wwPDB X-ray Structure Validation Summary Report (i)

May 29, 2020 – 06:35 am BST

PDB ID	:	4XJN
Title	:	Structure of the parainfluenza virus 5 nucleocapsid-RNA complex: an insight into paramyxovirus polymerase activity
Authors	:	Alayyoubi, M.; Leser, G.P.; Kors, C.A.; Lamb, R.A.
Deposited on	:	2015-01-08
Resolution	:	3.11 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 following versions of software and data (see references (1)) were used in the production of this report:

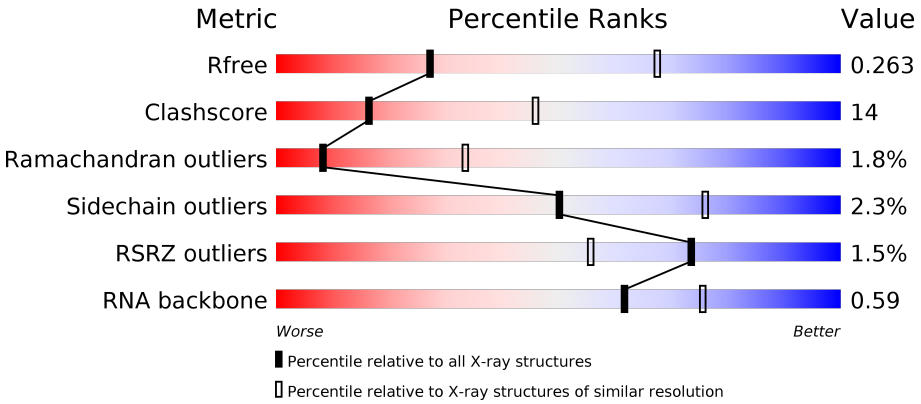
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)

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 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	A	525	2% 50% 23% • 25%
1	B	525	% 52% 22% • 25%
1	C	525	% 49% 24% • 25%
1	D	525	% 51% 23% • 25%

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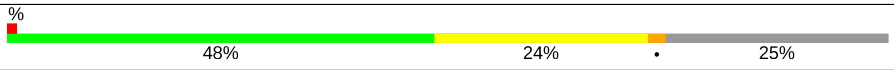
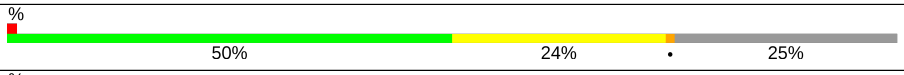
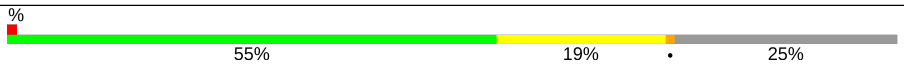
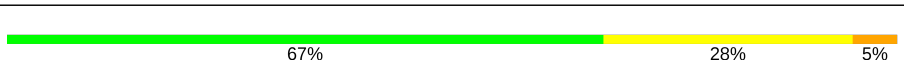
Mol	Chain	Length	Quality of chain
1	E	525	
1	F	525	
1	G	525	
1	H	525	
1	I	525	
1	J	525	
1	K	525	
1	L	525	
1	M	525	
2	N	78	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 42329 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 Nucleocapsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	B	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	C	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	D	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	E	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	F	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	G	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	H	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	I	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	J	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	K	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	L	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			
1	M	395	Total	C	N	O	S	16	0	0
			3135	1992	541	579	23			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	HIS	-	expression tag	UNP W5QKM4
A	-14	HIS	-	expression tag	UNP W5QKM4
A	-13	HIS	-	expression tag	UNP W5QKM4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	HIS	-	expression tag	UNP W5QKM4
A	-11	HIS	-	expression tag	UNP W5QKM4
A	-10	HIS	-	expression tag	UNP W5QKM4
A	-9	SER	-	expression tag	UNP W5QKM4
A	-8	SER	-	expression tag	UNP W5QKM4
A	-7	GLY	-	expression tag	UNP W5QKM4
A	-6	LEU	-	expression tag	UNP W5QKM4
A	-5	VAL	-	expression tag	UNP W5QKM4
A	-4	PRO	-	expression tag	UNP W5QKM4
A	-3	ARG	-	expression tag	UNP W5QKM4
A	-2	GLY	-	expression tag	UNP W5QKM4
A	-1	SER	-	expression tag	UNP W5QKM4
A	0	HIS	-	expression tag	UNP W5QKM4
B	-15	HIS	-	expression tag	UNP W5QKM4
B	-14	HIS	-	expression tag	UNP W5QKM4
B	-13	HIS	-	expression tag	UNP W5QKM4
B	-12	HIS	-	expression tag	UNP W5QKM4
B	-11	HIS	-	expression tag	UNP W5QKM4
B	-10	HIS	-	expression tag	UNP W5QKM4
B	-9	SER	-	expression tag	UNP W5QKM4
B	-8	SER	-	expression tag	UNP W5QKM4
B	-7	GLY	-	expression tag	UNP W5QKM4
B	-6	LEU	-	expression tag	UNP W5QKM4
B	-5	VAL	-	expression tag	UNP W5QKM4
B	-4	PRO	-	expression tag	UNP W5QKM4
B	-3	ARG	-	expression tag	UNP W5QKM4
B	-2	GLY	-	expression tag	UNP W5QKM4
B	-1	SER	-	expression tag	UNP W5QKM4
B	0	HIS	-	expression tag	UNP W5QKM4
C	-15	HIS	-	expression tag	UNP W5QKM4
C	-14	HIS	-	expression tag	UNP W5QKM4
C	-13	HIS	-	expression tag	UNP W5QKM4
C	-12	HIS	-	expression tag	UNP W5QKM4
C	-11	HIS	-	expression tag	UNP W5QKM4
C	-10	HIS	-	expression tag	UNP W5QKM4
C	-9	SER	-	expression tag	UNP W5QKM4
C	-8	SER	-	expression tag	UNP W5QKM4
C	-7	GLY	-	expression tag	UNP W5QKM4
C	-6	LEU	-	expression tag	UNP W5QKM4
C	-5	VAL	-	expression tag	UNP W5QKM4
C	-4	PRO	-	expression tag	UNP W5QKM4
C	-3	ARG	-	expression tag	UNP W5QKM4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP W5QKM4
C	-1	SER	-	expression tag	UNP W5QKM4
C	0	HIS	-	expression tag	UNP W5QKM4
D	-15	HIS	-	expression tag	UNP W5QKM4
D	-14	HIS	-	expression tag	UNP W5QKM4
D	-13	HIS	-	expression tag	UNP W5QKM4
D	-12	HIS	-	expression tag	UNP W5QKM4
D	-11	HIS	-	expression tag	UNP W5QKM4
D	-10	HIS	-	expression tag	UNP W5QKM4
D	-9	SER	-	expression tag	UNP W5QKM4
D	-8	SER	-	expression tag	UNP W5QKM4
D	-7	GLY	-	expression tag	UNP W5QKM4
D	-6	LEU	-	expression tag	UNP W5QKM4
D	-5	VAL	-	expression tag	UNP W5QKM4
D	-4	PRO	-	expression tag	UNP W5QKM4
D	-3	ARG	-	expression tag	UNP W5QKM4
D	-2	GLY	-	expression tag	UNP W5QKM4
D	-1	SER	-	expression tag	UNP W5QKM4
D	0	HIS	-	expression tag	UNP W5QKM4
E	-15	HIS	-	expression tag	UNP W5QKM4
E	-14	HIS	-	expression tag	UNP W5QKM4
E	-13	HIS	-	expression tag	UNP W5QKM4
E	-12	HIS	-	expression tag	UNP W5QKM4
E	-11	HIS	-	expression tag	UNP W5QKM4
E	-10	HIS	-	expression tag	UNP W5QKM4
E	-9	SER	-	expression tag	UNP W5QKM4
E	-8	SER	-	expression tag	UNP W5QKM4
E	-7	GLY	-	expression tag	UNP W5QKM4
E	-6	LEU	-	expression tag	UNP W5QKM4
E	-5	VAL	-	expression tag	UNP W5QKM4
E	-4	PRO	-	expression tag	UNP W5QKM4
E	-3	ARG	-	expression tag	UNP W5QKM4
E	-2	GLY	-	expression tag	UNP W5QKM4
E	-1	SER	-	expression tag	UNP W5QKM4
E	0	HIS	-	expression tag	UNP W5QKM4
F	-15	HIS	-	expression tag	UNP W5QKM4
F	-14	HIS	-	expression tag	UNP W5QKM4
F	-13	HIS	-	expression tag	UNP W5QKM4
F	-12	HIS	-	expression tag	UNP W5QKM4
F	-11	HIS	-	expression tag	UNP W5QKM4
F	-10	HIS	-	expression tag	UNP W5QKM4
F	-9	SER	-	expression tag	UNP W5QKM4

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-8	SER	-	expression tag	UNP W5QKM4
F	-7	GLY	-	expression tag	UNP W5QKM4
F	-6	LEU	-	expression tag	UNP W5QKM4
F	-5	VAL	-	expression tag	UNP W5QKM4
F	-4	PRO	-	expression tag	UNP W5QKM4
F	-3	ARG	-	expression tag	UNP W5QKM4
F	-2	GLY	-	expression tag	UNP W5QKM4
F	-1	SER	-	expression tag	UNP W5QKM4
F	0	HIS	-	expression tag	UNP W5QKM4
G	-15	HIS	-	expression tag	UNP W5QKM4
G	-14	HIS	-	expression tag	UNP W5QKM4
G	-13	HIS	-	expression tag	UNP W5QKM4
G	-12	HIS	-	expression tag	UNP W5QKM4
G	-11	HIS	-	expression tag	UNP W5QKM4
G	-10	HIS	-	expression tag	UNP W5QKM4
G	-9	SER	-	expression tag	UNP W5QKM4
G	-8	SER	-	expression tag	UNP W5QKM4
G	-7	GLY	-	expression tag	UNP W5QKM4
G	-6	LEU	-	expression tag	UNP W5QKM4
G	-5	VAL	-	expression tag	UNP W5QKM4
G	-4	PRO	-	expression tag	UNP W5QKM4
G	-3	ARG	-	expression tag	UNP W5QKM4
G	-2	GLY	-	expression tag	UNP W5QKM4
G	-1	SER	-	expression tag	UNP W5QKM4
G	0	HIS	-	expression tag	UNP W5QKM4
H	-15	HIS	-	expression tag	UNP W5QKM4
H	-14	HIS	-	expression tag	UNP W5QKM4
H	-13	HIS	-	expression tag	UNP W5QKM4
H	-12	HIS	-	expression tag	UNP W5QKM4
H	-11	HIS	-	expression tag	UNP W5QKM4
H	-10	HIS	-	expression tag	UNP W5QKM4
H	-9	SER	-	expression tag	UNP W5QKM4
H	-8	SER	-	expression tag	UNP W5QKM4
H	-7	GLY	-	expression tag	UNP W5QKM4
H	-6	LEU	-	expression tag	UNP W5QKM4
H	-5	VAL	-	expression tag	UNP W5QKM4
H	-4	PRO	-	expression tag	UNP W5QKM4
H	-3	ARG	-	expression tag	UNP W5QKM4
H	-2	GLY	-	expression tag	UNP W5QKM4
H	-1	SER	-	expression tag	UNP W5QKM4
H	0	HIS	-	expression tag	UNP W5QKM4
I	-15	HIS	-	expression tag	UNP W5QKM4

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-14	HIS	-	expression tag	UNP W5QKM4
I	-13	HIS	-	expression tag	UNP W5QKM4
I	-12	HIS	-	expression tag	UNP W5QKM4
I	-11	HIS	-	expression tag	UNP W5QKM4
I	-10	HIS	-	expression tag	UNP W5QKM4
I	-9	SER	-	expression tag	UNP W5QKM4
I	-8	SER	-	expression tag	UNP W5QKM4
I	-7	GLY	-	expression tag	UNP W5QKM4
I	-6	LEU	-	expression tag	UNP W5QKM4
I	-5	VAL	-	expression tag	UNP W5QKM4
I	-4	PRO	-	expression tag	UNP W5QKM4
I	-3	ARG	-	expression tag	UNP W5QKM4
I	-2	GLY	-	expression tag	UNP W5QKM4
I	-1	SER	-	expression tag	UNP W5QKM4
I	0	HIS	-	expression tag	UNP W5QKM4
J	-15	HIS	-	expression tag	UNP W5QKM4
J	-14	HIS	-	expression tag	UNP W5QKM4
J	-13	HIS	-	expression tag	UNP W5QKM4
J	-12	HIS	-	expression tag	UNP W5QKM4
J	-11	HIS	-	expression tag	UNP W5QKM4
J	-10	HIS	-	expression tag	UNP W5QKM4
J	-9	SER	-	expression tag	UNP W5QKM4
J	-8	SER	-	expression tag	UNP W5QKM4
J	-7	GLY	-	expression tag	UNP W5QKM4
J	-6	LEU	-	expression tag	UNP W5QKM4
J	-5	VAL	-	expression tag	UNP W5QKM4
J	-4	PRO	-	expression tag	UNP W5QKM4
J	-3	ARG	-	expression tag	UNP W5QKM4
J	-2	GLY	-	expression tag	UNP W5QKM4
J	-1	SER	-	expression tag	UNP W5QKM4
J	0	HIS	-	expression tag	UNP W5QKM4
K	-15	HIS	-	expression tag	UNP W5QKM4
K	-14	HIS	-	expression tag	UNP W5QKM4
K	-13	HIS	-	expression tag	UNP W5QKM4
K	-12	HIS	-	expression tag	UNP W5QKM4
K	-11	HIS	-	expression tag	UNP W5QKM4
K	-10	HIS	-	expression tag	UNP W5QKM4
K	-9	SER	-	expression tag	UNP W5QKM4
K	-8	SER	-	expression tag	UNP W5QKM4
K	-7	GLY	-	expression tag	UNP W5QKM4
K	-6	LEU	-	expression tag	UNP W5QKM4
K	-5	VAL	-	expression tag	UNP W5QKM4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP W5QKM4
K	-3	ARG	-	expression tag	UNP W5QKM4
K	-2	GLY	-	expression tag	UNP W5QKM4
K	-1	SER	-	expression tag	UNP W5QKM4
K	0	HIS	-	expression tag	UNP W5QKM4
L	-15	HIS	-	expression tag	UNP W5QKM4
L	-14	HIS	-	expression tag	UNP W5QKM4
L	-13	HIS	-	expression tag	UNP W5QKM4
L	-12	HIS	-	expression tag	UNP W5QKM4
L	-11	HIS	-	expression tag	UNP W5QKM4
L	-10	HIS	-	expression tag	UNP W5QKM4
L	-9	SER	-	expression tag	UNP W5QKM4
L	-8	SER	-	expression tag	UNP W5QKM4
L	-7	GLY	-	expression tag	UNP W5QKM4
L	-6	LEU	-	expression tag	UNP W5QKM4
L	-5	VAL	-	expression tag	UNP W5QKM4
L	-4	PRO	-	expression tag	UNP W5QKM4
L	-3	ARG	-	expression tag	UNP W5QKM4
L	-2	GLY	-	expression tag	UNP W5QKM4
L	-1	SER	-	expression tag	UNP W5QKM4
L	0	HIS	-	expression tag	UNP W5QKM4
M	-15	HIS	-	expression tag	UNP W5QKM4
M	-14	HIS	-	expression tag	UNP W5QKM4
M	-13	HIS	-	expression tag	UNP W5QKM4
M	-12	HIS	-	expression tag	UNP W5QKM4
M	-11	HIS	-	expression tag	UNP W5QKM4
M	-10	HIS	-	expression tag	UNP W5QKM4
M	-9	SER	-	expression tag	UNP W5QKM4
M	-8	SER	-	expression tag	UNP W5QKM4
M	-7	GLY	-	expression tag	UNP W5QKM4
M	-6	LEU	-	expression tag	UNP W5QKM4
M	-5	VAL	-	expression tag	UNP W5QKM4
M	-4	PRO	-	expression tag	UNP W5QKM4
M	-3	ARG	-	expression tag	UNP W5QKM4
M	-2	GLY	-	expression tag	UNP W5QKM4
M	-1	SER	-	expression tag	UNP W5QKM4
M	0	HIS	-	expression tag	UNP W5QKM4

- Molecule 2 is a RNA chain called RNA (78-MER).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	78	Total 1560	C 702	N 156	O 624	P 78	0	0	0

- Molecule 3 is LEAD (II) ION (three-letter code: PB) (formula: Pb).

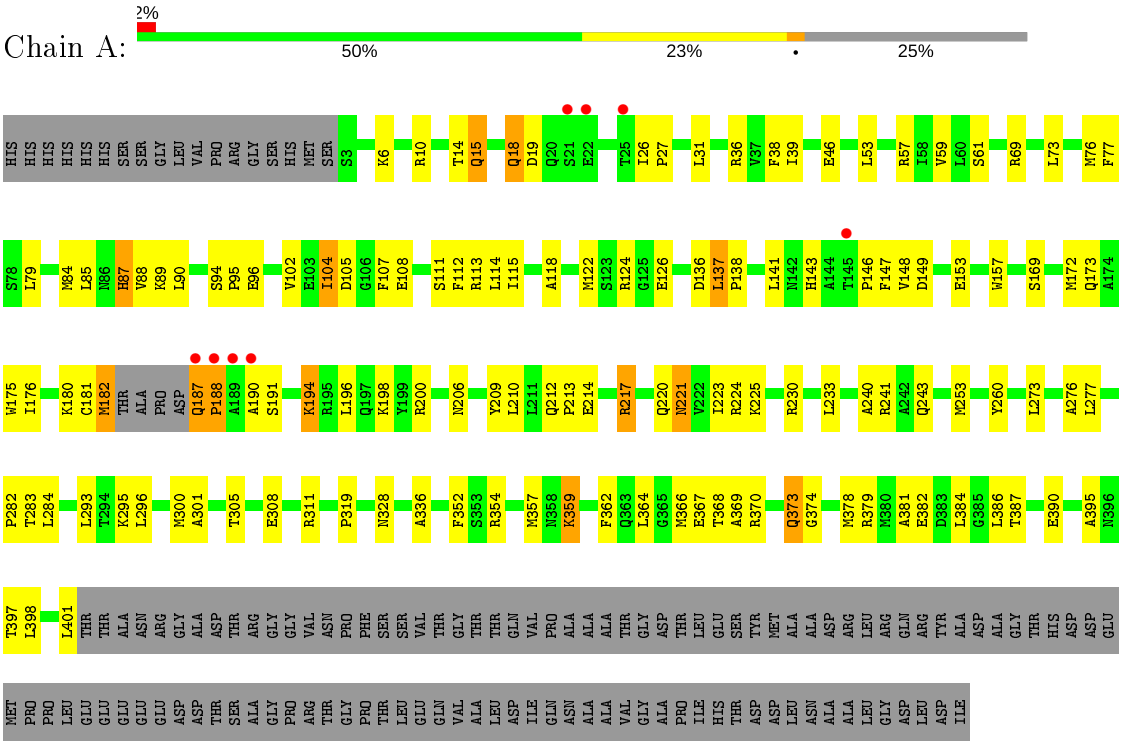
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Pb 1	0	0
3	D	1	Total 1	Pb 1	0	0
3	K	2	Total 2	Pb 2	0	0
3	H	1	Total 1	Pb 1	0	0
3	B	1	Total 1	Pb 1	0	0
3	I	2	Total 2	Pb 2	0	0
3	A	1	Total 1	Pb 1	0	0
3	N	1	Total 1	Pb 1	0	0
3	M	4	Total 4	Pb 4	0	0

3 Residue-property plots (i)

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

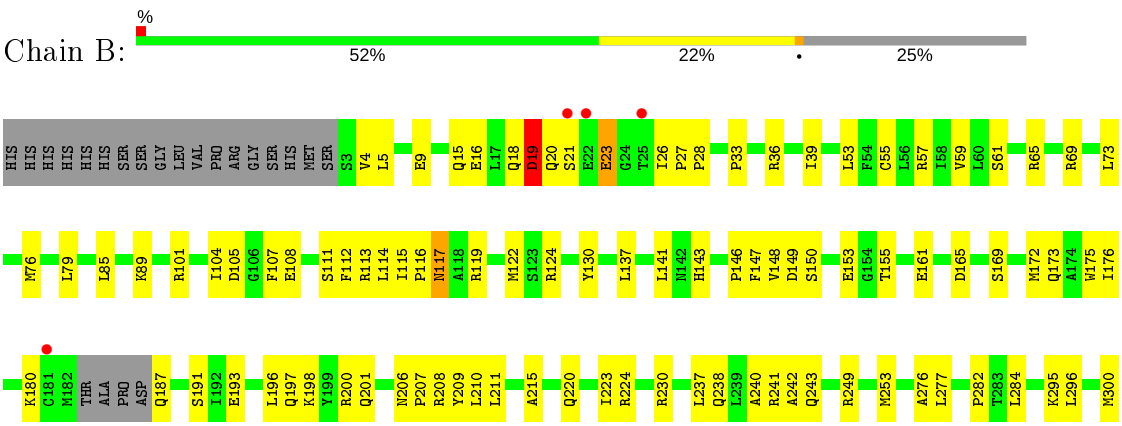
- Molecule 1: Nucleocapsid

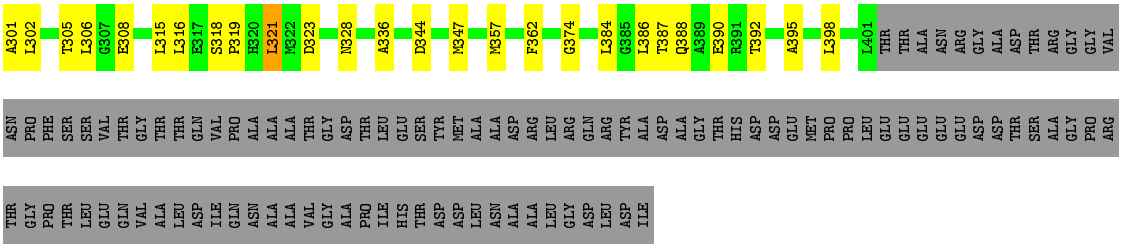
Chain A:



- Molecule 1: Nucleocapsid

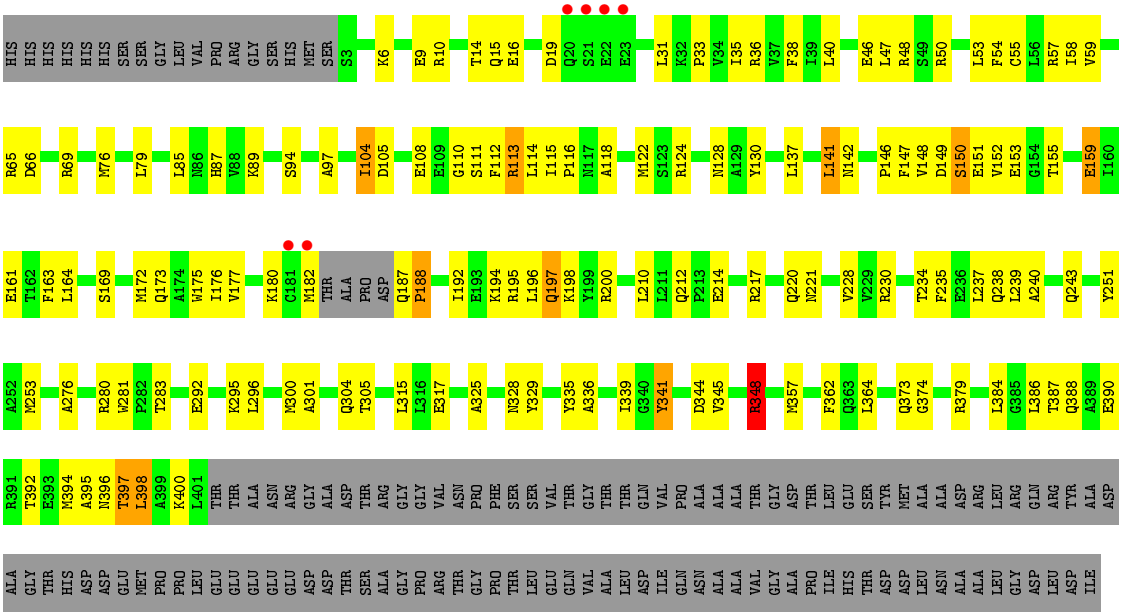
Chain B:





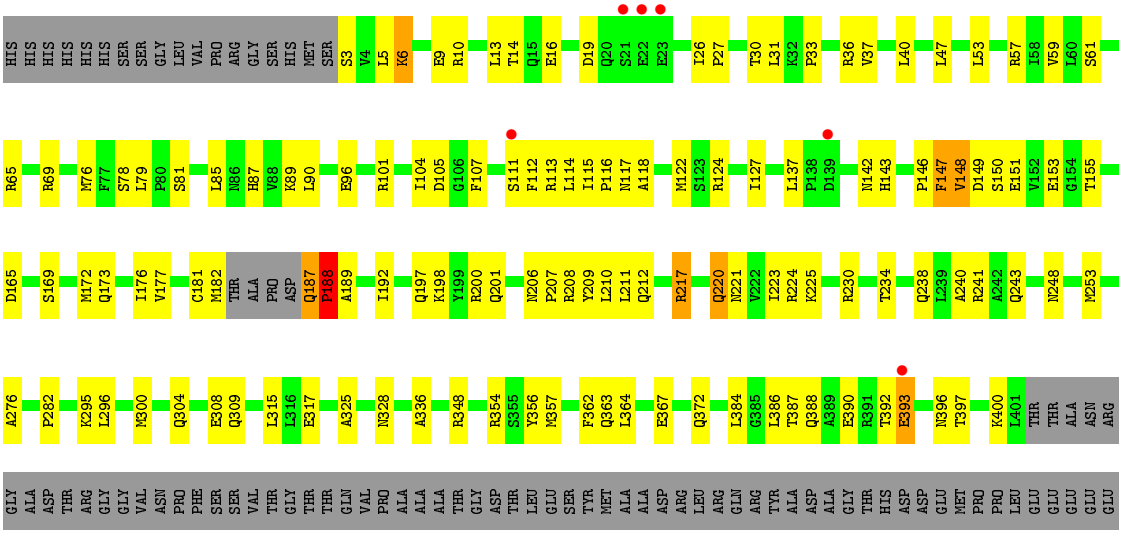
• Molecule 1: Nucleocapsid

Chain C:



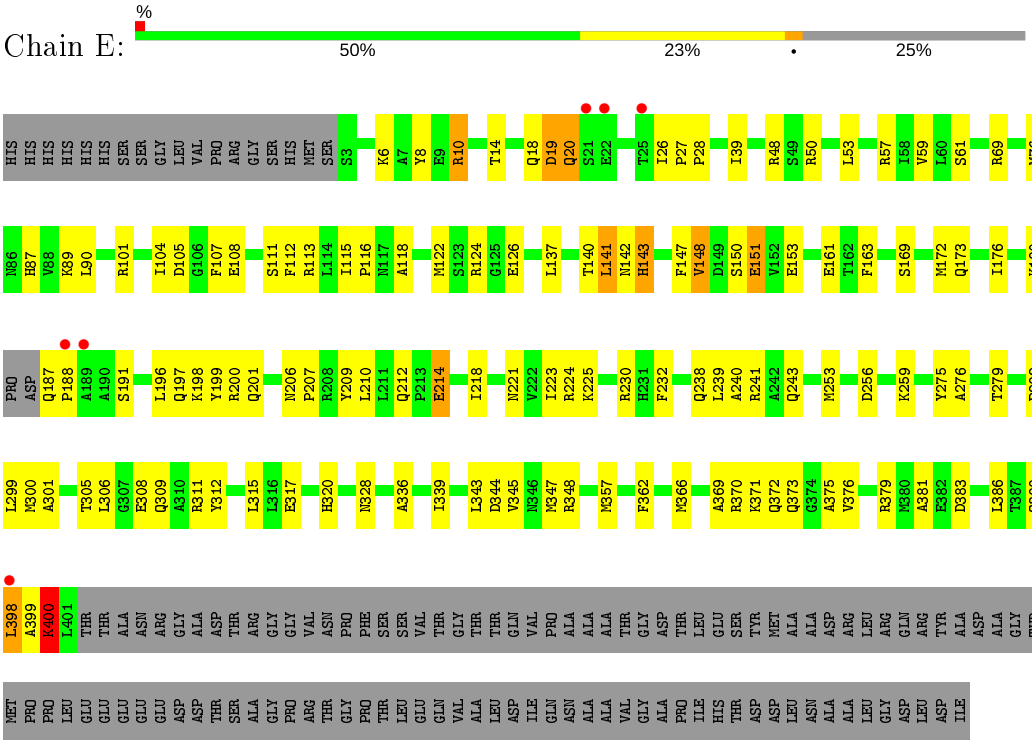
• Molecule 1: Nucleocapsid

Chain D:



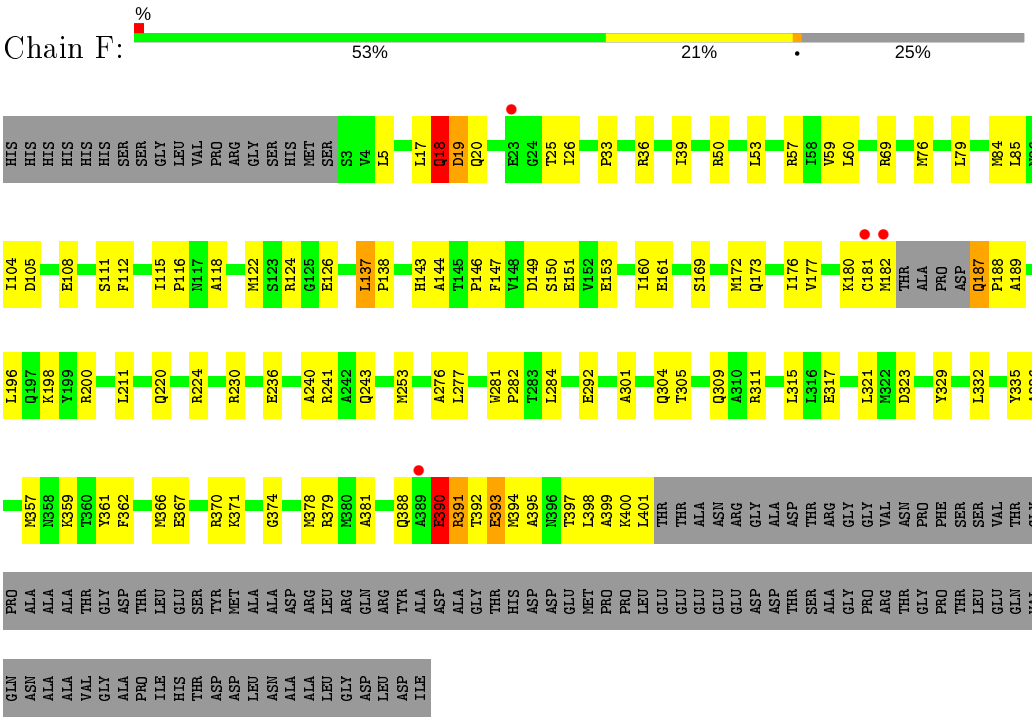
- Molecule 1: Nucleocapsid

Chain E:



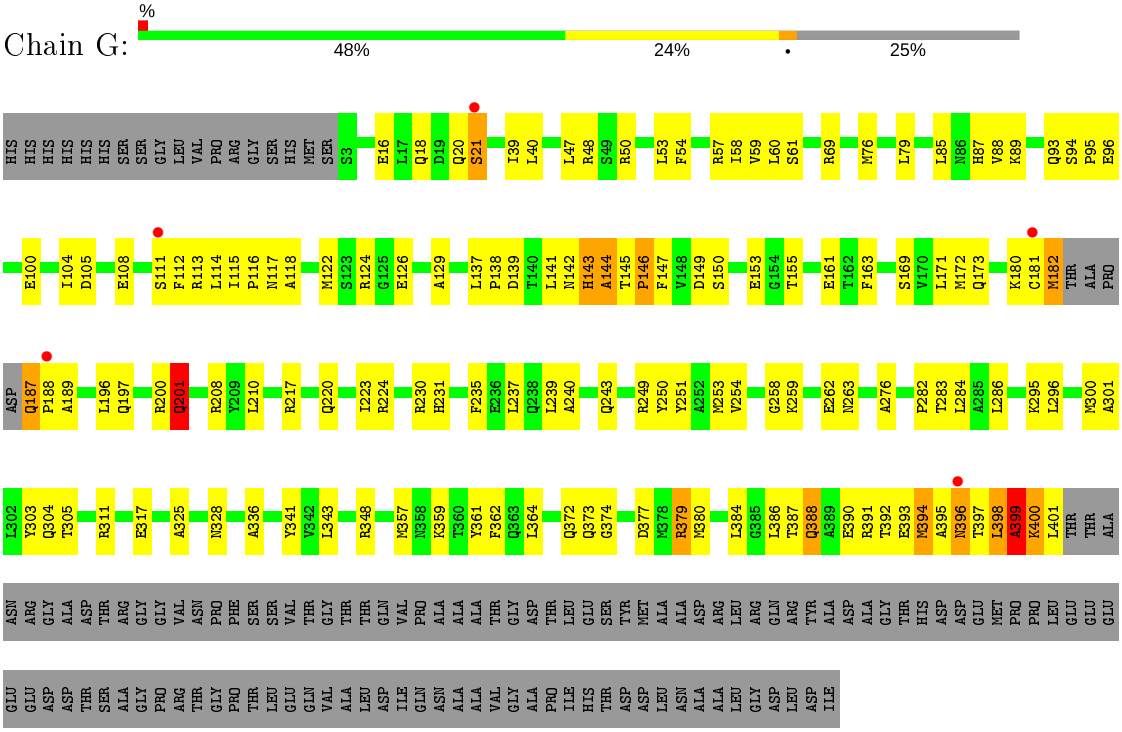
- Molecule 1: Nucleocapsid

Chain F:



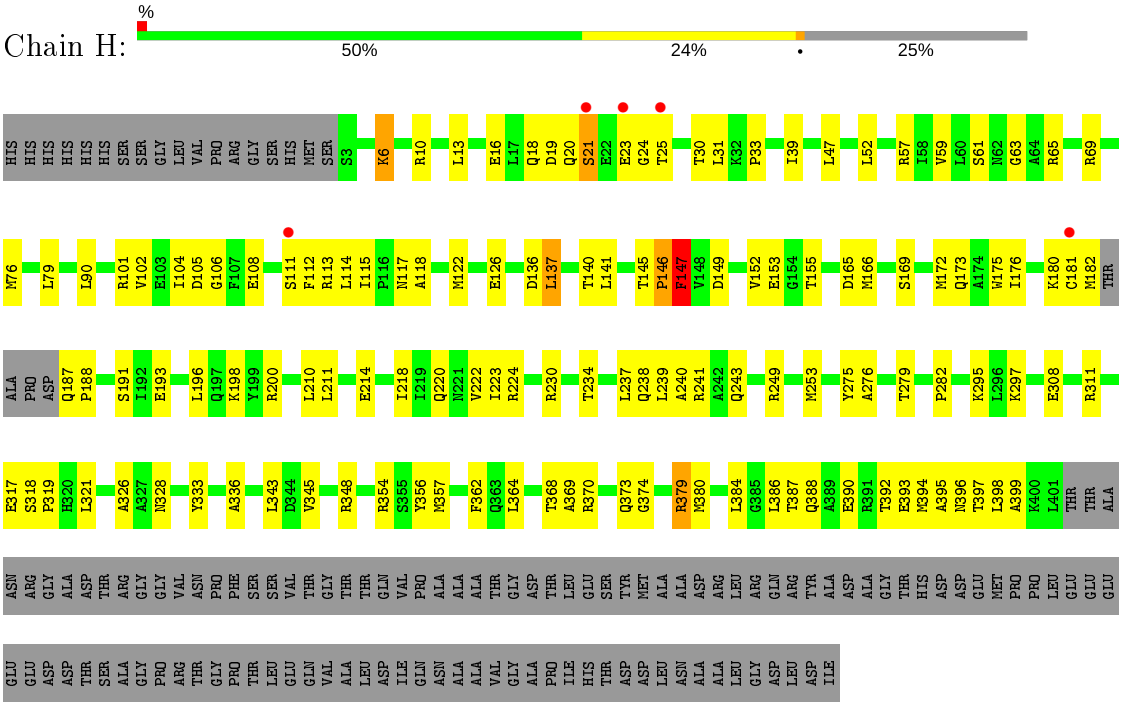
- Molecule 1: Nucleocapsid

Chain G:



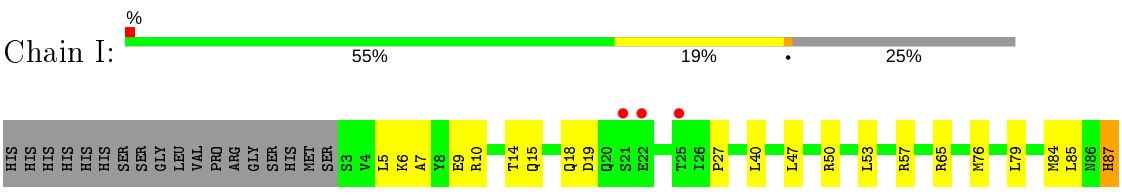
- Molecule 1: Nucleocapsid

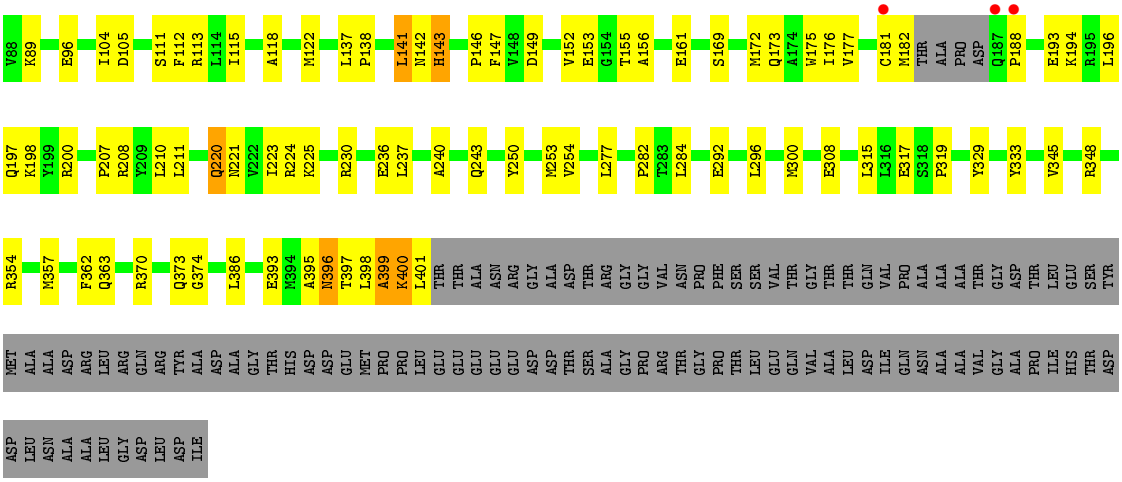
Chain H:



- Molecule 1: Nucleocapsid

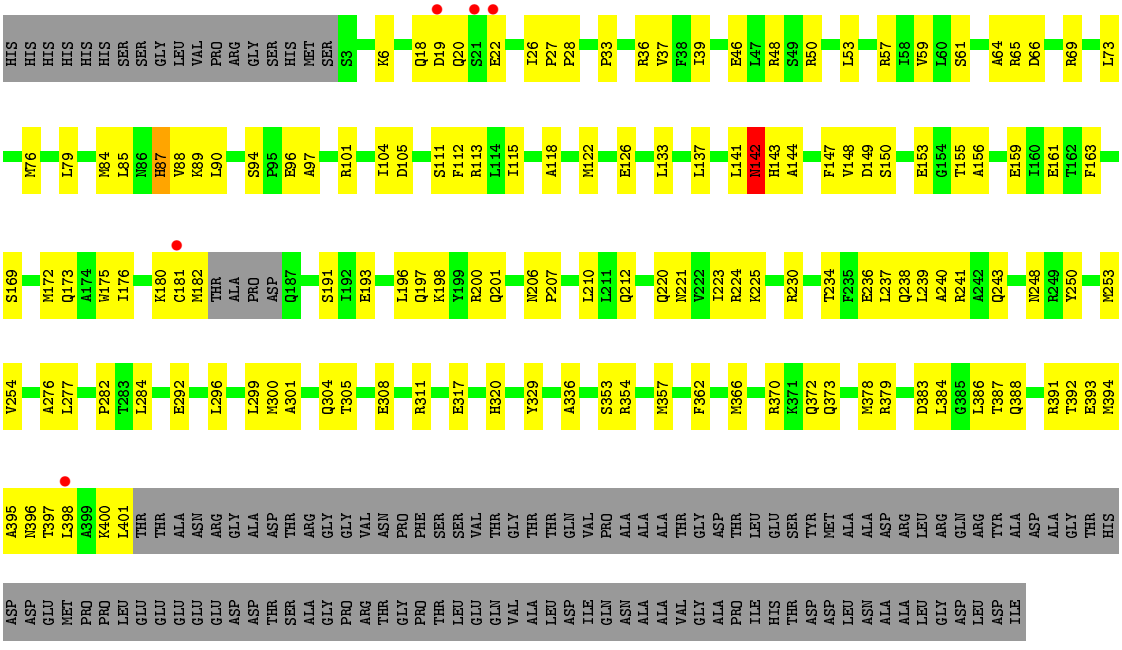
Chain I:





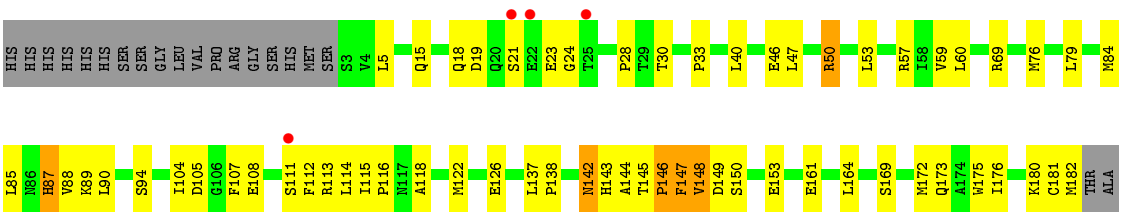
• Molecule 1: Nucleocapsid

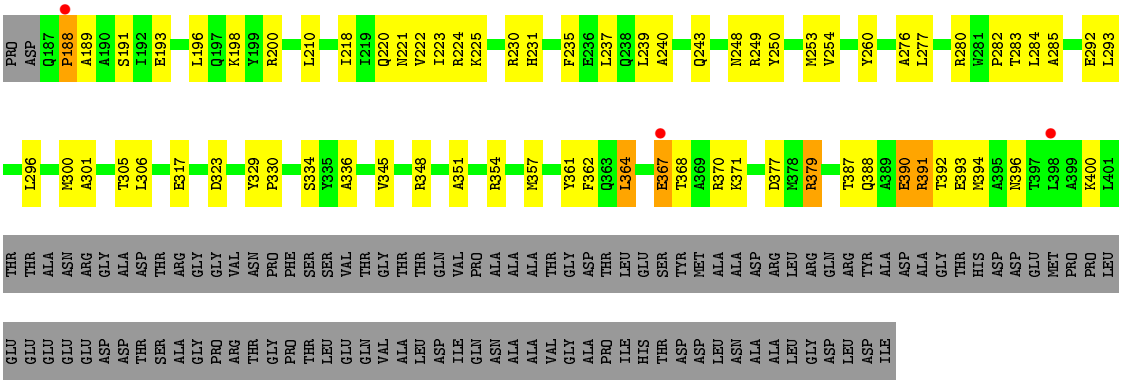
Chain J:



• Molecule 1: Nucleocapsid

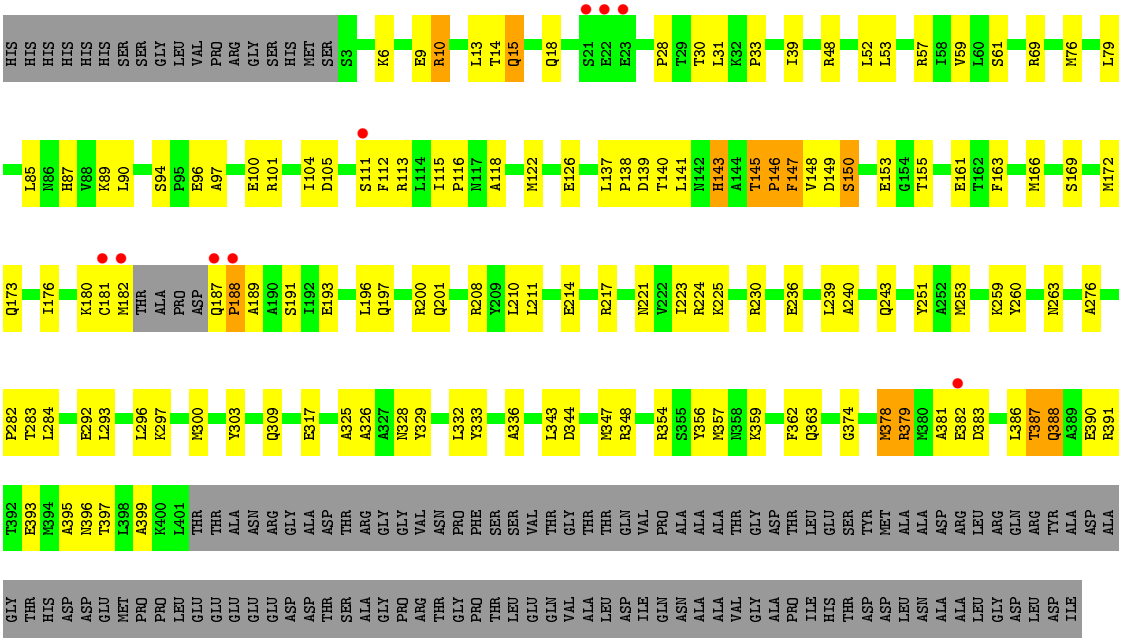
Chain K:





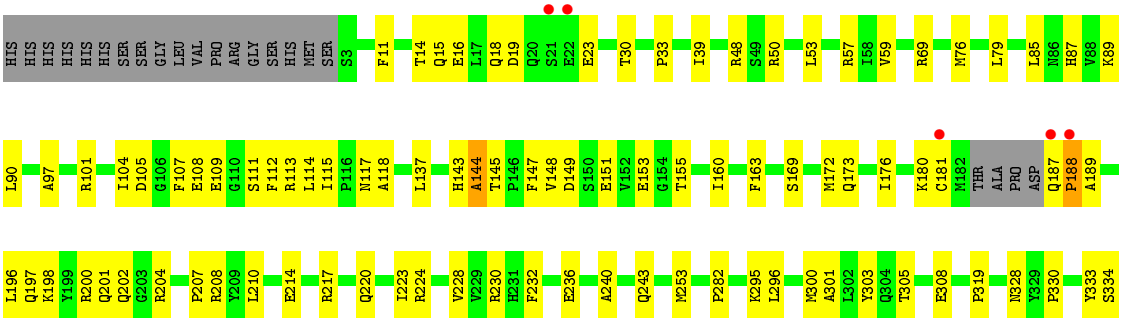
- Molecule 1: Nucleocapsid

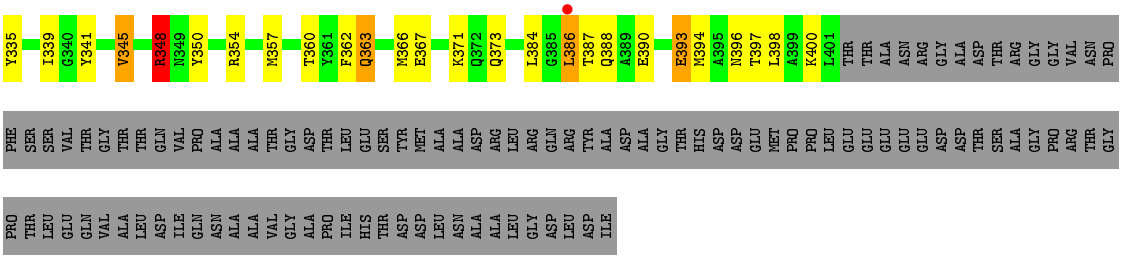
Chain L:



- Molecule 1: Nucleocapsid

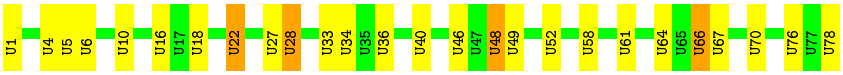
Chain M:





- Molecule 2: RNA (78-MER)

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	205.64Å 309.44Å 233.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.01 – 3.11 45.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.01-3.11) 99.6 (45.01-3.00)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.227 , 0.263 0.227 , 0.263	Depositor DCC
R_{free} test set	7159 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	42329	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.44	0/3194	0.69	2/4316 (0.0%)
1	B	0.44	0/3194	0.67	1/4316 (0.0%)
1	C	0.54	1/3194 (0.0%)	0.74	4/4316 (0.1%)
1	D	0.47	0/3194	0.66	0/4316
1	E	0.46	0/3194	0.72	2/4316 (0.0%)
1	F	0.48	1/3194 (0.0%)	0.71	3/4316 (0.1%)
1	G	0.49	0/3194	0.75	3/4316 (0.1%)
1	H	0.47	0/3194	0.70	2/4316 (0.0%)
1	I	0.45	0/3194	0.67	4/4316 (0.1%)
1	J	0.47	0/3194	0.69	0/4316
1	K	0.48	0/3194	0.69	1/4316 (0.0%)
1	L	0.48	0/3194	0.72	1/4316 (0.0%)
1	M	0.49	0/3194	0.70	3/4316 (0.1%)
2	N	0.42	0/1715	0.97	1/2648 (0.0%)
All	All	0.47	2/43237 (0.0%)	0.72	27/58756 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	2
1	F	0	2
1	G	0	4
1	I	0	2
1	M	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	341	TYR	CD2-CE2	-8.85	1.26	1.39
1	F	390	GLU	CB-CG	5.12	1.61	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	379	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	G	399	ALA	N-CA-C	7.74	131.90	111.00
1	M	348	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	M	388	GLN	CA-CB-CG	6.95	128.69	113.40
2	N	66	U	P-O3'-C3'	6.94	128.03	119.70

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	GLN	Peptide
1	B	117	ASN	Peptide
1	C	397	THR	Peptide
1	D	188	PRO	Peptide
1	E	19	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3135	0	3145	93	0
1	B	3135	0	3145	93	1
1	C	3135	0	3145	108	1
1	D	3135	0	3145	100	0
1	E	3135	0	3145	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3135	0	3145	90	0
1	G	3135	0	3145	111	2
1	H	3135	0	3145	104	0
1	I	3135	0	3145	82	2
1	J	3135	0	3145	111	0
1	K	3135	0	3145	101	0
1	L	3135	0	3145	102	1
1	M	3135	0	3144	86	0
2	N	1560	0	781	22	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	K	2	0	0	0	1
3	M	4	0	0	0	0
3	N	1	0	0	1	0
All	All	42329	0	41665	1193	4

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 1193 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:D:188:PRO:HB2	1:D:189:ALA:HA	1.42	1.00
1:M:341:TYR:O	1:M:348:ARG:NH1	1.96	0.98
1:A:369:ALA:O	1:A:373:GLN:NE2	1.99	0.95
1:I:396:ASN:HA	1:I:399:ALA:H	1.31	0.94
1:C:348:ARG:HD2	1:C:348:ARG:H	1.30	0.93

All (4) 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:L:100:GLU:OE2	3:K:601:PB:PB[3_555]	1.86	0.34
1:G:139:ASP:OD1	1:I:200:ARG:NH2[7_545]	2.13	0.07
1:B:119:ARG:NH1	1:G:100:GLU:OE1[3_555]	2.17	0.03
1:C:150:SER:OG	1:I:396:ASN:ND2[8_455]	2.18	0.02

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	A	391/525 (74%)	372 (95%)	12 (3%)	7 (2%)	8 33
1	B	391/525 (74%)	376 (96%)	13 (3%)	2 (0%)	29 63
1	C	391/525 (74%)	371 (95%)	13 (3%)	7 (2%)	8 33
1	D	391/525 (74%)	374 (96%)	11 (3%)	6 (2%)	10 38
1	E	391/525 (74%)	372 (95%)	9 (2%)	10 (3%)	5 25
1	F	391/525 (74%)	370 (95%)	13 (3%)	8 (2%)	7 30
1	G	391/525 (74%)	367 (94%)	15 (4%)	9 (2%)	6 28
1	H	391/525 (74%)	373 (95%)	11 (3%)	7 (2%)	8 33
1	I	391/525 (74%)	371 (95%)	14 (4%)	6 (2%)	10 38
1	J	391/525 (74%)	372 (95%)	15 (4%)	4 (1%)	15 48
1	K	391/525 (74%)	371 (95%)	12 (3%)	8 (2%)	7 30
1	L	391/525 (74%)	370 (95%)	12 (3%)	9 (2%)	6 28
1	M	391/525 (74%)	372 (95%)	12 (3%)	7 (2%)	8 33
All	All	5083/6825 (74%)	4831 (95%)	162 (3%)	90 (2%)	8 33

5 of 90 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	118	ALA
1	A	188	PRO
1	A	359	LYS
1	C	118	ALA

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	A	334/435 (77%)	325 (97%)	9 (3%)	44	73
1	B	334/435 (77%)	327 (98%)	7 (2%)	53	78
1	C	334/435 (77%)	327 (98%)	7 (2%)	53	78
1	D	334/435 (77%)	325 (97%)	9 (3%)	44	73
1	E	334/435 (77%)	328 (98%)	6 (2%)	59	82
1	F	334/435 (77%)	325 (97%)	9 (3%)	44	73
1	G	334/435 (77%)	327 (98%)	7 (2%)	53	78
1	H	334/435 (77%)	329 (98%)	5 (2%)	65	85
1	I	334/435 (77%)	327 (98%)	7 (2%)	53	78
1	J	334/435 (77%)	328 (98%)	6 (2%)	59	82
1	K	334/435 (77%)	323 (97%)	11 (3%)	38	68
1	L	334/435 (77%)	325 (97%)	9 (3%)	44	73
1	M	334/435 (77%)	328 (98%)	6 (2%)	59	82
All	All	4342/5655 (77%)	4244 (98%)	98 (2%)	50	76

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	390	GLU
1	H	6	LYS
1	L	382	GLU
1	F	393	GLU
1	G	182	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	143	HIS
1	H	220	GLN
1	M	220	GLN
1	G	201	GLN
1	G	304	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	N	77/78 (98%)	8 (10%)	2 (2%)

5 of 8 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	N	18	U
2	N	22	U
2	N	28	U
2	N	48	U
2	N	49	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	N	48	U
2	N	66	U

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

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	395/525 (75%)	-0.20	8 (2%)	65	45	23, 41, 107, 139	3 (0%)
1	B	395/525 (75%)	-0.28	4 (1%)	82	69	22, 40, 106, 140	3 (0%)
1	C	395/525 (75%)	-0.28	6 (1%)	73	56	22, 40, 107, 139	3 (0%)
1	D	395/525 (75%)	-0.30	6 (1%)	73	56	21, 39, 102, 137	3 (0%)
1	E	395/525 (75%)	-0.27	6 (1%)	73	56	22, 40, 109, 140	3 (0%)
1	F	395/525 (75%)	-0.30	4 (1%)	82	69	20, 40, 108, 137	3 (0%)
1	G	395/525 (75%)	-0.34	5 (1%)	77	60	21, 38, 103, 141	3 (0%)
1	H	395/525 (75%)	-0.29	5 (1%)	77	60	20, 39, 105, 140	3 (0%)
1	I	395/525 (75%)	-0.31	6 (1%)	73	56	21, 38, 106, 138	3 (0%)
1	J	395/525 (75%)	-0.30	5 (1%)	77	60	21, 39, 107, 141	3 (0%)
1	K	395/525 (75%)	-0.34	7 (1%)	68	48	21, 39, 105, 139	3 (0%)
1	L	395/525 (75%)	-0.27	9 (2%)	60	39	22, 40, 107, 137	3 (0%)
1	M	395/525 (75%)	-0.28	6 (1%)	73	56	24, 39, 104, 139	3 (0%)
2	N	78/78 (100%)	-0.48	0	100	100	35, 44, 50, 54	0
All	All	5213/6903 (75%)	-0.29	77 (1%)	73	56	20, 40, 106, 141	39 (0%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	187	GLN	6.0
1	J	21	SER	5.6
1	H	21	SER	5.1
1	A	187	GLN	4.8
1	L	181	CYS	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PB	A	601	1/1	0.77	0.14	70,70,70,70	1
3	PB	M	604	1/1	0.87	0.12	76,76,76,76	1
3	PB	H	601	1/1	0.92	0.12	59,59,59,59	1
3	PB	G	601	1/1	0.94	0.30	113,113,113,113	0
3	PB	M	603	1/1	0.94	0.08	83,83,83,83	1
3	PB	N	101	1/1	0.95	0.14	57,57,57,57	1
3	PB	M	602	1/1	0.96	0.53	171,171,171,171	0
3	PB	B	601	1/1	0.97	0.60	194,194,194,194	0
3	PB	M	601	1/1	0.97	0.18	83,83,83,83	0
3	PB	D	601	1/1	0.97	0.12	82,82,82,82	1
3	PB	K	602	1/1	0.99	0.11	62,62,62,62	0
3	PB	I	601	1/1	0.99	0.26	94,94,94,94	0
3	PB	K	601	1/1	0.99	0.08	56,56,56,56	0
3	PB	I	602	1/1	0.99	0.24	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.