



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:24 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

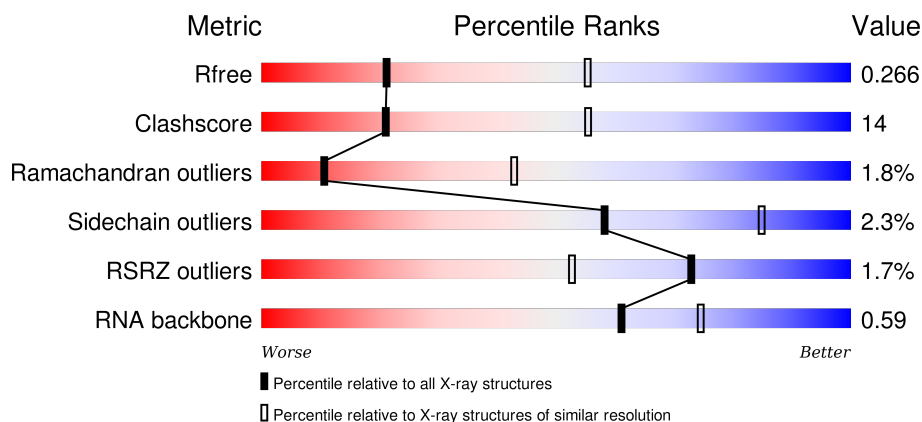
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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}	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)
RNA backbone	2183	1010 (3.54-2.70)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	525	
1	B	525	
1	C	525	
1	D	525	

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PB	B	601	-	-	-	X
3	PB	G	601	-	-	-	X
3	PB	M	602	-	-	-	X

2 Entry composition [i](#)

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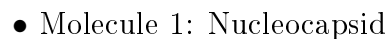
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	78	Total	C	N	O	P	0	0	0
			1560	702	156	624	78			

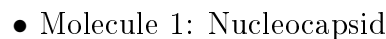
- Molecule 3 is LEAD (II) ION (three-letter code: Pb) (formula: Pb).

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

Response	Percentage
Yes	50%
No	23%
Don't know	25%

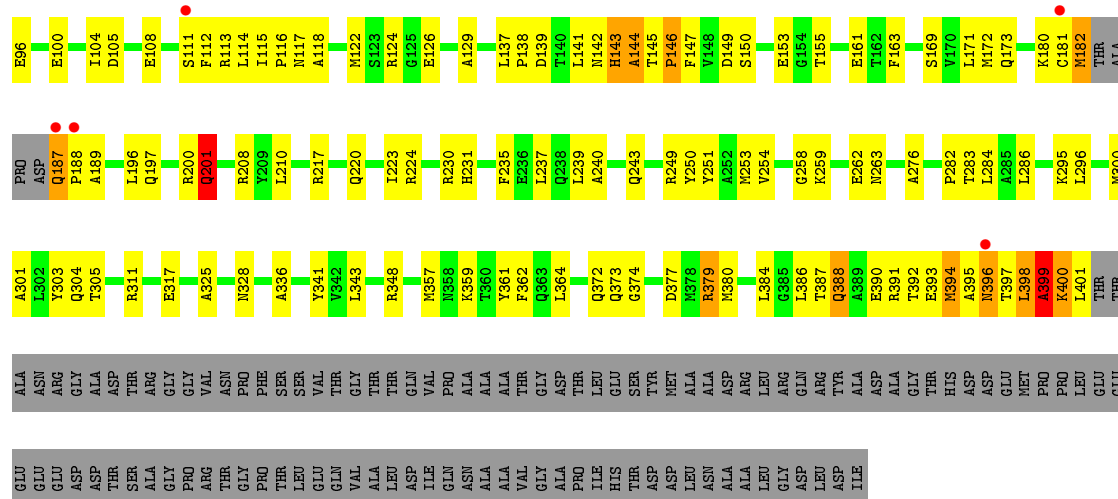


Category	Percentage
Very good	53%
Good	21%
Not good	25%
Very bad	1%

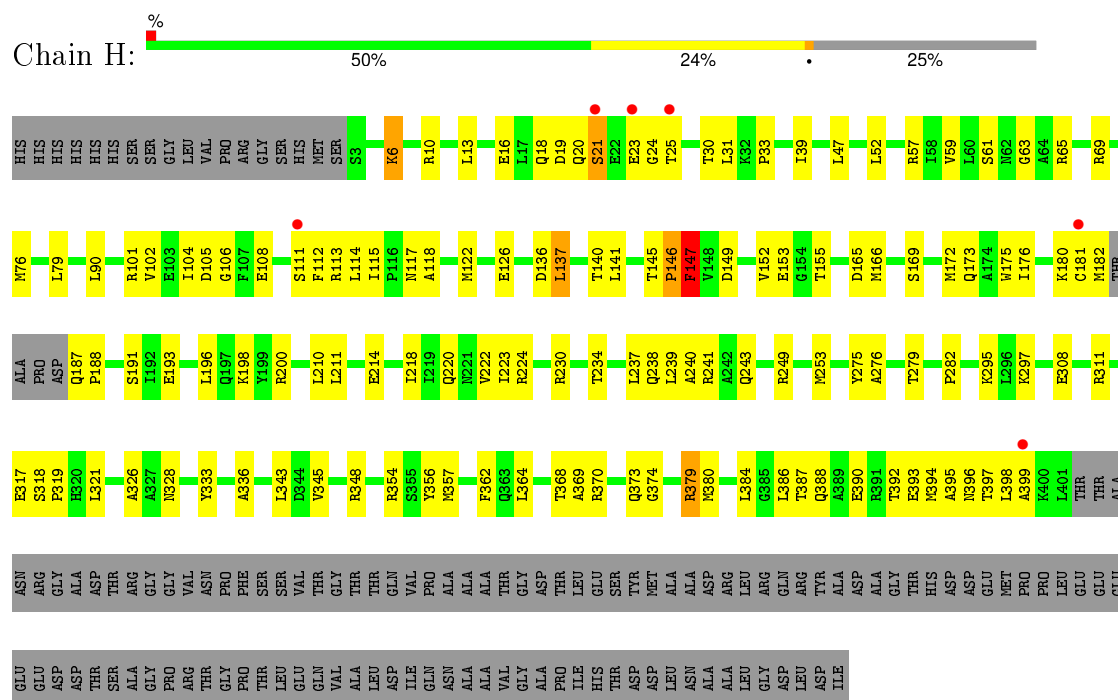


Category	Percentage
Very good	48%
Good	24%
Bad	25%
Very bad	3%

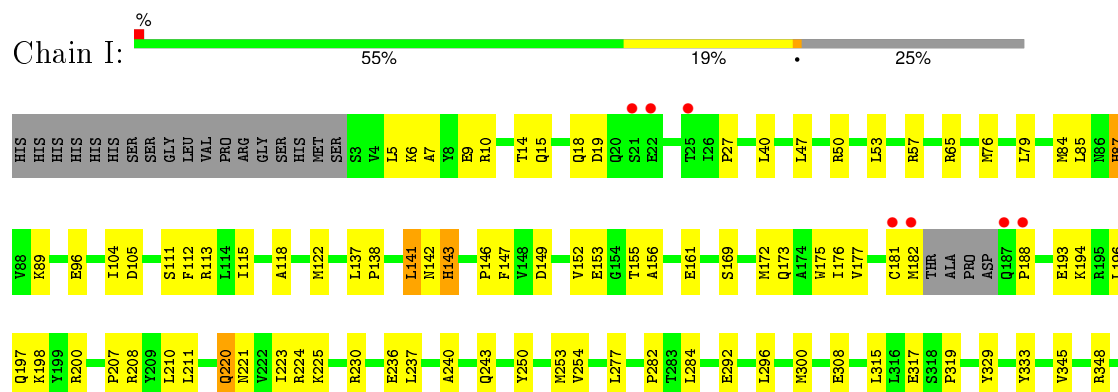


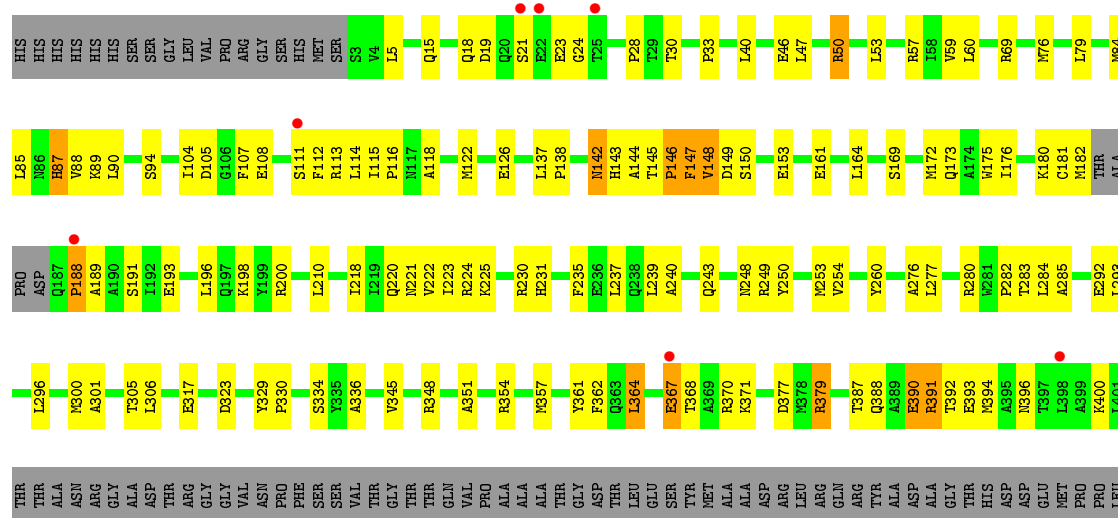


• Molecule 1: Nucleocapsid



• Molecule 1: Nucleocapsid

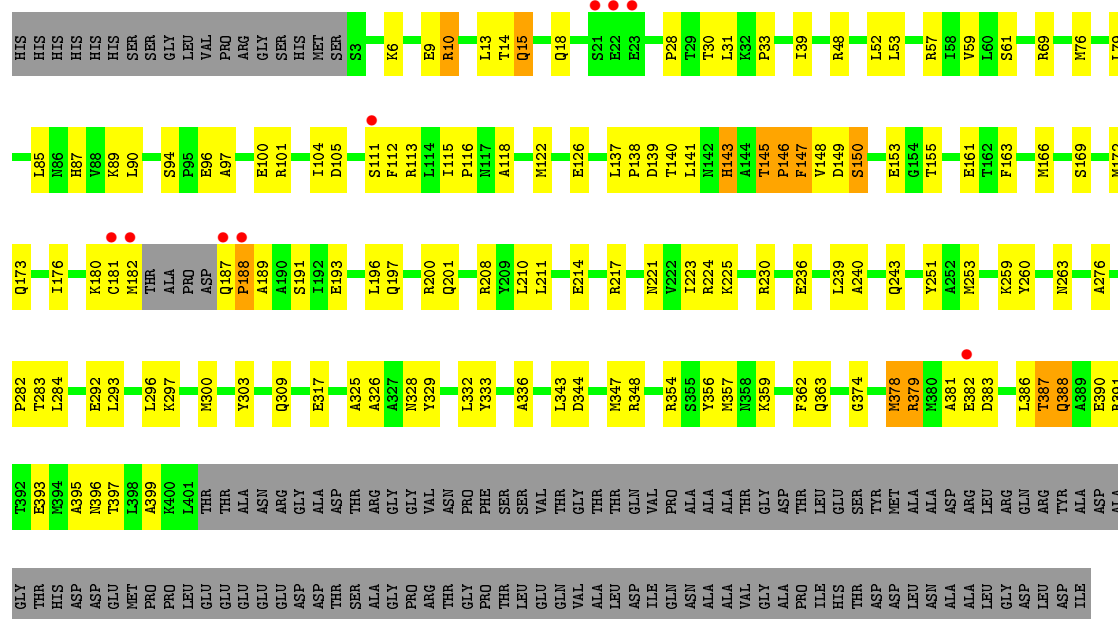




GLU
GLU
GLU
GLU
GLU
ASP
ASP
THR
SER
SER
GLY
ALA
LEU
PRO
ARG
THR
THR
GLY
PRO
GLY
THR
THR
LEU
GLU
GLN
VAL
VAL
ALA
LEU
LEU
ASP
ILE
GLN
ASN
ALA
ALA
VAL
VAL
GLY
ALA
ALA
PRO
ILE
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LEU
ASN
ALA
ALA
LEU
GLY
ASP
LEU
ASP
ILE

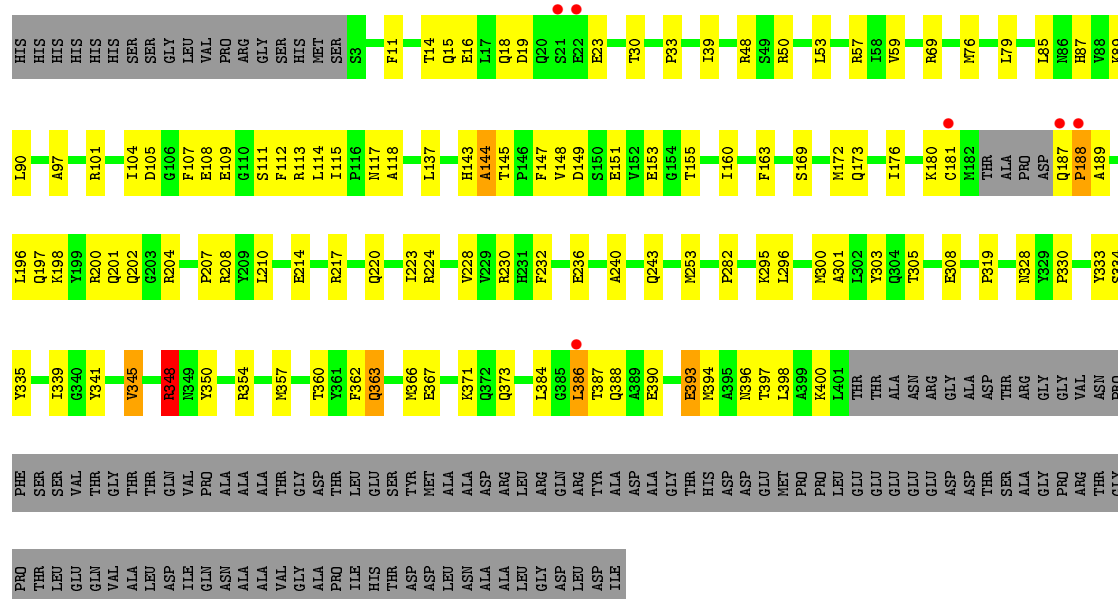
• Molecule 1: Nucleocapsid

Chain L: 



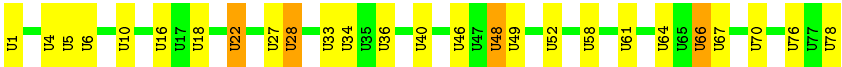
• Molecule 1: Nucleocapsid

Chain M: 



• Molecule 2: RNA (78-MER)

Chain N: 



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.263 0.231 , 0.266	Depositor DCC
R_{free} test set	6472 reflections (5.14%)	DCC
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 , 30.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	2 of 146767 reflections (0.001%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(°)	Ideal(°)
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

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 ⓘ

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	A	391/525 (74%)	372 (95%)	12 (3%)	7 (2%)	11	43
1	B	391/525 (74%)	376 (96%)	13 (3%)	2 (0%)	34	73
1	C	391/525 (74%)	371 (95%)	13 (3%)	7 (2%)	11	43
1	D	391/525 (74%)	374 (96%)	11 (3%)	6 (2%)	13	47
1	E	391/525 (74%)	372 (95%)	9 (2%)	10 (3%)	7	32
1	F	391/525 (74%)	370 (95%)	13 (3%)	8 (2%)	9	39
1	G	391/525 (74%)	367 (94%)	15 (4%)	9 (2%)	8	36
1	H	391/525 (74%)	373 (95%)	11 (3%)	7 (2%)	11	43
1	I	391/525 (74%)	371 (95%)	14 (4%)	6 (2%)	13	47
1	J	391/525 (74%)	372 (95%)	15 (4%)	4 (1%)	19	59
1	K	391/525 (74%)	371 (95%)	12 (3%)	8 (2%)	9	39
1	L	391/525 (74%)	370 (95%)	12 (3%)	9 (2%)	8	36
1	M	391/525 (74%)	372 (95%)	12 (3%)	7 (2%)	11	43
All	All	5083/6825 (74%)	4831 (95%)	162 (3%)	90 (2%)	11	43

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 ⓘ

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%)	52	83
1	B	334/435 (77%)	327 (98%)	7 (2%)	61	86
1	C	334/435 (77%)	327 (98%)	7 (2%)	61	86
1	D	334/435 (77%)	325 (97%)	9 (3%)	52	83
1	E	334/435 (77%)	328 (98%)	6 (2%)	66	89
1	F	334/435 (77%)	325 (97%)	9 (3%)	52	83
1	G	334/435 (77%)	327 (98%)	7 (2%)	61	86
1	H	334/435 (77%)	329 (98%)	5 (2%)	72	90
1	I	334/435 (77%)	327 (98%)	7 (2%)	61	86
1	J	334/435 (77%)	328 (98%)	6 (2%)	66	89
1	K	334/435 (77%)	323 (97%)	11 (3%)	45	79
1	L	334/435 (77%)	325 (97%)	9 (3%)	52	83
1	M	334/435 (77%)	328 (98%)	6 (2%)	66	89
All	All	4342/5655 (77%)	4244 (98%)	98 (2%)	58	85

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, 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	A	395/525 (75%)	-0.18	10 (2%) 61 39	23, 41, 107, 139	3 (0%)
1	B	395/525 (75%)	-0.27	5 (1%) 79 63	22, 40, 106, 140	3 (0%)
1	C	395/525 (75%)	-0.26	8 (2%) 68 47	22, 40, 107, 139	3 (0%)
1	D	395/525 (75%)	-0.28	6 (1%) 76 58	21, 39, 102, 137	3 (0%)
1	E	395/525 (75%)	-0.25	7 (1%) 71 50	22, 40, 109, 140	3 (0%)
1	F	395/525 (75%)	-0.28	4 (1%) 84 70	20, 40, 108, 137	3 (0%)
1	G	395/525 (75%)	-0.32	7 (1%) 71 50	21, 38, 103, 141	3 (0%)
1	H	395/525 (75%)	-0.27	6 (1%) 76 58	20, 39, 105, 140	3 (0%)
1	I	395/525 (75%)	-0.30	7 (1%) 71 50	21, 38, 106, 138	3 (0%)
1	J	395/525 (75%)	-0.29	6 (1%) 76 58	21, 39, 107, 141	3 (0%)
1	K	395/525 (75%)	-0.32	7 (1%) 71 50	21, 39, 105, 139	3 (0%)
1	L	395/525 (75%)	-0.25	9 (2%) 64 41	22, 40, 107, 137	3 (0%)
1	M	395/525 (75%)	-0.26	6 (1%) 76 58	24, 39, 104, 139	3 (0%)
2	N	78/78 (100%)	-0.46	0 100 100	35, 44, 50, 54	0
All	All	5213/6903 (75%)	-0.27	88 (1%) 73 53	20, 40, 106, 141	39 (0%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	187	GLN	6.2
1	J	21	SER	5.8
1	H	21	SER	5.2
1	A	187	GLN	4.8
1	L	181	CYS	4.8

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å ²)	Q<0.9
3	PB	B	601	1/1	0.97	0.60	9.45	194,194,194,194	0
3	PB	M	602	1/1	0.96	0.53	6.70	171,171,171,171	0
3	PB	G	601	1/1	0.94	0.30	2.64	113,113,113,113	0
3	PB	I	601	1/1	0.99	0.26	1.26	94,94,94,94	0
3	PB	I	602	1/1	0.99	0.24	0.95	94,94,94,94	0
3	PB	M	601	1/1	0.97	0.18	-0.31	83,83,83,83	0
3	PB	H	601	1/1	0.92	0.12	-0.91	59,59,59,59	1
3	PB	A	601	1/1	0.77	0.14	-1.02	70,70,70,70	1
3	PB	D	601	1/1	0.97	0.12	-1.73	82,82,82,82	1
3	PB	M	603	1/1	0.94	0.07	-1.77	83,83,83,83	1
3	PB	K	602	1/1	0.99	0.10	-1.82	62,62,62,62	0
3	PB	K	601	1/1	0.99	0.08	-2.09	56,56,56,56	0
3	PB	N	101	1/1	0.95	0.14	-	57,57,57,57	1
3	PB	M	604	1/1	0.87	0.12	-	76,76,76,76	1

6.5 Other polymers [i](#)

There are no such residues in this entry.