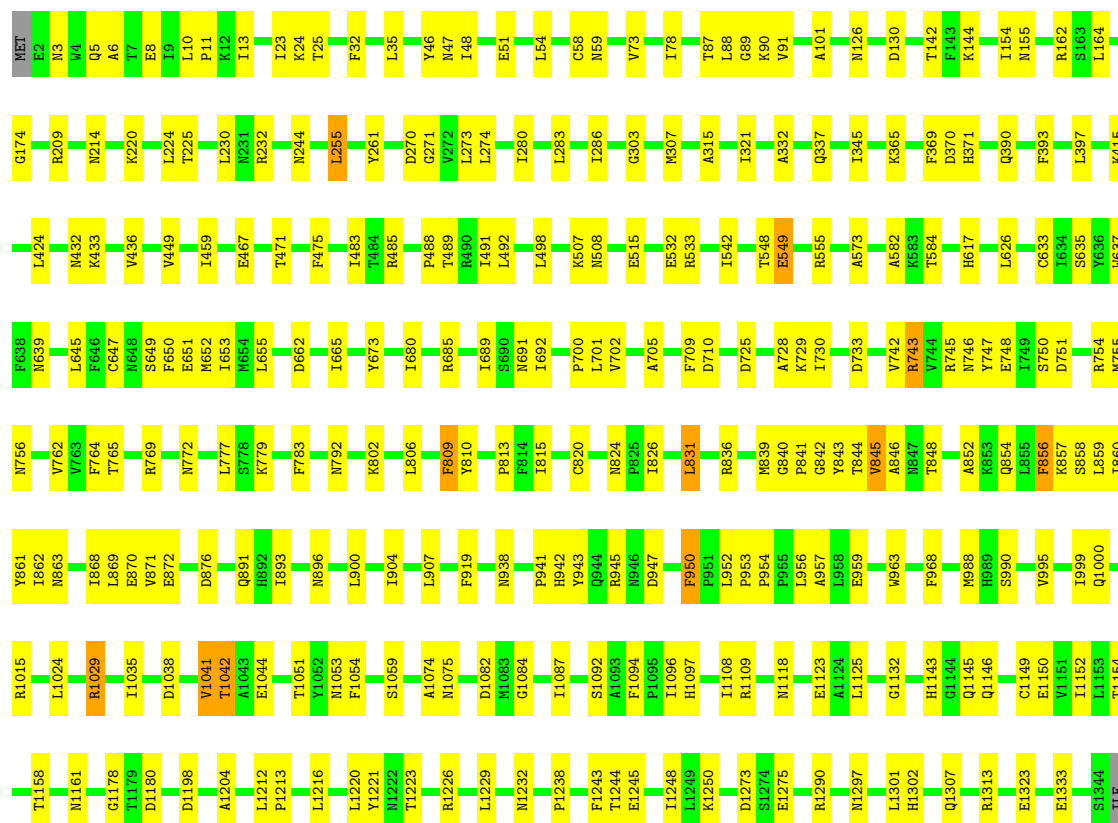
• Molecule 1: Major capsid protein

Chain C: 80% 18% ..




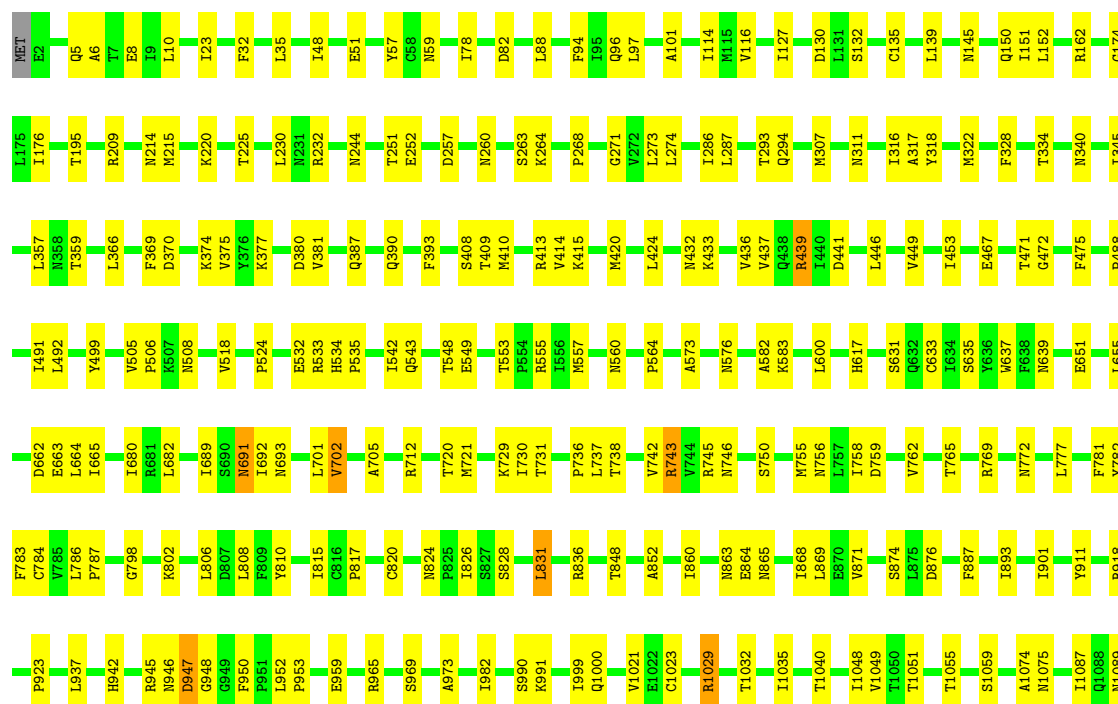
• Molecule 1: Major capsid protein

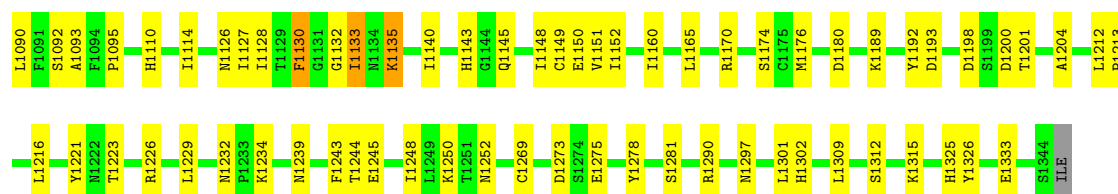
Chain D:  79% 20%



• Molecule 1: Major capsid protein

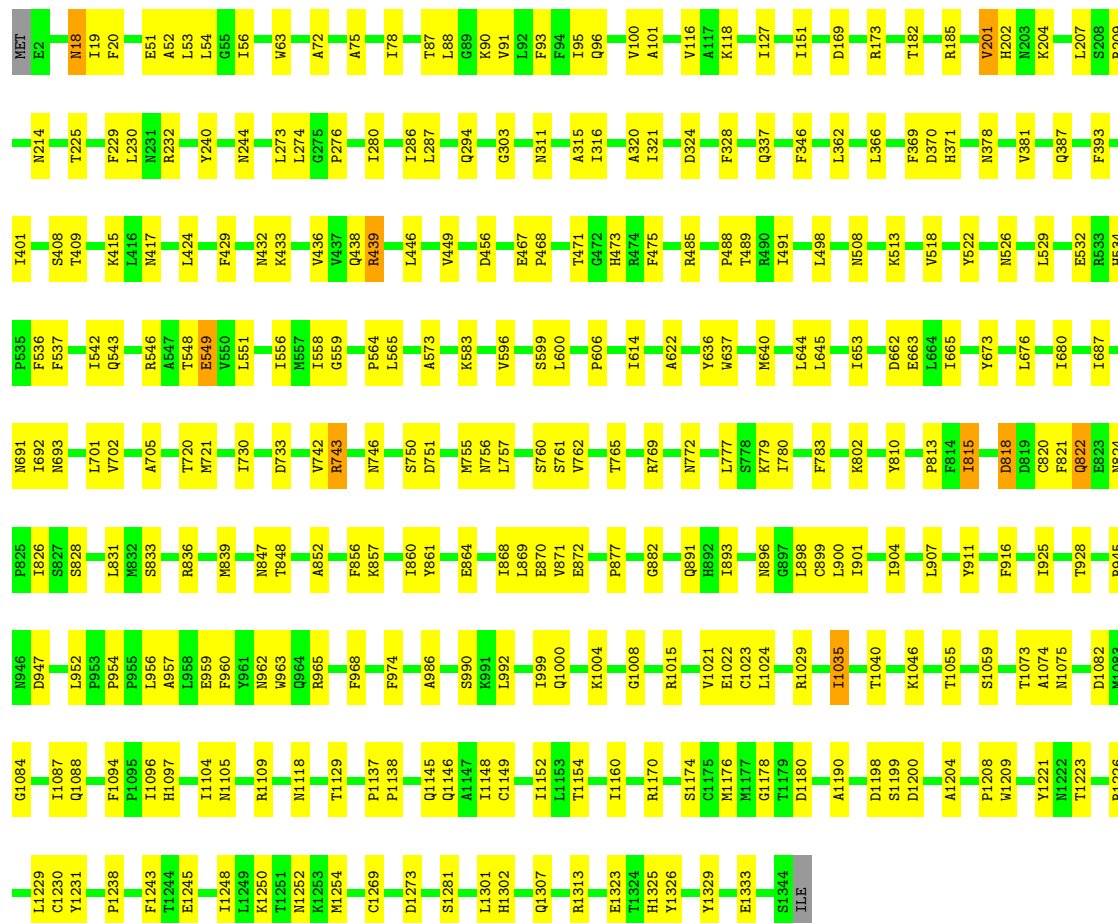
Chain E:  77% 22%





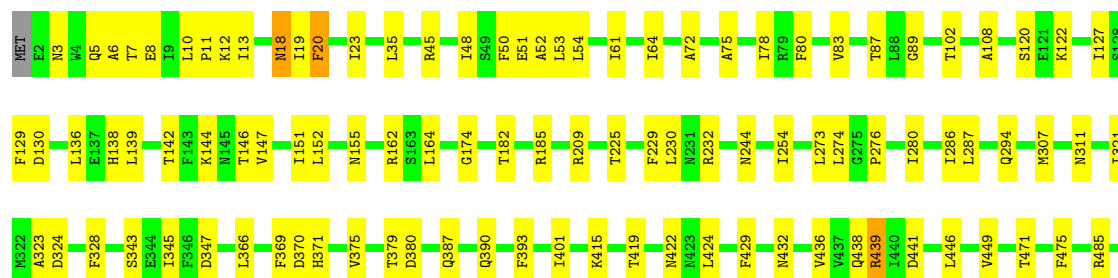
• Molecule 1: Major capsid protein

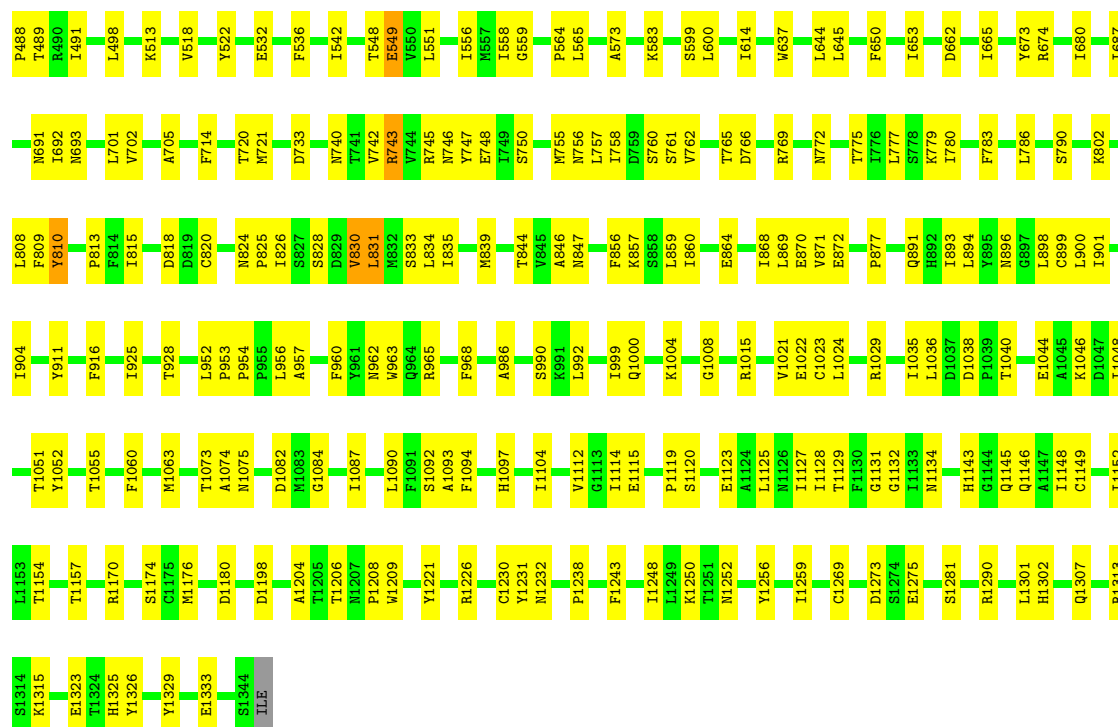
Chain F: 78% 21% .



• Molecule 1: Major capsid protein

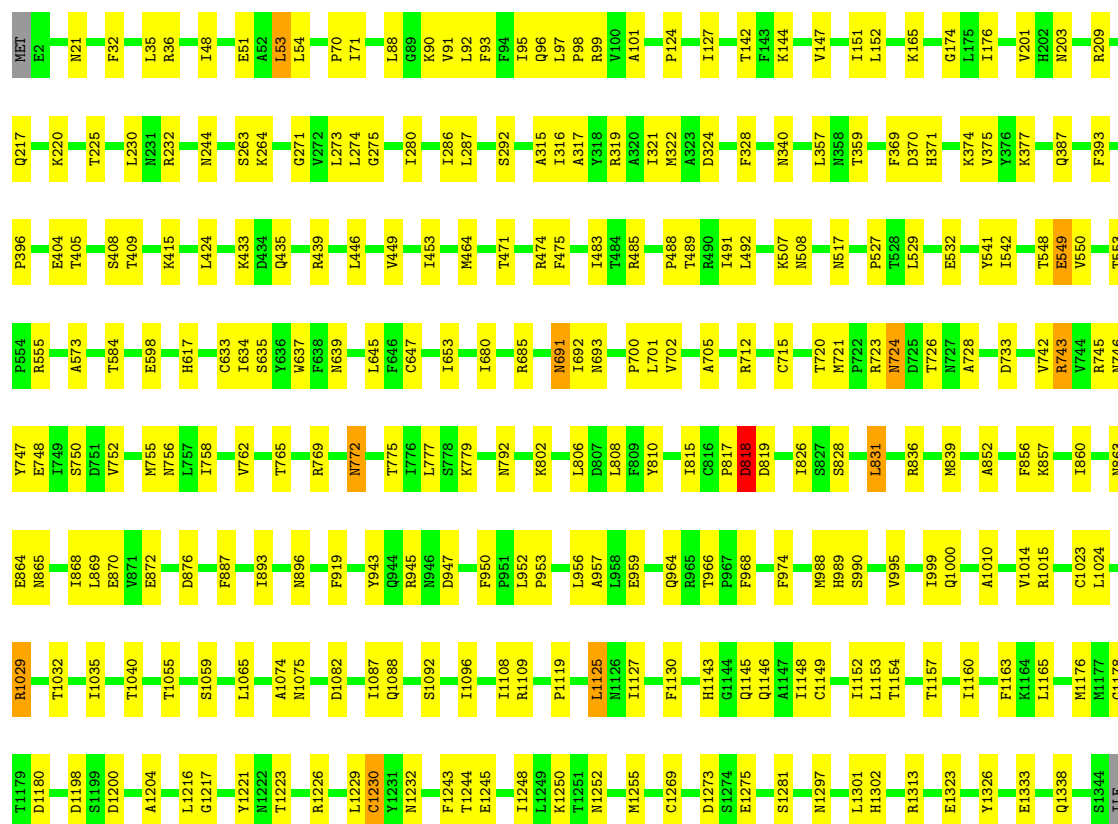
Chain G: 76% 23% .






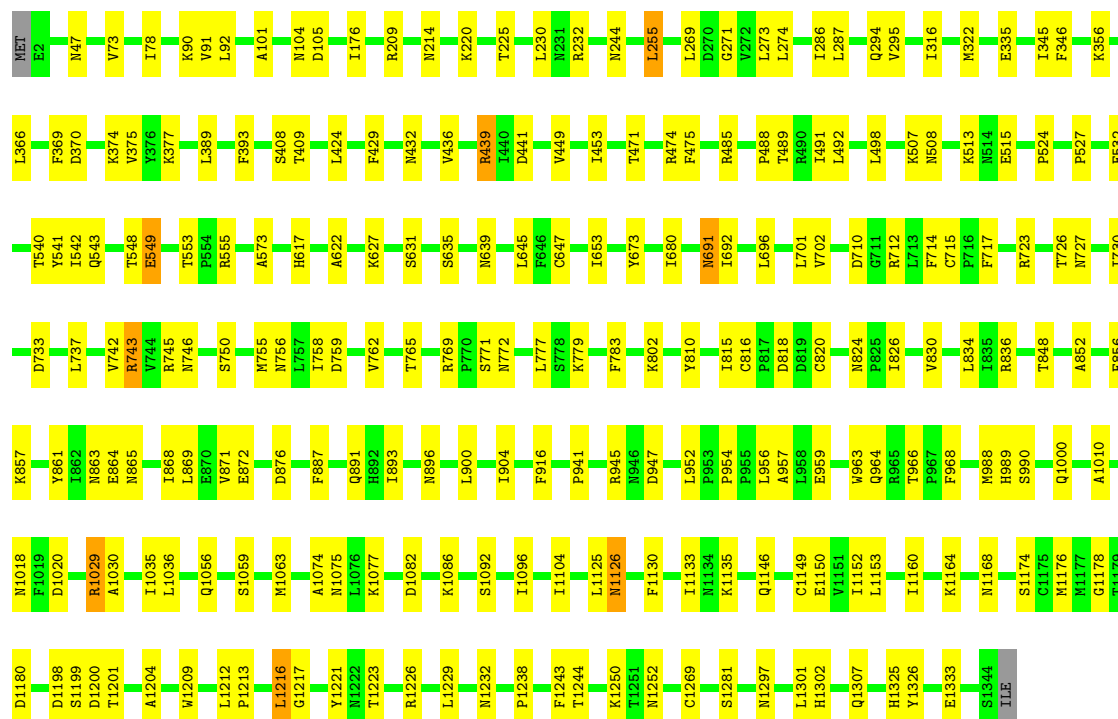
• Molecule 1: Major capsid protein

Chain H: 80% 19%



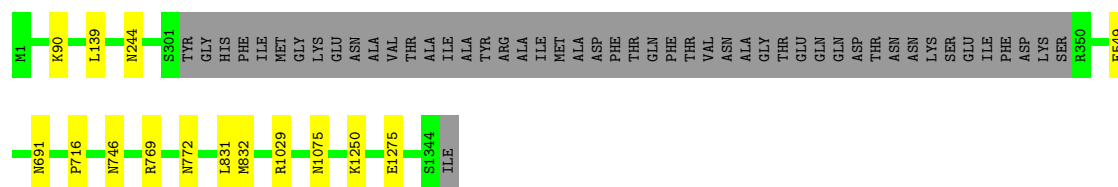
• Molecule 1: Major capsid protein

Chain I:  83% 17%



• Molecule 1: Major capsid protein

Chain q:  95%



• Molecule 1: Major capsid protein

Chain r:  99%



• Molecule 1: Major capsid protein

Chain s:  99%



• Molecule 1: Major capsid protein

Chain t:  99%



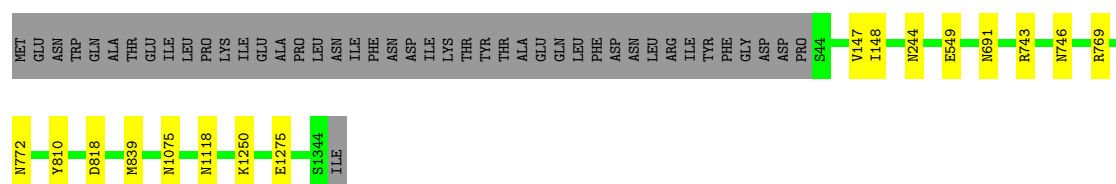
- Molecule 1: Major capsid protein

Chain u:  99%



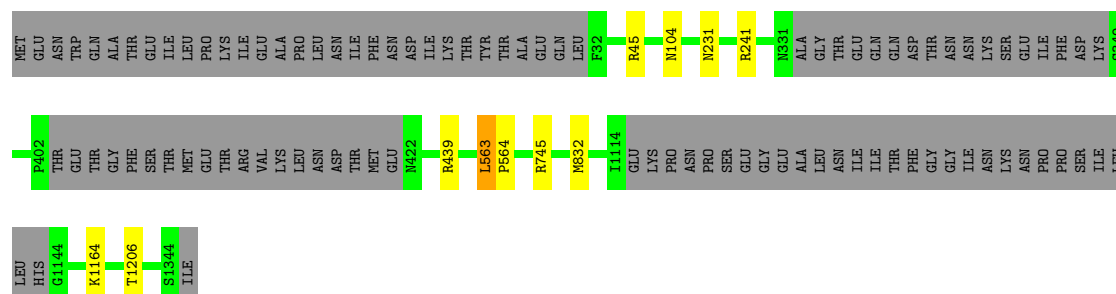
- Molecule 1: Major capsid protein

Chain v:  96%



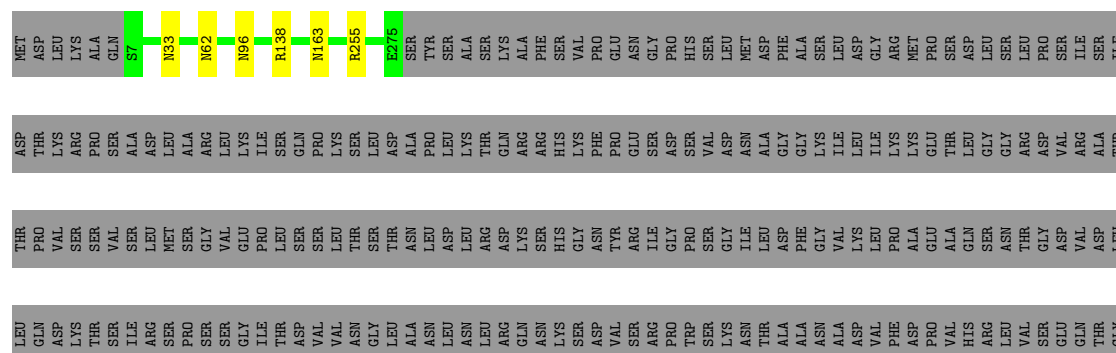
- Molecule 1: Major capsid protein

Chain w: 92% • 7%



- Molecule 2: Large structural phosphoprotein

Chain e: 31% . 69%



[illegible]

- Molecule 2: Large structural phosphoprotein

Chain f:  31% 69%

[illegible]

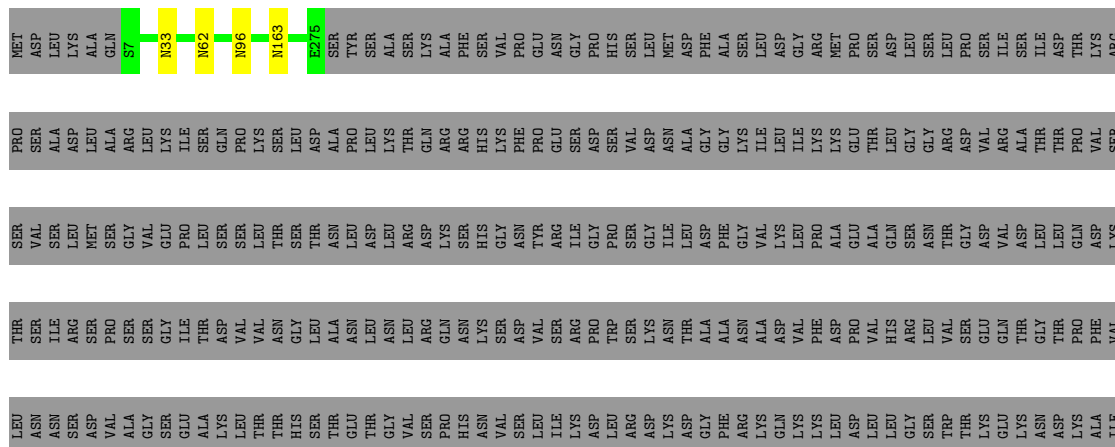
- Molecule 2: Large structural phosphoprotein

Chain g:  30% 69%



- Molecule 2: Large structural phosphoprotein

Chain h:  31% 69%



GLU	THR	SER	ILE	GLY	ASN	VAL
THR	LEU	VAL	LEU	GLY	ASN	HIS
LEU	GLN	GLN	LEU	LEU	ALA	SER
ILE	SER	SER	GLY	GLU	GLU	ARG
PRO	PRO	PRO	GLU	LYS	LYS	VAL
THR	THR	PHE	LYS	GLY	THR	THR
GLN	GLN	ARG	GLY	GLU	GLY	GLY
LEU	LEU	LEU	ILE	GLN	SER	ASP
MET	MET	PRO	GLN	SER	GLY	SER
GLY	VAL	ALA	ILE	LEU	PHE	GLY
THR	THR	LEU	HIS	LEU	ASN	ALA
PRO	PRO	SER	ASN	VAL	VAL	THR
GLU	GLU	ARG	GLN	ASP	GLU	GLU
GLU	GLU	ASP	SER	LYS	THR	THR
LYS	LYS	LEU	GLY	GLU	VAL	VAL
ASP	ASP	ASP	THR	MET	THR	THR
ASP	ASP	SER	GLU	THR	ALA	ALA
VAL	VAL	VAL	LEU	GLN	ARG	ARG
ILE	SER	SER	LYS	ASN	ASP	ASP
GLU	GLU	PHE	LEU	GLU	SER	SER
LYS	LYS	LYS	PRO	GLN	PRO	PRO
MET	MET	ASP	THR	GLU	VAL	VAL
VAL	VAL	ALA	GLU	PRO	LEU	LEU
LEU	LEU	LEU	ASN	LEU	ARG	ARG
ARG	ARG	ASP	LYS	PRO	LYS	LYS
ILE	ILE	VAL	LEU	ASN	THR	THR
ARG	ARG	LYS	GLY	LEU	LYS	LYS
GLN	GLN	LEU	ARG	MET	HIS	HIS
ASP	ASP	PRO	GLU	GLU	ALA	ALA
GLY	GLY	GLY	SER	ALA	ASN	ASN
THR	THR	ASN	GLU	ALA	ASP	ASP
GLU	GLU	GLY	GLU	ARG	ILE	ILE
ASP	ASP	GLU	ALA	ASN	PHE	PHE
GLU	GLU	ARG	ASN	ALA	ALA	ALA
GLU	GLU	GLU	VAL	GLY	LEU	LEU
VAL	VAL	LYS	ASP	GLN	VAL	VAL
SER	SER	ALA	GLN	GLY	SER	SER
LEU	LEU	GLY	ASN	GLN	ARG	ARG
ILE	ILE	ARG	PHE	VAL	GLY	GLY
ALA	ALA	GLU	LYS	ASN	LYS	LYS
ALA	ALA	THR	ASN	GLY	GLY	GLY
LYS	LYS	SER	PHE	ILE	ASN	ASN
ASP	ASP	ASP	LYS	LEU	SER	SER
LYS	LYS	PHE	LEU	ALA	ARG	ARG
SER	SER	LYS	GLN	GLU	LEU	LEU
VAL	VAL	VAL	ASN	PHE	THR	THR
ILE	ILE	GLY	ASP	THR	TYR	TYR
ALA	ALA	GLN	LEU	ASN	SER	SER
ASP	ASP	ASP	LEU	LEU	GLY	GLY

- Molecule 2: Large structural phosphoprotein

Chain i: 

[illegible]

- Molecule 2: Large structural phosphoprotein

Chain j:  30% . 69%

[illegible]

- Molecule 2: Large structural phosphoprotein

Chain k:  30% 69%

[illegible]

[illegible]

- Molecule 2: Large structural phosphoprotein

Chain 1: 30% 69%

ALA	LYS	THR	ASN	LYS	GLY	THR	SER	ASN	LYS	THR	SER	GLY	THR	ASP	PRO	MET
LYS	ASP	SER	PHE	LYS	LEU	GLY	LEU	LYS	LEU	GLU	GLN	ASP	VAL	VAL	SER	ASP
SER	SER	PHE	GLN	LEU	ALA	ASN	GLY	ARG	GLY	ASN	GLY	THR	THR	THR	ILE	ALA
VAL	VAL	VAL	ASN	PHE	THR	THR	LEU	THR	TYR	LYS	PRO	GLN	THR	THR	ASP	GLN
ILE	ALA	GLY	ASP	LEU	ASN	ALA	PHE	THR	THR	ALA	PHE	ASP	VAL	VAL	THR	GLN
ALA	ALA	GLN	LEU	ASN	GLY	GLY	SER	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLN
SER	SER	ASP	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	GLN
THR	THR	THR	VAL	SER	ASN	HIS	ASN	SER	ASN	ASN	ASN	SER	VAL	VAL	SER	THR
ILE	ILE	ILE	SER	GLY	GLY	ARG	SER	SER	SER	SER	SER	ARG	LEU	LEU	ASP	ALA
PRO	PRO	THR	PHE	LYS	LYS	GLU	ASP	GLU	ASP	GLU	ASP	SER	MET	MET	LEU	ALA
GLN	GLN	GLN	ARG	GLY	THR	THR	THR	THR	THR	THR	THR	SER	GLY	GLY	ARG	ALA
LEU	LEU	LEU	LEU	ILE	ILE	GLY	GLY	GLY	GLY	GLY	GLY	SER	VAL	VAL	LEU	LYS
MET	MET	MET	PRO	GLN	SER	ASP	SER	ASP	SER	ASP	SER	GLY	GLY	GLY	LYS	LYS
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THR	THR	THR	SER	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS
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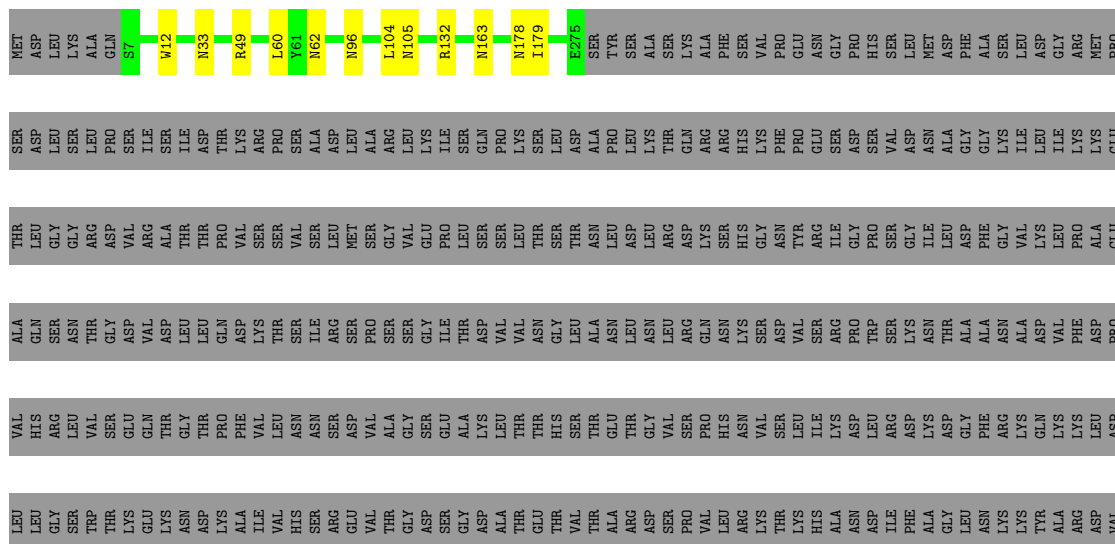
- Molecule 2: Large structural phosphoprotein

Chain m: 31% 69%



- Molecule 2: Large structural phosphoprotein

Chain n:  30% . 69%



SER	ALA	GLN	GLY	SER
LEU	GLY	ASN	GLN	ARG
ILE	ARG	LEU	VAL	GLY
ALA	GLU	PHE	ASN	LYS
ALA	THR	ASN	LYS	GLY
LYS	SER	PHE	ILE	ASN
ASP	ASP	LYS	LEU	SER
LYS	PHE	LEU	ALA	ARG
SER	LYS	GLN	GLU	ASP
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SER	ASP	ASP	LEU	GLY
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	THR	GLN	SER	ALA
	LEU	LEU	LEU	GLY
	ILE	SER	GLY	GLU
	PRO	PRO	GLU	LYS
	THR	PHE	GLU	LYS
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	VAL	ALA	ILE	LYS
	GLU	ASP	LEU	PHE
	THR	LEU	HIS	ASN
	PRO	SER	ASN	VAL
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	GLU	ASP	SER	LYS
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	ASP	ASP	THR	MET
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	VAL	VAL	LEU	GLN
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	VAL	ALA	GLU	PRO
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	THR	LEU	ARG	MET
	ASP	GLY	GLU	ALA
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	THR	ASN	GLU	ARG
	VAL	GLY	GLU	ASN
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	GLU	GLU	ASN	ALA
	THR	GLU	VAL	GLY
	ASP	ILE	ARG	GLY
	GLU	LEU	ILE	GLU
	VAL	ASP	THR	GLN
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	PRO	LEU	GLU	GLN
	GLY	GLN	VAL	ALA
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- Molecule 2: Large structural phosphoprotein

Chain o:  30% . 69%

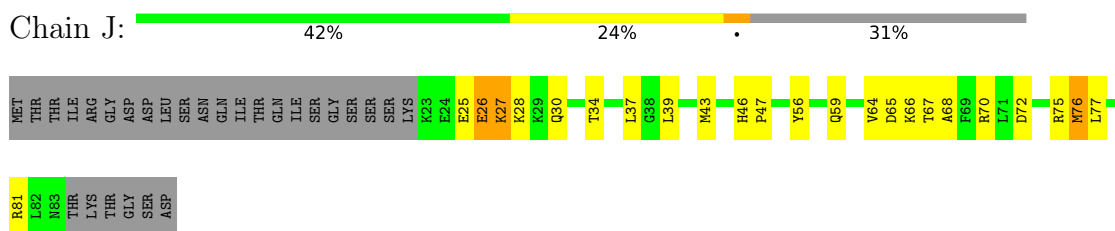
[illegible]

- Molecule 2: Large structural phosphoprotein

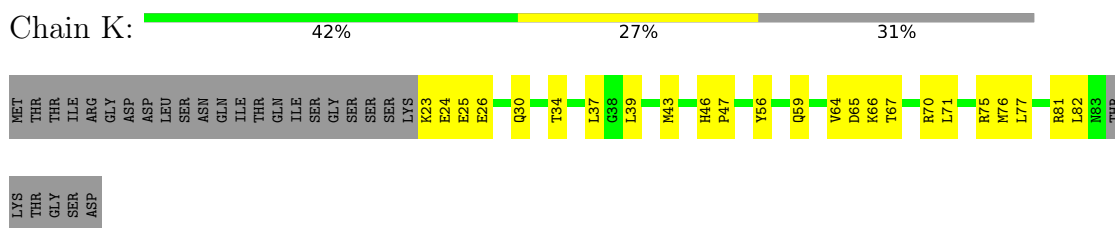
Chain p:  31% . 69%



- Molecule 3: Small capsomere-interacting protein

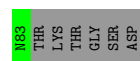


- Molecule 3: Small capsomere-interacting protein



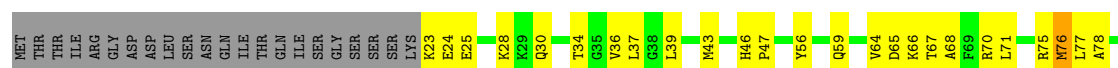
- Molecule 3: Small capsomere-interacting protein

Chain L: 



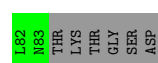
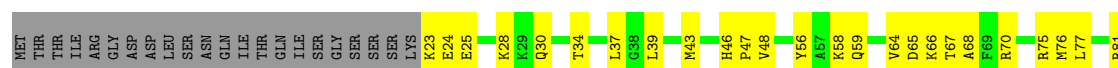
- Molecule 3: Small capsomere-interacting protein

Chain M: 



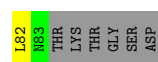
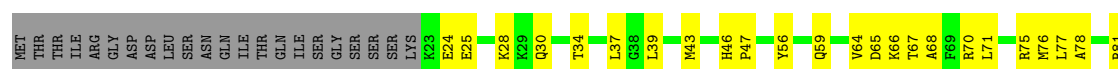
- Molecule 3: Small capsomere-interacting protein

Chain N: 



- Molecule 3: Small capsomere-interacting protein

Chain O: 

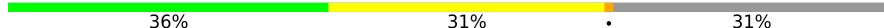


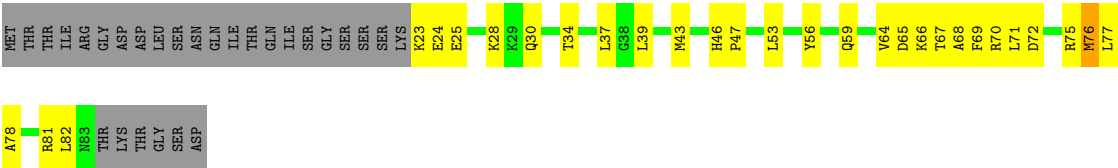
- Molecule 3: Small capsomere-interacting protein

Chain P: 

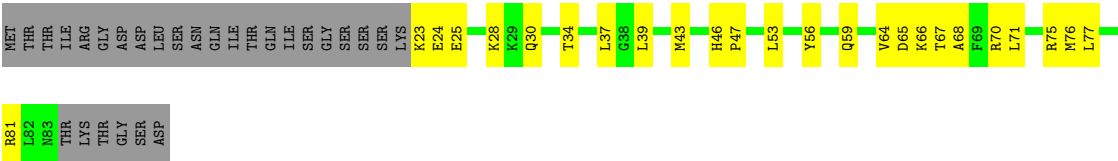


- Molecule 3: Small capsomere-interacting protein

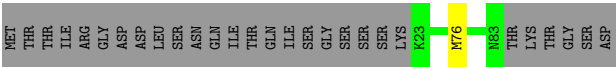
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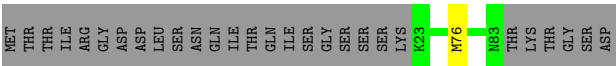
● Molecule 3: Small capsomere-interacting protein



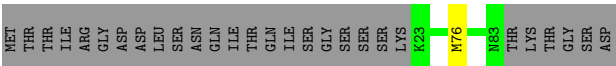
● Molecule 3: Small capsomere-interacting protein



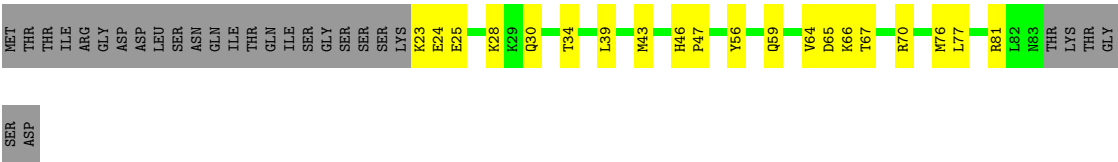
● Molecule 3: Small capsomere-interacting protein



● Molecule 3: Small capsomere-interacting protein

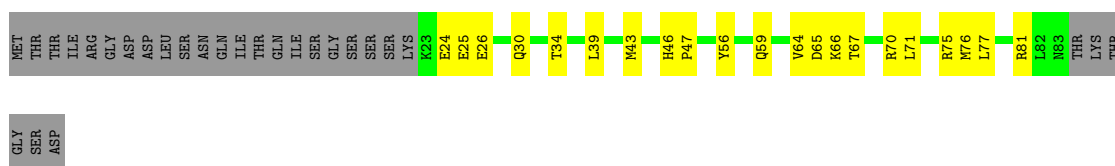


● Molecule 3: Small capsomere-interacting protein

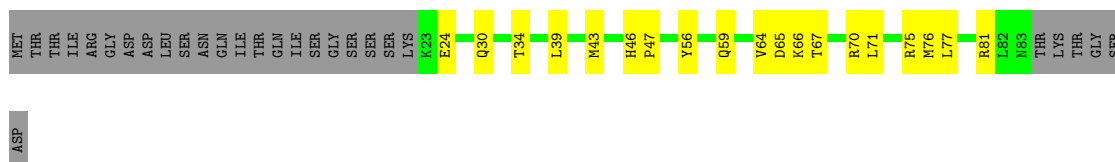


● Molecule 3: Small capsomere-interacting protein

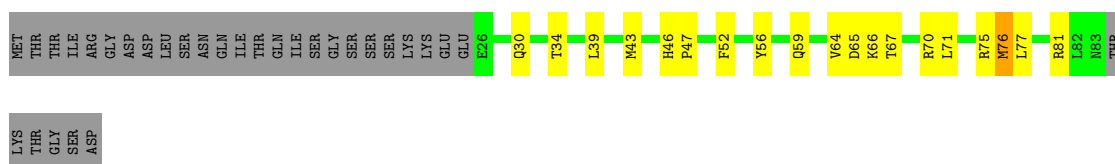




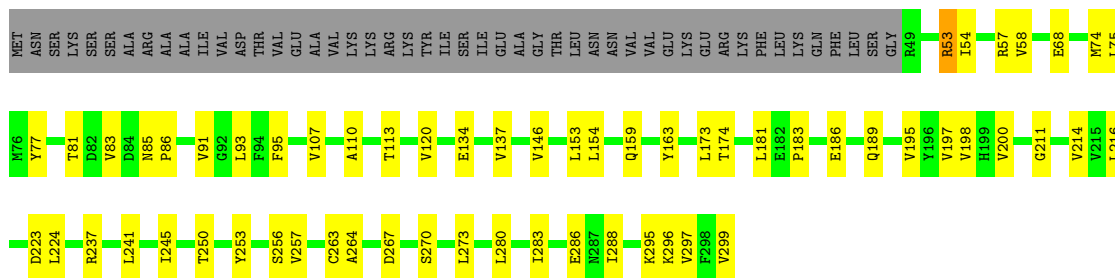
- Molecule 3: Small capsomere-interacting protein



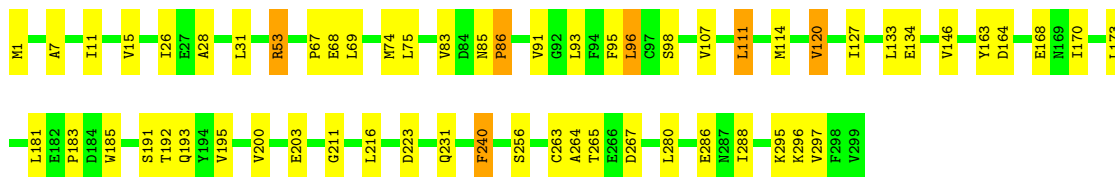
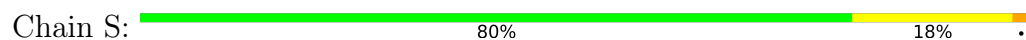
- Molecule 3: Small capsomere-interacting protein



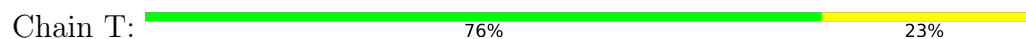
- Molecule 4: Triplex capsid protein 1

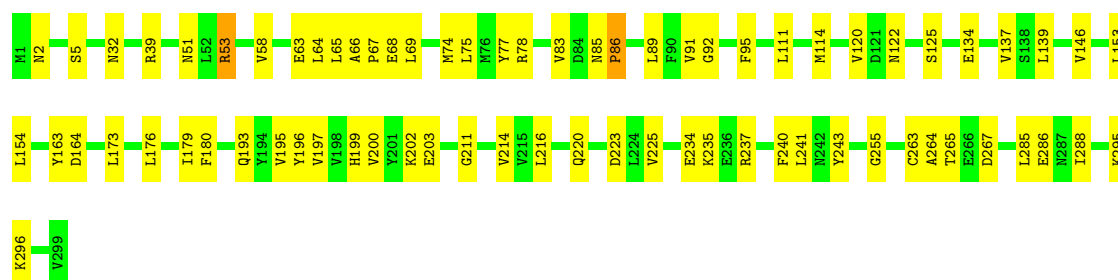


- Molecule 4: Triplex capsid protein 1



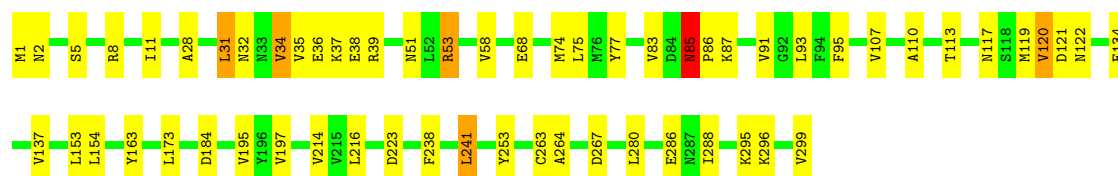
- Molecule 4: Triplex capsid protein 1





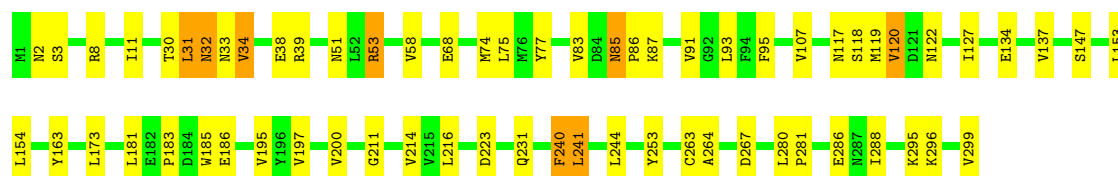
- Molecule 4: Triplex capsid protein 1

Chain U: 80% 18% .



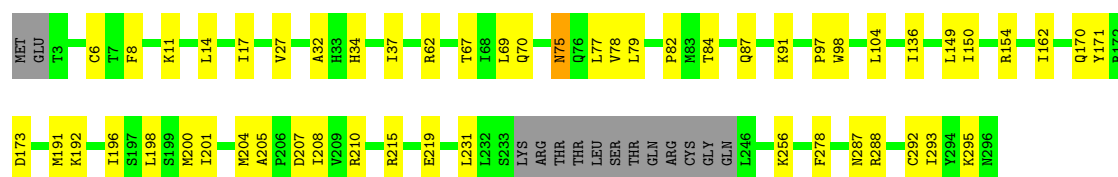
- Molecule 4: Triplex capsid protein 1

Chain V: 78% 19% .



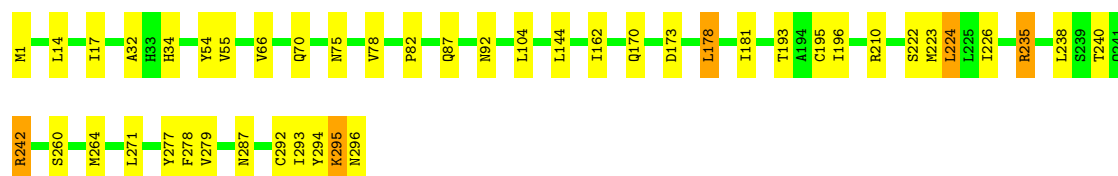
- Molecule 5: Triplex capsid protein 2

Chain 6: 77% 18% 5%




- Molecule 5: Triplex capsid protein 2

Chain W: 85% 14% .




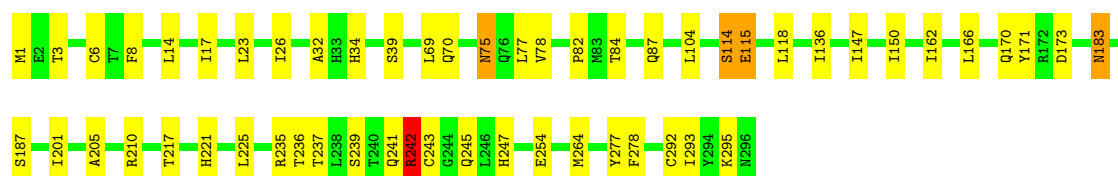
- Molecule 5: Triplex capsid protein 2

Chain X:  82% 17%




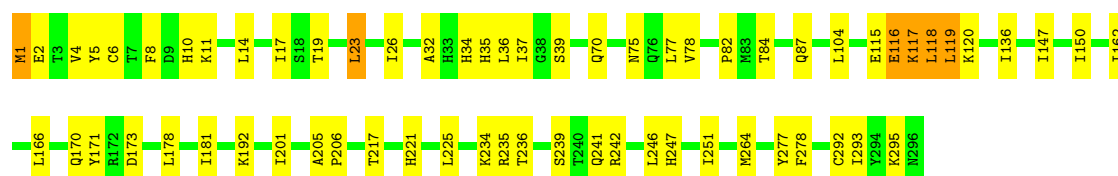
- Molecule 5: Triplex capsid protein 2

Chain Y:  81% 17%




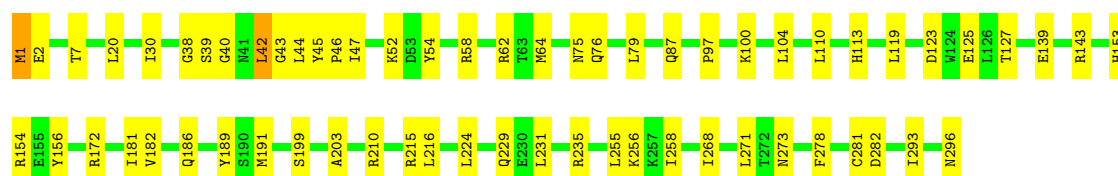
- Molecule 5: Triplex capsid protein 2

Chain Z:  78% 20%



- Molecule 5: Triplex capsid protein 2

Chain 7:  79% 21%



- Molecule 5: Triplex capsid protein 2

Chain a:  98%



- Molecule 5: Triplex capsid protein 2

Chain b:  97%



- Molecule 5: Triplex capsid protein 2

Chain c:  98% .



- Molecule 5: Triplex capsid protein 2

Chain d:  97% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	6443	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 ($e^-/\text{\AA}^2$)	23	Depositor
Minimum defocus (nm)	2200	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	64000	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	0.51	0/10927	0.68	0/14860
1	B	0.46	0/10927	0.66	0/14860
1	C	0.46	0/10793	0.63	0/14676
1	D	0.46	0/10927	0.64	1/14860 (0.0%)
1	E	0.50	0/10927	0.66	0/14860
1	F	0.42	0/10927	0.65	0/14860
1	G	0.42	1/10927 (0.0%)	0.66	0/14860
1	H	0.50	0/10927	0.66	0/14860
1	I	0.47	0/10927	0.64	0/14860
1	q	0.42	0/10550	0.64	0/14349
1	r	0.38	0/10927	0.62	0/14860
1	s	0.39	0/10927	0.64	0/14860
1	t	0.40	0/10927	0.63	0/14860
1	u	0.38	0/10935	0.62	0/14870
1	v	0.38	0/10566	0.62	0/14366
1	w	0.38	0/10161	0.66	1/13814 (0.0%)
2	e	0.32	0/2272	0.54	0/3084
2	f	0.34	0/2272	0.62	0/3084
2	g	0.35	0/2272	0.62	0/3084
2	h	0.31	0/2272	0.56	0/3084
2	i	0.32	0/2272	0.63	0/3084
2	j	0.32	0/2272	0.59	0/3084
2	k	0.33	0/2272	0.58	0/3084
2	l	0.32	0/2272	0.57	1/3084 (0.0%)
2	m	0.36	0/2272	0.60	1/3084 (0.0%)
2	n	0.34	0/2272	0.63	1/3084 (0.0%)
2	o	0.40	0/2272	0.66	0/3084
2	p	0.34	0/2272	0.60	0/3084
3	1	0.29	0/490	0.44	0/656
3	2	0.29	0/490	0.44	0/656
3	3	0.28	0/490	0.44	0/656
3	4	0.29	0/463	0.44	0/621
3	J	0.28	0/490	0.44	0/656
3	K	0.28	0/490	0.44	0/656

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
3	L	0.29	0/490	0.44	0/656
3	M	0.29	0/490	0.44	0/656
3	N	0.29	0/490	0.44	0/656
3	O	0.29	0/490	0.44	0/656
3	P	0.29	0/490	0.44	0/656
3	Q	0.28	0/490	0.44	0/656
3	R	0.29	0/490	0.44	0/656
3	x	0.29	0/490	0.44	0/656
3	y	0.29	0/490	0.44	0/656
3	z	0.29	0/490	0.44	0/656
4	5	0.39	0/2062	0.67	0/2793
4	S	0.49	0/2440	0.67	0/3297
4	T	0.48	0/2440	0.70	0/3297
4	U	0.41	0/2440	0.67	0/3297
4	V	0.41	0/2440	0.66	0/3297
5	6	0.39	0/2262	0.67	0/3069
5	7	0.33	0/2374	0.66	0/3219
5	W	0.42	0/2374	0.68	0/3219
5	X	0.38	0/2374	0.62	0/3219
5	Y	0.39	0/2374	0.68	0/3219
5	Z	0.41	0/2374	0.72	0/3219
5	a	0.44	0/2366	0.73	0/3209
5	b	0.44	0/2366	0.73	0/3209
5	c	0.52	0/2366	0.77	0/3209
5	d	0.41	0/2366	0.75	0/3209
All	All	0.42	1/243697 (0.0%)	0.64	5/330985 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1115	GLU	C-N	-5.30	1.21	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	563	LEU	C-N-CD	-8.35	102.23	120.60
2	l	181	ASP	N-CA-C	5.66	126.28	111.00
2	m	154	ALA	N-CA-C	5.37	125.51	111.00
2	n	179	ILE	N-CA-C	-5.11	97.21	111.00
1	D	255	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	o	7	SER	Mainchain

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	10682	0	10575	240	0
1	B	10682	0	10575	257	0
1	C	10552	0	10444	226	0
1	D	10682	0	10575	249	0
1	E	10682	0	10574	297	0
1	F	10682	0	10574	288	0
1	G	10682	0	10575	334	0
1	H	10682	0	10574	260	0
1	I	10682	0	10575	192	0
1	q	10313	0	10230	0	0
1	r	10682	0	10575	0	0
1	s	10682	0	10574	0	0
1	t	10682	0	10575	0	0
1	u	10690	0	10587	0	0
1	v	10331	0	10242	0	0
1	w	9933	0	9844	0	0
2	e	2224	0	2186	0	0
2	f	2224	0	2186	0	0
2	g	2224	0	2186	0	0
2	h	2224	0	2186	0	0
2	i	2224	0	2186	0	0
2	j	2224	0	2186	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	k	2224	0	2186	0	0
2	l	2224	0	2186	0	0
2	m	2224	0	2186	0	0
2	n	2224	0	2186	0	0
2	o	2224	0	2186	0	0
2	p	2224	0	2186	0	0
3	1	483	0	513	16	0
3	2	483	0	513	13	0
3	3	483	0	513	12	0
3	4	456	0	488	11	0
3	J	483	0	513	57	0
3	K	483	0	513	34	0
3	L	483	0	513	34	0
3	M	483	0	513	50	0
3	N	483	0	513	54	0
3	O	483	0	513	43	0
3	P	483	0	513	45	0
3	Q	483	0	513	64	0
3	R	483	0	513	52	0
3	x	483	0	513	0	0
3	y	483	0	513	0	0
3	z	483	0	513	0	0
4	5	2023	0	2034	39	0
4	S	2398	0	2438	82	0
4	T	2398	0	2438	63	0
4	U	2398	0	2438	59	0
4	V	2398	0	2438	91	0
5	6	2226	0	2318	39	0
5	7	2337	0	2437	61	0
5	W	2337	0	2436	84	0
5	X	2337	0	2437	82	0
5	Y	2337	0	2437	37	0
5	Z	2337	0	2437	46	0
5	a	2329	0	2425	0	0
5	b	2329	0	2419	0	0
5	c	2329	0	2425	0	0
5	d	2329	0	2425	0	0
All	All	238552	0	238065	2801	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 12.

The worst 5 of 2801 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:I:810:TYR:CE2	3:R:37:LEU:HD12	1.33	1.59
1:F:1109:ARG:NH1	5:X:223:MET:CE	1.70	1.51
1:H:810:TYR:CZ	3:Q:37:LEU:HD12	1.47	1.49
1:I:335:GLU:CD	4:V:31:LEU:HG	1.20	1.48
1:D:862:ILE:HD11	3:M:75:ARG:NH1	1.24	1.46

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	1341/1345 (100%)	1238 (92%)	102 (8%)	1 (0%)	53	88
1	B	1341/1345 (100%)	1251 (93%)	87 (6%)	3 (0%)	49	85
1	C	1321/1345 (98%)	1239 (94%)	80 (6%)	2 (0%)	49	85
1	D	1341/1345 (100%)	1248 (93%)	89 (7%)	4 (0%)	43	81
1	E	1341/1345 (100%)	1243 (93%)	94 (7%)	4 (0%)	43	81
1	F	1341/1345 (100%)	1243 (93%)	96 (7%)	2 (0%)	53	88
1	G	1341/1345 (100%)	1253 (93%)	83 (6%)	5 (0%)	36	77
1	H	1341/1345 (100%)	1253 (93%)	84 (6%)	4 (0%)	43	81
1	I	1341/1345 (100%)	1242 (93%)	98 (7%)	1 (0%)	53	88
1	q	1292/1345 (96%)	1190 (92%)	99 (8%)	3 (0%)	49	85
1	r	1341/1345 (100%)	1235 (92%)	103 (8%)	3 (0%)	49	85
1	s	1341/1345 (100%)	1246 (93%)	93 (7%)	2 (0%)	53	88
1	t	1341/1345 (100%)	1240 (92%)	98 (7%)	3 (0%)	49	85
1	u	1342/1345 (100%)	1234 (92%)	106 (8%)	2 (0%)	53	88
1	v	1299/1345 (97%)	1204 (93%)	89 (7%)	6 (0%)	31	74
1	w	1240/1345 (92%)	1141 (92%)	98 (8%)	1 (0%)	53	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	e	267/858 (31%)	254 (95%)	13 (5%)	0	100	100
2	f	267/858 (31%)	248 (93%)	16 (6%)	3 (1%)	16	58
2	g	267/858 (31%)	255 (96%)	9 (3%)	3 (1%)	16	58
2	h	267/858 (31%)	248 (93%)	19 (7%)	0	100	100
2	i	267/858 (31%)	245 (92%)	17 (6%)	5 (2%)	9	45
2	j	267/858 (31%)	249 (93%)	16 (6%)	2 (1%)	24	67
2	k	267/858 (31%)	249 (93%)	17 (6%)	1 (0%)	36	77
2	l	267/858 (31%)	247 (92%)	19 (7%)	1 (0%)	36	77
2	m	267/858 (31%)	248 (93%)	18 (7%)	1 (0%)	36	77
2	n	267/858 (31%)	244 (91%)	18 (7%)	5 (2%)	9	45
2	o	267/858 (31%)	247 (92%)	16 (6%)	4 (2%)	11	51
2	p	267/858 (31%)	249 (93%)	18 (7%)	0	100	100
3	1	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	2	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	3	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	4	56/89 (63%)	49 (88%)	7 (12%)	0	100	100
3	J	59/89 (66%)	51 (86%)	7 (12%)	1 (2%)	10	49
3	K	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	L	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	M	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	N	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	O	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	P	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	Q	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	R	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	x	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	y	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
3	z	59/89 (66%)	52 (88%)	7 (12%)	0	100	100
4	5	249/299 (83%)	226 (91%)	23 (9%)	0	100	100
4	S	297/299 (99%)	269 (91%)	27 (9%)	1 (0%)	43	81
4	T	297/299 (99%)	275 (93%)	21 (7%)	1 (0%)	43	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	U	297/299 (99%)	267 (90%)	29 (10%)	1 (0%)	43	81
4	V	297/299 (99%)	268 (90%)	27 (9%)	2 (1%)	24	67
5	6	278/296 (94%)	260 (94%)	18 (6%)	0	100	100
5	7	294/296 (99%)	259 (88%)	32 (11%)	3 (1%)	17	60
5	W	294/296 (99%)	277 (94%)	17 (6%)	0	100	100
5	X	294/296 (99%)	273 (93%)	20 (7%)	1 (0%)	43	81
5	Y	294/296 (99%)	269 (92%)	22 (8%)	3 (1%)	17	60
5	Z	294/296 (99%)	274 (93%)	19 (6%)	1 (0%)	43	81
5	a	293/296 (99%)	262 (89%)	28 (10%)	3 (1%)	17	60
5	b	293/296 (99%)	268 (92%)	24 (8%)	1 (0%)	43	81
5	c	293/296 (99%)	259 (88%)	33 (11%)	1 (0%)	43	81
5	d	293/296 (99%)	258 (88%)	30 (10%)	5 (2%)	10	49
All	All	29747/37695 (79%)	27475 (92%)	2177 (7%)	95 (0%)	47	81

5 of 95 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	GLY
1	F	19	ILE
1	G	810	TYR
1	H	21	ASN
1	H	818	ASP

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	1218/1220 (100%)	1202 (99%)	16 (1%)	71	86
1	B	1218/1220 (100%)	1201 (99%)	17 (1%)	69	85
1	C	1204/1220 (99%)	1191 (99%)	13 (1%)	76	88
1	D	1218/1220 (100%)	1197 (98%)	21 (2%)	63	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	1218/1220 (100%)	1200 (98%)	18 (2%)	67	85
1	F	1218/1220 (100%)	1198 (98%)	20 (2%)	65	84
1	G	1218/1220 (100%)	1199 (98%)	19 (2%)	65	84
1	H	1218/1220 (100%)	1197 (98%)	21 (2%)	63	83
1	I	1218/1220 (100%)	1204 (99%)	14 (1%)	76	88
1	q	1180/1220 (97%)	1168 (99%)	12 (1%)	78	89
1	r	1218/1220 (100%)	1204 (99%)	14 (1%)	76	88
1	s	1218/1220 (100%)	1202 (99%)	16 (1%)	71	86
1	t	1218/1220 (100%)	1207 (99%)	11 (1%)	81	90
1	u	1219/1220 (100%)	1205 (99%)	14 (1%)	76	88
1	v	1180/1220 (97%)	1170 (99%)	10 (1%)	83	92
1	w	1133/1220 (93%)	1123 (99%)	10 (1%)	81	90
2	e	253/761 (33%)	247 (98%)	6 (2%)	52	75
2	f	253/761 (33%)	253 (100%)	0	100	100
2	g	253/761 (33%)	246 (97%)	7 (3%)	47	71
2	h	253/761 (33%)	249 (98%)	4 (2%)	65	84
2	i	253/761 (33%)	245 (97%)	8 (3%)	42	68
2	j	253/761 (33%)	246 (97%)	7 (3%)	47	71
2	k	253/761 (33%)	246 (97%)	7 (3%)	47	71
2	l	253/761 (33%)	246 (97%)	7 (3%)	47	71
2	m	253/761 (33%)	249 (98%)	4 (2%)	65	84
2	n	253/761 (33%)	247 (98%)	6 (2%)	52	75
2	o	253/761 (33%)	247 (98%)	6 (2%)	52	75
2	p	253/761 (33%)	248 (98%)	5 (2%)	58	79
3	1	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	2	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	3	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	4	49/77 (64%)	48 (98%)	1 (2%)	58	79
3	J	52/77 (68%)	49 (94%)	3 (6%)	22	52
3	K	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	L	52/77 (68%)	50 (96%)	2 (4%)	36	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	N	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	O	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	P	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	Q	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	R	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	x	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	y	52/77 (68%)	51 (98%)	1 (2%)	60	80
3	z	52/77 (68%)	51 (98%)	1 (2%)	60	80
4	5	232/273 (85%)	230 (99%)	2 (1%)	81	90
4	S	273/273 (100%)	268 (98%)	5 (2%)	62	82
4	T	273/273 (100%)	271 (99%)	2 (1%)	85	93
4	U	273/273 (100%)	265 (97%)	8 (3%)	45	70
4	V	273/273 (100%)	266 (97%)	7 (3%)	49	73
5	6	261/274 (95%)	260 (100%)	1 (0%)	92	95
5	7	274/274 (100%)	270 (98%)	4 (2%)	67	85
5	W	274/274 (100%)	268 (98%)	6 (2%)	55	77
5	X	274/274 (100%)	272 (99%)	2 (1%)	85	93
5	Y	274/274 (100%)	269 (98%)	5 (2%)	62	82
5	Z	274/274 (100%)	264 (96%)	10 (4%)	38	65
5	a	273/274 (100%)	269 (98%)	4 (2%)	67	85
5	b	273/274 (100%)	266 (97%)	7 (3%)	49	73
5	c	273/274 (100%)	268 (98%)	5 (2%)	62	82
5	d	273/274 (100%)	269 (98%)	4 (2%)	67	85
All	All	27226/33989 (80%)	26822 (98%)	404 (2%)	70	85

5 of 404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	r	1029	ARG
1	v	244	ASN
5	Z	117	LYS
1	s	244	ASN
1	t	743	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 534 such sidechains are listed below:

Mol	Chain	Res	Type
1	s	435	GLN
1	v	211	GLN
5	Z	34	HIS
1	s	772	ASN
1	t	1000	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.