wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 09:28 AM EDT

PDB ID	:	4V5V
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 (i) 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 (1)) were used in the production of this report:

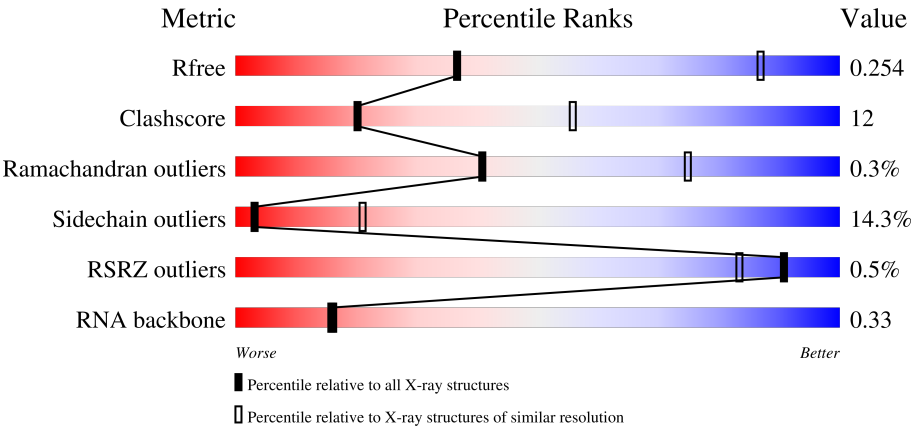
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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 <=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	68% 27% 5%
1	AB	375	68% 27% 5%
1	AC	375	% 69% 26% 5%
1	AD	375	71% 24% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AE	375	70% 25% 5%
1	AF	375	2% 70% 25% 5%
1	AG	375	69% 25% 6%
1	AH	375	69% 26% 5%
1	AI	375	67% 28% 5%
1	AJ	375	69% 25% 5%
1	AL	375	% 69% 26% 5%
1	AN	375	68% 27% 5%
1	AO	375	69% 26% 5%
1	AP	375	68% 27% 5%
1	AQ	375	68% 27% 5%
1	AR	375	69% 26% 5%
1	AS	375	70% 25% 5%
1	AT	375	% 70% 25% 5%
1	AU	375	70% 26% 5%
1	AV	375	% 70% 25% 5%
1	BA	375	2% 68% 28%
1	BB	375	68% 27% 5%
1	BC	375	% 68% 27% 5%
1	BD	375	% 69% 26% 5%
1	BE	375	70% 26% 5%
1	BF	375	% 69% 26% 5%
1	BG	375	% 69% 27%
1	BH	375	69% 26% 5%
1	BI	375	% 69% 26% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	BJ	375	70% 25% 5%
1	BK	375	69% 26% 5%
1	BL	375	70% 25% 5%
1	BM	375	68% 27% 5%
1	BN	375	69% 26%
1	BO	375	68% 27% 5%
1	BP	375	69% 27% 5%
1	BQ	375	70% 25% 5%
1	BW	375	68% 27% 5%
1	BY	375	68% 27% 5%
1	BZ	375	68% 27%
2	AK	70	19% 63% 19%
2	AM	70	11% 63% 24%
2	BR	70	10% 66% 23%
2	BX	70	11% 56% 33%

2 Entry composition (i)

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.

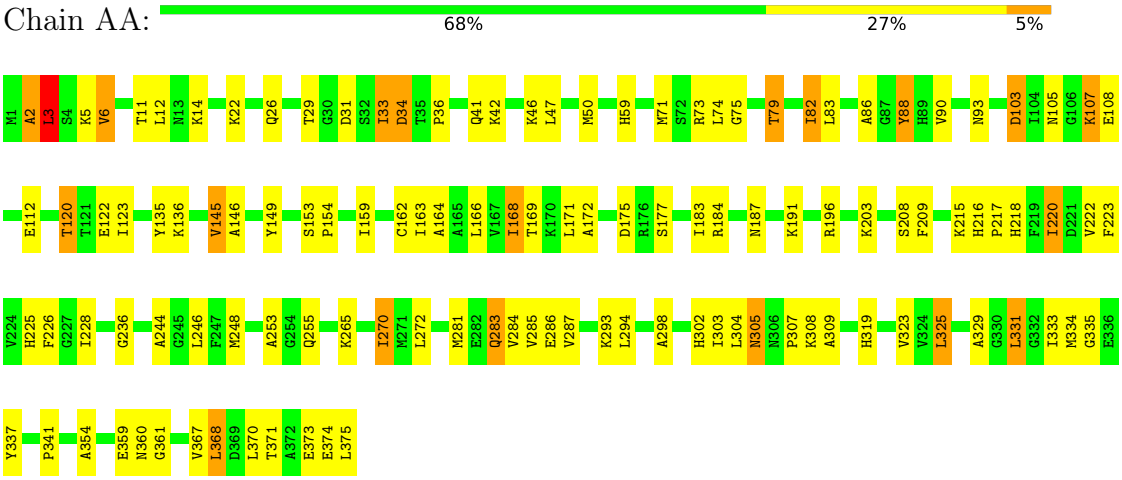
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AK	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	AM	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	BR	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	BX	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			

3 Residue-property plots (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 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.

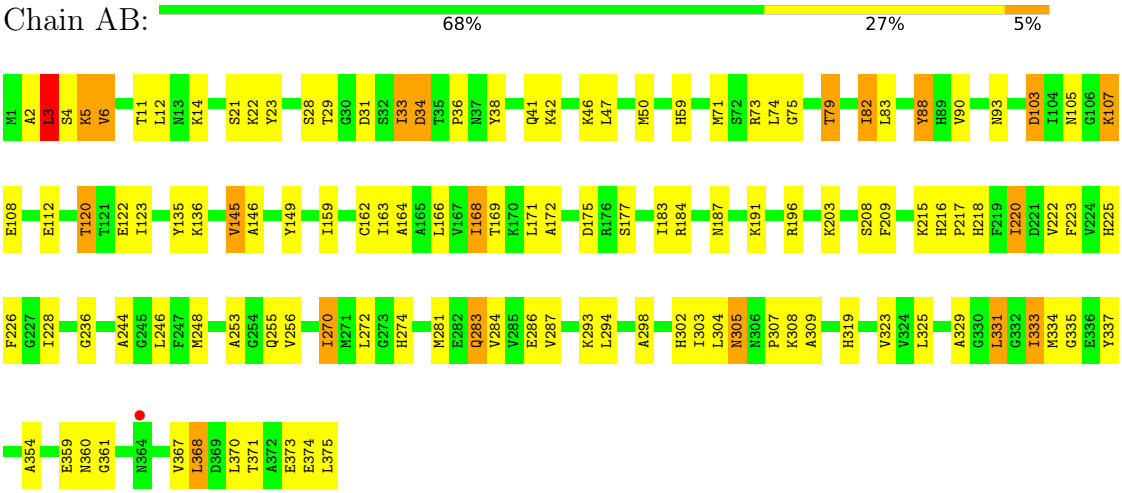
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AA:



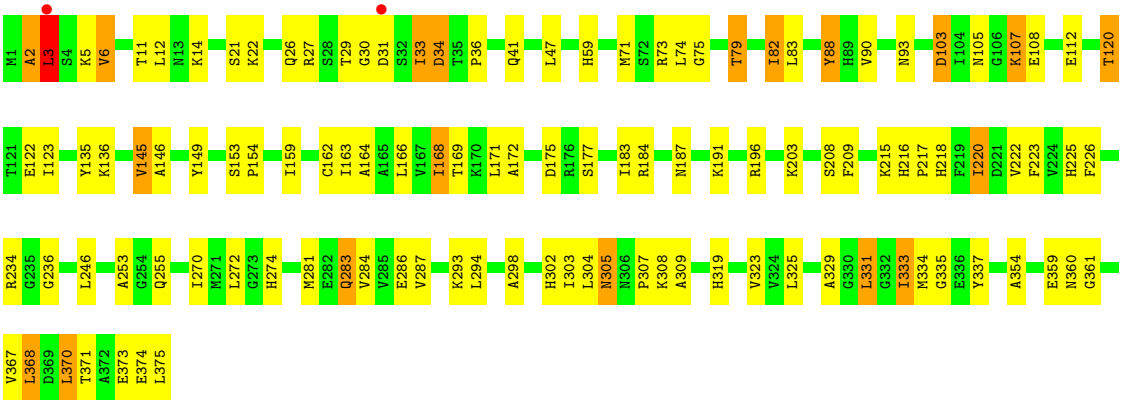
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AB:



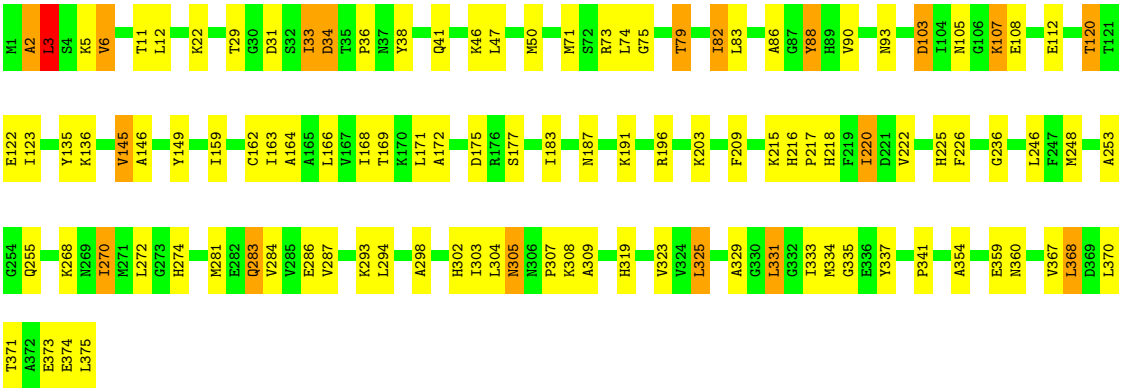
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AC:



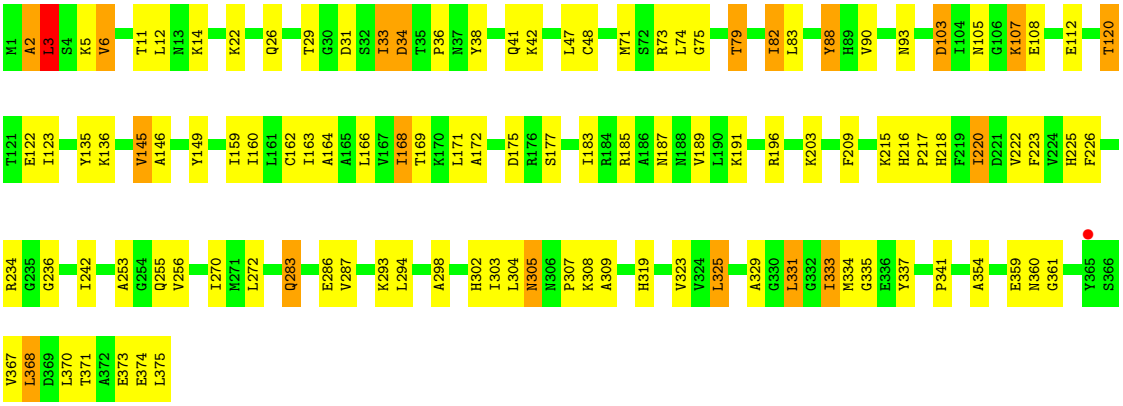
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AD:



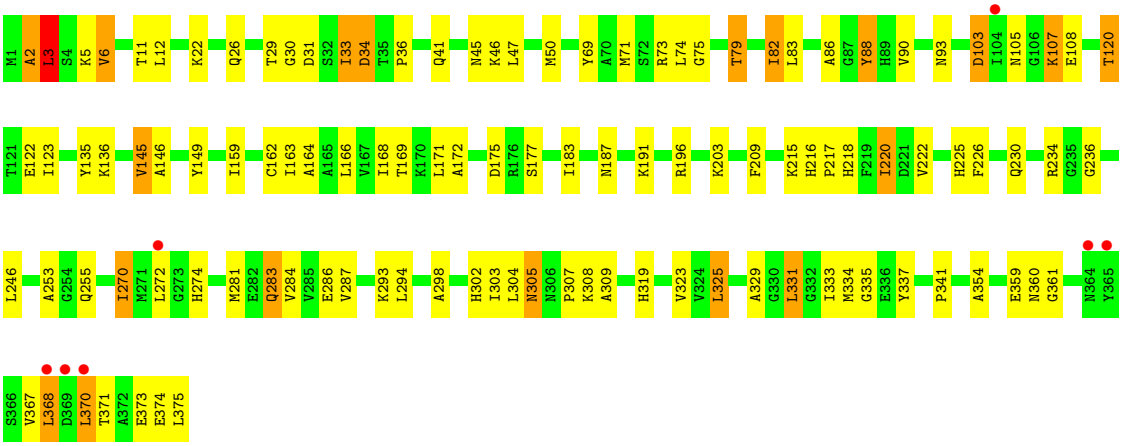
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AE:



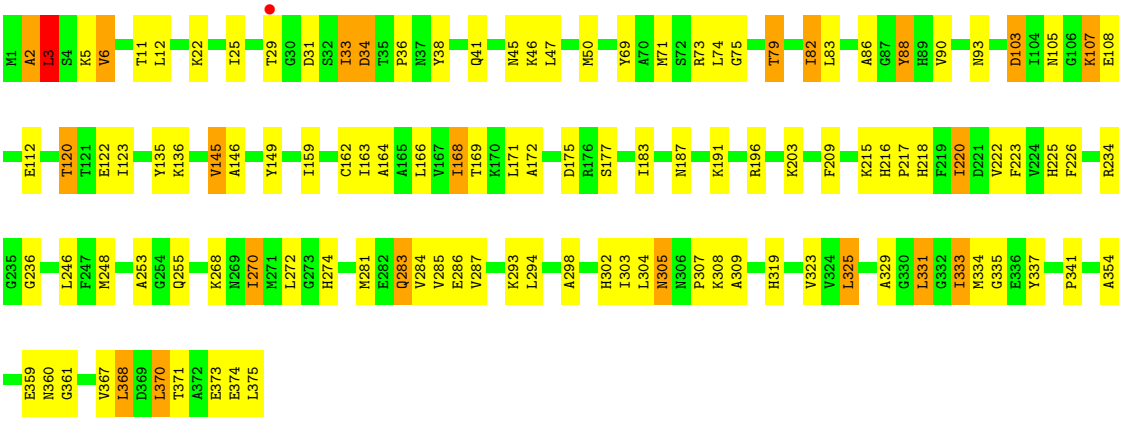
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AF:



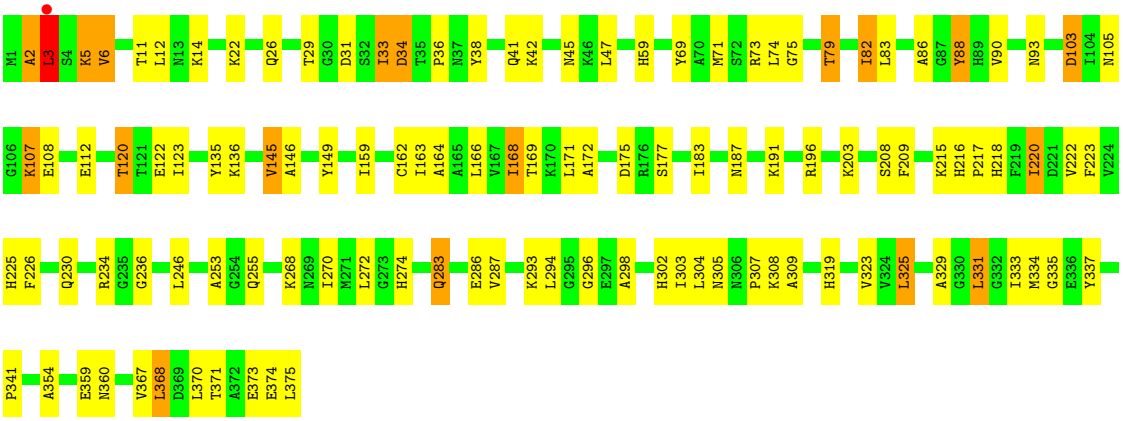
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AG:



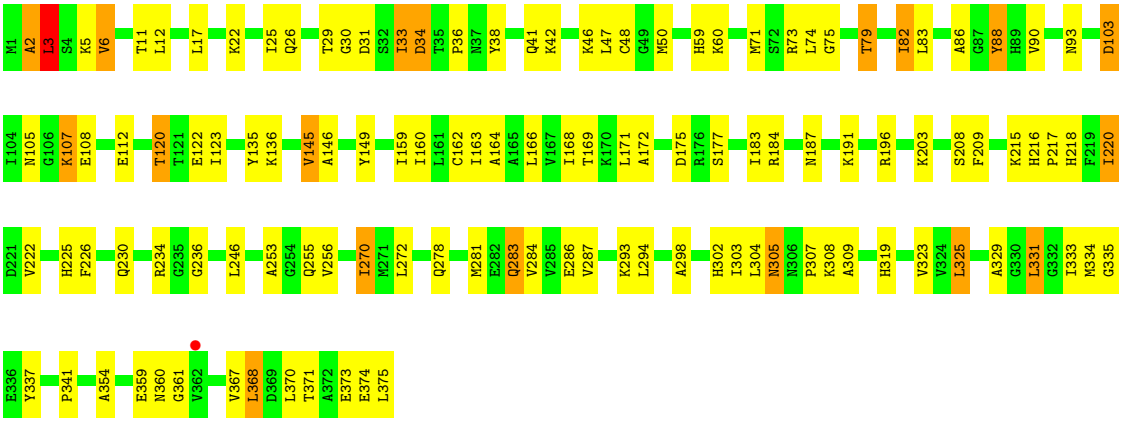
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AH:



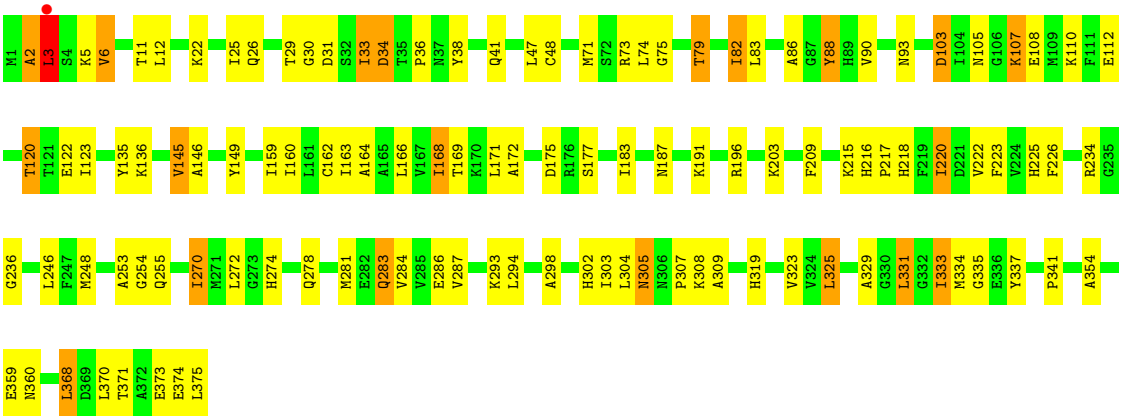
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AI:



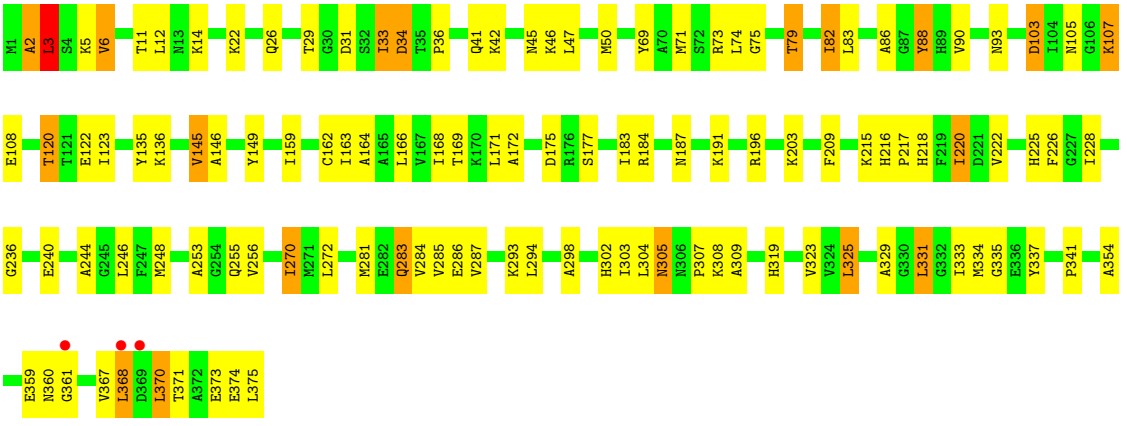
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AJ:



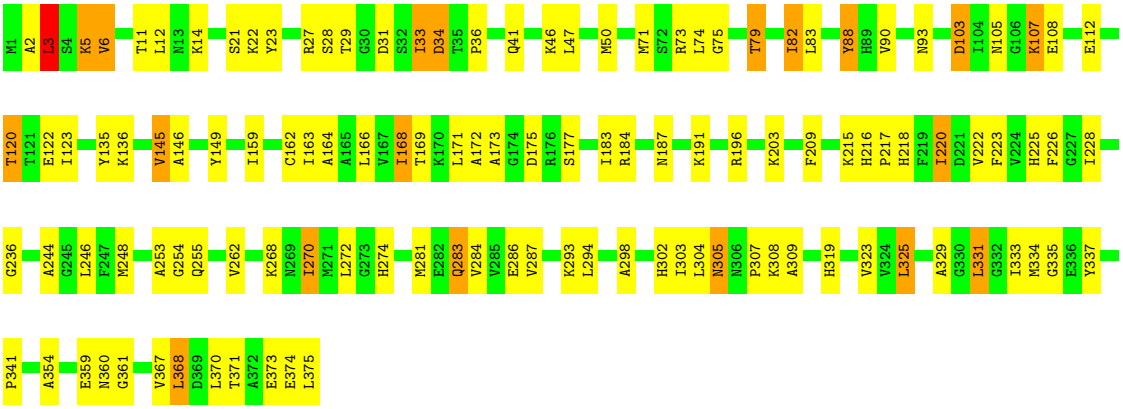
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AL:



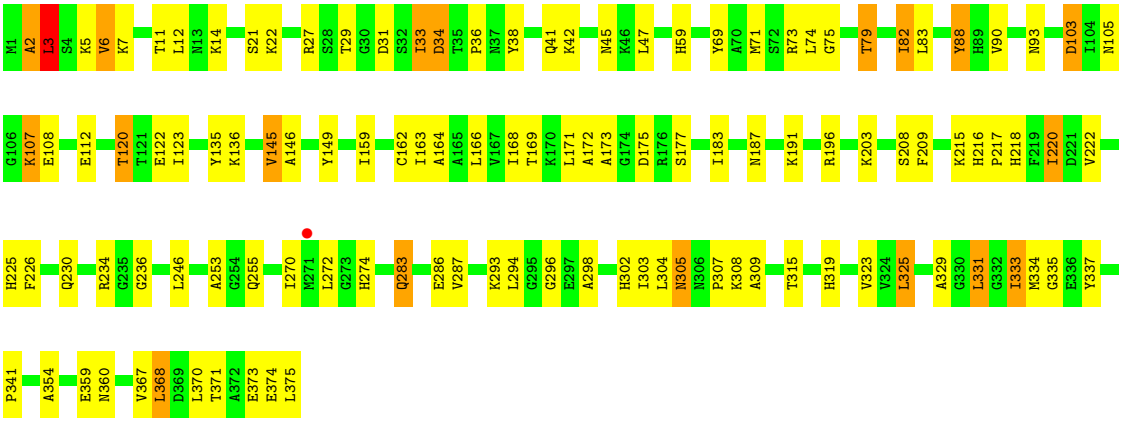
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AN:



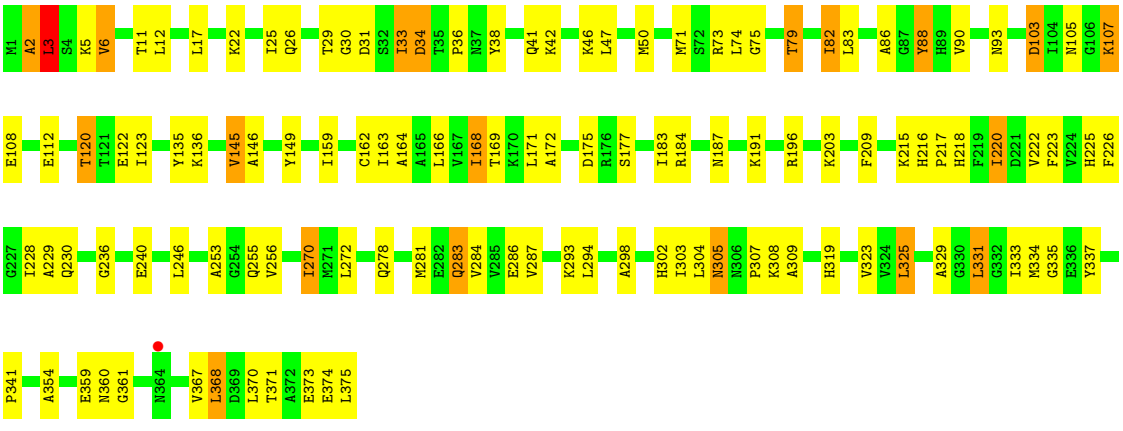
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AO:



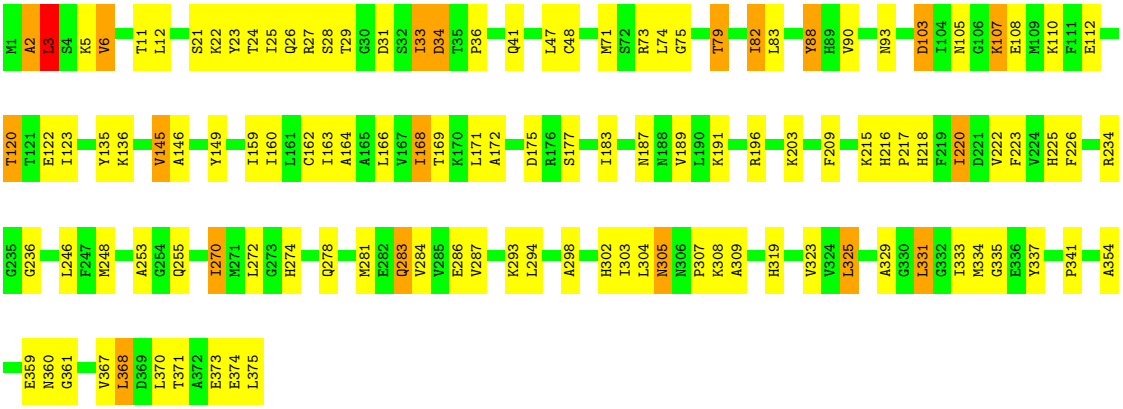
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AP:



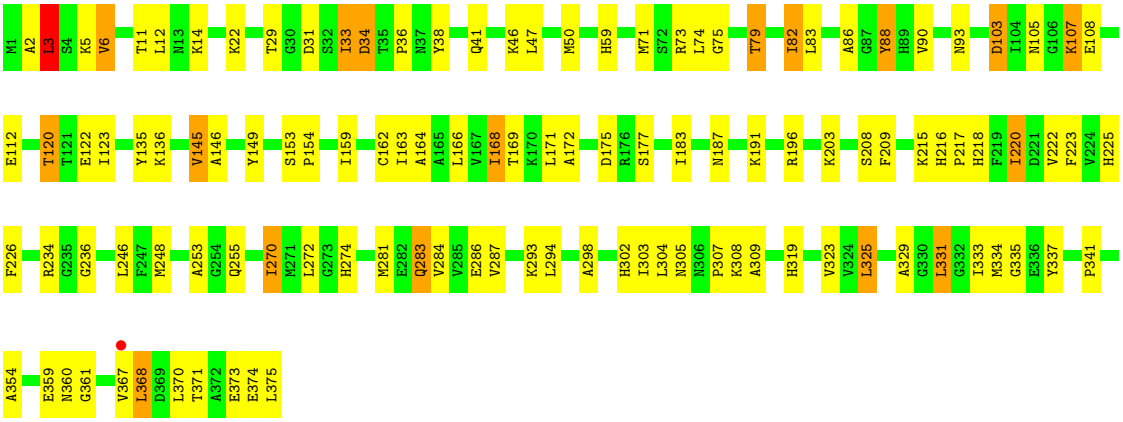
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AQ:



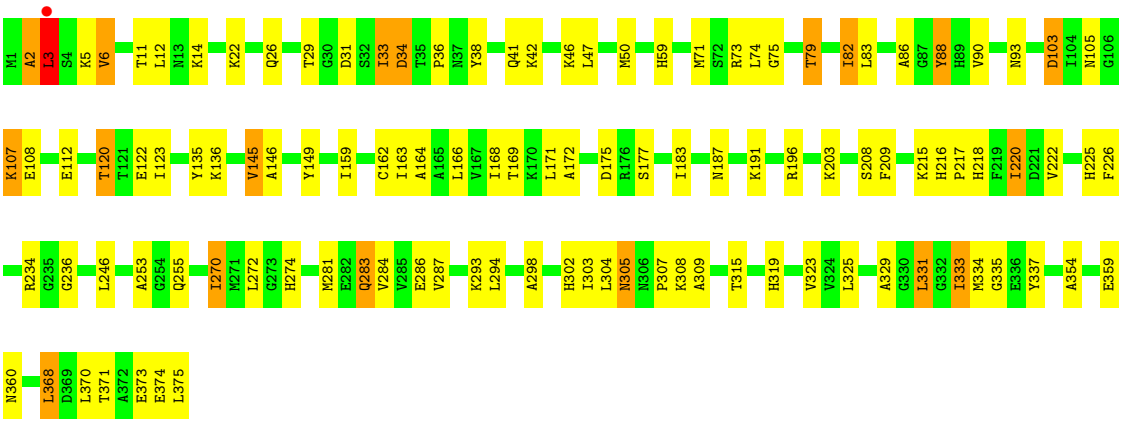
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AR:



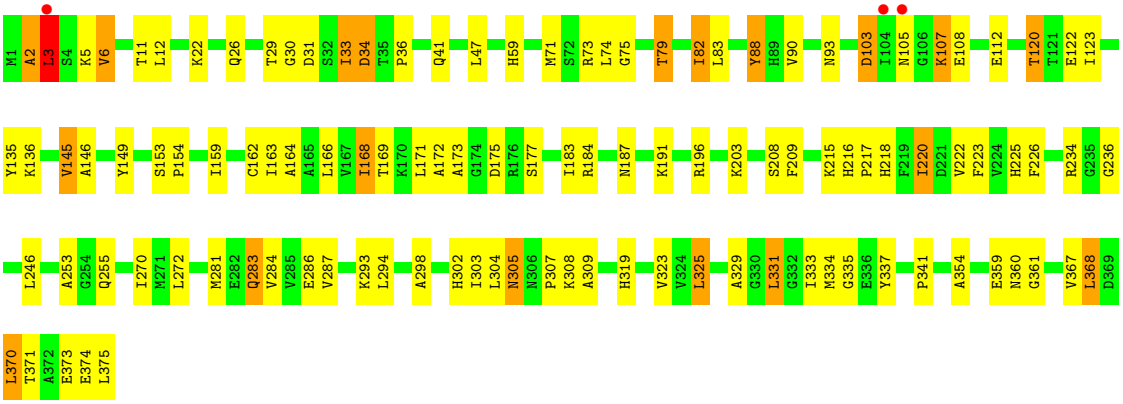
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AS:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AT:

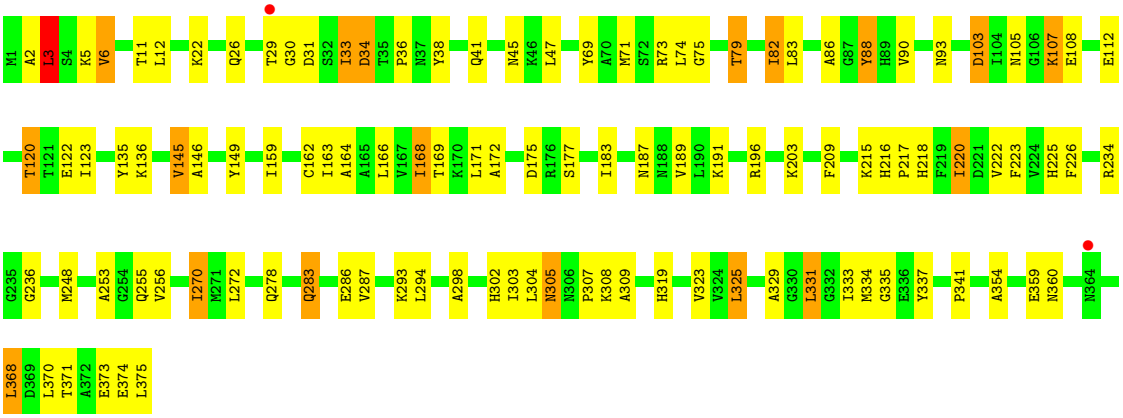


• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AU:

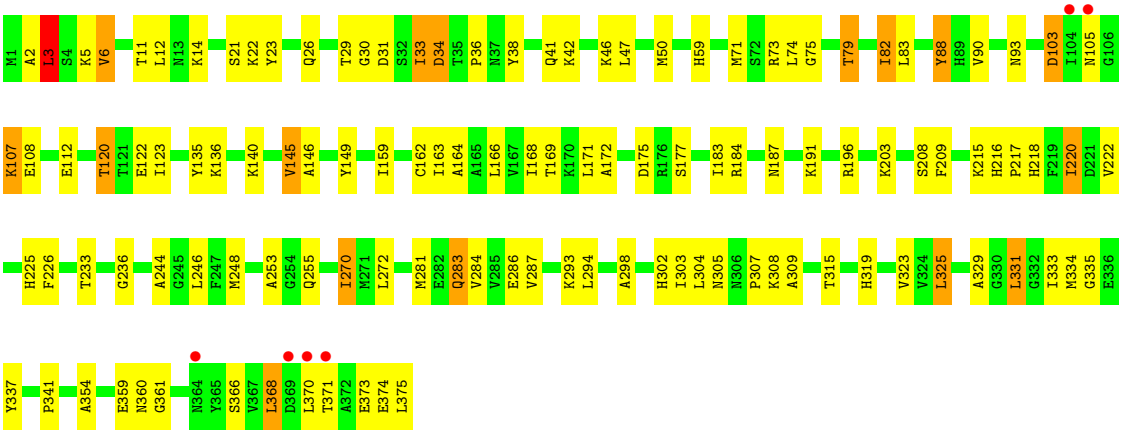
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AV:



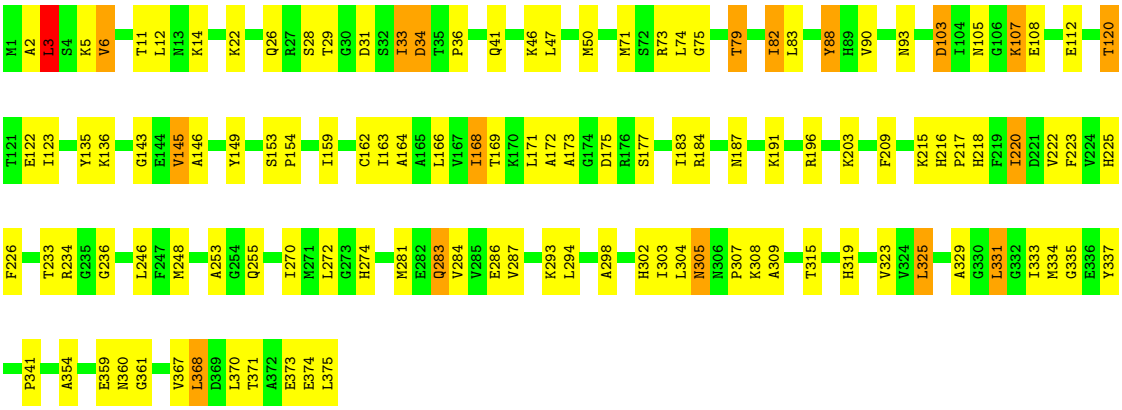
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BA:



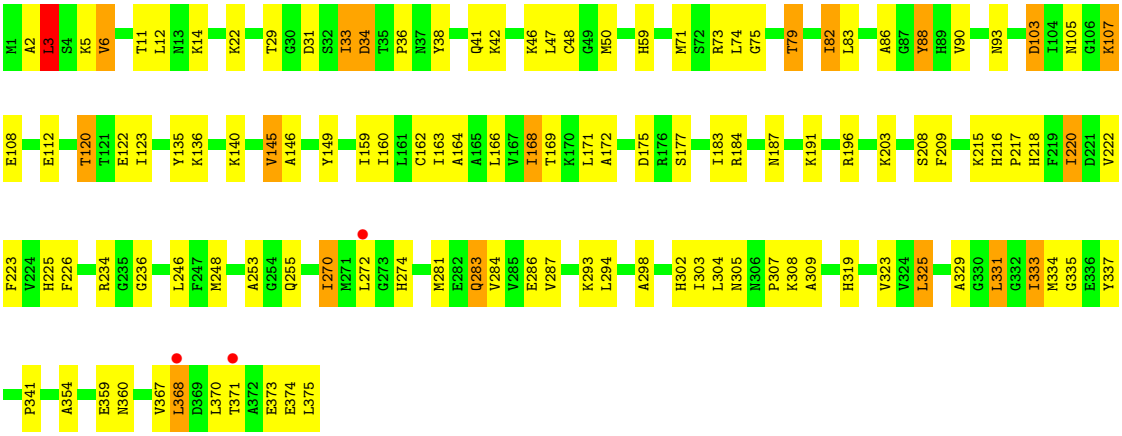
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BB:



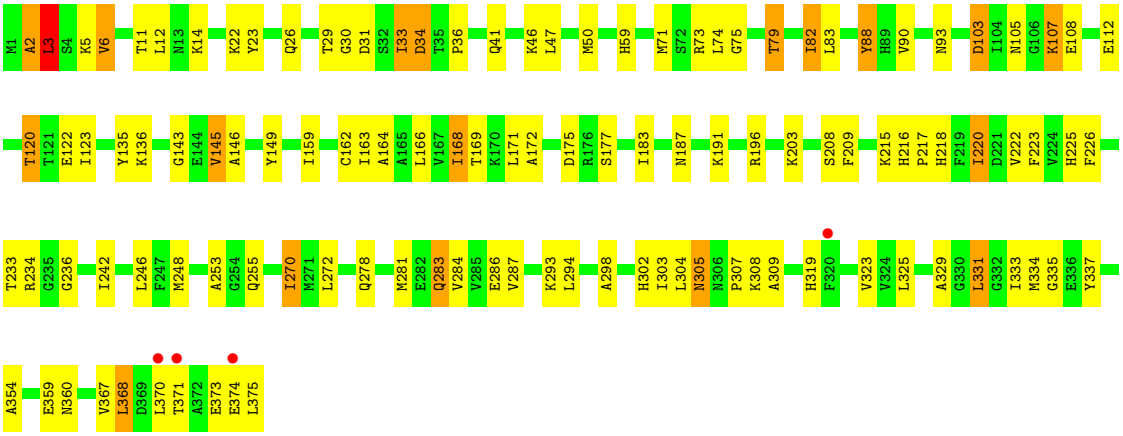
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BC:



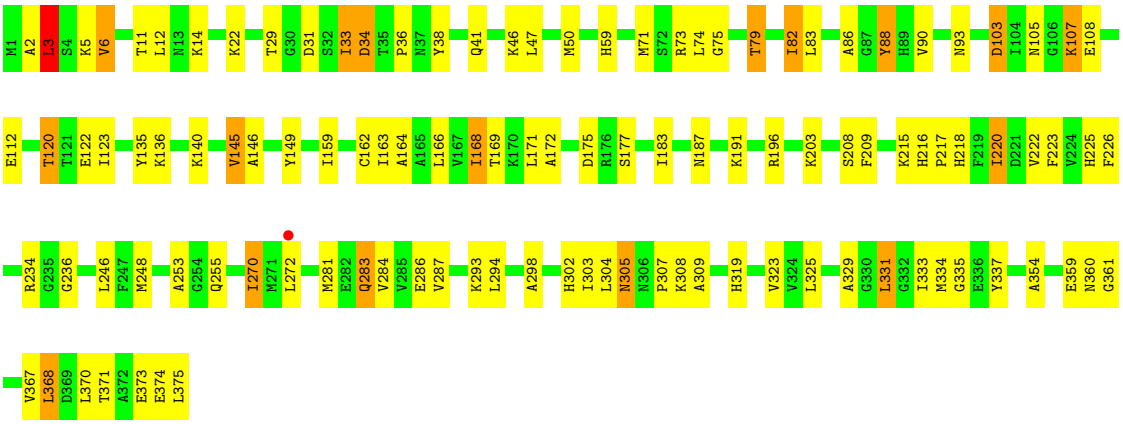
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BD:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BE:

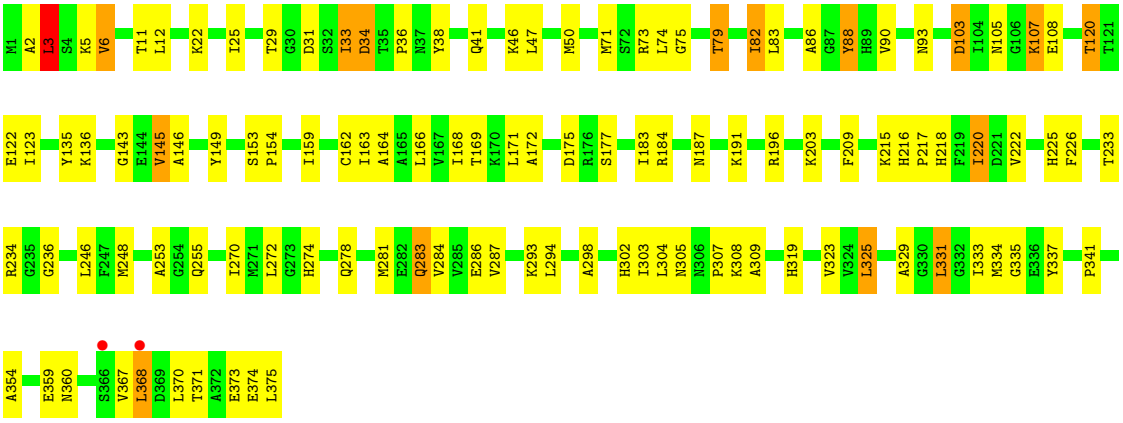


• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BF:

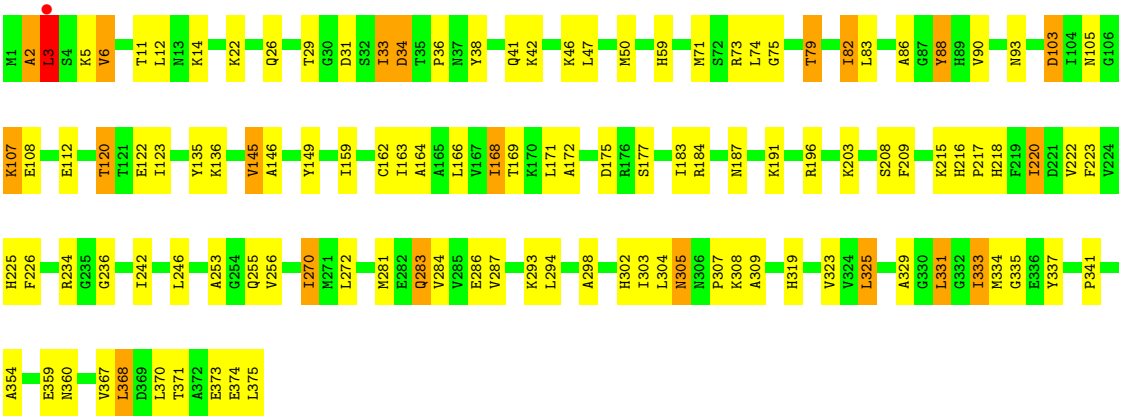
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BG:



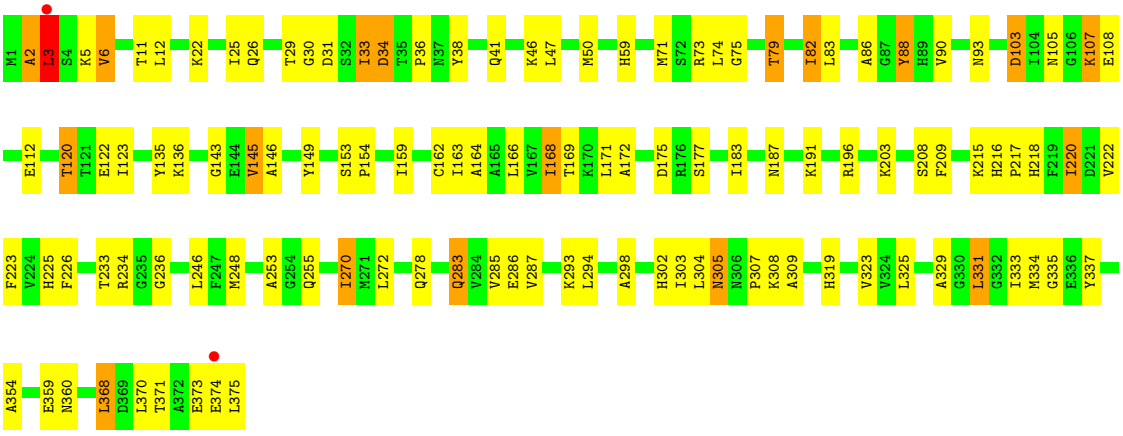
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BH:



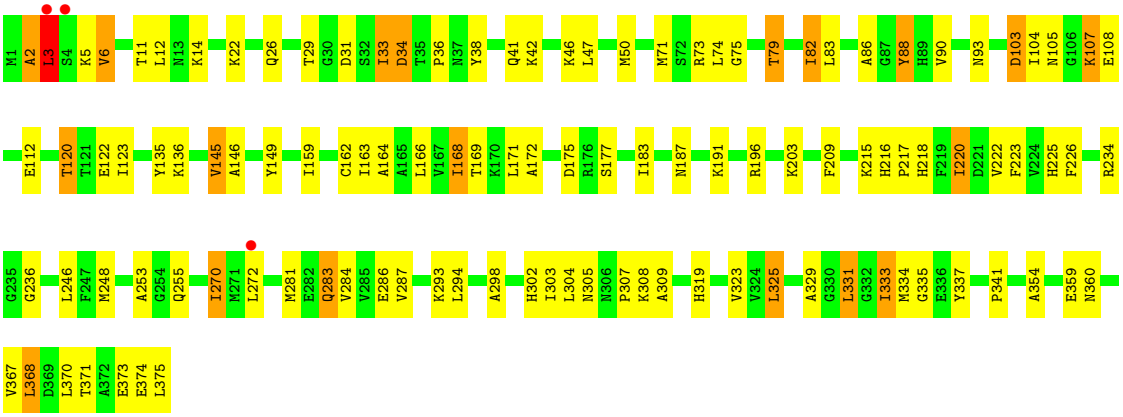
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BI:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BJ:

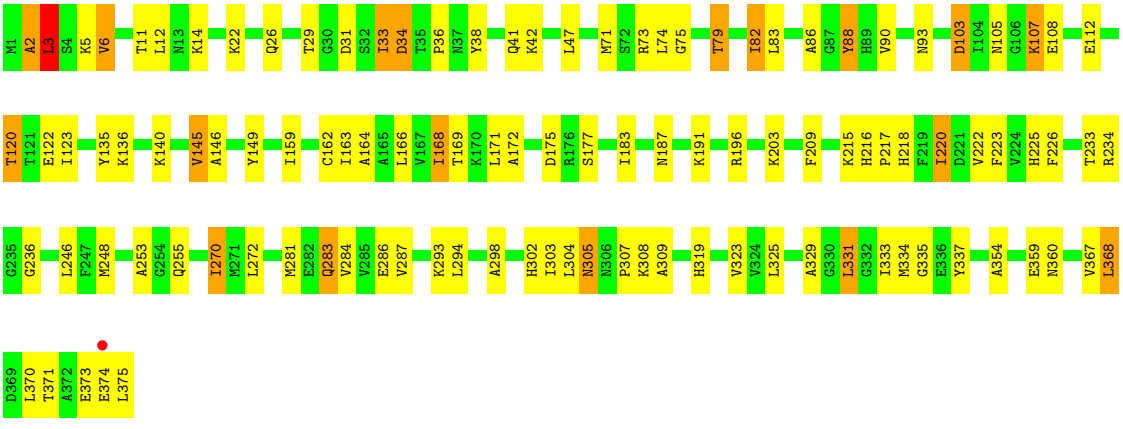


• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BK:

• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BL:

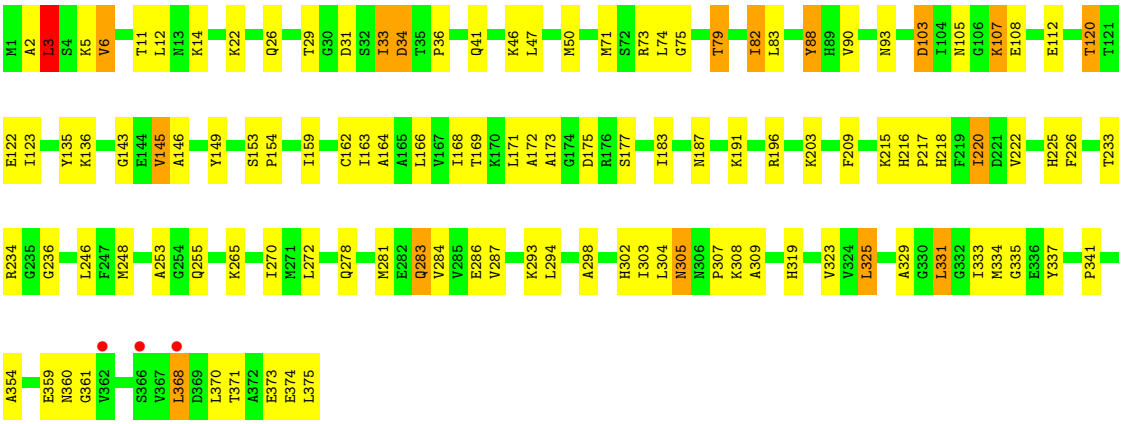


• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BM:

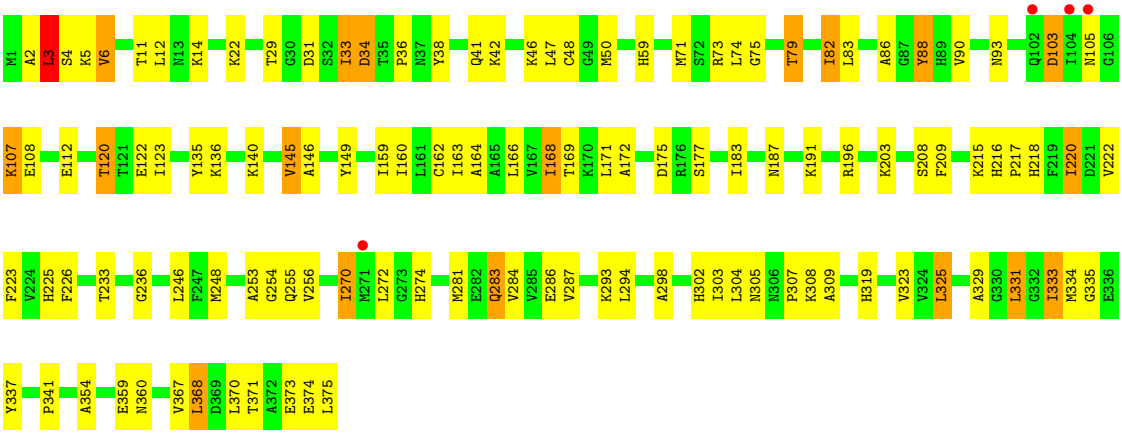
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BN:



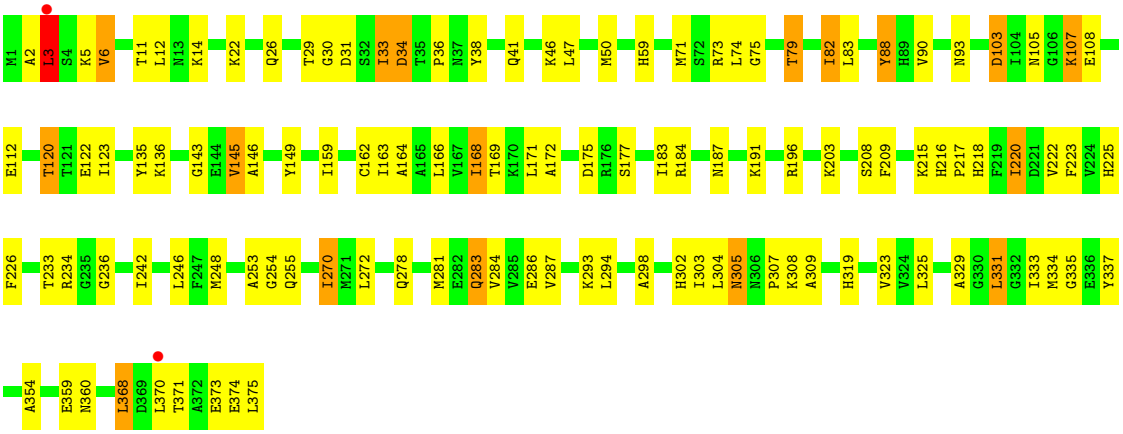
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BO:



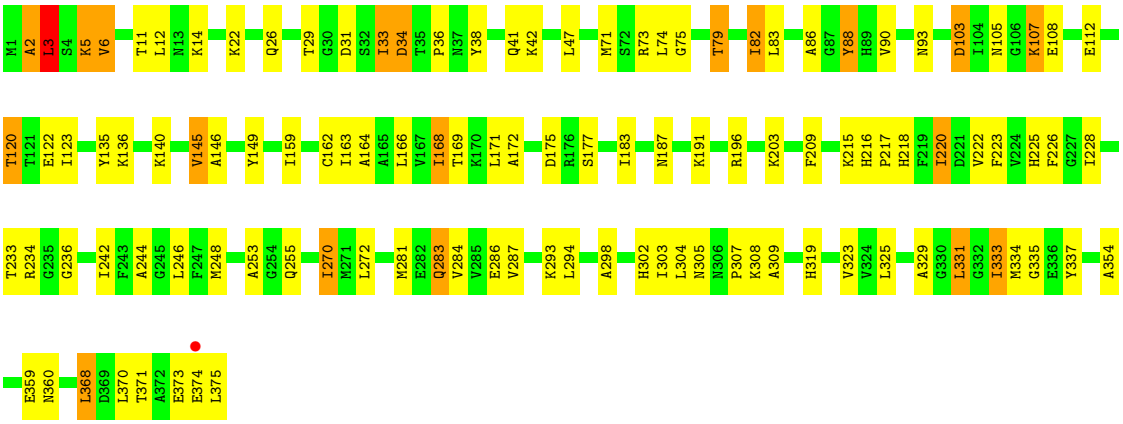
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BP:



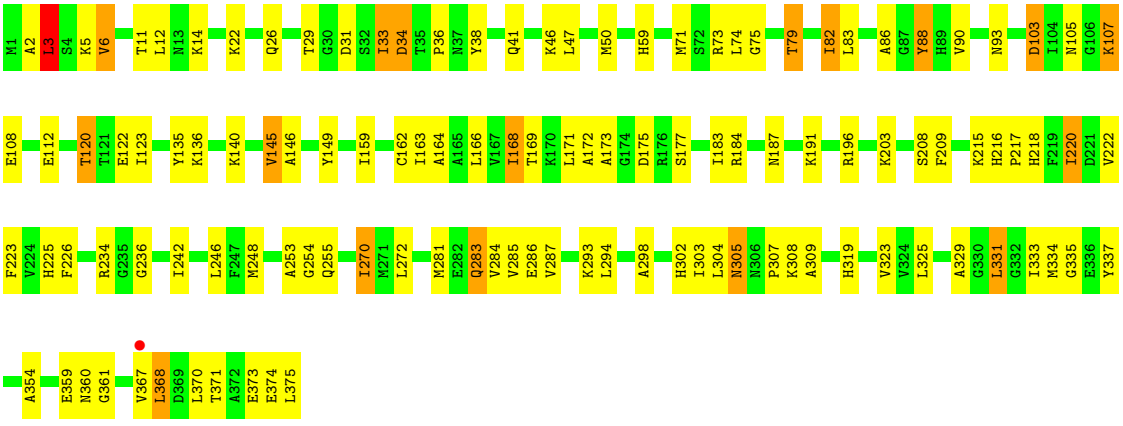
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BQ:



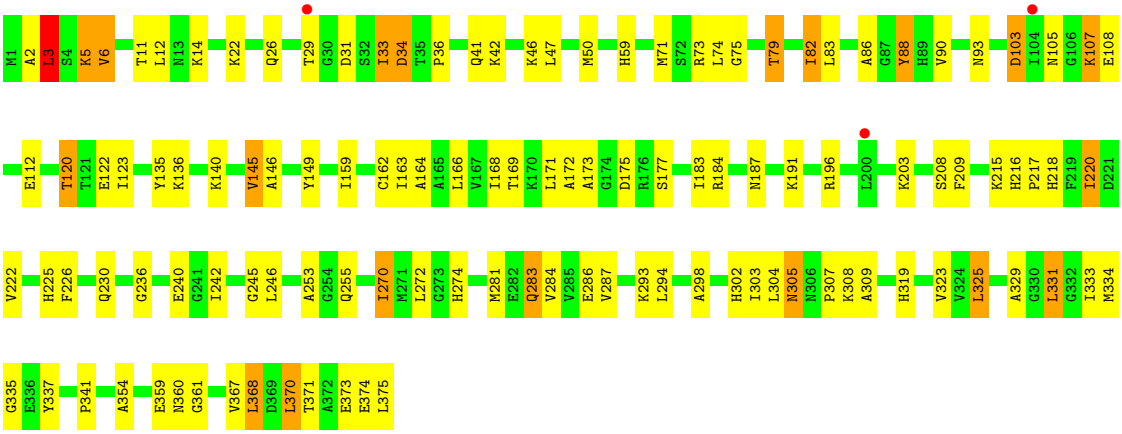
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BW:



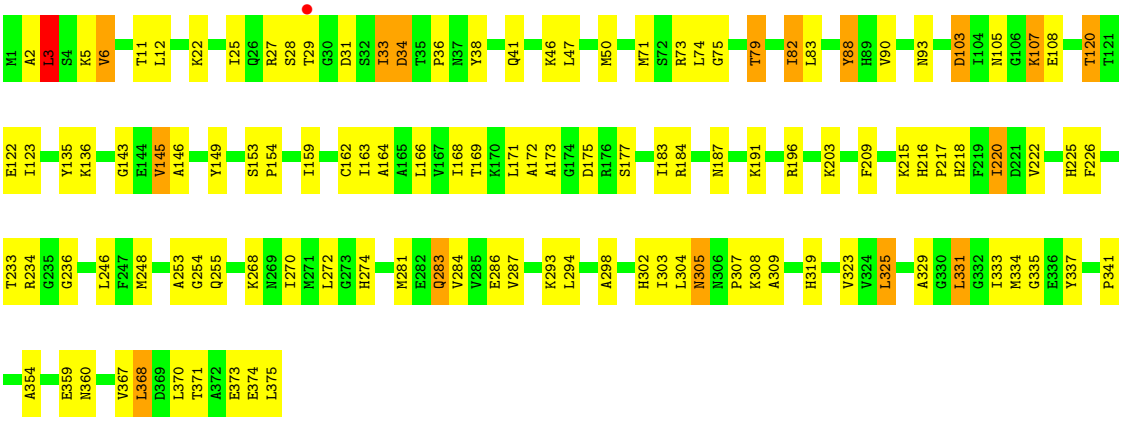
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BY:



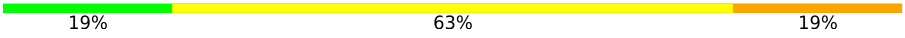
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

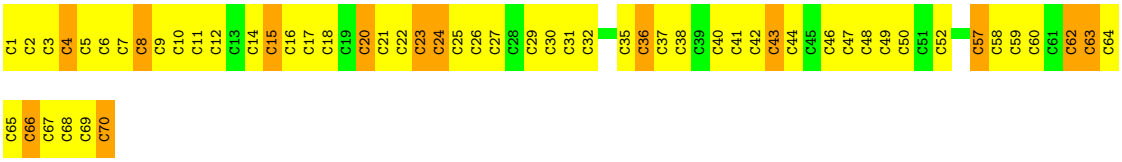
Chain BZ:



• Molecule 2: RNA

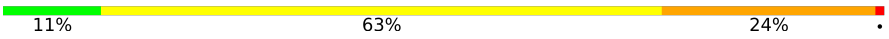
Chain AK:





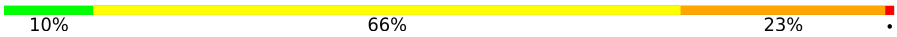
• Molecule 2: RNA

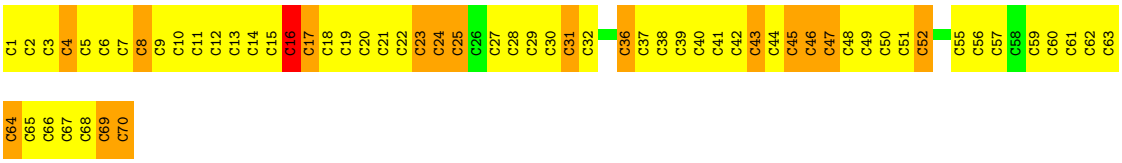
Chain AM:



• Molecule 2: RNA

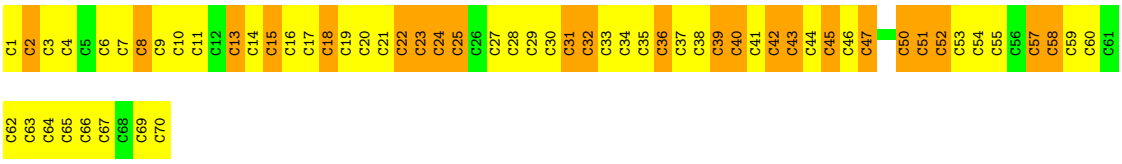
Chain BR:





• Molecule 2: RNA

Chain BX:



4 Data and refinement statistics (i)

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 48.03 – 3.46	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-3.60) 72.7 (48.03-3.46)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0070	Depositor
R, R_{free}	0.234 , 0.269 0.253 , 0.254	Depositor DCC
R_{free} test set	12956 reflections (5.02%)	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)	0.27 , 69.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	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	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.45	0/2968	0.63	2/3998 (0.1%)
1	AB	0.45	0/2968	0.63	2/3998 (0.1%)
1	AC	0.45	0/2968	0.63	2/3998 (0.1%)
1	AD	0.45	0/2968	0.63	2/3998 (0.1%)
1	AE	0.45	0/2968	0.63	2/3998 (0.1%)
1	AF	0.45	0/2968	0.63	2/3998 (0.1%)
1	AG	0.45	0/2968	0.63	2/3998 (0.1%)
1	AH	0.45	0/2968	0.63	2/3998 (0.1%)
1	AI	0.45	0/2968	0.63	2/3998 (0.1%)
1	AJ	0.45	0/2968	0.63	2/3998 (0.1%)
1	AL	0.45	0/2968	0.63	2/3998 (0.1%)
1	AN	0.45	0/2968	0.63	2/3998 (0.1%)
1	AO	0.45	0/2968	0.63	2/3998 (0.1%)
1	AP	0.45	0/2968	0.63	2/3998 (0.1%)
1	AQ	0.45	0/2968	0.63	2/3998 (0.1%)
1	AR	0.45	0/2968	0.63	2/3998 (0.1%)
1	AS	0.45	0/2968	0.63	2/3998 (0.1%)
1	AT	0.45	0/2968	0.63	2/3998 (0.1%)
1	AU	0.45	0/2968	0.63	2/3998 (0.1%)
1	AV	0.45	0/2968	0.63	2/3998 (0.1%)
1	BA	0.45	0/2968	0.63	2/3998 (0.1%)
1	BB	0.45	0/2968	0.63	2/3998 (0.1%)
1	BC	0.45	0/2968	0.63	2/3998 (0.1%)
1	BD	0.45	0/2968	0.63	2/3998 (0.1%)
1	BE	0.45	0/2968	0.63	2/3998 (0.1%)
1	BF	0.45	0/2968	0.63	2/3998 (0.1%)
1	BG	0.45	0/2968	0.63	2/3998 (0.1%)
1	BH	0.45	0/2968	0.63	2/3998 (0.1%)
1	BI	0.45	0/2968	0.63	2/3998 (0.1%)
1	BJ	0.45	0/2968	0.63	2/3998 (0.1%)
1	BK	0.45	0/2968	0.63	2/3998 (0.1%)
1	BL	0.45	0/2968	0.63	2/3998 (0.1%)
1	BM	0.45	0/2968	0.63	2/3998 (0.1%)
1	BN	0.45	0/2968	0.63	2/3998 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	BO	0.45	0/2968	0.63	2/3998 (0.1%)
1	BP	0.45	0/2968	0.63	2/3998 (0.1%)
1	BQ	0.45	0/2968	0.63	2/3998 (0.1%)
1	BW	0.45	0/2968	0.63	2/3998 (0.1%)
1	BY	0.45	0/2968	0.63	2/3998 (0.1%)
1	BZ	0.45	0/2968	0.63	2/3998 (0.1%)
2	AK	0.38	0/1539	0.93	8/2376 (0.3%)
2	AM	0.37	0/1539	0.91	8/2376 (0.3%)
2	BR	0.35	0/1539	0.88	2/2376 (0.1%)
2	BX	0.35	0/1539	0.91	6/2376 (0.3%)
All	All	0.45	0/124876	0.65	104/169424 (0.1%)

There are no bond length outliers.

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BR	69	C	P-O3'-C3'	-7.37	110.86	119.70
2	AK	62	C	P-O3'-C3'	-7.10	111.18	119.70
2	BX	2	C	P-O3'-C3'	-7.06	111.23	119.70
2	BX	16	C	P-O3'-C3'	-6.21	112.25	119.70
2	AK	8	C	P-O3'-C3'	6.08	127.00	119.70

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	AA	2920	0	2955	81	1
1	AB	2920	0	2955	87	0
1	AC	2920	0	2955	76	6
1	AD	2920	0	2955	66	1
1	AE	2920	0	2955	69	3
1	AF	2920	0	2955	71	2
1	AG	2920	0	2955	80	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	74	0
1	AI	2920	0	2955	85	2
1	AJ	2920	0	2955	74	5
1	AL	2920	0	2955	85	2
1	AN	2920	0	2955	93	0
1	AO	2920	0	2955	79	0
1	AP	2920	0	2955	88	1
1	AQ	2920	0	2955	79	5
1	AR	2920	0	2955	70	1
1	AS	2920	0	2955	71	0
1	AT	2920	0	2955	71	5
1	AU	2920	0	2955	71	1
1	AV	2920	0	2955	69	4
1	BA	2920	0	2955	84	3
1	BB	2920	0	2955	76	1
1	BC	2920	0	2955	79	5
1	BD	2920	0	2955	76	2
1	BE	2920	0	2955	75	4
1	BF	2920	0	2955	76	1
1	BG	2920	0	2955	74	1
1	BH	2920	0	2955	78	0
1	BI	2920	0	2955	77	1
1	BJ	2920	0	2955	73	1
1	BK	2920	0	2955	76	1
1	BL	2920	0	2955	74	3
1	BM	2920	0	2955	78	3
1	BN	2920	0	2955	70	1
1	BO	2920	0	2955	82	6
1	BP	2920	0	2955	86	2
1	BQ	2920	0	2955	87	3
1	BW	2920	0	2955	85	3
1	BY	2920	0	2955	77	1
1	BZ	2920	0	2955	75	1
2	AK	1400	0	771	81	0
2	AM	1400	0	771	112	0
2	BR	1400	0	771	87	0
2	BX	1400	0	771	121	0
All	All	122400	0	121284	3044	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 12.

The worst 5 of 3044 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 (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 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%)	41	75
1	AB	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	AC	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	AD	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AE	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	AF	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AG	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AH	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AI	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	AJ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75

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%)	41	75
1	AN	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AO	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AP	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	AQ	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AR	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AS	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	AT	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AU	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	AV	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BA	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BB	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BC	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BD	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BE	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BF	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BG	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BH	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BI	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BJ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BK	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BL	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BM	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BN	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BO	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BP	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BQ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BW	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
1	BY	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	41	75
1	BZ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	41	75
All	All	14920/15000 (100%)	14421 (97%)	459 (3%)	40 (0%)	41	75

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%)	268 (86%)	45 (14%)	3	20
1	AB	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AC	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AD	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AE	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AF	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AG	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AH	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	AI	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AJ	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AL	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AN	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AO	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AP	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AQ	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AR	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	AS	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AT	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	AU	313/313 (100%)	268 (86%)	45 (14%)	3	20

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AV	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BA	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	BB	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BC	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	BD	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BE	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BF	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BG	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	BH	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BI	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BJ	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	BK	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	BL	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BM	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BN	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BO	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	BP	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BQ	313/313 (100%)	269 (86%)	44 (14%)	3	21
1	BW	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BY	313/313 (100%)	268 (86%)	45 (14%)	3	20
1	BZ	313/313 (100%)	268 (86%)	45 (14%)	3	20
All	All	12520/12520 (100%)	10729 (86%)	1791 (14%)	3	21

5 of 1791 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BA	272	LEU
1	BZ	270	ILE
1	BF	220	ILE
1	BZ	34	ASP
1	BP	304	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 133 such sidechains are listed below:

Mol	Chain	Res	Type
1	BO	216	HIS
1	BP	216	HIS
1	BZ	151	HIS
1	AR	216	HIS
1	AR	187	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	AK	69/70 (98%)	16 (23%)	2 (2%)
2	AM	69/70 (98%)	14 (20%)	2 (2%)
2	BR	69/70 (98%)	19 (27%)	7 (10%)
2	BX	69/70 (98%)	19 (27%)	4 (5%)
All	All	276/280 (98%)	68 (24%)	15 (5%)

5 of 68 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	AK	8	C
2	AK	15	C
2	AK	17	C
2	AK	22	C
2	AK	25	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 (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 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, 95^{th} 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%)	-0.35	0 100 100	77, 135, 189, 218	0
1	AB	375/375 (100%)	-0.34	1 (0%) 94 88	77, 135, 189, 218	0
1	AC	375/375 (100%)	-0.30	2 (0%) 91 83	77, 135, 189, 218	0
1	AD	375/375 (100%)	-0.28	0 100 100	77, 135, 189, 218	0
1	AE	375/375 (100%)	-0.34	1 (0%) 94 88	77, 135, 189, 218	0
1	AF	375/375 (100%)	-0.27	7 (1%) 66 51	77, 135, 189, 218	0
1	AG	375/375 (100%)	-0.44	1 (0%) 94 88	77, 135, 189, 218	0
1	AH	375/375 (100%)	-0.42	1 (0%) 94 88	77, 135, 189, 218	0
1	AI	375/375 (100%)	-0.27	1 (0%) 94 88	77, 135, 189, 218	0
1	AJ	375/375 (100%)	-0.34	1 (0%) 94 88	77, 135, 189, 218	0
1	AL	375/375 (100%)	-0.31	3 (0%) 86 75	77, 135, 189, 218	0
1	AN	375/375 (100%)	-0.40	0 100 100	77, 135, 189, 218	0
1	AO	375/375 (100%)	-0.35	1 (0%) 94 88	77, 135, 189, 218	0
1	AP	375/375 (100%)	-0.31	1 (0%) 94 88	77, 135, 189, 218	0
1	AQ	375/375 (100%)	-0.30	0 100 100	77, 135, 189, 218	0
1	AR	375/375 (100%)	-0.32	1 (0%) 94 88	77, 135, 189, 218	0
1	AS	375/375 (100%)	-0.42	1 (0%) 94 88	77, 135, 189, 218	0
1	AT	375/375 (100%)	-0.37	3 (0%) 86 75	77, 135, 189, 218	0
1	AU	375/375 (100%)	-0.27	0 100 100	77, 135, 189, 218	0
1	AV	375/375 (100%)	-0.36	2 (0%) 91 83	77, 135, 189, 218	0
1	BA	375/375 (100%)	-0.29	6 (1%) 72 57	77, 135, 189, 218	0
1	BB	375/375 (100%)	-0.36	0 100 100	77, 135, 189, 218	0
1	BC	375/375 (100%)	-0.26	3 (0%) 86 75	77, 135, 189, 218	0
1	BD	375/375 (100%)	-0.28	4 (1%) 80 68	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%)	-0.35	1 (0%) 94 88	77, 135, 189, 218	0
1	BF	375/375 (100%)	-0.40	5 (1%) 77 63	77, 135, 189, 218	0
1	BG	375/375 (100%)	-0.37	2 (0%) 91 83	77, 135, 189, 218	0
1	BH	375/375 (100%)	-0.26	1 (0%) 94 88	77, 135, 189, 218	0
1	BI	375/375 (100%)	-0.29	2 (0%) 91 83	77, 135, 189, 218	0
1	BJ	375/375 (100%)	-0.27	3 (0%) 86 75	77, 135, 189, 218	0
1	BK	375/375 (100%)	-0.30	0 100 100	77, 135, 189, 218	0
1	BL	375/375 (100%)	-0.31	1 (0%) 94 88	77, 135, 189, 218	0
1	BM	375/375 (100%)	-0.38	4 (1%) 80 68	77, 135, 189, 218	0
1	BN	375/375 (100%)	-0.34	3 (0%) 86 75	77, 135, 189, 218	0
1	BO	375/375 (100%)	-0.23	4 (1%) 80 68	77, 135, 189, 218	0
1	BP	375/375 (100%)	-0.29	2 (0%) 91 83	77, 135, 189, 218	0
1	BQ	375/375 (100%)	-0.34	1 (0%) 94 88	77, 135, 189, 218	0
1	BW	375/375 (100%)	-0.34	1 (0%) 94 88	77, 135, 189, 218	0
1	BY	375/375 (100%)	-0.34	3 (0%) 86 75	77, 135, 189, 218	0
1	BZ	375/375 (100%)	-0.37	1 (0%) 94 88	77, 135, 189, 218	0
2	AK	70/70 (100%)	-0.36	0 100 100	120, 142, 159, 162	0
2	AM	70/70 (100%)	-0.33	0 100 100	112, 143, 161, 165	0
2	BR	70/70 (100%)	-0.31	0 100 100	129, 145, 158, 162	0
2	BX	70/70 (100%)	-0.32	0 100 100	119, 145, 156, 159	0
All	All	15280/15280 (100%)	-0.33	74 (0%) 91 83	77, 136, 189, 218	0

The worst 5 of 74 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AF	368	LEU	6.4
1	AF	369	ASP	5.0
1	BM	374	GLU	5.0
1	AF	364	ASN	4.8
1	AC	31	ASP	4.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.