



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:14 PM GMT

PDB ID : 4O6H  
Title : 2.8Å crystal structure of Lymphocytic Choriomeningitis Virus Nucleoprotein C-terminal Domain  
Authors : West, B.R.; Hastie, K.M.; Sapphire, E.O.  
Deposited on : 2013-12-20  
Resolution : 2.80 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](mailto: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.

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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

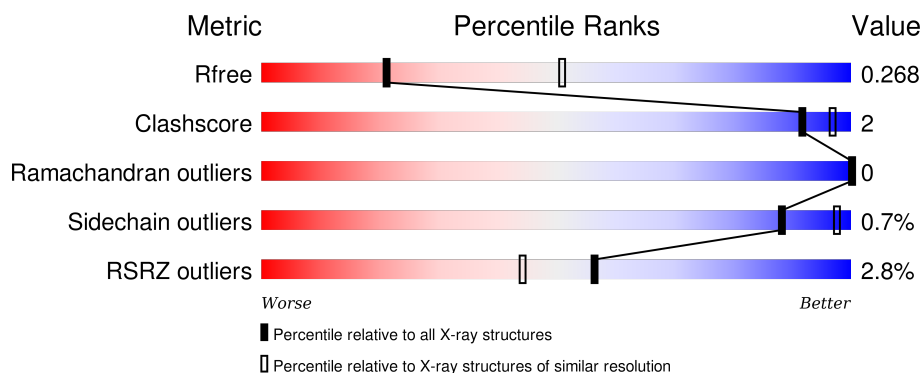
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	233	<div> <div>2%</div> <div>82% 5% 13%</div> </div>
1	B	233	<div> <div>%</div> <div>83% 5% 12%</div> </div>
1	C	233	<div> <div>%</div> <div>79% 8% 13%</div> </div>
1	D	233	<div> <div>%</div> <div>80% 7% 12%</div> </div>
1	E	233	<div> <div>2%</div> <div>80% • 16%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	233	
1	G	233	
1	H	233	

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
4	MG	G	602	-	-	-	X
4	MG	H	602	-	-	-	X
5	K	G	603	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24479 atoms, of which 11980 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 Nucleoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	H	N	O	S	0	0	0
			3096	1000	1513	270	302	11			
1	B	204	Total	C	H	N	O	S	0	0	0
			3054	994	1488	261	300	11			
1	C	203	Total	C	H	N	O	S	0	0	0
			3129	1007	1543	271	297	11			
1	D	204	Total	C	H	N	O	S	0	0	0
			3133	1009	1543	272	299	10			
1	E	196	Total	C	H	N	O	S	0	0	0
			2924	952	1427	249	286	10			
1	F	195	Total	C	H	N	O	S	0	0	0
			2930	950	1431	252	287	10			
1	G	203	Total	C	H	N	O	S	0	0	0
			3072	996	1503	266	296	11			
1	H	203	Total	C	H	N	O	S	0	0	0
			3085	994	1512	269	299	11			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	MET	-	EXPRESSION TAG	UNP P09992
A	327	ALA	-	EXPRESSION TAG	UNP P09992
A	328	HIS	-	EXPRESSION TAG	UNP P09992
A	329	HIS	-	EXPRESSION TAG	UNP P09992
A	330	HIS	-	EXPRESSION TAG	UNP P09992
A	331	HIS	-	EXPRESSION TAG	UNP P09992
A	332	HIS	-	EXPRESSION TAG	UNP P09992
A	333	HIS	-	EXPRESSION TAG	UNP P09992
A	334	VAL	-	EXPRESSION TAG	UNP P09992
A	335	ASP	-	EXPRESSION TAG	UNP P09992
A	336	ASP	-	EXPRESSION TAG	UNP P09992
A	337	ASP	-	EXPRESSION TAG	UNP P09992
A	338	ASP	-	EXPRESSION TAG	UNP P09992

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Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ARG	-	EXPRESSION TAG	UNP P09992
A	340	MET	-	EXPRESSION TAG	UNP P09992
B	326	MET	-	EXPRESSION TAG	UNP P09992
B	327	ALA	-	EXPRESSION TAG	UNP P09992
B	328	HIS	-	EXPRESSION TAG	UNP P09992
B	329	HIS	-	EXPRESSION TAG	UNP P09992
B	330	HIS	-	EXPRESSION TAG	UNP P09992
B	331	HIS	-	EXPRESSION TAG	UNP P09992
B	332	HIS	-	EXPRESSION TAG	UNP P09992
B	333	HIS	-	EXPRESSION TAG	UNP P09992
B	334	VAL	-	EXPRESSION TAG	UNP P09992
B	335	ASP	-	EXPRESSION TAG	UNP P09992
B	336	ASP	-	EXPRESSION TAG	UNP P09992
B	337	ASP	-	EXPRESSION TAG	UNP P09992
B	338	ASP	-	EXPRESSION TAG	UNP P09992
B	339	ARG	-	EXPRESSION TAG	UNP P09992
B	340	MET	-	EXPRESSION TAG	UNP P09992
C	326	MET	-	EXPRESSION TAG	UNP P09992
C	327	ALA	-	EXPRESSION TAG	UNP P09992
C	328	HIS	-	EXPRESSION TAG	UNP P09992
C	329	HIS	-	EXPRESSION TAG	UNP P09992
C	330	HIS	-	EXPRESSION TAG	UNP P09992
C	331	HIS	-	EXPRESSION TAG	UNP P09992
C	332	HIS	-	EXPRESSION TAG	UNP P09992
C	333	HIS	-	EXPRESSION TAG	UNP P09992
C	334	VAL	-	EXPRESSION TAG	UNP P09992
C	335	ASP	-	EXPRESSION TAG	UNP P09992
C	336	ASP	-	EXPRESSION TAG	UNP P09992
C	337	ASP	-	EXPRESSION TAG	UNP P09992
C	338	ASP	-	EXPRESSION TAG	UNP P09992
C	339	ARG	-	EXPRESSION TAG	UNP P09992
C	340	MET	-	EXPRESSION TAG	UNP P09992
D	326	MET	-	EXPRESSION TAG	UNP P09992
D	327	ALA	-	EXPRESSION TAG	UNP P09992
D	328	HIS	-	EXPRESSION TAG	UNP P09992
D	329	HIS	-	EXPRESSION TAG	UNP P09992
D	330	HIS	-	EXPRESSION TAG	UNP P09992
D	331	HIS	-	EXPRESSION TAG	UNP P09992
D	332	HIS	-	EXPRESSION TAG	UNP P09992
D	333	HIS	-	EXPRESSION TAG	UNP P09992
D	334	VAL	-	EXPRESSION TAG	UNP P09992
D	335	ASP	-	EXPRESSION TAG	UNP P09992

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Chain	Residue	Modelled	Actual	Comment	Reference
D	336	ASP	-	EXPRESSION TAG	UNP P09992
D	337	ASP	-	EXPRESSION TAG	UNP P09992
D	338	ASP	-	EXPRESSION TAG	UNP P09992
D	339	ARG	-	EXPRESSION TAG	UNP P09992
D	340	MET	-	EXPRESSION TAG	UNP P09992
E	326	MET	-	EXPRESSION TAG	UNP P09992
E	327	ALA	-	EXPRESSION TAG	UNP P09992
E	328	HIS	-	EXPRESSION TAG	UNP P09992
E	329	HIS	-	EXPRESSION TAG	UNP P09992
E	330	HIS	-	EXPRESSION TAG	UNP P09992
E	331	HIS	-	EXPRESSION TAG	UNP P09992
E	332	HIS	-	EXPRESSION TAG	UNP P09992
E	333	HIS	-	EXPRESSION TAG	UNP P09992
E	334	VAL	-	EXPRESSION TAG	UNP P09992
E	335	ASP	-	EXPRESSION TAG	UNP P09992
E	336	ASP	-	EXPRESSION TAG	UNP P09992
E	337	ASP	-	EXPRESSION TAG	UNP P09992
E	338	ASP	-	EXPRESSION TAG	UNP P09992
E	339	ARG	-	EXPRESSION TAG	UNP P09992
E	340	MET	-	EXPRESSION TAG	UNP P09992
F	326	MET	-	EXPRESSION TAG	UNP P09992
F	327	ALA	-	EXPRESSION TAG	UNP P09992
F	328	HIS	-	EXPRESSION TAG	UNP P09992
F	329	HIS	-	EXPRESSION TAG	UNP P09992
F	330	HIS	-	EXPRESSION TAG	UNP P09992
F	331	HIS	-	EXPRESSION TAG	UNP P09992
F	332	HIS	-	EXPRESSION TAG	UNP P09992
F	333	HIS	-	EXPRESSION TAG	UNP P09992
F	334	VAL	-	EXPRESSION TAG	UNP P09992
F	335	ASP	-	EXPRESSION TAG	UNP P09992
F	336	ASP	-	EXPRESSION TAG	UNP P09992
F	337	ASP	-	EXPRESSION TAG	UNP P09992
F	338	ASP	-	EXPRESSION TAG	UNP P09992
F	339	ARG	-	EXPRESSION TAG	UNP P09992
F	340	MET	-	EXPRESSION TAG	UNP P09992
G	326	MET	-	EXPRESSION TAG	UNP P09992
G	327	ALA	-	EXPRESSION TAG	UNP P09992
G	328	HIS	-	EXPRESSION TAG	UNP P09992
G	329	HIS	-	EXPRESSION TAG	UNP P09992
G	330	HIS	-	EXPRESSION TAG	UNP P09992
G	331	HIS	-	EXPRESSION TAG	UNP P09992
G	332	HIS	-	EXPRESSION TAG	UNP P09992

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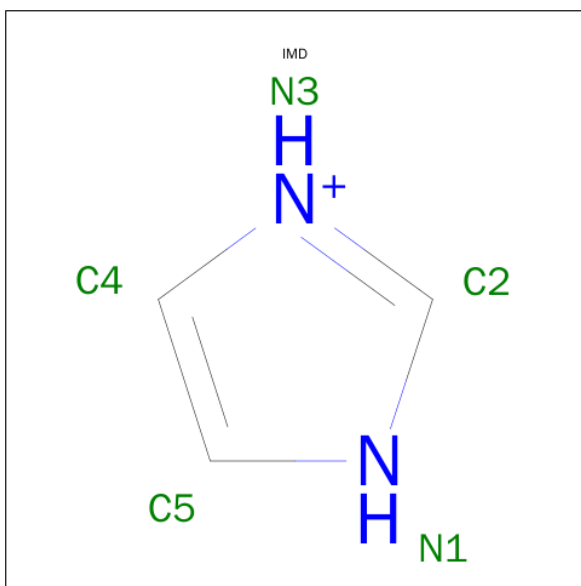
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Chain	Residue	Modelled	Actual	Comment	Reference
G	333	HIS	-	EXPRESSION TAG	UNP P09992
G	334	VAL	-	EXPRESSION TAG	UNP P09992
G	335	ASP	-	EXPRESSION TAG	UNP P09992
G	336	ASP	-	EXPRESSION TAG	UNP P09992
G	337	ASP	-	EXPRESSION TAG	UNP P09992
G	338	ASP	-	EXPRESSION TAG	UNP P09992
G	339	ARG	-	EXPRESSION TAG	UNP P09992
G	340	MET	-	EXPRESSION TAG	UNP P09992
H	326	MET	-	EXPRESSION TAG	UNP P09992
H	327	ALA	-	EXPRESSION TAG	UNP P09992
H	328	HIS	-	EXPRESSION TAG	UNP P09992
H	329	HIS	-	EXPRESSION TAG	UNP P09992
H	330	HIS	-	EXPRESSION TAG	UNP P09992
H	331	HIS	-	EXPRESSION TAG	UNP P09992
H	332	HIS	-	EXPRESSION TAG	UNP P09992
H	333	HIS	-	EXPRESSION TAG	UNP P09992
H	334	VAL	-	EXPRESSION TAG	UNP P09992
H	335	ASP	-	EXPRESSION TAG	UNP P09992
H	336	ASP	-	EXPRESSION TAG	UNP P09992
H	337	ASP	-	EXPRESSION TAG	UNP P09992
H	338	ASP	-	EXPRESSION TAG	UNP P09992
H	339	ARG	-	EXPRESSION TAG	UNP P09992
H	340	MET	-	EXPRESSION TAG	UNP P09992

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			10	3	5	2		
3	B	1	Total	C	H	N	0	0
			10	3	5	2		
3	E	1	Total	C	H	N	0	0
			10	3	5	2		
3	F	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	K	0	0
			1	1		

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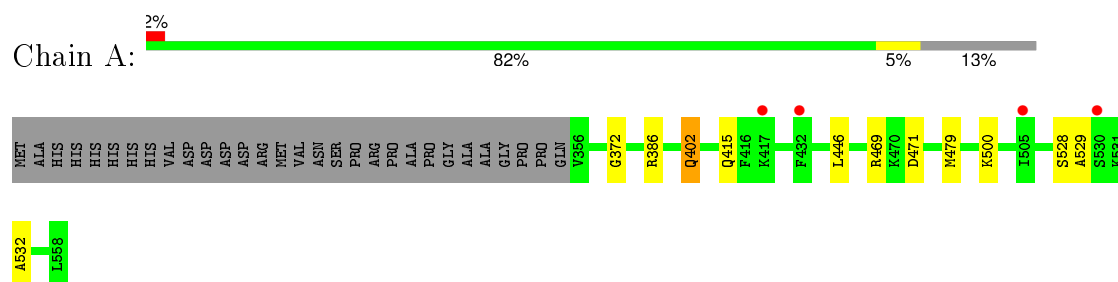
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0

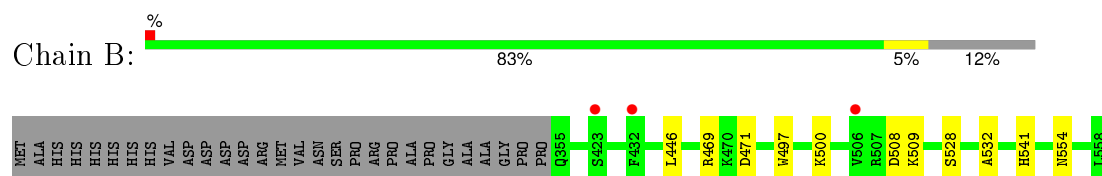
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

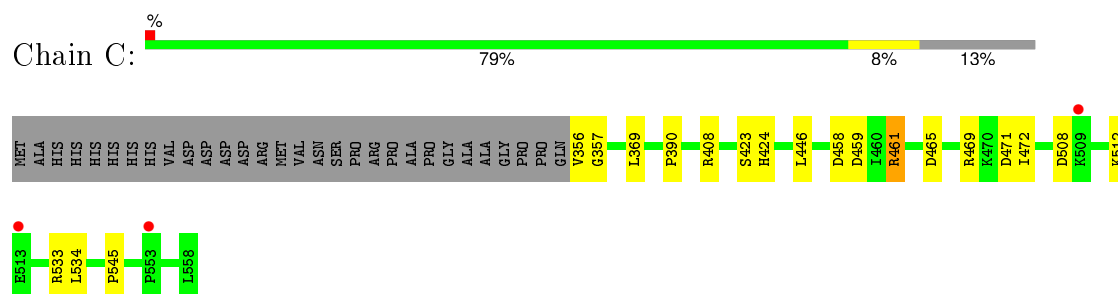
#### ● Molecule 1: Nucleoprotein



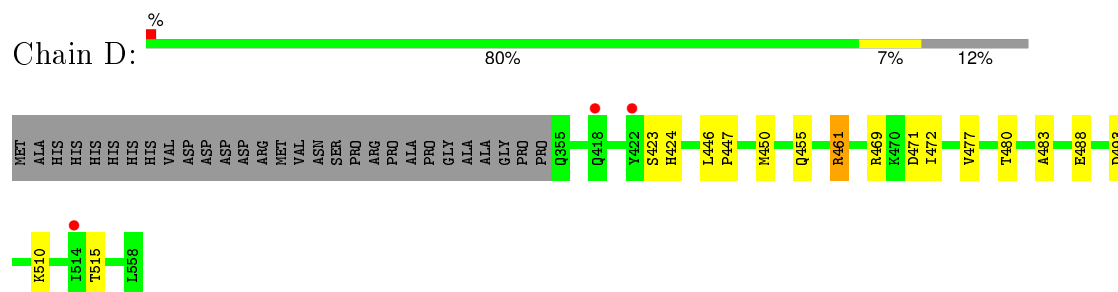
#### ● Molecule 1: Nucleoprotein



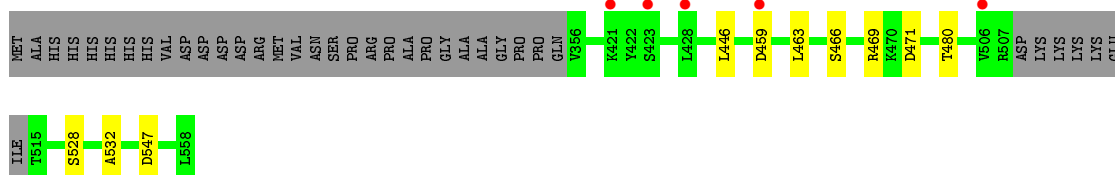
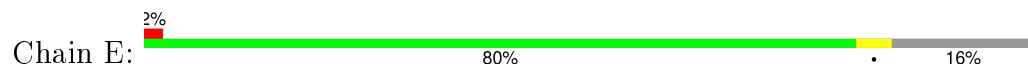
#### ● Molecule 1: Nucleoprotein



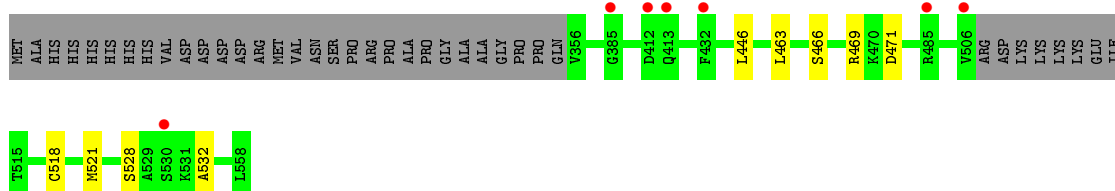
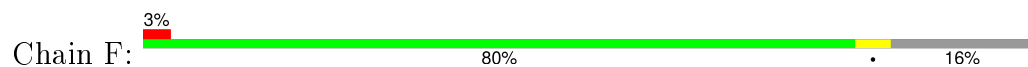
#### ● Molecule 1: Nucleoprotein



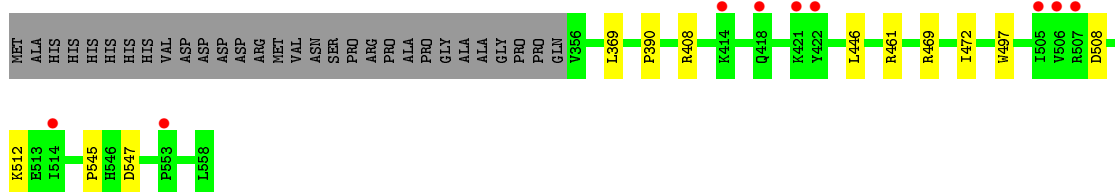
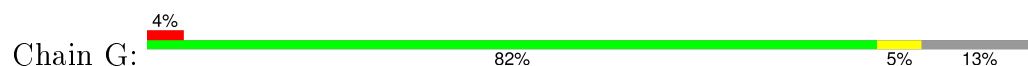
## • Molecule 1: Nucleoprotein



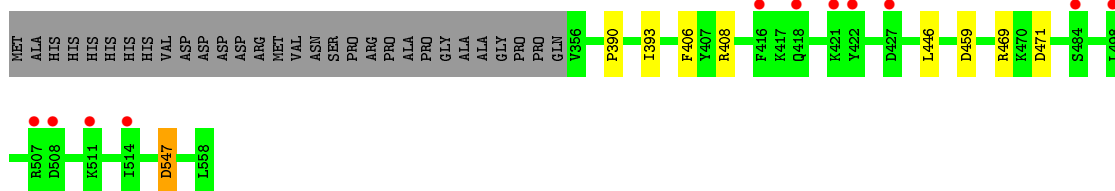
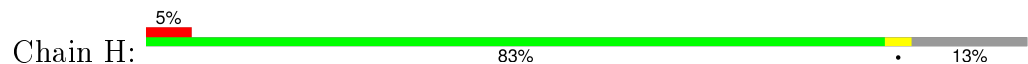
## • Molecule 1: Nucleoprotein



## • Molecule 1: Nucleoprotein



## • Molecule 1: Nucleoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.86 Å 94.40 Å 145.12 Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	47.26 – 2.80 47.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.26-2.80) 97.2 (47.26-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.81 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.227 , 0.261 0.238 , 0.268	Depositor DCC
$R_{free}$ test set	2991 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	73.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Outliers	2 of 58930 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24479	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	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 48.82 % 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 8.1519e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, K, MG, IMD

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	0.22	0/1618	0.39	0/2195
1	B	0.22	0/1601	0.37	0/2176
1	C	0.22	0/1621	0.37	0/2195
1	D	0.22	0/1625	0.37	0/2202
1	E	0.21	0/1530	0.37	0/2078
1	F	0.21	0/1532	0.37	0/2079
1	G	0.22	0/1604	0.37	0/2177
1	H	0.21	0/1607	0.37	0/2179
All	All	0.22	0/12738	0.37	0/17281

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1583	1513	1514	7	0
1	B	1566	1488	1488	6	0
1	C	1586	1543	1543	11	0
1	D	1590	1543	1543	9	0
1	E	1497	1427	1427	5	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1499	1431	1431	5	0
1	G	1569	1503	1503	5	2
1	H	1573	1512	1512	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	5	5	5	0	0
3	B	5	5	5	0	0
3	E	5	5	5	0	0
3	F	5	5	5	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	12499	11980	11981	52	2

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 2.

The worst 5 of 52 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:461:ARG:NH2	1:D:472:ILE:O	2.17	0.78
1:C:446:LEU:O	1:C:469:ARG:NH2	2.17	0.77
1:C:461:ARG:NH2	1:C:472:ILE:O	2.19	0.75
1:B:446:LEU:O	1:B:469:ARG:NH2	2.22	0.72
1:D:446:LEU:O	1:D:469:ARG:NH2	2.23	0.71

All (2) 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:E:480:THR:HG1	1:G:547:ASP:OD2[2_555]	1.54	0.06
1:E:480:THR:OG1	1:G:547:ASP:OD2[2_555]	2.17	0.03

### 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	201/233 (86%)	198 (98%)	3 (2%)	0	100	100
1	B	202/233 (87%)	196 (97%)	6 (3%)	0	100	100
1	C	201/233 (86%)	195 (97%)	6 (3%)	0	100	100
1	D	202/233 (87%)	193 (96%)	9 (4%)	0	100	100
1	E	192/233 (82%)	189 (98%)	3 (2%)	0	100	100
1	F	191/233 (82%)	187 (98%)	4 (2%)	0	100	100
1	G	201/233 (86%)	193 (96%)	8 (4%)	0	100	100
1	H	201/233 (86%)	188 (94%)	13 (6%)	0	100	100
All	All	1591/1864 (85%)	1539 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	171/205 (83%)	170 (99%)	1 (1%)	90	98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	168/205 (82%)	167 (99%)	1 (1%)	90	98
1	C	172/205 (84%)	169 (98%)	3 (2%)	68	92
1	D	172/205 (84%)	170 (99%)	2 (1%)	78	95
1	E	160/205 (78%)	159 (99%)	1 (1%)	90	98
1	F	162/205 (79%)	162 (100%)	0	100	100
1	G	168/205 (82%)	167 (99%)	1 (1%)	90	98
1	H	170/205 (83%)	169 (99%)	1 (1%)	90	98
All	All	1343/1640 (82%)	1333 (99%)	10 (1%)	88	97

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	534	LEU
1	D	461	ARG
1	E	459	ASP
1	C	533	ARG
1	D	493	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.



In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	IMD	A	602	-	5,5,5	1.34	2 (40%)	4,5,5	0.18	0
3	IMD	B	602	-	5,5,5	1.35	2 (40%)	4,5,5	0.20	0
3	IMD	E	602	-	5,5,5	1.34	2 (40%)	4,5,5	0.19	0
3	IMD	F	602	-	5,5,5	1.33	1 (20%)	4,5,5	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	A	602	-	-	0/0/0/0	0/1/1/1
3	IMD	B	602	-	-	0/0/0/0	0/1/1/1
3	IMD	E	602	-	-	0/0/0/0	0/1/1/1
3	IMD	F	602	-	-	0/0/0/0	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	602	IMD	C2-N3	2.00	1.35	1.31
3	A	602	IMD	C2-N3	2.00	1.35	1.31
3	B	602	IMD	C2-N1	2.01	1.35	1.31
3	A	602	IMD	C2-N1	2.01	1.35	1.31
3	F	602	IMD	C2-N1	2.01	1.35	1.31

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	203/233 (87%)	0.24	4 (1%) 68 58	42, 65, 102, 129	0
1	B	204/233 (87%)	0.22	3 (1%) 76 68	43, 68, 100, 122	0
1	C	203/233 (87%)	0.27	3 (1%) 76 68	46, 65, 102, 116	0
1	D	204/233 (87%)	0.19	3 (1%) 76 68	44, 63, 95, 125	0
1	E	196/233 (84%)	0.23	5 (2%) 59 47	51, 78, 108, 119	0
1	F	195/233 (83%)	0.31	7 (3%) 46 34	55, 83, 110, 126	0
1	G	203/233 (87%)	0.41	9 (4%) 38 26	55, 78, 114, 126	0
1	H	203/233 (87%)	0.47	11 (5%) 29 19	58, 84, 118, 132	0
All	All	1611/1864 (86%)	0.29	45 (2%) 56 44	42, 74, 112, 132	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	514	ILE	5.4
1	G	422	TYR	5.0
1	C	509	LYS	4.4
1	C	553	PRO	4.4
1	G	421	LYS	4.2

### 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MG	H	602	1/1	0.86	0.44	3.61	85,85,85,85	0
4	MG	G	602	1/1	0.66	0.33	2.36	78,78,78,78	0
5	K	G	603	1/1	0.94	0.29	2.05	85,85,85,85	0
5	K	H	603	1/1	0.95	0.35	1.46	89,89,89,89	0
5	K	C	603	1/1	0.96	0.25	1.25	63,63,63,63	0
3	IMD	B	602	5/5	0.93	0.30	1.04	63,75,87,91	0
2	ZN	G	601	1/1	0.95	0.21	0.76	72,72,72,72	0
2	ZN	B	601	1/1	0.99	0.21	0.49	61,61,61,61	0
4	MG	D	602	1/1	0.96	0.23	0.49	65,65,65,65	0
2	ZN	D	601	1/1	1.00	0.19	0.48	51,51,51,51	0
5	K	D	603	1/1	0.95	0.20	0.20	71,71,71,71	0
2	ZN	A	601	1/1	0.99	0.22	0.16	53,53,53,53	0
2	ZN	E	601	1/1	0.98	0.21	0.08	77,77,77,77	0
2	ZN	F	601	1/1	0.99	0.19	0.03	78,78,78,78	0
3	IMD	A	602	5/5	0.89	0.19	-0.21	65,74,81,89	0
3	IMD	F	602	5/5	0.88	0.19	-0.32	88,92,110,111	0
3	IMD	E	602	5/5	0.82	0.17	-0.32	84,95,110,114	0
2	ZN	C	601	1/1	0.99	0.18	-0.56	54,54,54,54	0
2	ZN	H	601	1/1	0.99	0.17	-0.63	83,83,83,83	0
4	MG	C	602	1/1	0.98	0.14	-1.73	70,70,70,70	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.