



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:45 AM UTC

PDB ID : 4V5V / pdb_00004v5v
Title : Structure of respiratory syncytial virus nucleocapsid protein, P1 crystal form
Authors : El Omari, K.; Dhaliwal, B.; Ren, J.; Abrescia, N.G.A.; Lockyer, M.; Powell, K.L.; Hawkins, A.R.; Stammers, D.K.
Deposited on : 2011-05-04
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

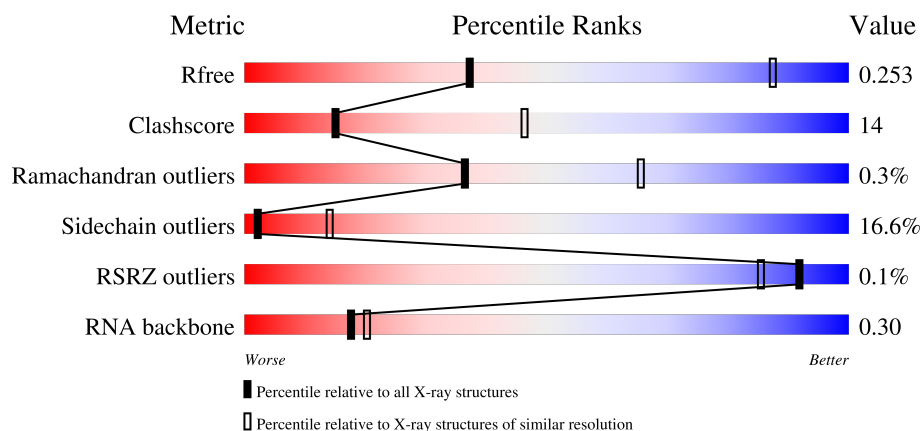
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	375	66% 27% 6%
1	AB	375	66% 27% 7%
1	AC	375	67% 26% 6%
1	AD	375	68% 25% 6%

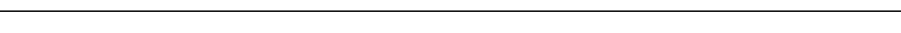
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AE	375	 67% 26% 6% .
1	AF	375	 68% 25% 6% .
1	AG	375	 67% 25% 7% .
1	AH	375	 67% 26% 6% .
1	AI	375	 65% 28% 6% .
1	AJ	375	 67% 26% 6% .
1	AL	375	 % 66% 27% 6% .
1	AN	375	 66% 27% 7% .
1	AO	375	 66% 27% 6% .
1	AP	375	 66% 27% 7% .
1	AQ	375	 66% 26% 7% .
1	AR	375	 67% 26% 6% .
1	AS	375	 67% 26% 6% .
1	AT	375	 67% 26% 6% .
1	AU	375	 67% 26% 6% .
1	AV	375	 68% 26% 6% .
1	BA	375	 65% 29% 6% .
1	BB	375	 66% 27% 6% .
1	BC	375	 66% 27% 6% .
1	BD	375	 67% 26% 6% .
1	BE	375	 68% 26% 6% .
1	BF	375	 66% 27% 6% .
1	BG	375	 67% 26% 6% .
1	BH	375	 67% 26% 7% .
1	BI	375	 66% 27% 6% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BJ	375	 68% 25% 7% .
1	BK	375	 67% 26% 6% .
1	BL	375	 68% 25% 6% .
1	BM	375	 66% 28% 6% .
1	BN	375	 66% 28% 5% .
1	BO	375	 66% 27% 6% .
1	BP	375	 66% 28% 6% .
1	BQ	375	 67% 26% 7% .
1	BW	375	 66% 28% 6% .
1	BY	375	 66% 27% 6% .
1	BZ	375	 66% 27% 6% .
2	AK	70	 19% 70% 11%
2	AM	70	 11% 70% 16% .
2	BR	70	 10% 66% 24%
2	BX	70	 9% 63% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 122400 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AB	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AC	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AD	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AE	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AF	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AG	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AH	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AI	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AJ	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AL	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AN	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AO	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AP	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AQ	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AR	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AS	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AT	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AU	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	AV	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BA	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BB	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BC	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BD	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BE	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BF	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BG	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BH	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BI	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BJ	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BK	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BL	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BM	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BN	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BO	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BP	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BQ	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BW	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BY	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			
1	BZ	375	Total	C	N	O	S	0	0	0
			2920	1848	506	549	17			

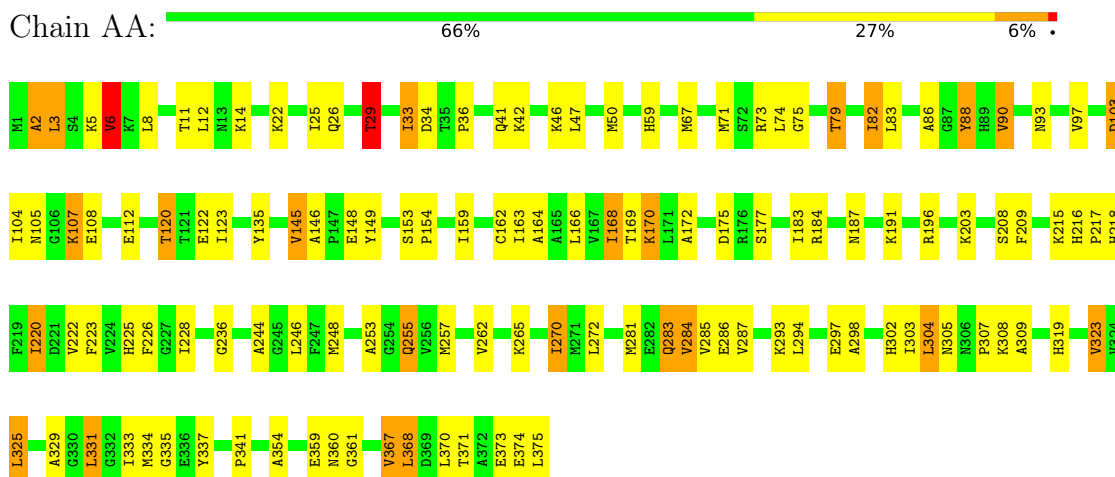
- Molecule 2 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AK	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	AM	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	BR	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	BX	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			

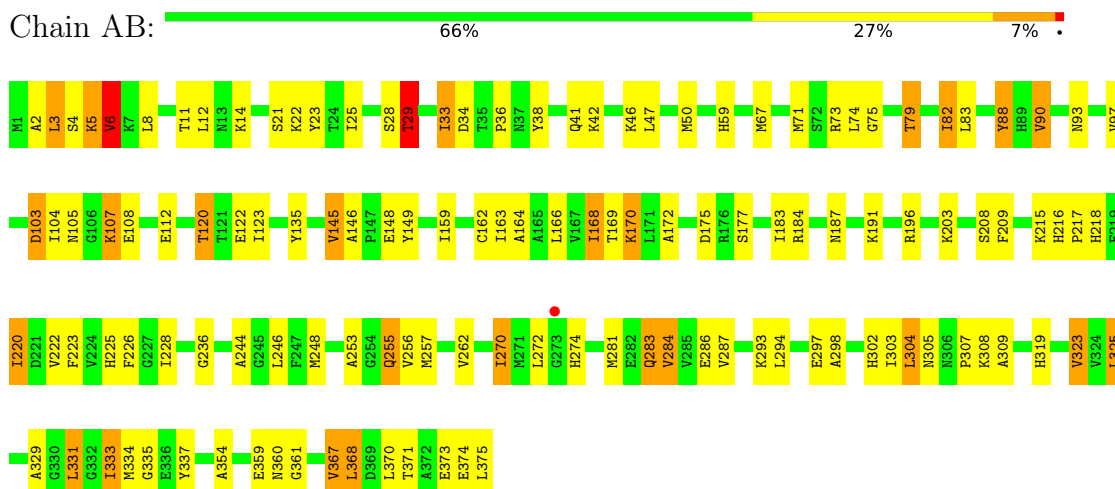
3 Residue-property plots

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

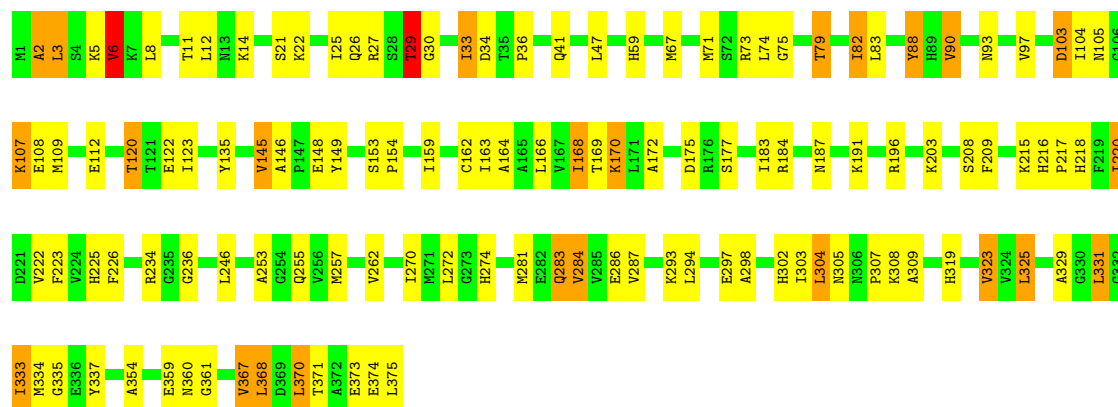


• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN



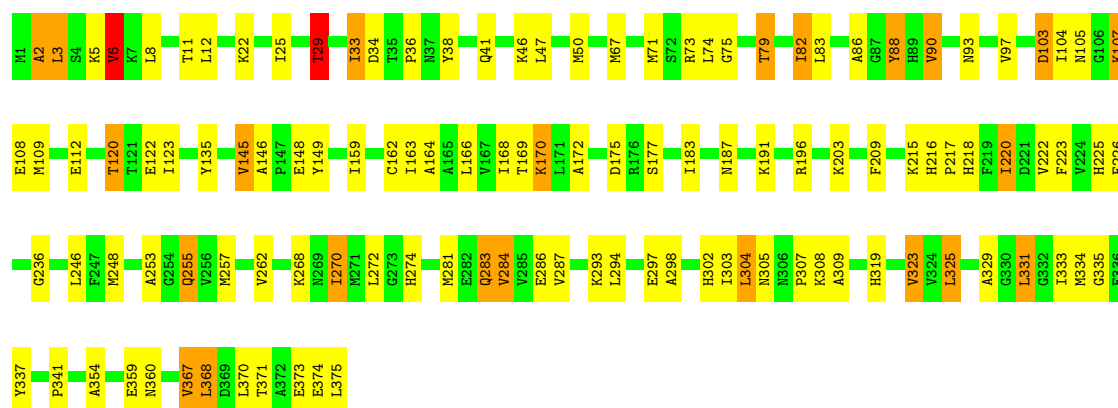
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN





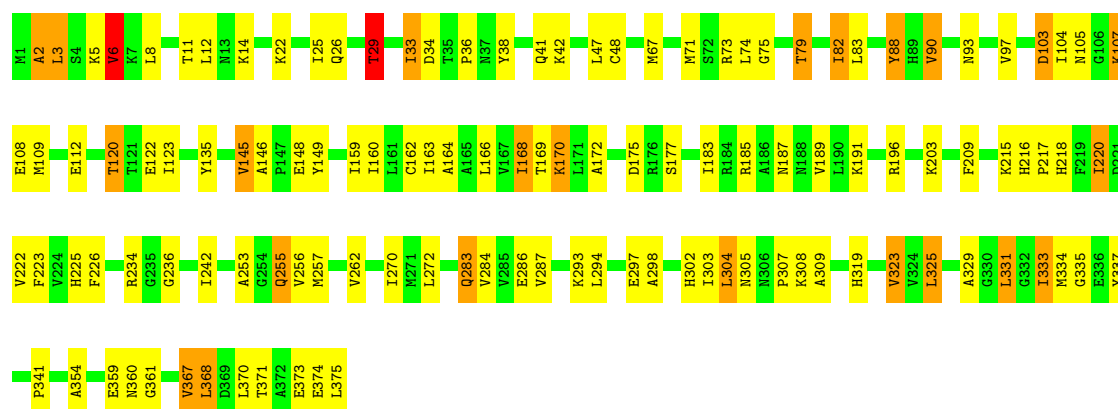
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AD: 68% 25% 6% .



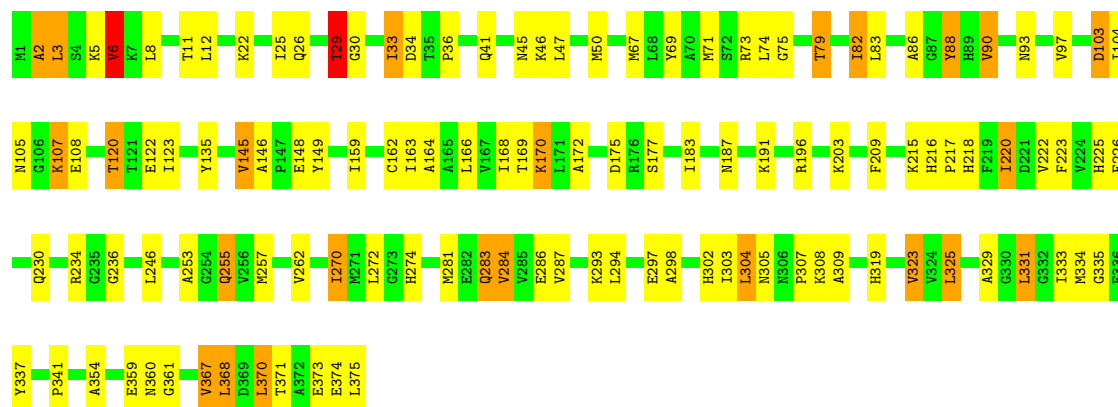
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AE: 67% 26% 6% .



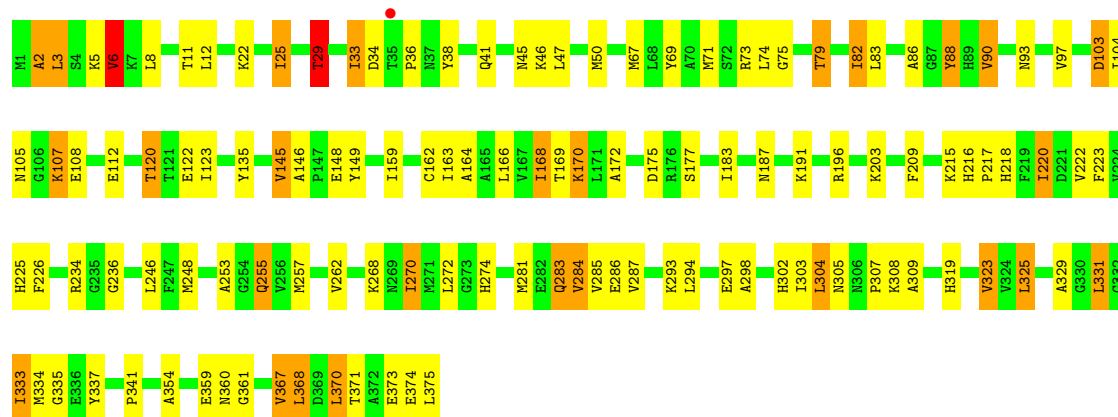
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AF: 68% 25% 6% .



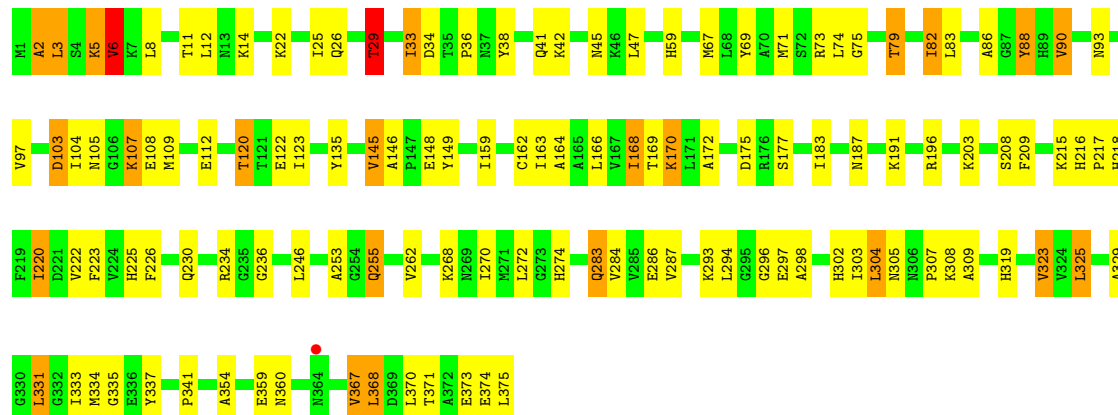
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AG: 67% 25% 7% .



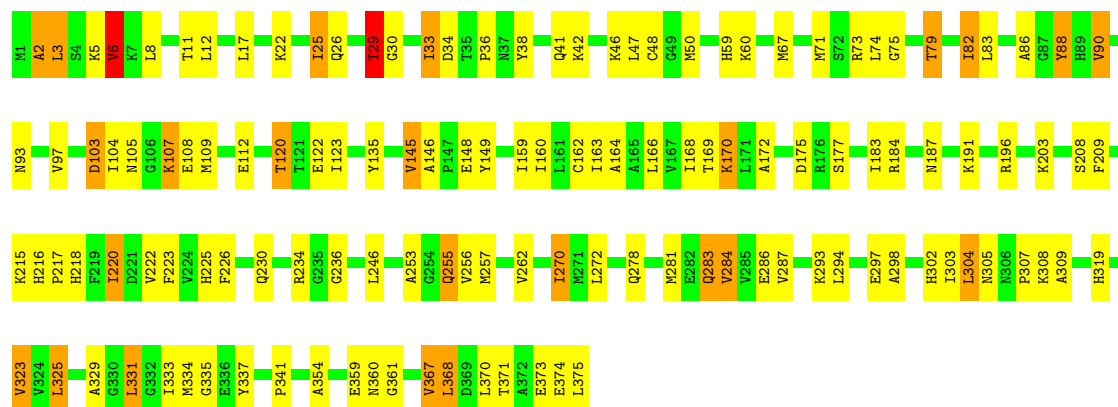
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AH: 67% 26% 6% .



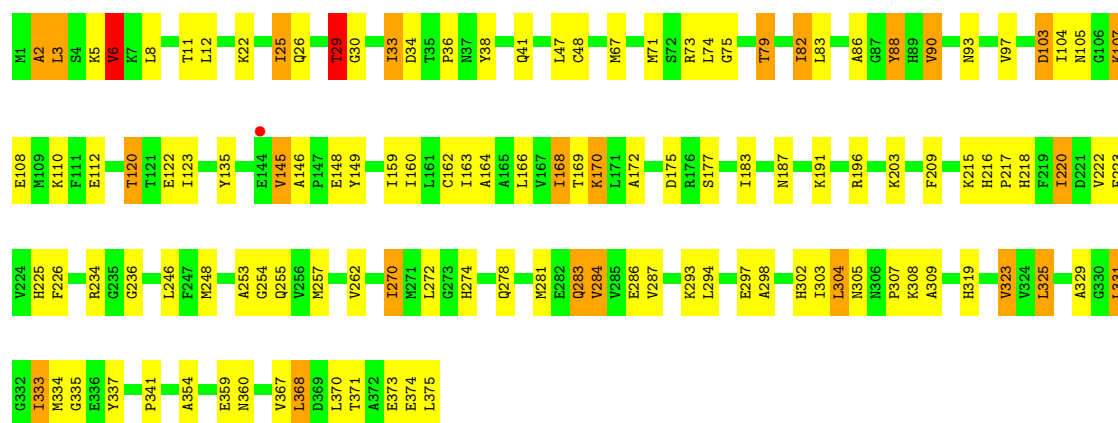
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AI: 65% 28% 6% .



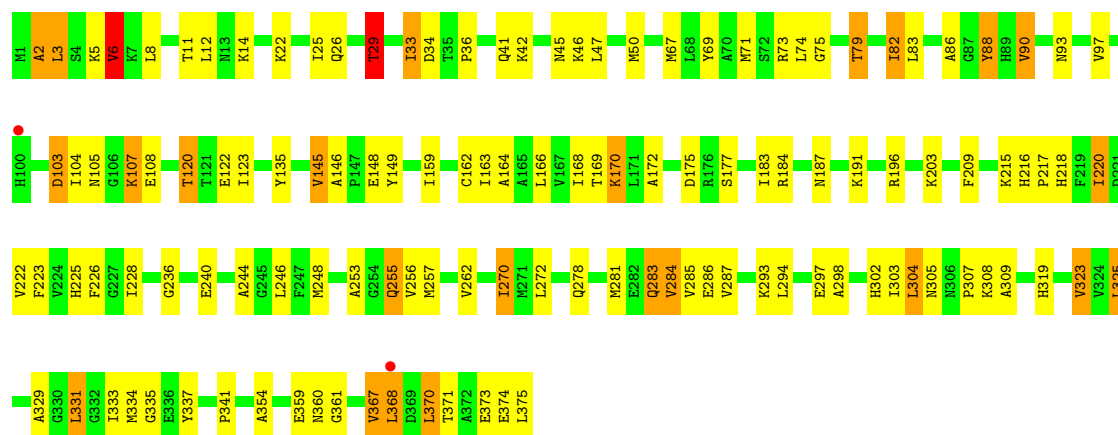
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AJ: 67% 26% 6%



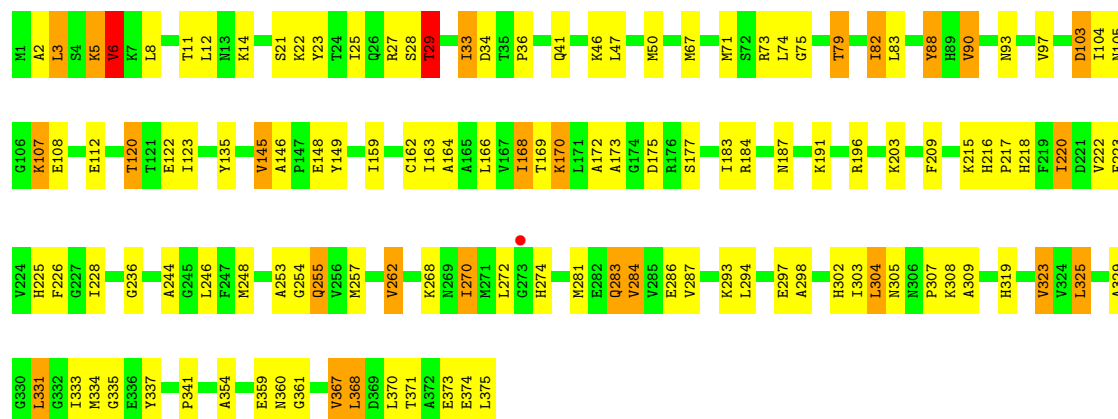
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AL: 66% 27% 6%



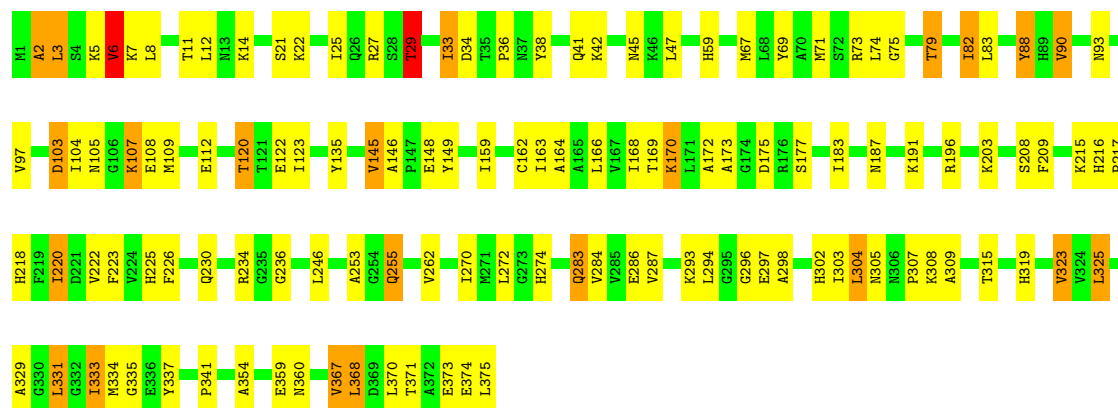
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AN: 66% 27% 7%



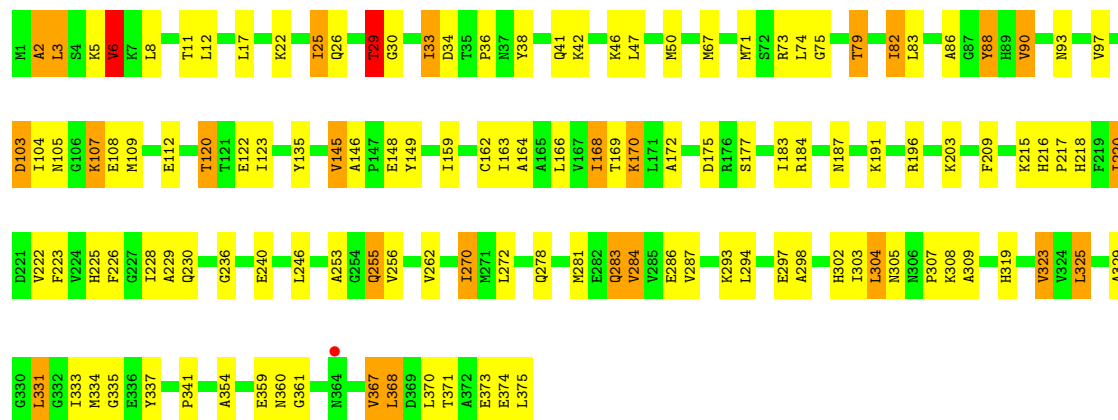
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AO: 66% 27% 6%



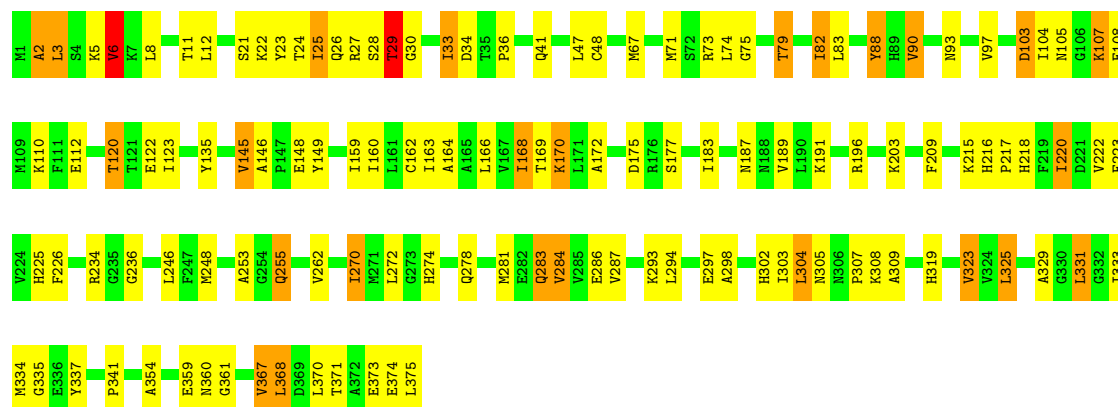
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AP: 66% 27% 7%



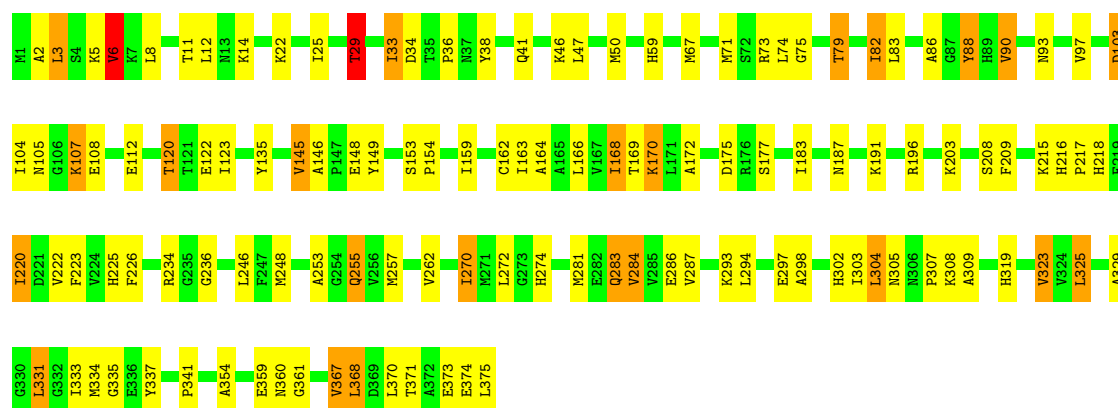
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AQ: 66% 26% 7%



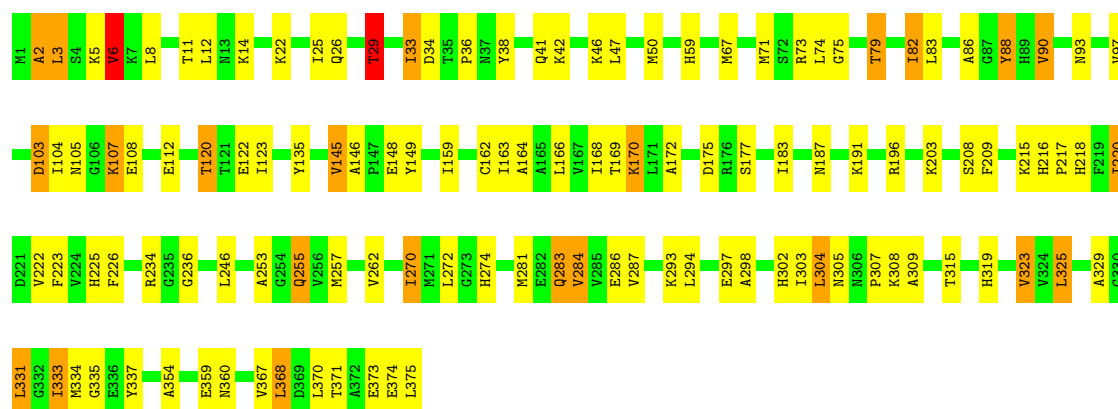
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AR: 67% 26% 6% .



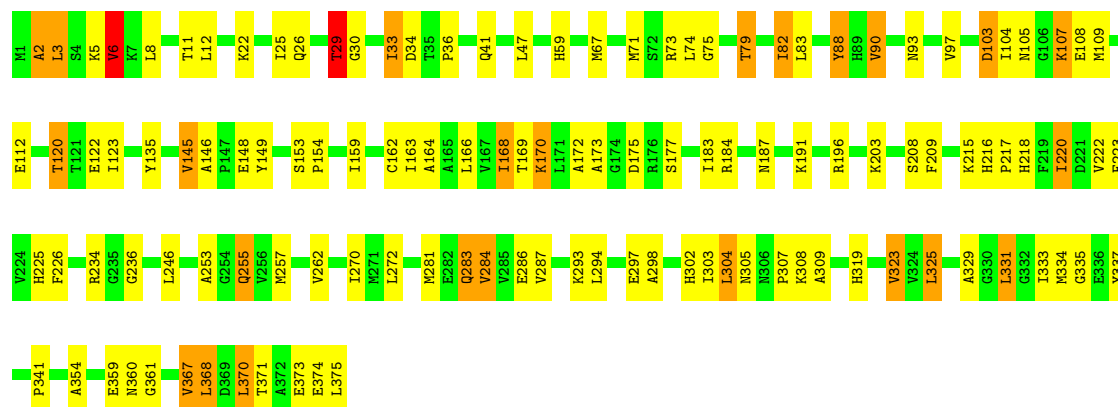
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AS: 67% 26% 6% .



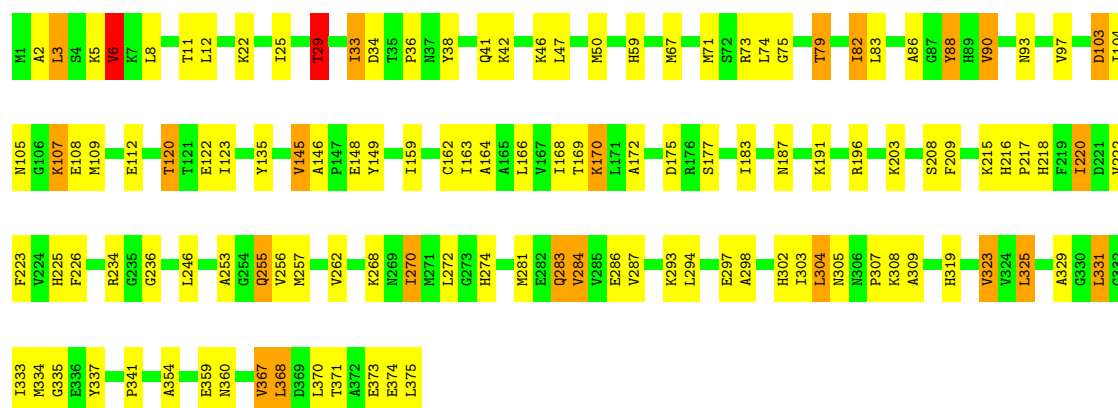
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AT: 67% 26% 6% .



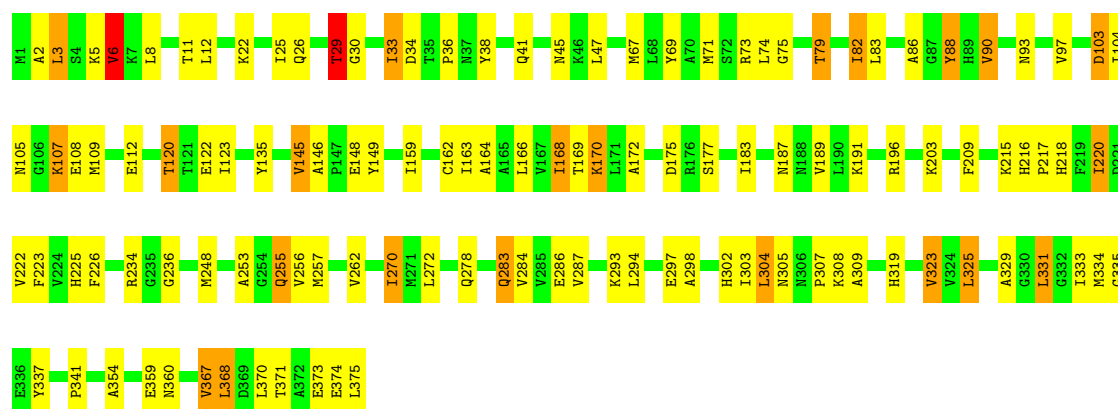
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AU: 67% 26% 6% •



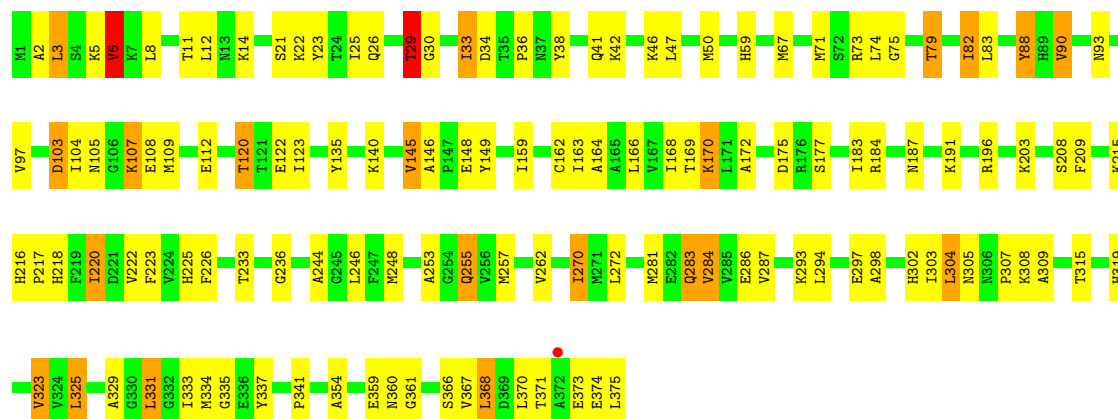
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AV: 68% 26% 6% •



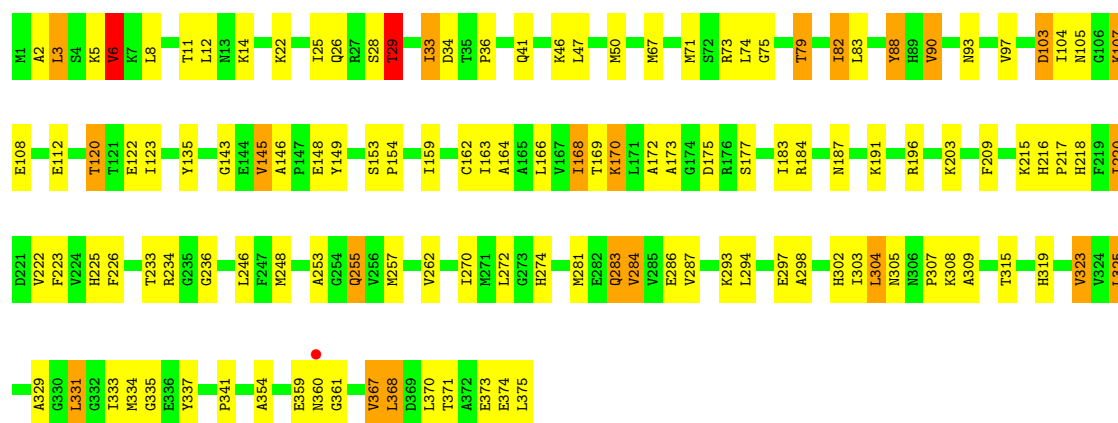
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BA: 65% 29% 6% •



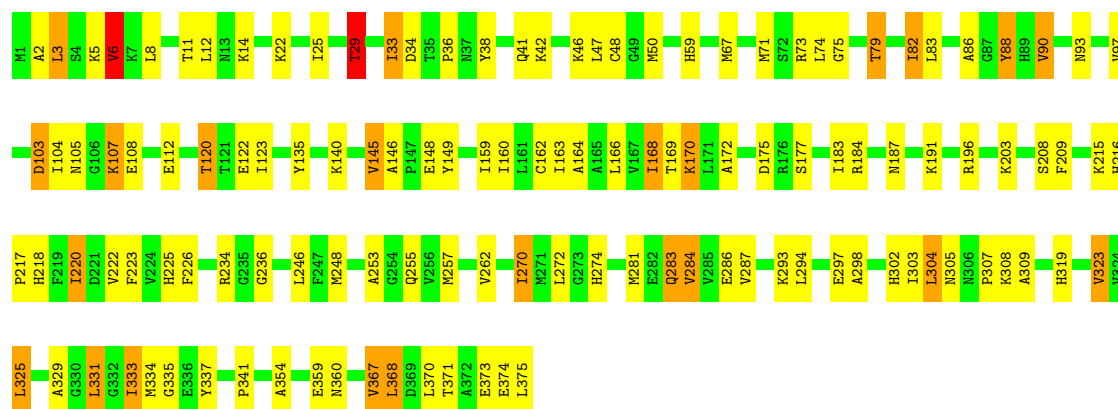
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BB: 66% 27% 6% •



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BC: 66% 27% 6% •



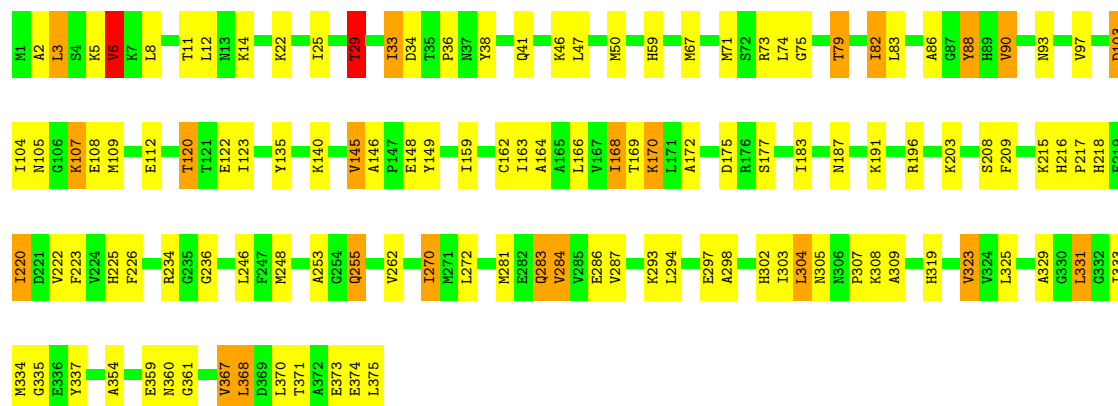
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BD: 67% 26% 6% •



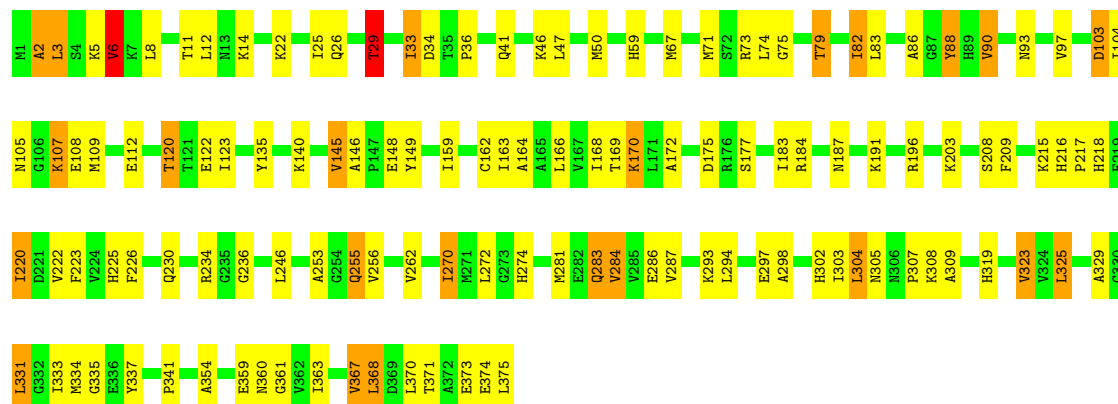
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BE: 68% 26% 6% •



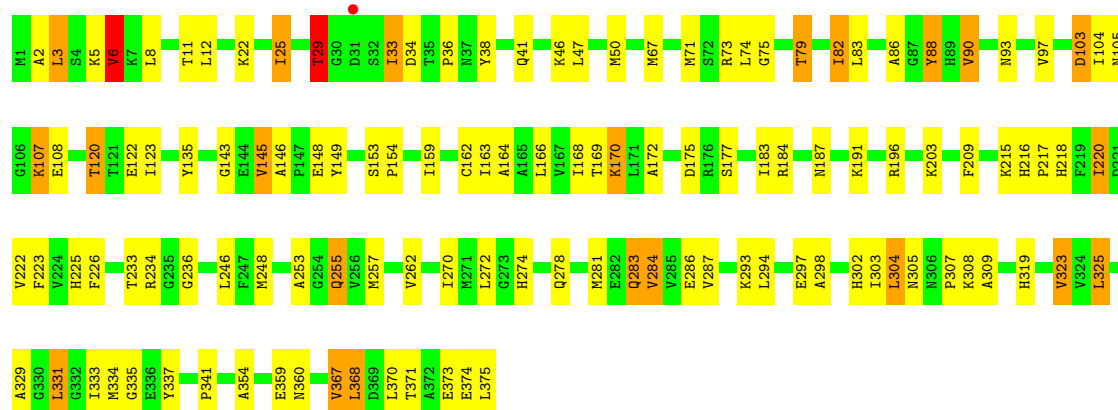
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BF: 66% 27% 6% •



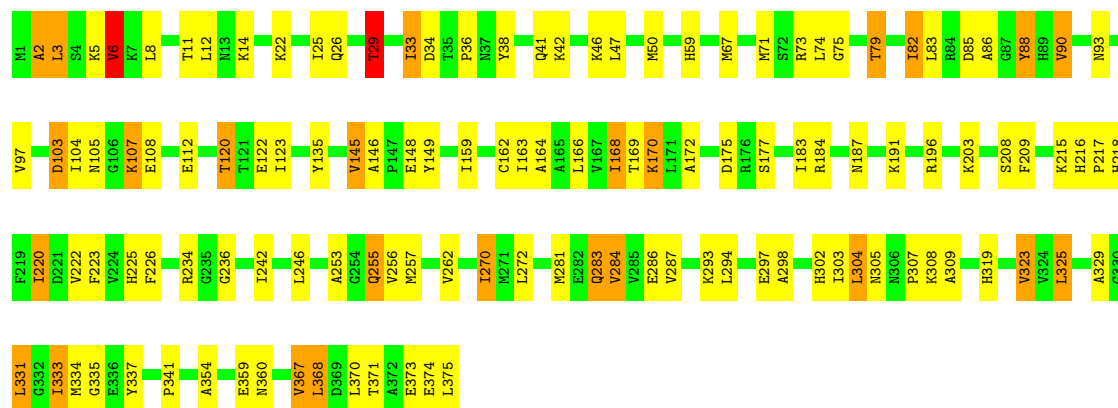
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BG: 67% 26% 6% •



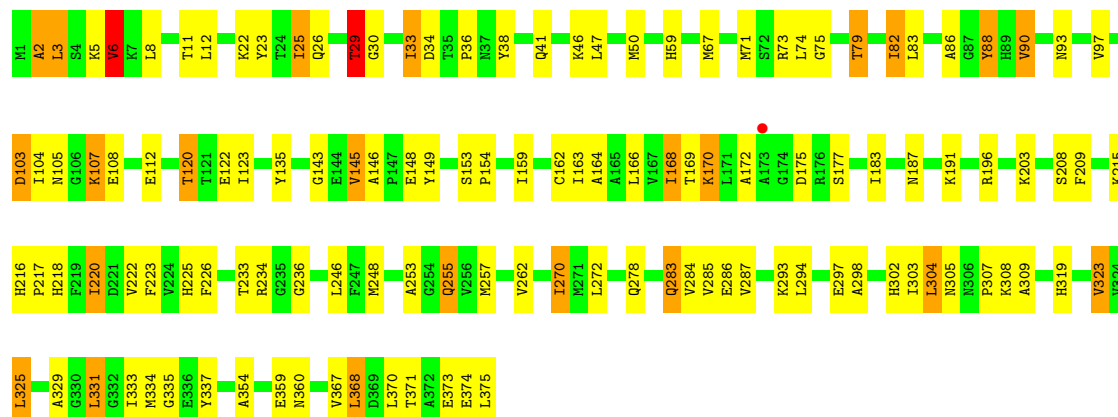
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BH: 67% 26% 7%



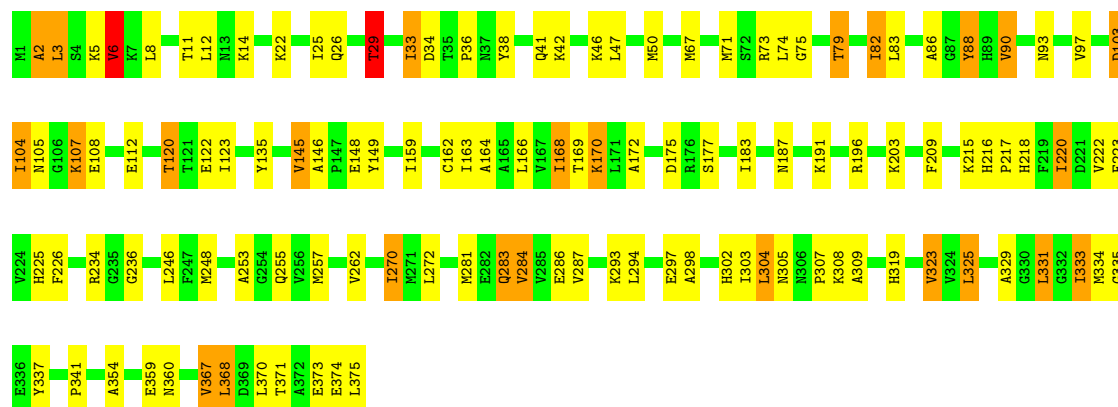
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BI: 66% 27% 6%



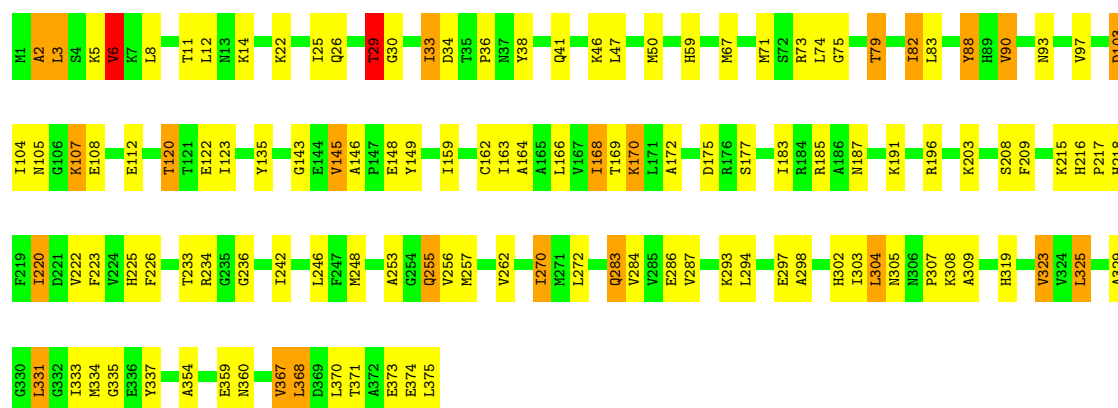
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BJ: 68% 25% 7%



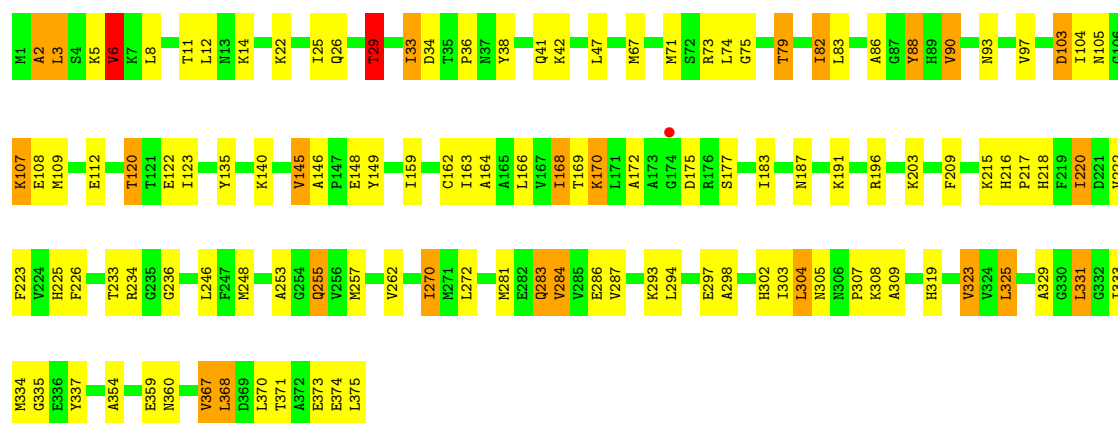
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BK: 67% 26% 6% .



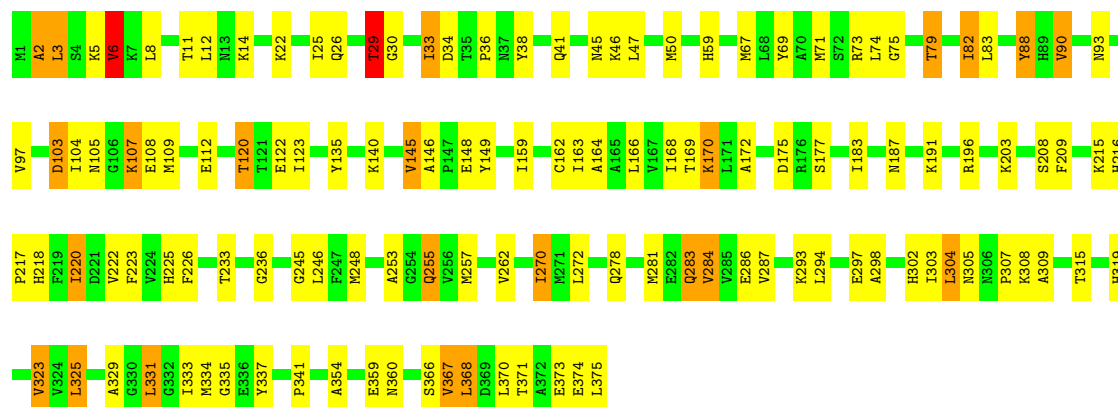
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BL: 68% 25% 6% .



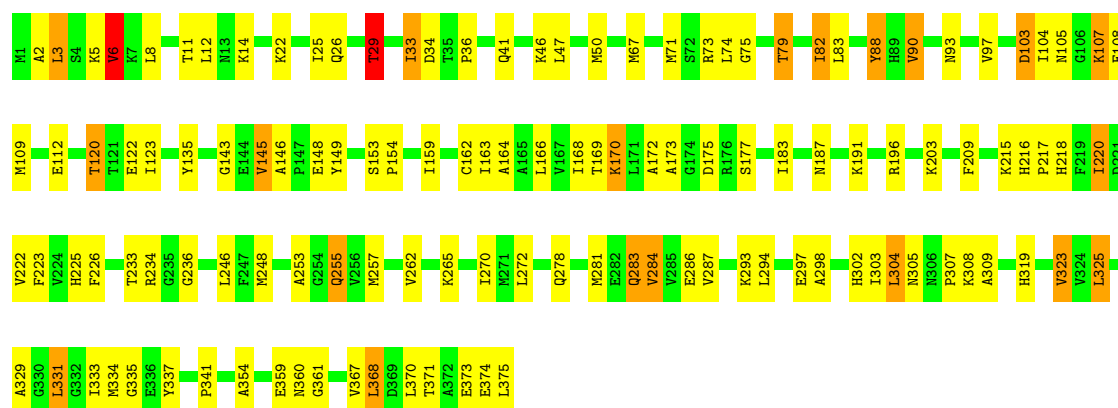
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BM: 66% 28% 6% .



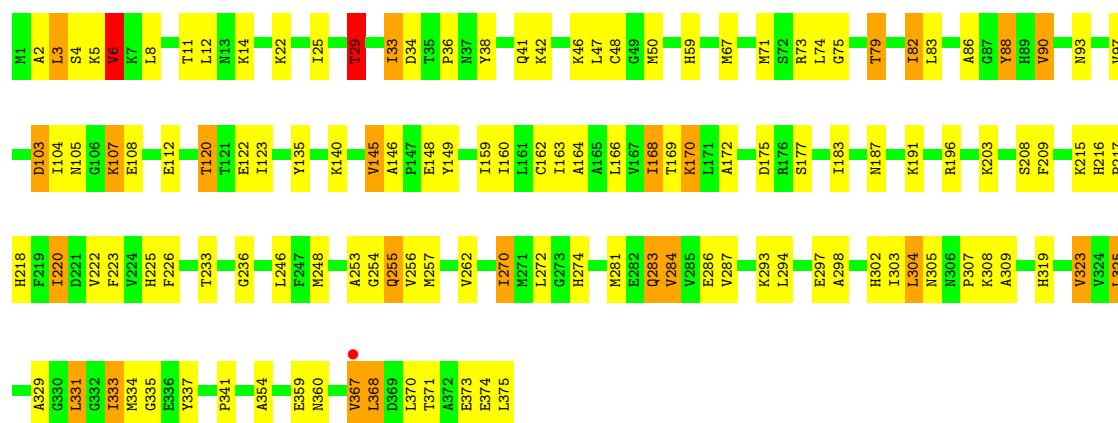
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BN: 66% 28% 5% .



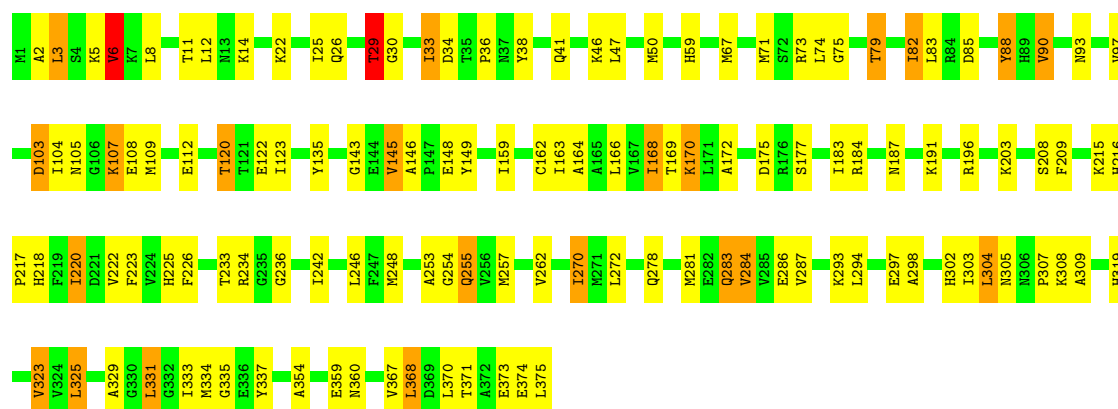
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BO: 66% 27% 6% .



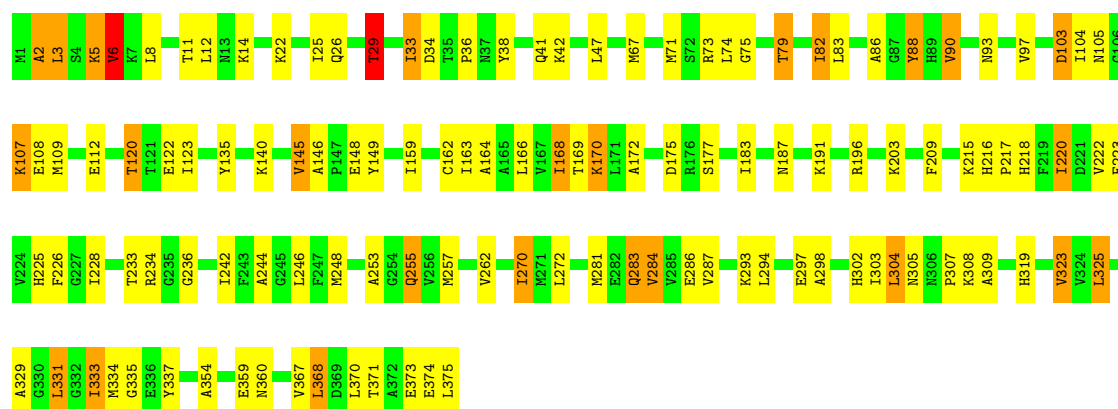
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BP: 66% 28% 6% .



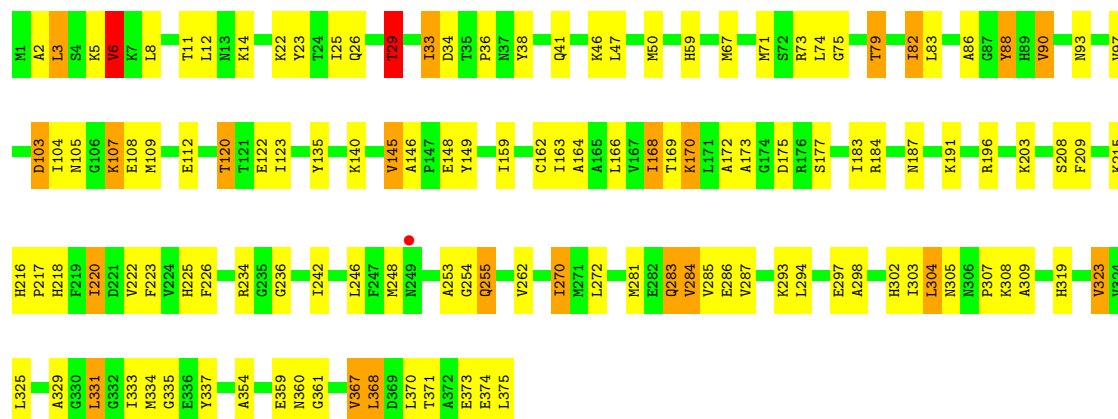
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BQ: 67% 26% 7% .



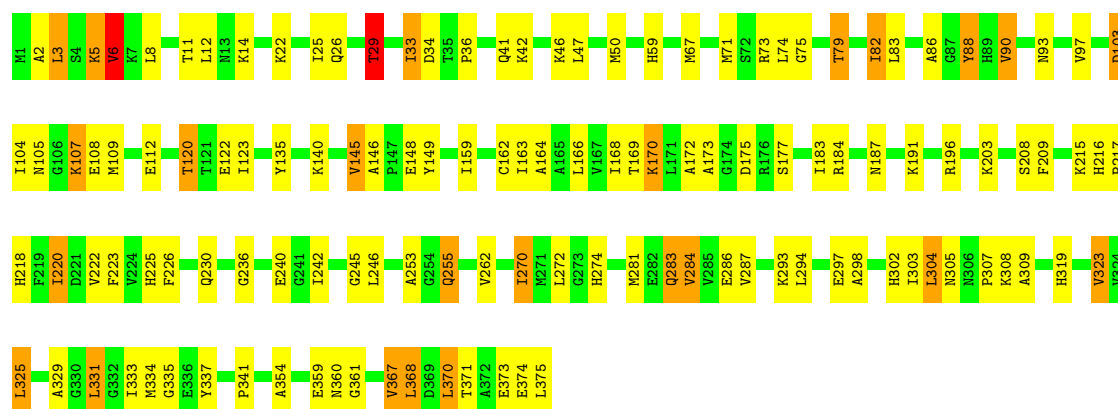
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BW: 66% 28% 6% .



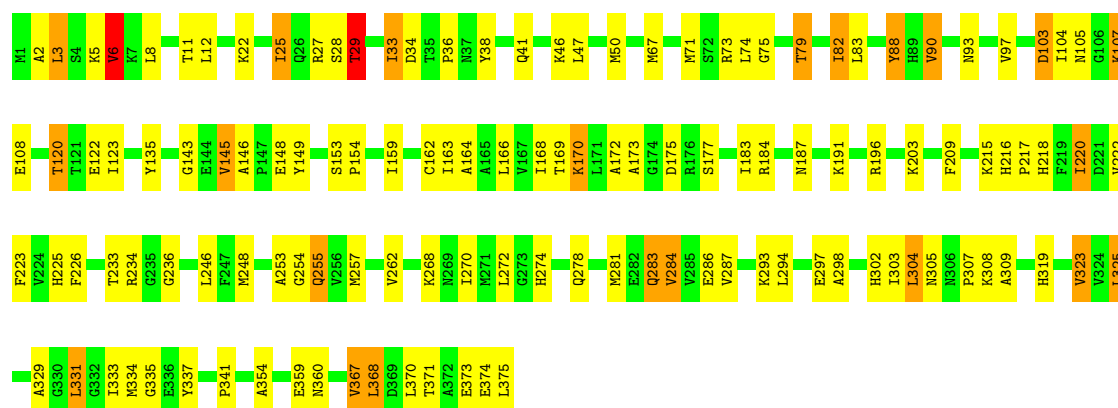
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BY: 66% 27% 6% .



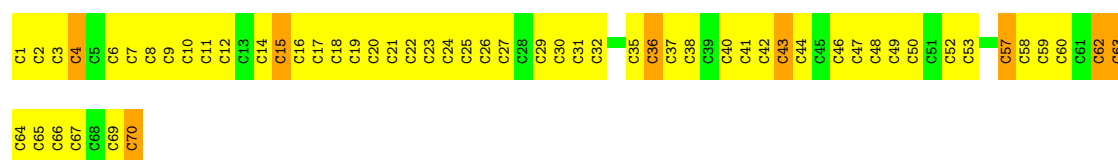
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BZ: 66% 27% 6% .



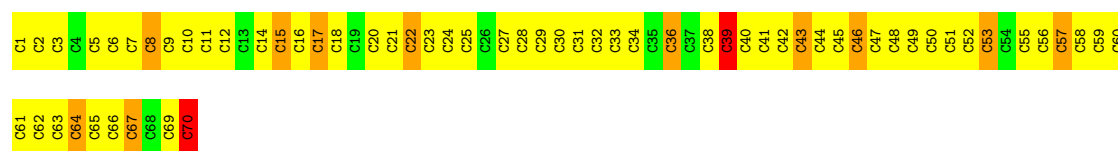
• Molecule 2: RNA

Chain AK: 19% 70% 11% .



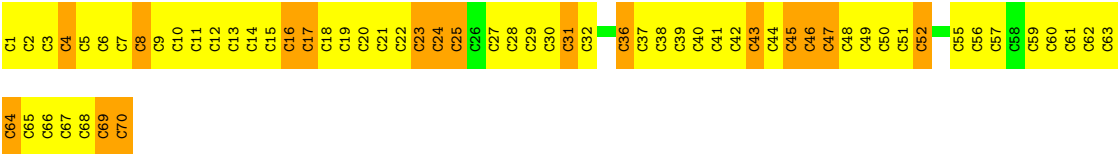
• Molecule 2: RNA

Chain AM: 11% 70% 16% .

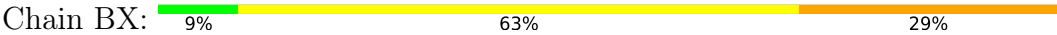


• Molecule 2: RNA

Chain BR: 10% 66% 24%



● Molecule 2: RNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	164.35Å 175.74Å 241.98Å 90.09° 89.96° 89.92°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-3.60) 75.1 (50.00-3.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0070	Depositor
R, R_{free}	0.234 , 0.269 0.252 , 0.253	Depositor DCC
R_{free} test set	12956 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 180.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.297 for h,-k,-l 0.058 for -h,k,-l 0.057 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	122400	wwPDB-VP
Average B, all atoms (Å ²)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7195e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	AA	0.60	0/2968	1.01	6/3998 (0.2%)
1	AB	0.60	0/2968	1.01	6/3998 (0.2%)
1	AC	0.60	0/2968	1.01	5/3998 (0.1%)
1	AD	0.60	0/2968	1.01	6/3998 (0.2%)
1	AE	0.60	0/2968	1.01	6/3998 (0.2%)
1	AF	0.60	0/2968	1.01	6/3998 (0.2%)
1	AG	0.60	0/2968	1.02	6/3998 (0.2%)
1	AH	0.60	0/2968	1.01	6/3998 (0.2%)
1	AI	0.60	0/2968	1.02	6/3998 (0.2%)
1	AJ	0.60	0/2968	1.01	5/3998 (0.1%)
1	AL	0.60	0/2968	1.02	6/3998 (0.2%)
1	AN	0.60	0/2968	1.01	6/3998 (0.2%)
1	AO	0.60	0/2968	1.01	6/3998 (0.2%)
1	AP	0.60	0/2968	1.01	6/3998 (0.2%)
1	AQ	0.60	0/2968	1.02	6/3998 (0.2%)
1	AR	0.60	0/2968	1.01	6/3998 (0.2%)
1	AS	0.60	0/2968	1.02	6/3998 (0.2%)
1	AT	0.60	0/2968	1.02	6/3998 (0.2%)
1	AU	0.60	0/2968	1.01	6/3998 (0.2%)
1	AV	0.60	0/2968	1.01	6/3998 (0.2%)
1	BA	0.60	0/2968	1.02	6/3998 (0.2%)
1	BB	0.60	0/2968	1.01	6/3998 (0.2%)
1	BC	0.60	0/2968	1.02	5/3998 (0.1%)
1	BD	0.60	0/2968	1.02	6/3998 (0.2%)
1	BE	0.60	0/2968	1.02	6/3998 (0.2%)
1	BF	0.60	0/2968	1.02	6/3998 (0.2%)
1	BG	0.60	0/2968	1.02	6/3998 (0.2%)
1	BH	0.60	0/2968	1.01	6/3998 (0.2%)
1	BI	0.60	0/2968	1.02	6/3998 (0.2%)
1	BJ	0.60	0/2968	1.01	5/3998 (0.1%)
1	BK	0.60	0/2968	1.02	6/3998 (0.2%)
1	BL	0.60	0/2968	1.01	6/3998 (0.2%)
1	BM	0.60	0/2968	1.02	6/3998 (0.2%)
1	BN	0.60	0/2968	1.01	6/3998 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	BO	0.60	0/2968	1.01	6/3998 (0.2%)
1	BP	0.60	0/2968	1.01	6/3998 (0.2%)
1	BQ	0.60	0/2968	1.02	6/3998 (0.2%)
1	BW	0.60	0/2968	1.01	6/3998 (0.2%)
1	BY	0.60	0/2968	1.01	6/3998 (0.2%)
1	BZ	0.60	0/2968	1.01	6/3998 (0.2%)
2	AK	0.48	0/1539	0.96	2/2376 (0.1%)
2	AM	0.47	0/1539	0.96	4/2376 (0.2%)
2	BR	0.45	0/1539	0.92	1/2376 (0.0%)
2	BX	0.45	0/1539	0.94	3/2376 (0.1%)
All	All	0.59	0/124876	1.01	246/169424 (0.1%)

There are no bond length outliers.

The worst 5 of 246 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	2	ALA	N-CA-C	14.44	126.73	111.14
1	BY	2	ALA	N-CA-C	14.43	126.73	111.14
1	AN	2	ALA	N-CA-C	14.43	126.72	111.14
1	AT	2	ALA	N-CA-C	14.43	126.72	111.14
1	BK	2	ALA	N-CA-C	14.42	126.72	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2920	0	2955	89	1
1	AB	2920	0	2955	94	0
1	AC	2920	0	2955	84	6
1	AD	2920	0	2955	75	1
1	AE	2920	0	2955	79	3
1	AF	2920	0	2955	78	2
1	AG	2920	0	2955	88	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AH	2920	0	2955	83	0
1	AI	2920	0	2955	95	2
1	AJ	2920	0	2955	82	5
1	AL	2920	0	2955	93	2
1	AN	2920	0	2955	101	0
1	AO	2920	0	2955	87	0
1	AP	2920	0	2955	98	1
1	AQ	2920	0	2955	86	5
1	AR	2920	0	2955	75	1
1	AS	2920	0	2955	78	0
1	AT	2920	0	2955	79	5
1	AU	2920	0	2955	81	1
1	AV	2920	0	2955	79	4
1	BA	2920	0	2955	89	3
1	BB	2920	0	2955	83	1
1	BC	2920	0	2955	87	5
1	BD	2920	0	2955	84	2
1	BE	2920	0	2955	82	4
1	BF	2920	0	2955	83	1
1	BG	2920	0	2955	81	1
1	BH	2920	0	2955	87	0
1	BI	2920	0	2955	84	1
1	BJ	2920	0	2955	82	1
1	BK	2920	0	2955	85	1
1	BL	2920	0	2955	83	3
1	BM	2920	0	2955	86	3
1	BN	2920	0	2955	78	1
1	BO	2920	0	2955	89	6
1	BP	2920	0	2955	94	2
1	BQ	2920	0	2955	94	3
1	BW	2920	0	2955	93	3
1	BY	2920	0	2955	86	1
1	BZ	2920	0	2955	84	1
2	AK	1400	0	771	81	0
2	AM	1400	0	771	112	0
2	BR	1400	0	771	88	0
2	BX	1400	0	771	121	0
All	All	122400	0	121284	3346	41

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 14.

The worst 5 of 3346 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:BK:253:ALA:HB3	1:BK:303:ILE:HD11	1.27	1.17
1:AQ:253:ALA:HB3	1:AQ:303:ILE:HD11	1.27	1.16
1:BI:253:ALA:HB3	1:BI:303:ILE:HD11	1.27	1.16
1:AJ:253:ALA:HB3	1:AJ:303:ILE:HD11	1.27	1.16
1:BF:253:ALA:HB3	1:BF:303:ILE:HD11	1.27	1.16

The worst 5 of 41 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AQ:149:TYR:OH	1:BQ:140:LYS:NZ[1_445]	0.38	1.82
1:AC:149:TYR:OH	1:BO:140:LYS:NZ[1_455]	0.56	1.64
1:AT:149:TYR:OH	1:BC:140:LYS:NZ[1_444]	0.68	1.52
1:AJ:149:TYR:OH	1:BL:140:LYS:NZ[1_454]	0.77	1.43
1:AE:149:TYR:OH	1:BW:140:LYS:NZ[1_445]	0.83	1.37

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AA	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AB	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AC	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AD	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AE	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AF	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AG	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AH	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AI	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AJ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AL	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AN	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AO	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AP	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AQ	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AR	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AS	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	AT	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AU	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	AV	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BA	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BB	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BC	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BD	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BE	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BF	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BG	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BH	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BI	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BJ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BK	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BL	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BM	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BN	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BO	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BP	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BQ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BW	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
1	BY	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	36	65
1	BZ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	36	65
All	All	14920/15000 (100%)	14421 (97%)	459 (3%)	40 (0%)	36	65

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	308	LYS
1	AB	308	LYS
1	AC	308	LYS
1	AD	308	LYS
1	AE	308	LYS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AA	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AB	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AC	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AD	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AE	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AF	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AG	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AH	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AI	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AJ	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AL	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AN	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AO	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AP	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AQ	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AR	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AS	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AT	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	AU	313/313 (100%)	261 (83%)	52 (17%)	2	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AV	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BA	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BB	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BC	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BD	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BE	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BF	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BG	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BH	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BI	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BJ	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BK	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BL	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BM	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BN	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BO	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BP	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BQ	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BW	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BY	313/313 (100%)	261 (83%)	52 (17%)	2	14
1	BZ	313/313 (100%)	261 (83%)	52 (17%)	2	14
All	All	12520/12520 (100%)	10440 (83%)	2080 (17%)	2	14

5 of 2080 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BP	272	LEU
1	BQ	287	VAL
1	BP	262	VAL
1	AQ	373	GLU
1	AQ	220	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 310 such sidechains are listed below:

Mol	Chain	Res	Type
1	BK	43	HIS
1	BW	26	GLN
1	BL	26	GLN
1	BN	305	ASN
1	BY	305	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	AK	69/70 (98%)	18 (26%)	2 (2%)
2	AM	69/70 (98%)	15 (21%)	2 (2%)
2	BR	69/70 (98%)	20 (28%)	7 (10%)
2	BX	69/70 (98%)	24 (34%)	4 (5%)
All	All	276/280 (98%)	77 (27%)	15 (5%)

5 of 77 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	AK	8	C
2	AK	15	C
2	AK	17	C
2	AK	18	C
2	AK	19	C

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	BR	25	C
2	BX	32	C
2	BR	32	C
2	BX	39	C
2	BX	18	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	375/375 (100%)	-0.44	0 100 100	77, 135, 189, 218	0
1	AB	375/375 (100%)	-0.51	1 (0%) 90 75	77, 135, 189, 218	0
1	AC	375/375 (100%)	-0.47	0 100 100	77, 135, 189, 218	0
1	AD	375/375 (100%)	-0.51	0 100 100	77, 135, 189, 218	0
1	AE	375/375 (100%)	-0.50	0 100 100	77, 135, 189, 218	0
1	AF	375/375 (100%)	-0.43	0 100 100	77, 135, 189, 218	0
1	AG	375/375 (100%)	-0.42	1 (0%) 90 75	77, 135, 189, 218	0
1	AH	375/375 (100%)	-0.46	1 (0%) 90 75	77, 135, 189, 218	0
1	AI	375/375 (100%)	-0.44	0 100 100	77, 135, 189, 218	0
1	AJ	375/375 (100%)	-0.49	1 (0%) 90 75	77, 135, 189, 218	0
1	AL	375/375 (100%)	-0.44	2 (0%) 87 66	77, 135, 189, 218	0
1	AN	375/375 (100%)	-0.47	1 (0%) 90 75	77, 135, 189, 218	0
1	AO	375/375 (100%)	-0.47	0 100 100	77, 135, 189, 218	0
1	AP	375/375 (100%)	-0.41	1 (0%) 90 75	77, 135, 189, 218	0
1	AQ	375/375 (100%)	-0.48	0 100 100	77, 135, 189, 218	0
1	AR	375/375 (100%)	-0.49	0 100 100	77, 135, 189, 218	0
1	AS	375/375 (100%)	-0.51	0 100 100	77, 135, 189, 218	0
1	AT	375/375 (100%)	-0.52	0 100 100	77, 135, 189, 218	0
1	AU	375/375 (100%)	-0.50	0 100 100	77, 135, 189, 218	0
1	AV	375/375 (100%)	-0.53	0 100 100	77, 135, 189, 218	0
1	BA	375/375 (100%)	-0.51	1 (0%) 90 75	77, 135, 189, 218	0
1	BB	375/375 (100%)	-0.51	1 (0%) 90 75	77, 135, 189, 218	0
1	BC	375/375 (100%)	-0.49	0 100 100	77, 135, 189, 218	0
1	BD	375/375 (100%)	-0.46	1 (0%) 90 75	77, 135, 189, 218	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	BE	375/375 (100%)	-0.41	0 100 100	77, 135, 189, 218	0
1	BF	375/375 (100%)	-0.50	0 100 100	77, 135, 189, 218	0
1	BG	375/375 (100%)	-0.44	1 (0%) 90 75	77, 135, 189, 218	0
1	BH	375/375 (100%)	-0.47	0 100 100	77, 135, 189, 218	0
1	BI	375/375 (100%)	-0.54	1 (0%) 90 75	77, 135, 189, 218	0
1	BJ	375/375 (100%)	-0.50	0 100 100	77, 135, 189, 218	0
1	BK	375/375 (100%)	-0.48	0 100 100	77, 135, 189, 218	0
1	BL	375/375 (100%)	-0.42	1 (0%) 90 75	77, 135, 189, 218	0
1	BM	375/375 (100%)	-0.50	0 100 100	77, 135, 189, 218	0
1	BN	375/375 (100%)	-0.49	0 100 100	77, 135, 189, 218	0
1	BO	375/375 (100%)	-0.48	1 (0%) 90 75	77, 135, 189, 218	0
1	BP	375/375 (100%)	-0.50	0 100 100	77, 135, 189, 218	0
1	BQ	375/375 (100%)	-0.44	0 100 100	77, 135, 189, 218	0
1	BW	375/375 (100%)	-0.42	1 (0%) 90 75	77, 135, 189, 218	0
1	BY	375/375 (100%)	-0.52	0 100 100	77, 135, 189, 218	0
1	BZ	375/375 (100%)	-0.47	0 100 100	77, 135, 189, 218	0
2	AK	70/70 (100%)	-0.33	0 100 100	120, 142, 159, 162	0
2	AM	70/70 (100%)	-0.24	0 100 100	112, 143, 161, 165	0
2	BR	70/70 (100%)	-0.34	0 100 100	129, 145, 158, 162	0
2	BX	70/70 (100%)	-0.37	0 100 100	119, 145, 156, 159	0
All	All	15280/15280 (100%)	-0.47	16 (0%) 92 85	77, 136, 189, 218	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AN	273	GLY	4.2
1	BB	360	ASN	2.8
1	BI	173	ALA	2.7
1	BG	31	ASP	2.7
1	AL	368	LEU	2.6

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.