



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 05:54 PM BST

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 validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

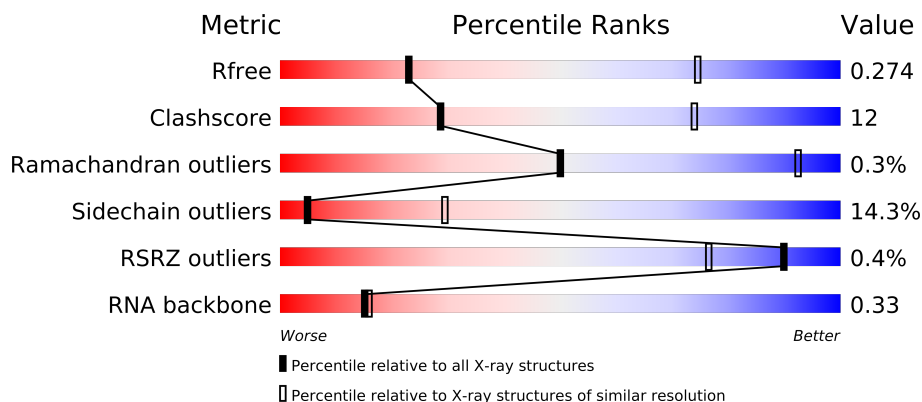
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

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}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AB	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AC	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AD	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AE	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AF	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AG	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AH	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AI	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AJ	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AL	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	AN	375	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
1	AO	375	
1	AP	375	
1	AQ	375	
1	AR	375	
1	AS	375	
1	AT	375	
1	AU	375	
1	AV	375	
1	BA	375	
1	BB	375	
1	BC	375	
1	BD	375	
1	BE	375	
1	BF	375	
1	BG	375	
1	BH	375	
1	BI	375	
1	BJ	375	
1	BK	375	
1	BL	375	
1	BM	375	
1	BN	375	
1	BO	375	
1	BP	375	
1	BQ	375	
1	BW	375	
1	BY	375	
1	BZ	375	
2	AK	70	
2	AM	70	
2	BR	70	
2	BX	70	

2 Entry composition

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

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			

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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			

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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.

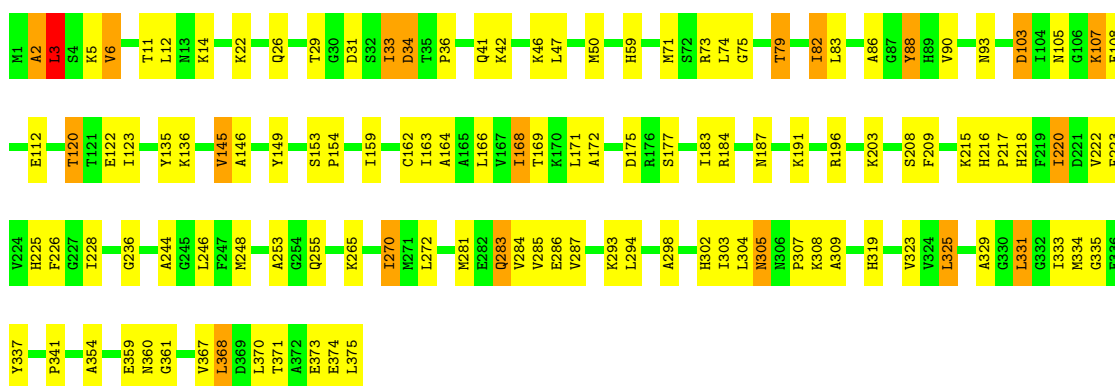
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AK	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	AM	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	BR	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			
2	BX	70	Total	C	N	O	P	0	0	0
			1400	630	210	490	70			

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

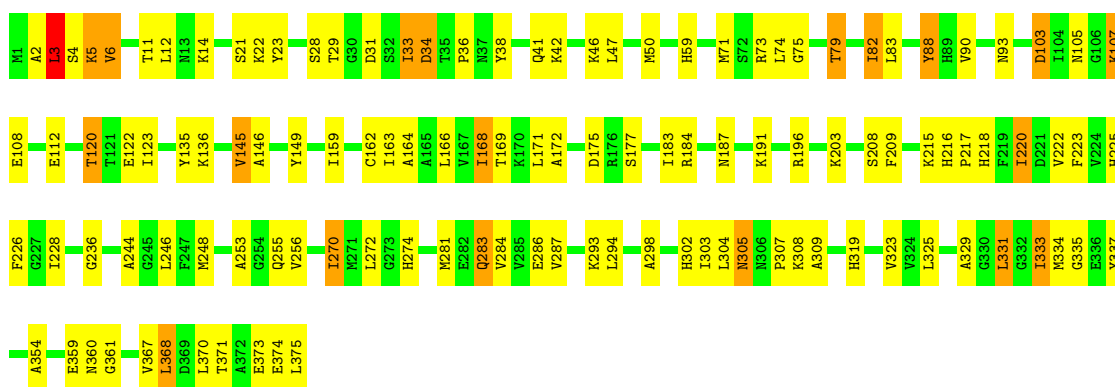
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AA: 



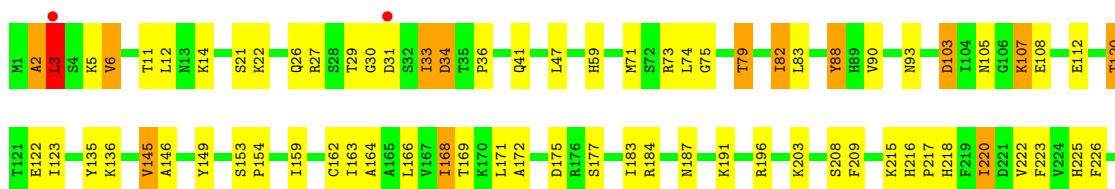
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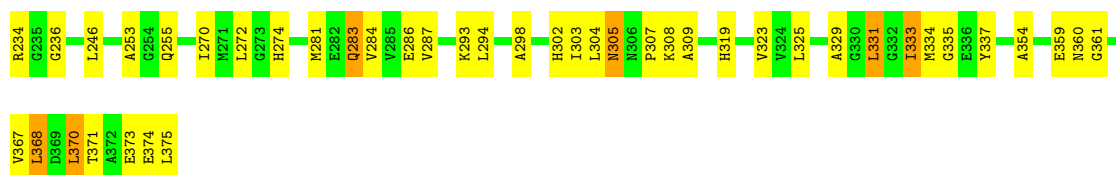
Chain AB: 



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

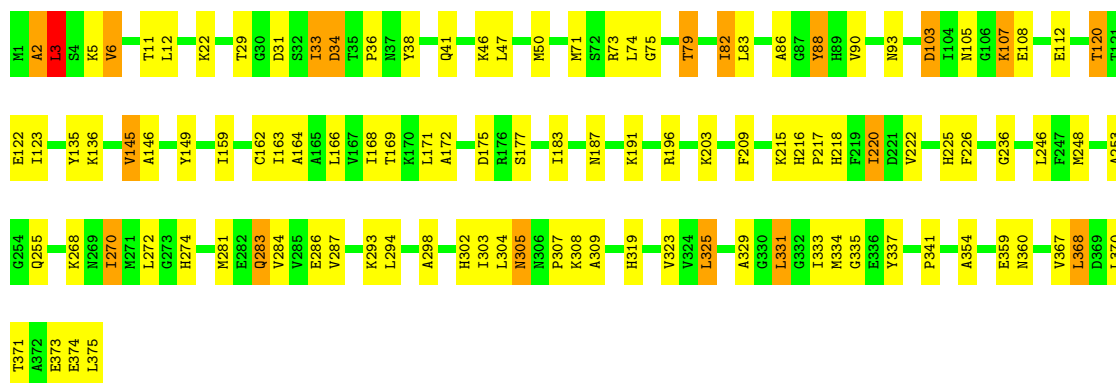
Chain AC: 





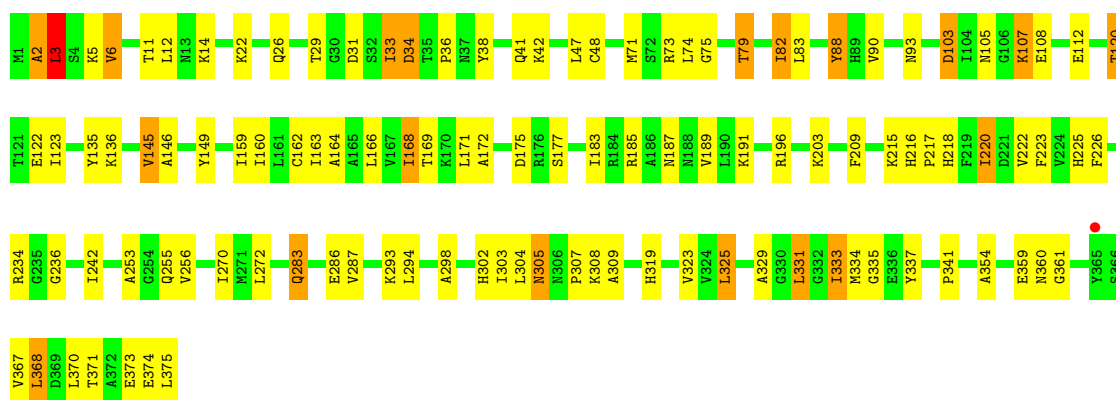
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AD:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

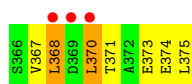
Chain AE:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

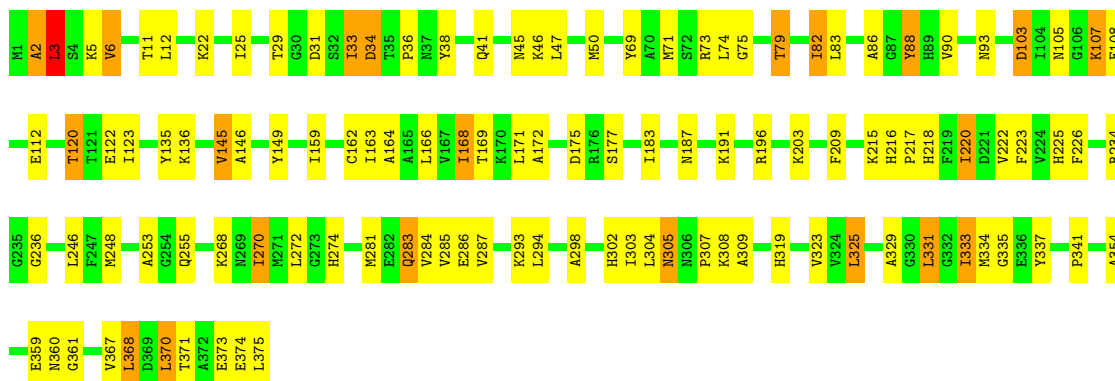
Chain AF:





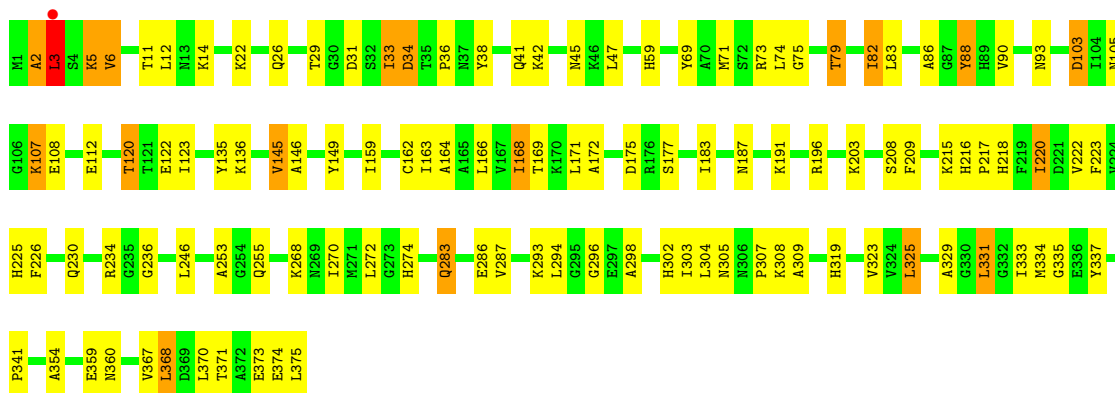
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AG:



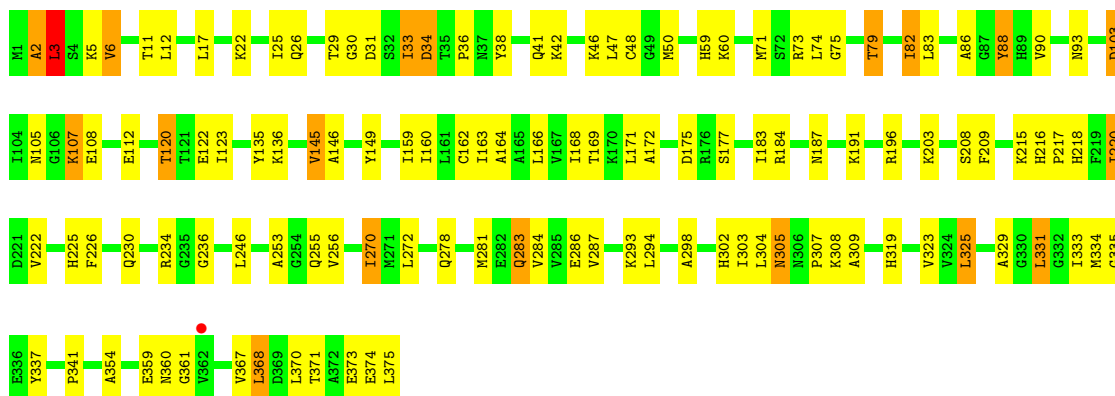
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AH:



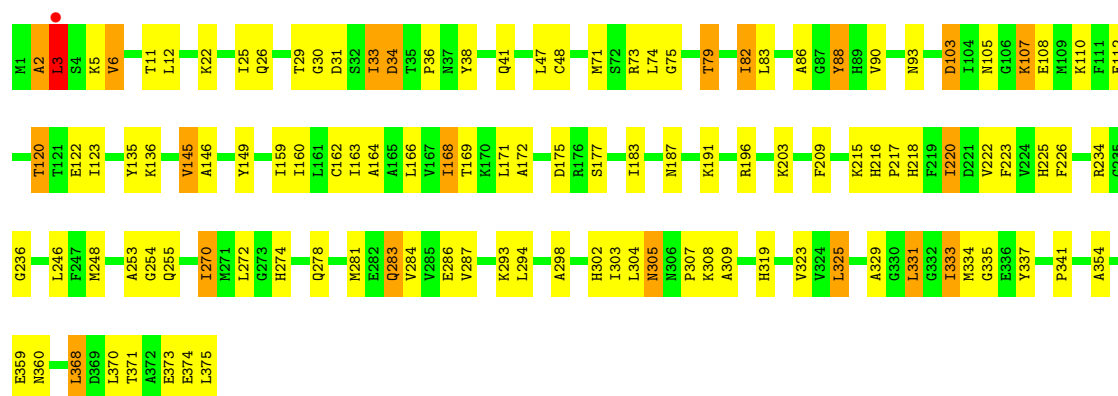
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AI:



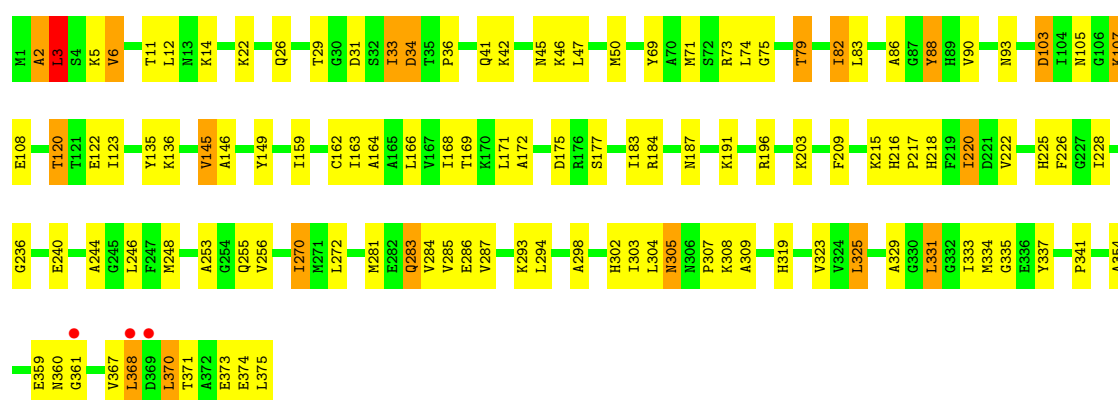
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AJ:



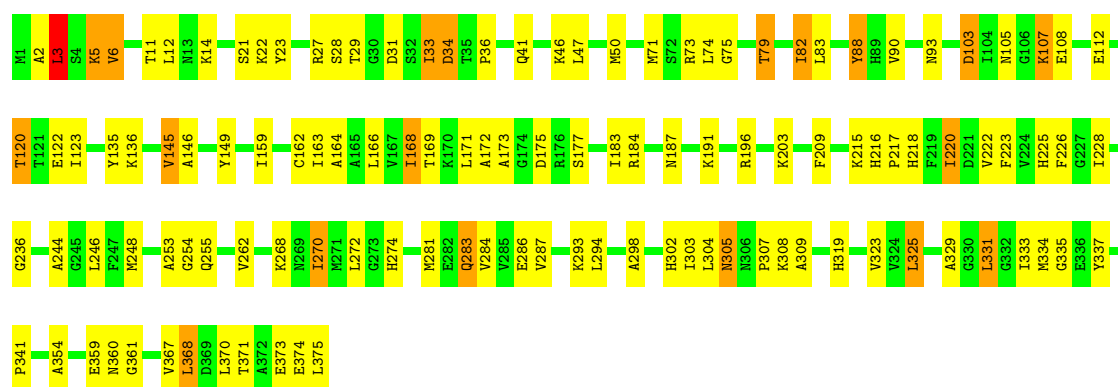
- Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AL:



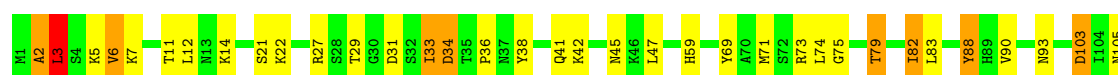
- Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

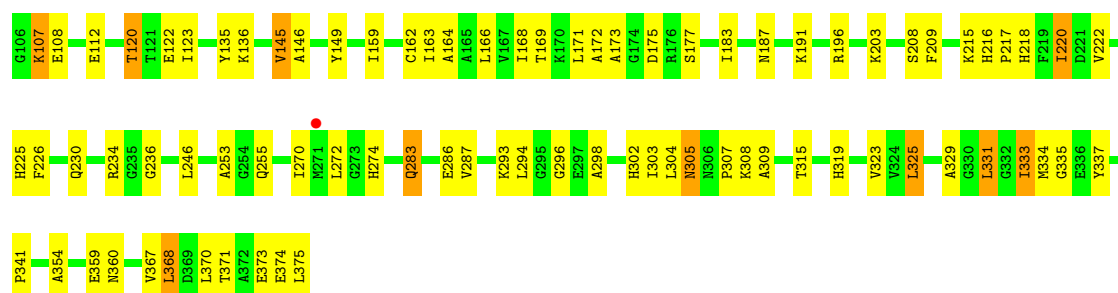
Chain AN:



- Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

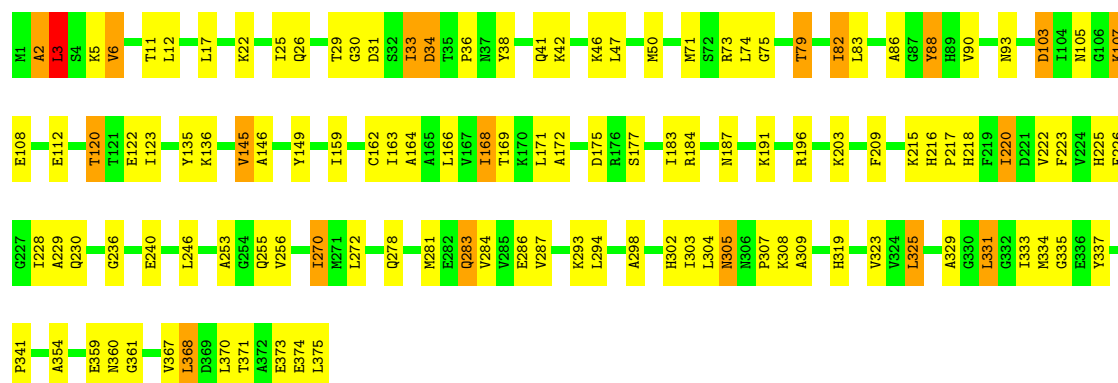
Chain AO:





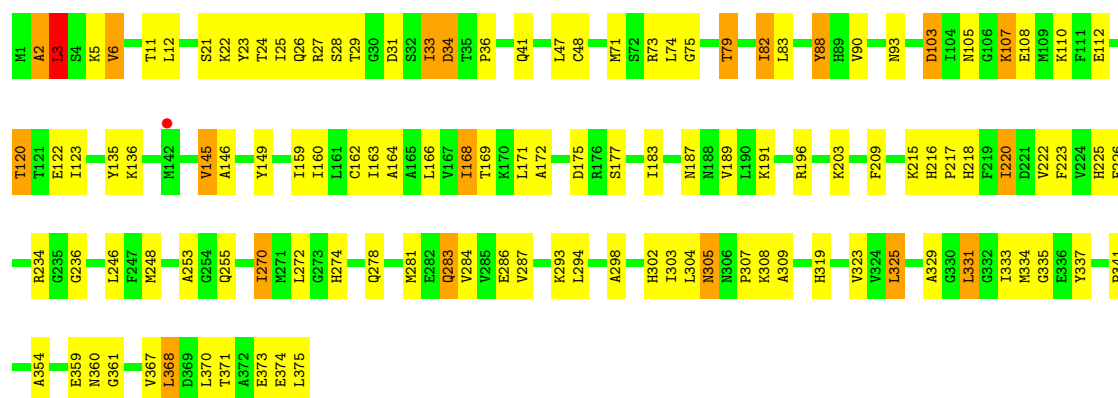
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AP:



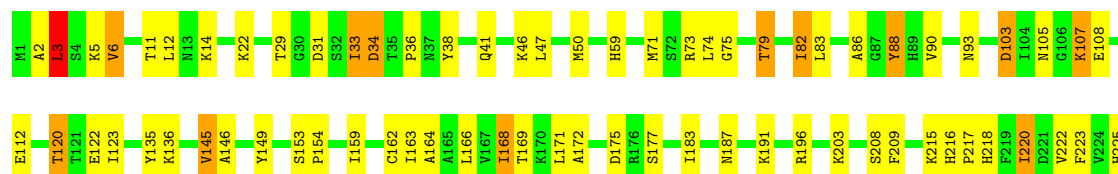
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AQ:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

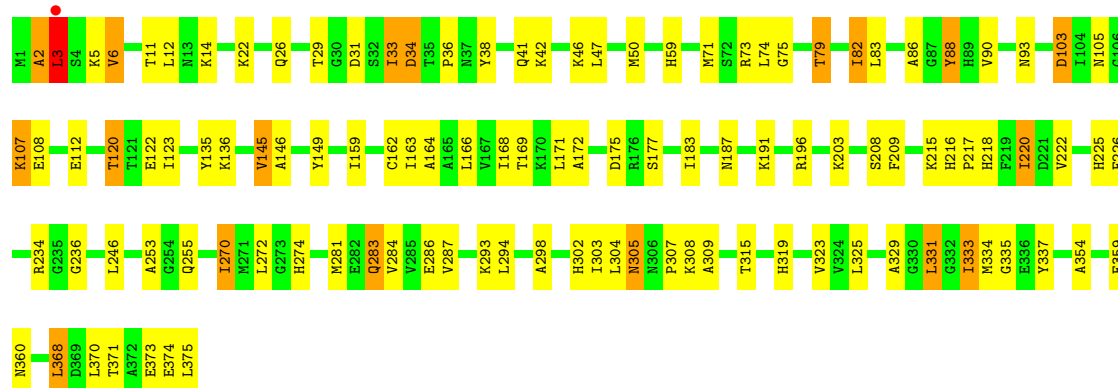
Chain AR:





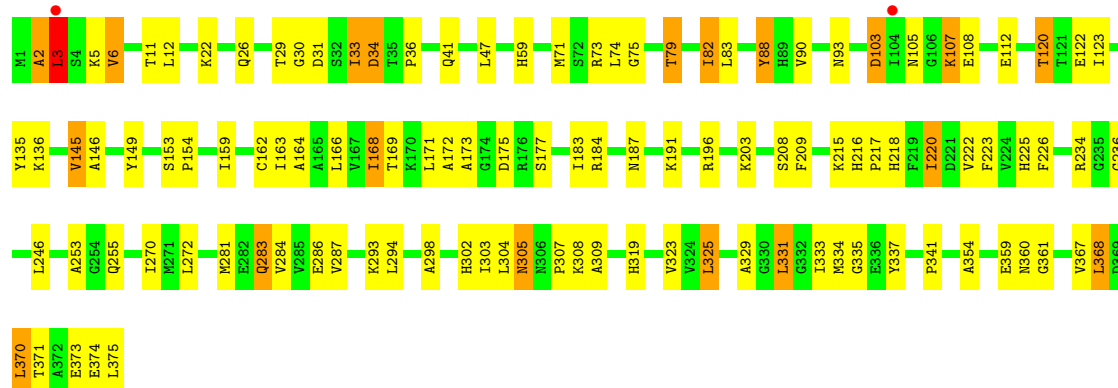
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AS:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

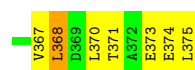
Chain AT:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

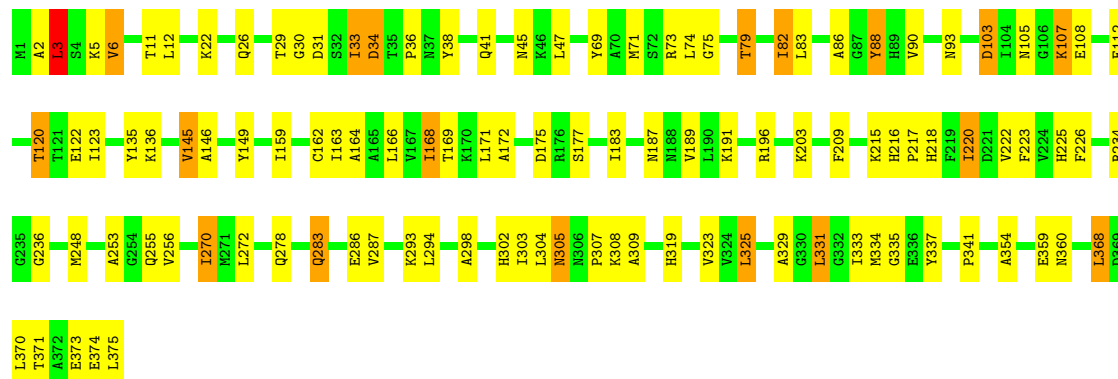
Chain AU:





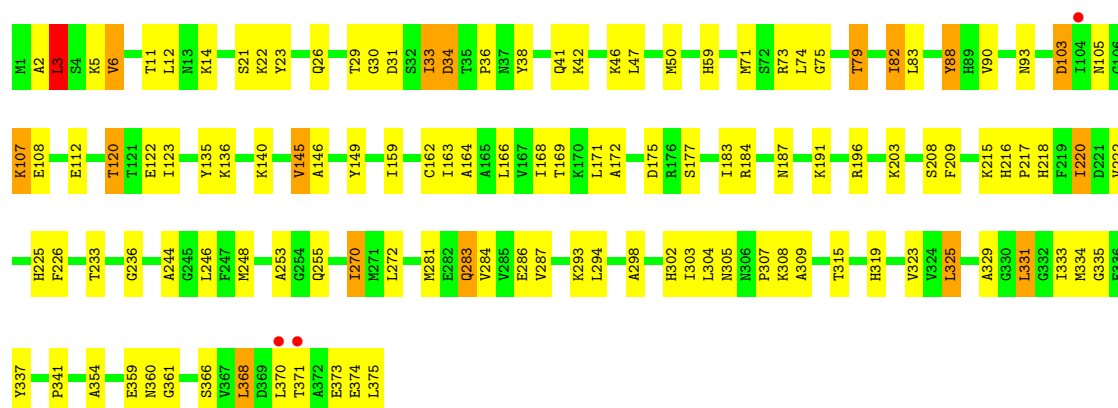
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain AV:



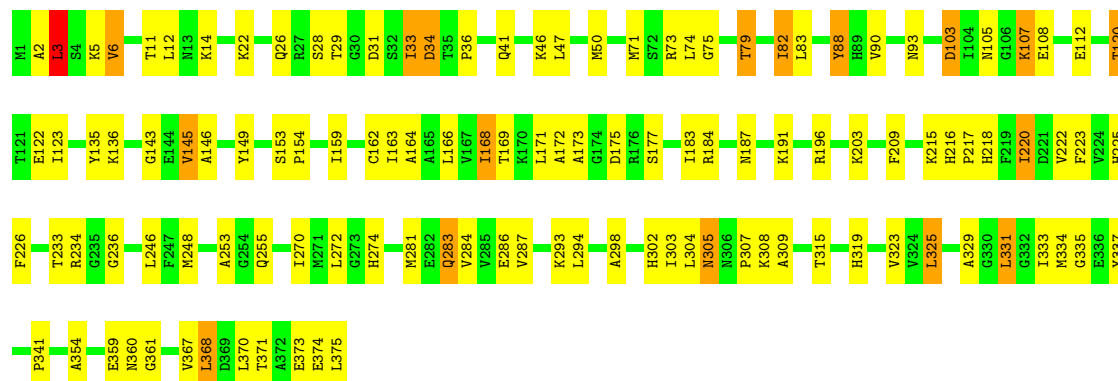
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BA:

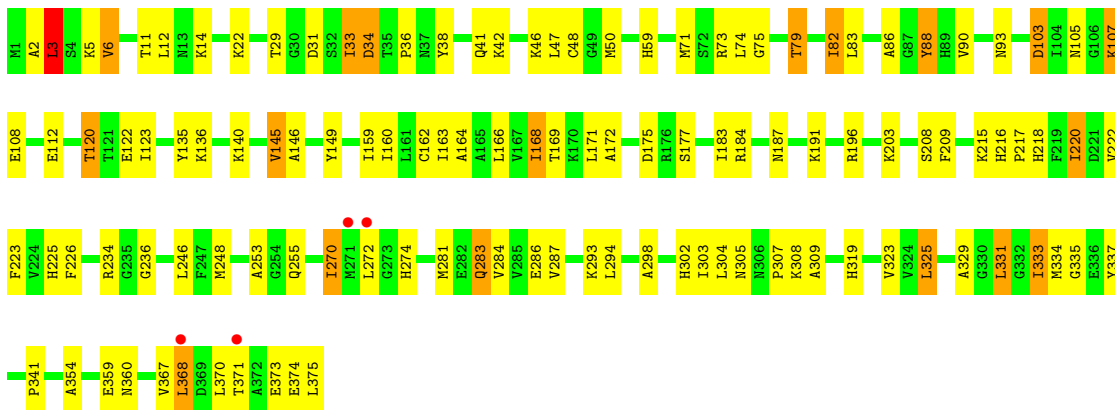


• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

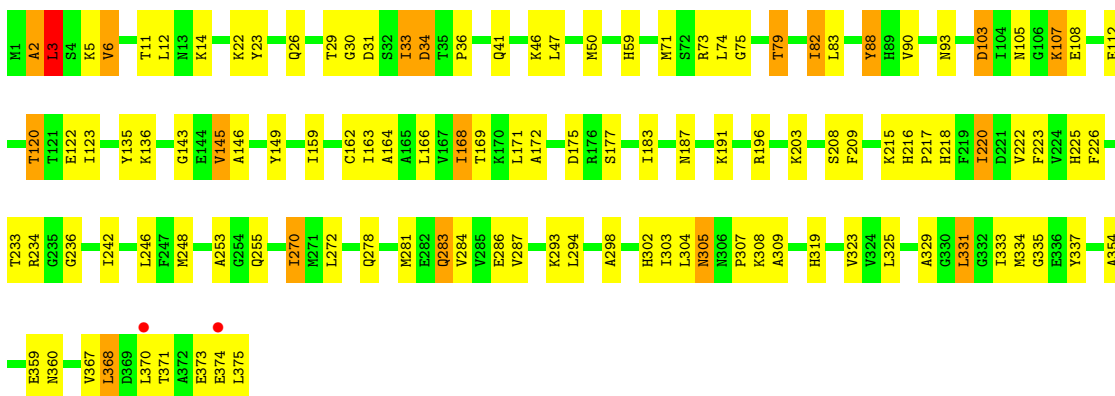
Chain BB:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

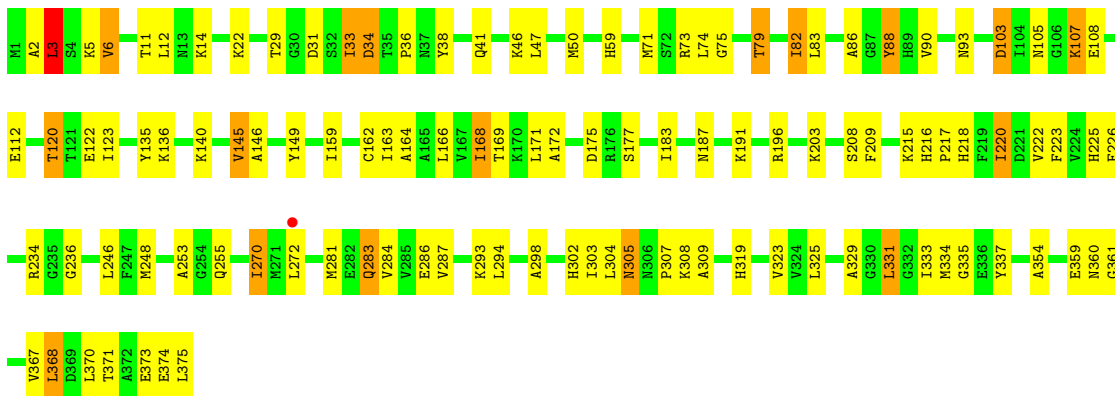


● Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN



- Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Age Group	Percentage
18-24	35%
25-34	25%
35-44	20%
45-54	10%
55-64	5%
65-74	2%
75-84	1%
85+	1%



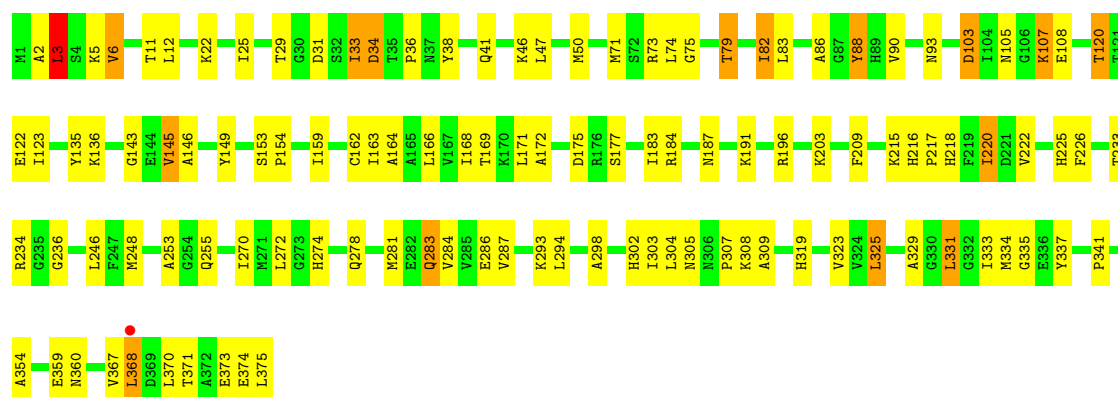
● Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN





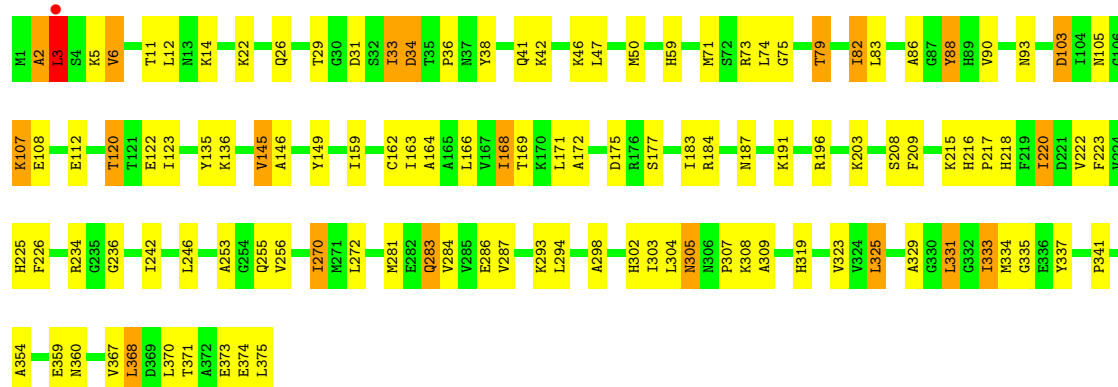
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BG:



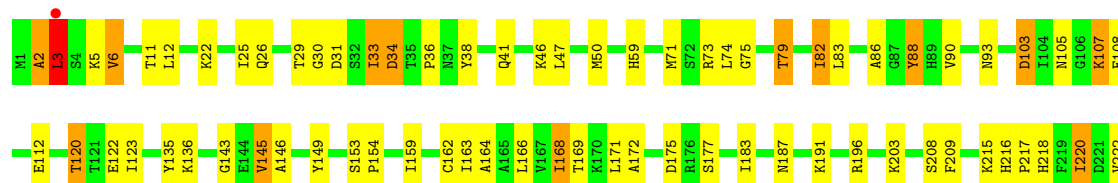
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

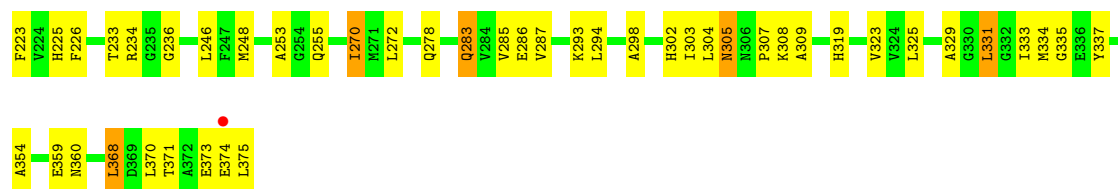
Chain BH:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

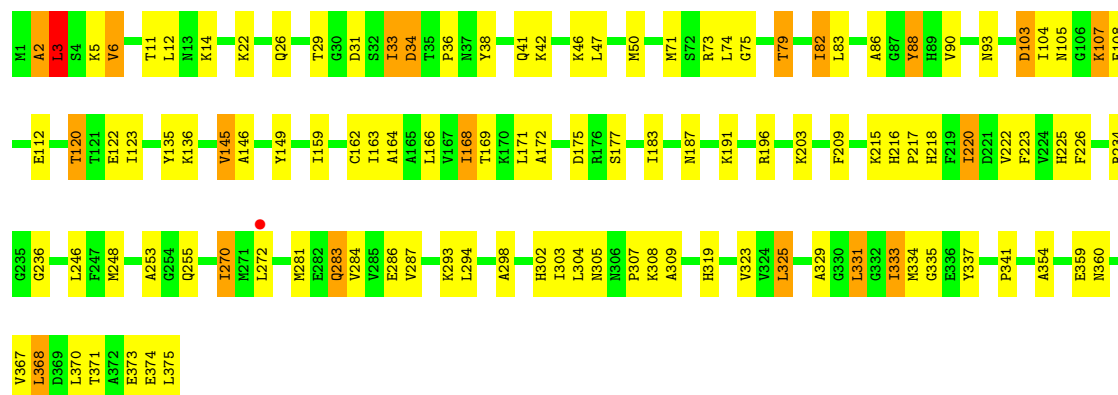
Chain BI:





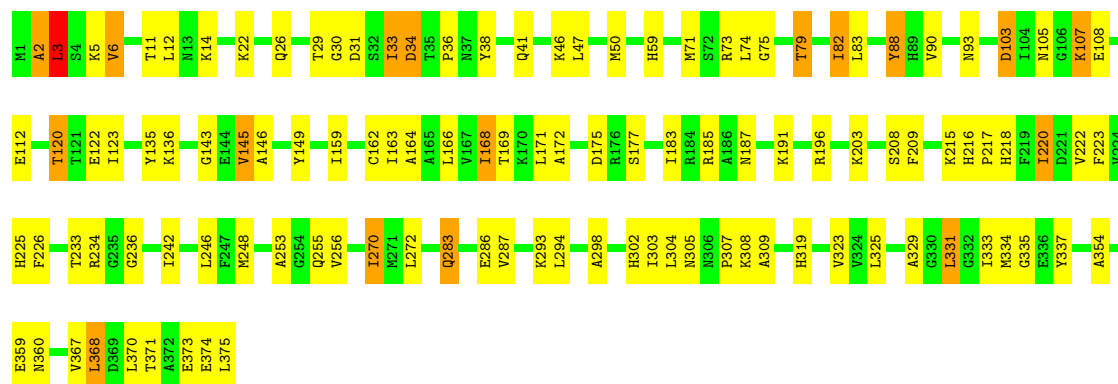
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

Chain BJ:



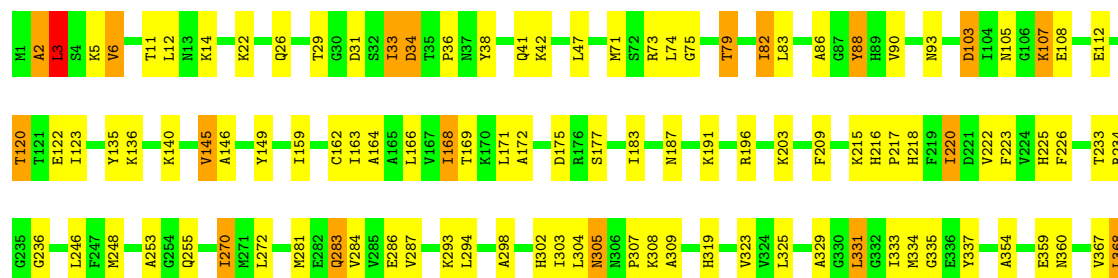
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Chain BK:




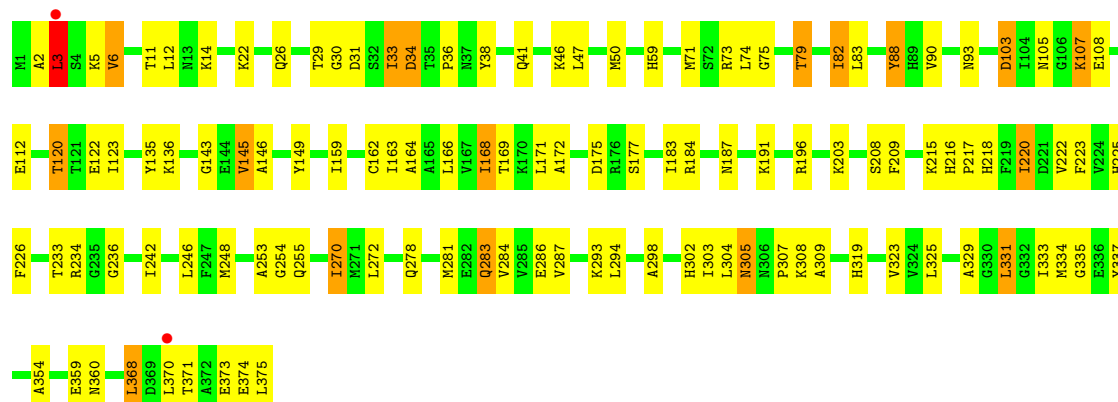
• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

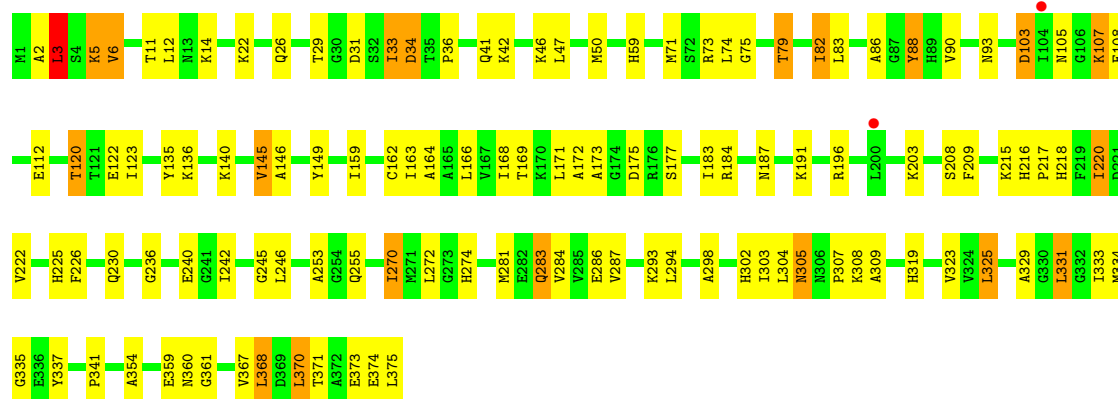
Chain BL:



• Molecule 1: RESPIRATORY SYNCYTIAL VIRUS NUCLEOCAPSID PROTEIN

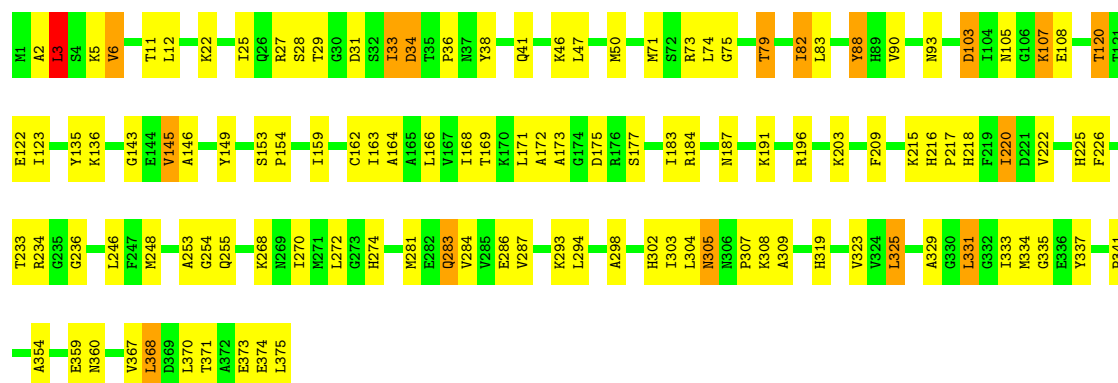
Chain BP: 





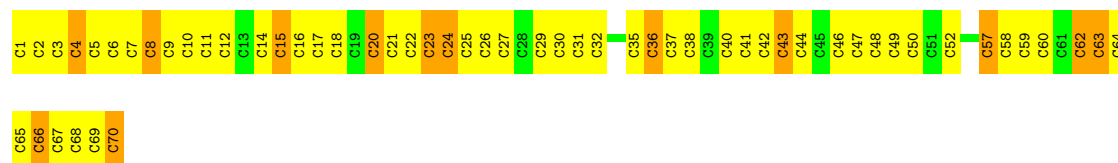
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Chain BZ:



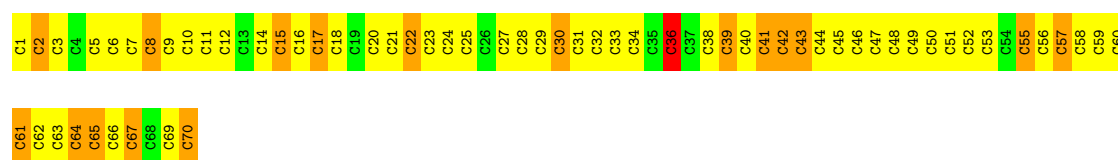
• Molecule 2: RNA

Chain AK:



• Molecule 2: RNA

Chain AM:




• Molecule 2: RNA

Chain BR:





● Molecule 2: RNA

Chain BX: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0070	Depositor
R, R_{free}	0.234 , 0.269 0.273 , 0.274	Depositor DCC
R_{free} test set	12956 reflections (5.29%)	DCC
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 , 65.8	EDS
Estimated twinning fraction	0.297 for h,-k,-l 0.058 for -h,k,-l 0.057 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 258134 reflections	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.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AG	2920	0	2955	80	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 3044 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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%)	50	92
1	AB	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	AC	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	AD	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AE	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	AF	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AG	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AH	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AI	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	AJ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AL	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	AN	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AO	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AP	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	AQ	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AR	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AS	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	AT	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AU	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	AV	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BA	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BB	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BC	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BD	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BE	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BF	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BG	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BH	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BI	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BJ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BK	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BL	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BM	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BN	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BO	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BP	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BQ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BW	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
1	BY	373/375 (100%)	360 (96%)	12 (3%)	1 (0%)	50	92
1	BZ	373/375 (100%)	361 (97%)	11 (3%)	1 (0%)	50	92
All	All	14920/15000 (100%)	14421 (97%)	459 (3%)	40 (0%)	50	92

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 ⓘ

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%)	5	28
1	AB	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AC	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AD	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AE	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AF	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AG	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AH	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	AI	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AJ	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AL	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AN	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AO	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AP	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AQ	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AR	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	AS	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AT	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AU	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	AV	313/313 (100%)	268 (86%)	45 (14%)	5	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	BB	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BC	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	BD	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BE	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BF	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BG	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	BH	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BI	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BJ	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	BK	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	BL	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BM	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BN	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BO	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	BP	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BQ	313/313 (100%)	269 (86%)	44 (14%)	5	30
1	BW	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BY	313/313 (100%)	268 (86%)	45 (14%)	5	28
1	BZ	313/313 (100%)	268 (86%)	45 (14%)	5	28
All	All	12520/12520 (100%)	10729 (86%)	1791 (14%)	5	29

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

Mol	Chain	Res	Type
1	AU	6	VAL
1	BC	103	ASP
1	BQ	375	LEU
1	AU	220	ILE
1	BA	82	ILE

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

Mol	Chain	Res	Type
1	AV	216	HIS
1	BD	216	HIS
1	BQ	216	HIS
1	BA	151	HIS
1	BB	216	HIS

5.3.3 RNA ⓘ

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	23	C
2	BR	25	C
2	BX	25	C
2	BR	11	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.04	0 100 100	77, 135, 189, 218	0
1	AB	375/375 (100%)	-0.04	0 100 100	77, 135, 189, 218	0
1	AC	375/375 (100%)	-0.01	2 (0%) 88 71	77, 135, 189, 218	0
1	AD	375/375 (100%)	0.01	0 100 100	77, 135, 189, 218	0
1	AE	375/375 (100%)	-0.04	1 (0%) 91 81	77, 135, 189, 218	0
1	AF	375/375 (100%)	0.02	8 (2%) 60 35	77, 135, 189, 218	0
1	AG	375/375 (100%)	-0.11	0 100 100	77, 135, 189, 218	0
1	AH	375/375 (100%)	-0.09	1 (0%) 91 81	77, 135, 189, 218	0
1	AI	375/375 (100%)	0.02	1 (0%) 91 81	77, 135, 189, 218	0
1	AJ	375/375 (100%)	-0.04	1 (0%) 91 81	77, 135, 189, 218	0
1	AL	375/375 (100%)	-0.01	3 (0%) 83 60	77, 135, 189, 218	0
1	AN	375/375 (100%)	-0.07	0 100 100	77, 135, 189, 218	0
1	AO	375/375 (100%)	-0.04	1 (0%) 91 81	77, 135, 189, 218	0
1	AP	375/375 (100%)	-0.01	0 100 100	77, 135, 189, 218	0
1	AQ	375/375 (100%)	-0.00	1 (0%) 91 81	77, 135, 189, 218	0
1	AR	375/375 (100%)	-0.02	0 100 100	77, 135, 189, 218	0
1	AS	375/375 (100%)	-0.10	1 (0%) 91 81	77, 135, 189, 218	0
1	AT	375/375 (100%)	-0.06	2 (0%) 88 71	77, 135, 189, 218	0
1	AU	375/375 (100%)	0.02	0 100 100	77, 135, 189, 218	0
1	AV	375/375 (100%)	-0.05	0 100 100	77, 135, 189, 218	0
1	BA	375/375 (100%)	0.01	3 (0%) 83 60	77, 135, 189, 218	0
1	BB	375/375 (100%)	-0.05	0 100 100	77, 135, 189, 218	0
1	BC	375/375 (100%)	0.03	4 (1%) 77 50	77, 135, 189, 218	0
1	BD	375/375 (100%)	0.01	2 (0%) 88 71	77, 135, 189, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	BE	375/375 (100%)	-0.04	1 (0%) 91 81	77, 135, 189, 218	0
1	BF	375/375 (100%)	-0.08	3 (0%) 83 60	77, 135, 189, 218	0
1	BG	375/375 (100%)	-0.06	1 (0%) 91 81	77, 135, 189, 218	0
1	BH	375/375 (100%)	0.02	1 (0%) 91 81	77, 135, 189, 218	0
1	BI	375/375 (100%)	0.00	2 (0%) 88 71	77, 135, 189, 218	0
1	BJ	375/375 (100%)	0.01	1 (0%) 91 81	77, 135, 189, 218	0
1	BK	375/375 (100%)	-0.00	0 100 100	77, 135, 189, 218	0
1	BL	375/375 (100%)	-0.01	1 (0%) 91 81	77, 135, 189, 218	0
1	BM	375/375 (100%)	-0.07	4 (1%) 77 50	77, 135, 189, 218	0
1	BN	375/375 (100%)	-0.04	1 (0%) 91 81	77, 135, 189, 218	0
1	BO	375/375 (100%)	0.05	4 (1%) 77 50	77, 135, 189, 218	0
1	BP	375/375 (100%)	0.01	2 (0%) 88 71	77, 135, 189, 218	0
1	BQ	375/375 (100%)	-0.03	1 (0%) 91 81	77, 135, 189, 218	0
1	BW	375/375 (100%)	-0.04	0 100 100	77, 135, 189, 218	0
1	BY	375/375 (100%)	-0.04	2 (0%) 88 71	77, 135, 189, 218	0
1	BZ	375/375 (100%)	-0.06	0 100 100	77, 135, 189, 218	0
2	AK	70/70 (100%)	-0.33	0 100 100	120, 142, 159, 163	0
2	AM	70/70 (100%)	-0.30	0 100 100	112, 143, 161, 165	0
2	BR	70/70 (100%)	-0.28	0 100 100	129, 145, 158, 162	0
2	BX	70/70 (100%)	-0.30	0 100 100	119, 145, 156, 159	0
All	All	15280/15280 (100%)	-0.03	55 (0%) 90 76	77, 136, 189, 218	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AF	368	LEU	5.8
1	BM	374	GLU	4.5
1	BC	272	LEU	3.6
1	AL	368	LEU	3.4
1	AF	369	ASP	3.4

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.