wwPDB X-ray Structure Validation Summary Report (i)

May 15, 2020 – 09:44 am BST

PDB ID	:	6QPF
Title	:	Influenza A virus Polymerase Heterotrimer A/duck/Fujian/01/2002(H5N1)
Authors	:	Fan, H.T.; Keown, J.R.; Fodor, E.; Grimes, J.M.
Deposited on	:	2019-02-13
Resolution	:	3.63 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:

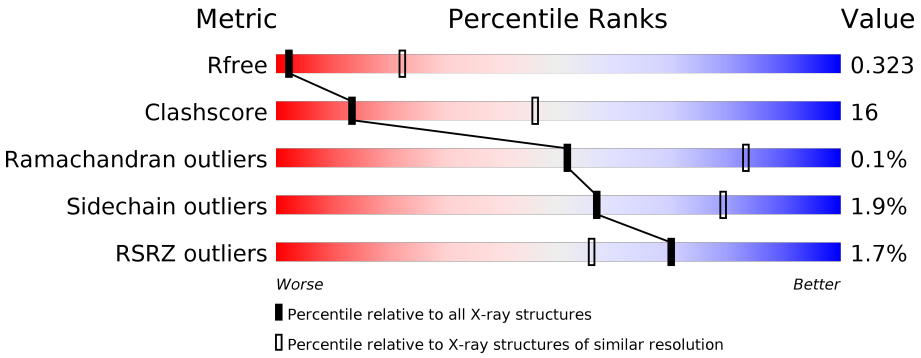
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.63 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	1341 (3.78-3.50)
Clashscore	141614	1439 (3.78-3.50)
Ramachandran outliers	138981	1391 (3.78-3.50)
Sidechain outliers	138945	1391 (3.78-3.50)
RSRZ outliers	127900	1242 (3.78-3.50)

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	716	62% 36%
1	D	716	3% 67% 32%
1	G	716	64% 35%
1	J	716	2% 63% 34%
2	B	757	2% 57% 33% 10%
2	E	757	2% 54% 33% 13%

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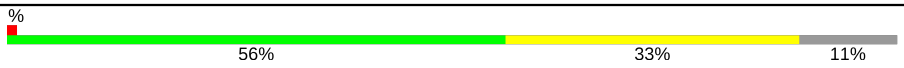
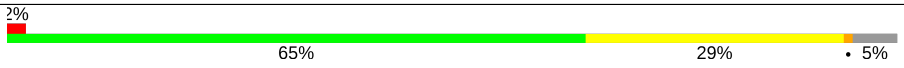
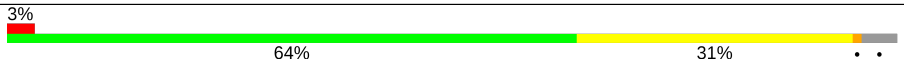
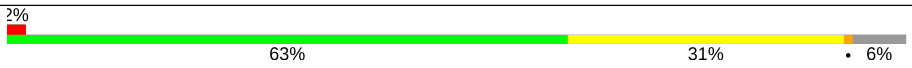
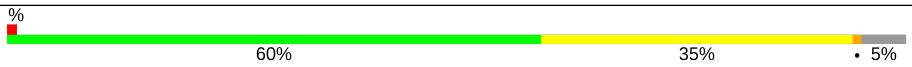
Mol	Chain	Length	Quality of chain
2	H	757	
2	K	757	
3	C	765	
3	F	765	
3	I	765	
3	L	765	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 67760 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	716	Total	C	N	O	S	0	0	0
			5796	3671	985	1099	41			
1	D	716	Total	C	N	O	S	0	0	0
			5796	3671	985	1099	41			
1	G	716	Total	C	N	O	S	0	0	0
			5796	3671	985	1099	41			
1	J	710	Total	C	N	O	S	0	0	0
			5751	3643	978	1089	41			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	685	Total	C	N	O	S	0	0	0
			5474	3446	950	1037	41			
2	E	661	Total	C	N	O	S	0	0	0
			5283	3328	909	1005	41			
2	H	673	Total	C	N	O	S	0	0	0
			5389	3393	936	1020	40			
2	K	662	Total	C	N	O	S	0	0	0
			5290	3339	913	998	40			

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	727	Total	C	N	O	S	0	0	0
			5790	3643	1042	1066	39			
3	F	731	Total	C	N	O	S	0	0	0
			5824	3661	1050	1074	39			
3	I	722	Total	C	N	O	S	0	0	0
			5755	3620	1038	1058	39			
3	L	730	Total	C	N	O	S	0	0	0
			5816	3657	1048	1072	39			

There are 24 discrepancies between the modelled and reference sequences:

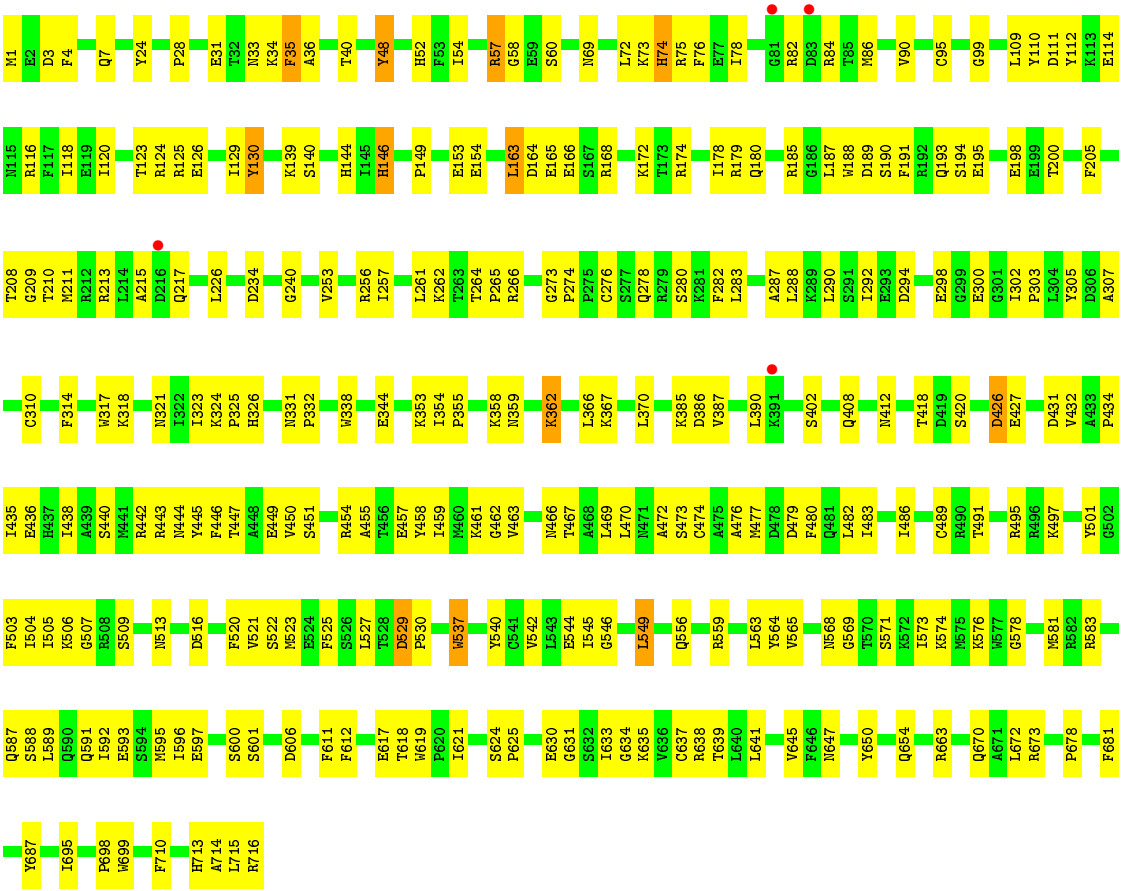
Chain	Residue	Modelled	Actual	Comment	Reference
C	760	GLU	-	expression tag	UNP D3YNB5
C	761	ASN	-	expression tag	UNP D3YNB5
C	762	LEU	-	expression tag	UNP D3YNB5
C	763	TYR	-	expression tag	UNP D3YNB5
C	764	PHE	-	expression tag	UNP D3YNB5
C	765	GLN	-	expression tag	UNP D3YNB5
F	760	GLU	-	expression tag	UNP D3YNB5
F	761	ASN	-	expression tag	UNP D3YNB5
F	762	LEU	-	expression tag	UNP D3YNB5
F	763	TYR	-	expression tag	UNP D3YNB5
F	764	PHE	-	expression tag	UNP D3YNB5
F	765	GLN	-	expression tag	UNP D3YNB5
I	760	GLU	-	expression tag	UNP D3YNB5
I	761	ASN	-	expression tag	UNP D3YNB5
I	762	LEU	-	expression tag	UNP D3YNB5
I	763	TYR	-	expression tag	UNP D3YNB5
I	764	PHE	-	expression tag	UNP D3YNB5
I	765	GLN	-	expression tag	UNP D3YNB5
L	760	GLU	-	expression tag	UNP D3YNB5
L	761	ASN	-	expression tag	UNP D3YNB5
L	762	LEU	-	expression tag	UNP D3YNB5
L	763	TYR	-	expression tag	UNP D3YNB5
L	764	PHE	-	expression tag	UNP D3YNB5
L	765	GLN	-	expression tag	UNP D3YNB5

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.

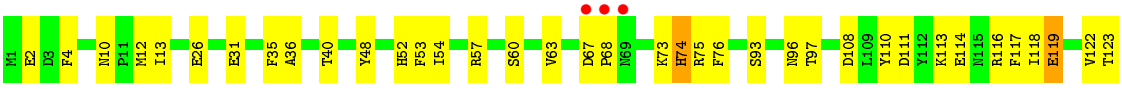
- Molecule 1: Polymerase acidic protein

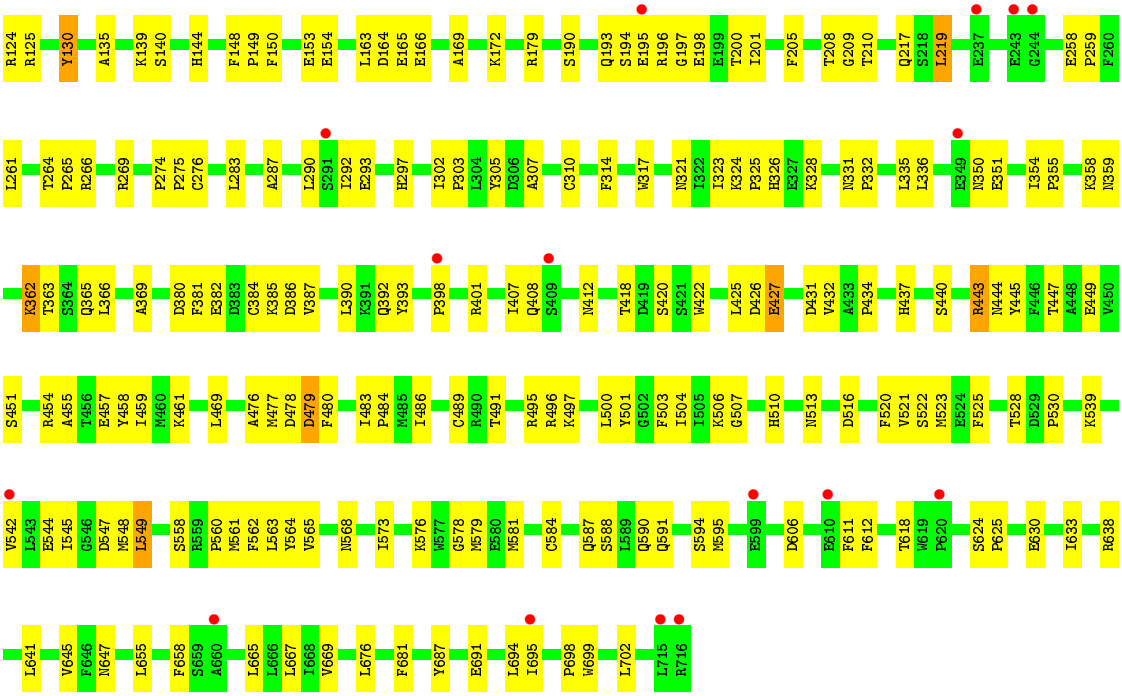
Chain A:



- Molecule 1: Polymerase acidic protein

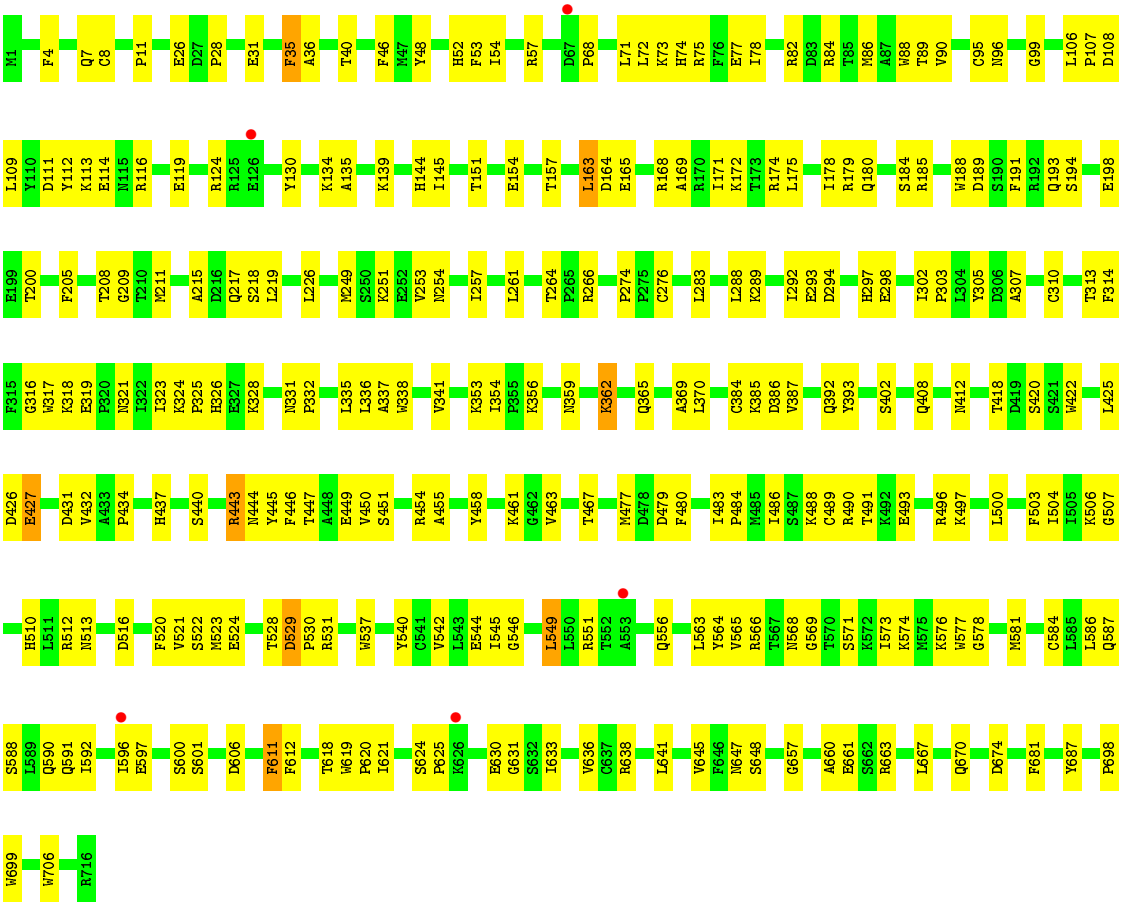
Chain D:





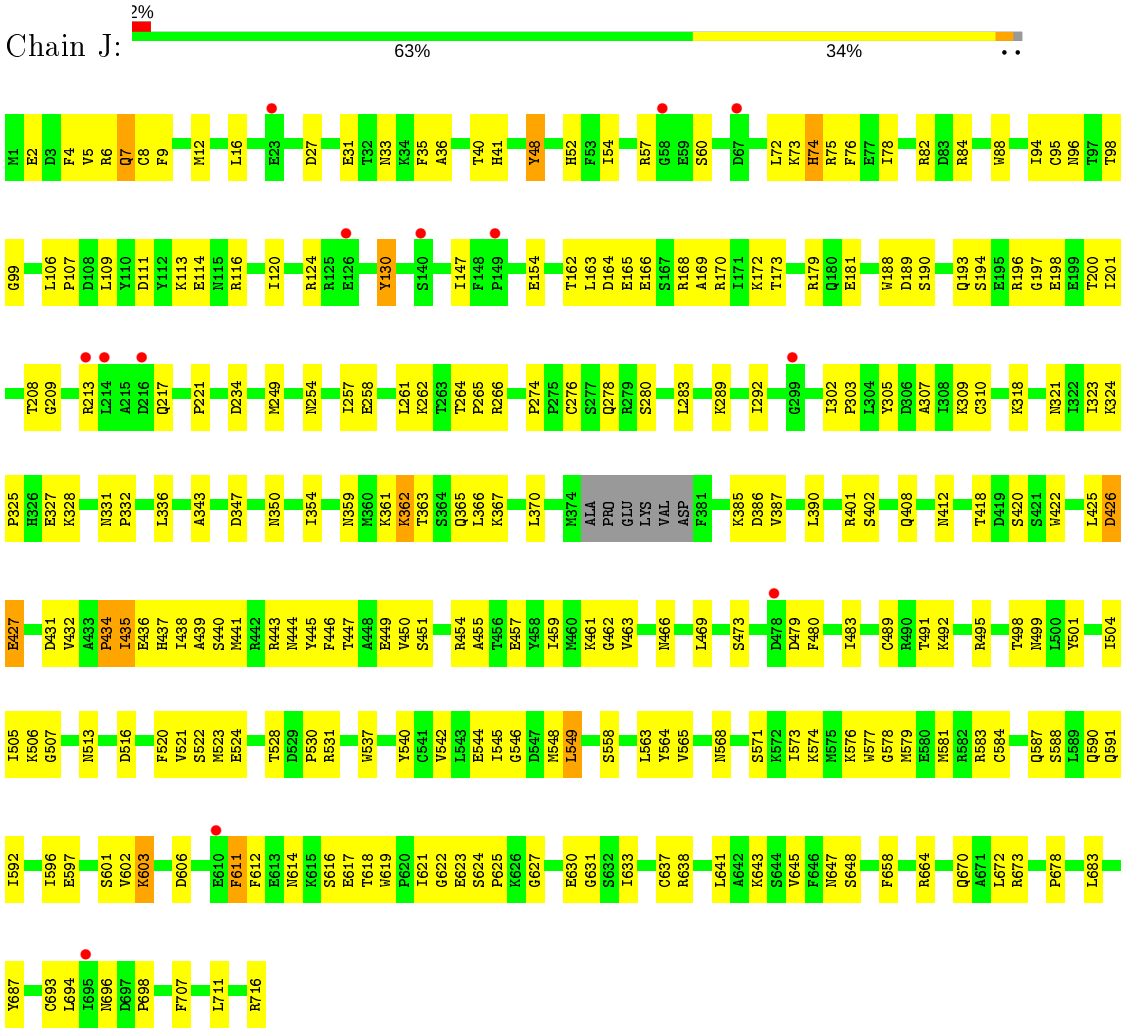
• Molecule 1: Polymerase acidic protein

Chain G:



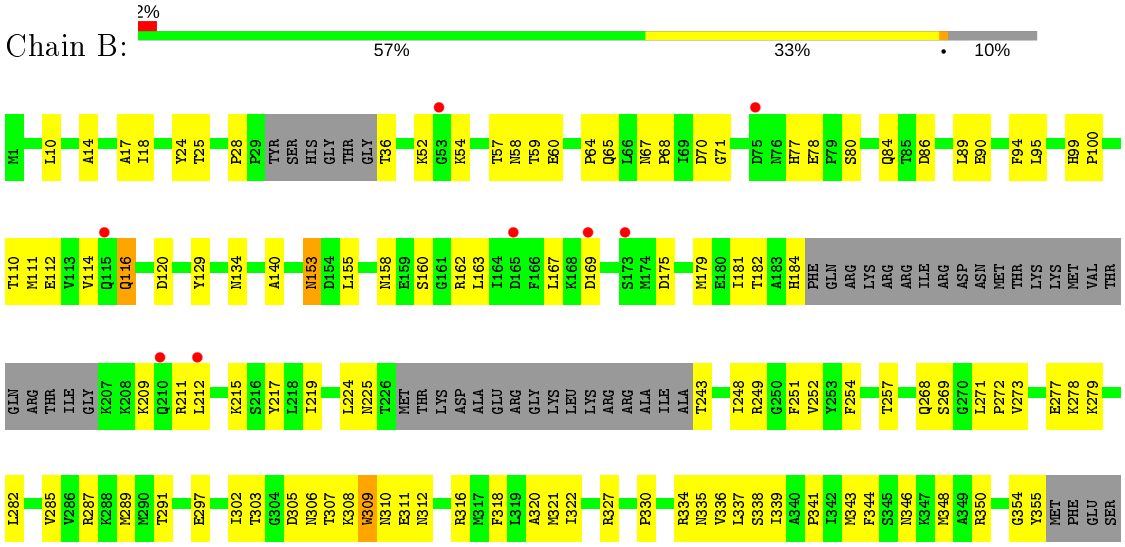
• Molecule 1: Polymerase acidic protein

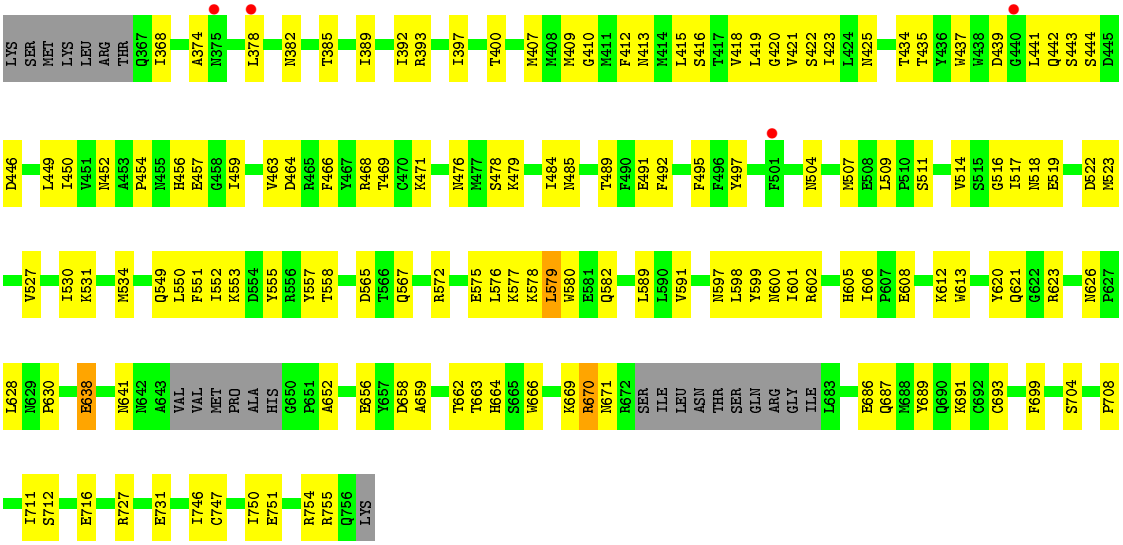
Chain J:



• Molecule 2: RNA-directed RNA polymerase catalytic subunit

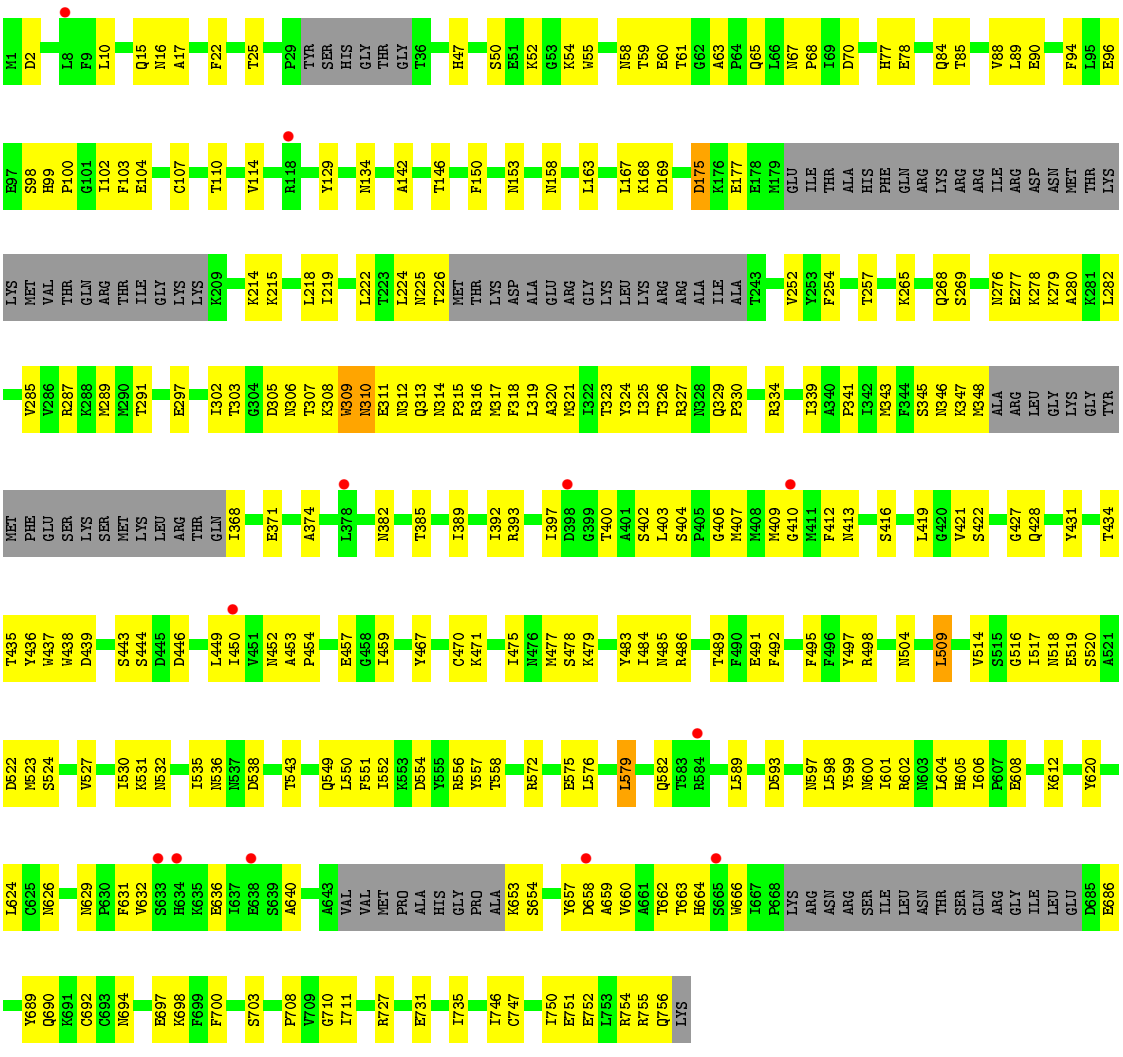
Chain B:





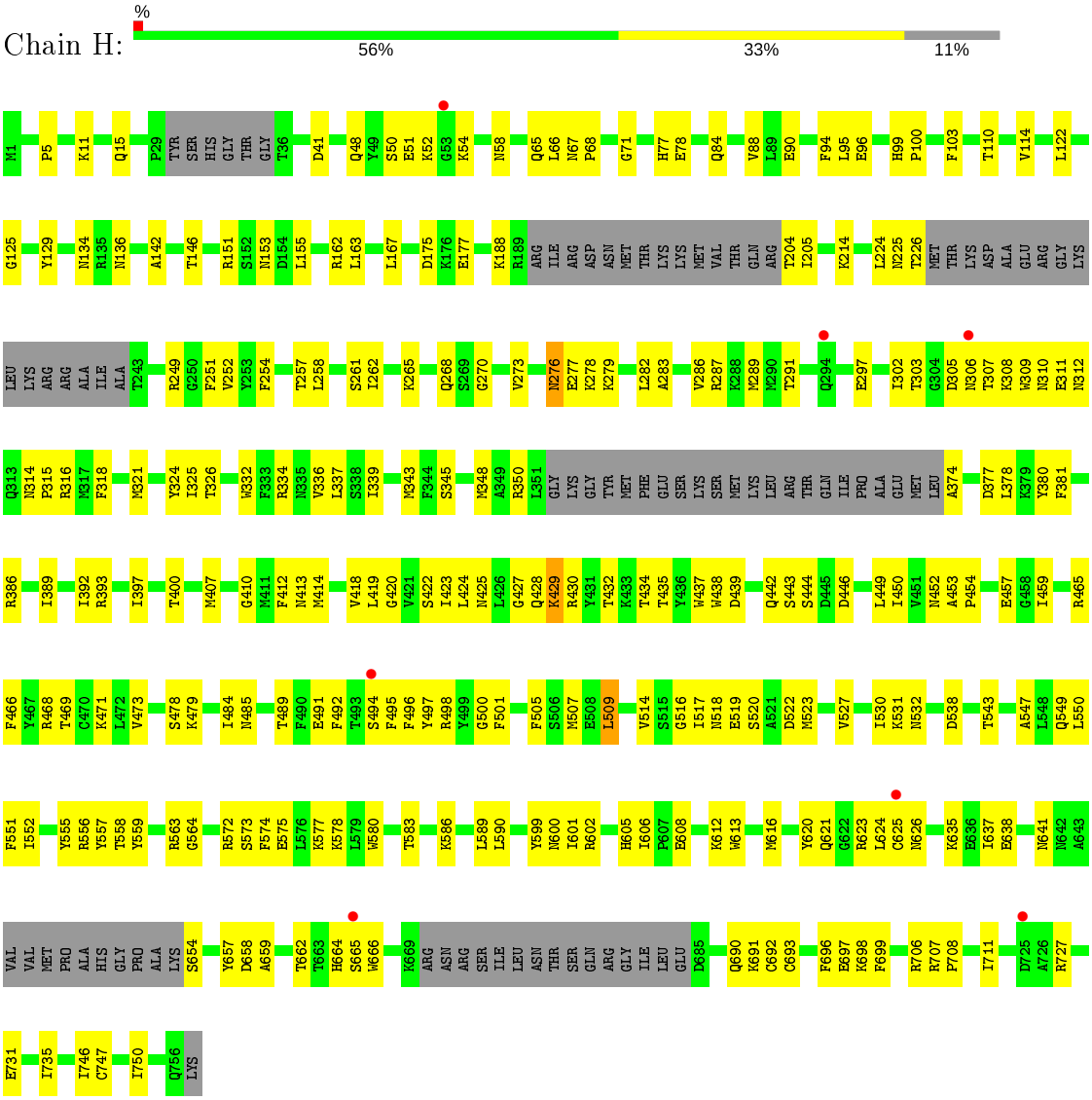
• Molecule 2: RNA-directed RNA polymerase catalytic subunit

Chain E:



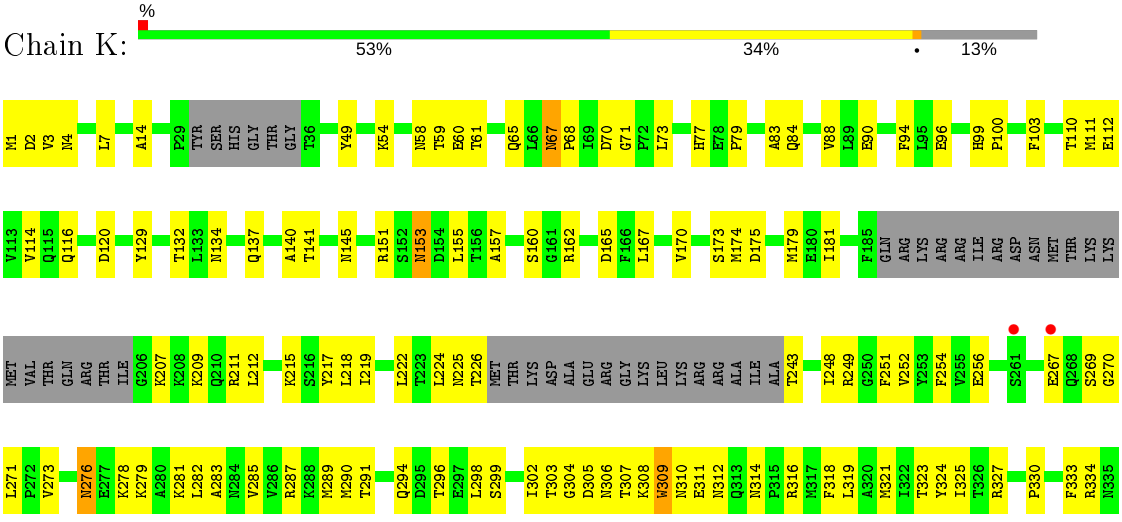
- Molecule 2: RNA-directed RNA polymerase catalytic subunit

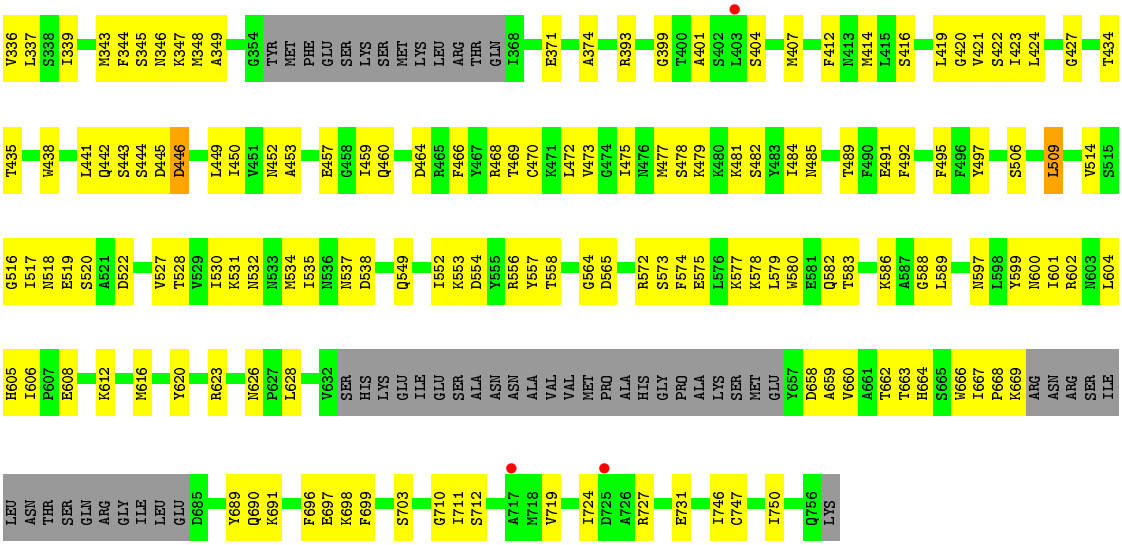
Chain H:



- Molecule 2: RNA-directed RNA polymerase catalytic subunit

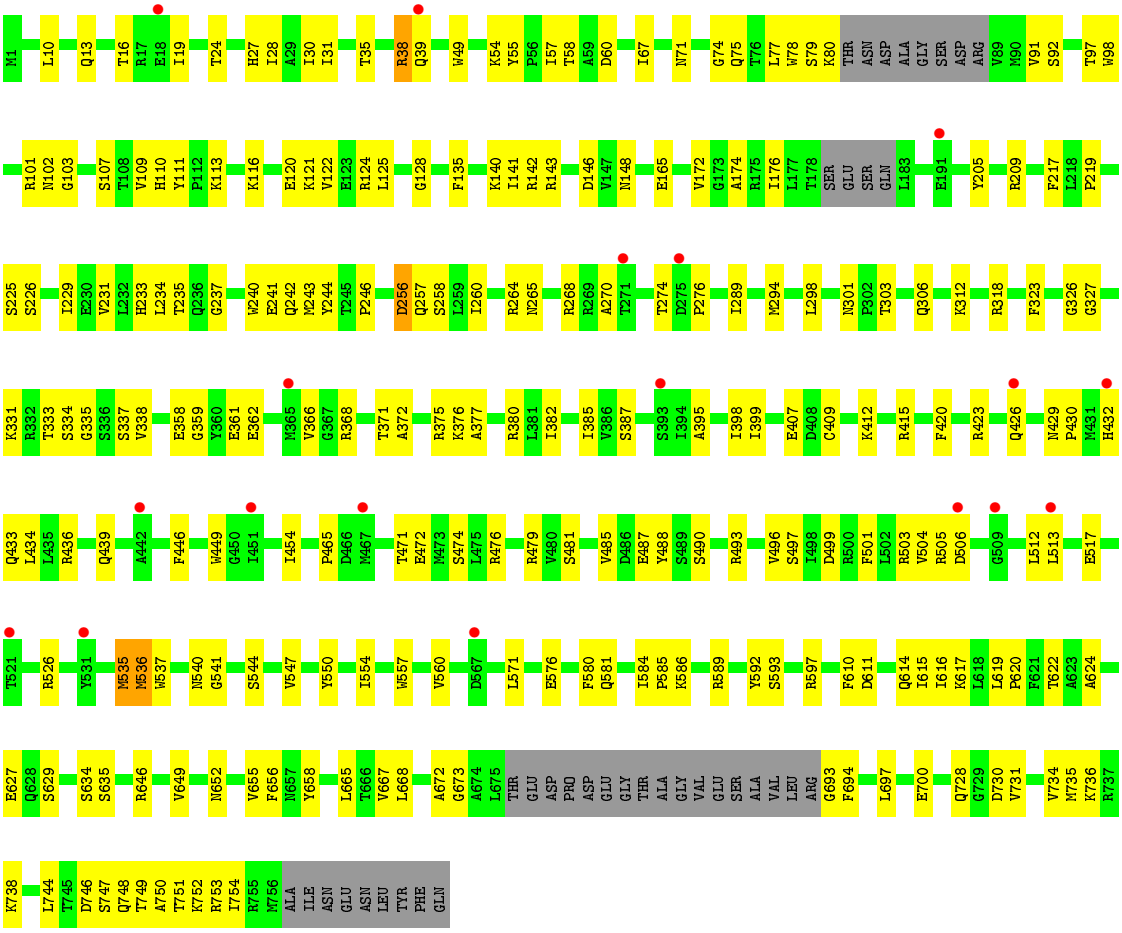
Chain K:





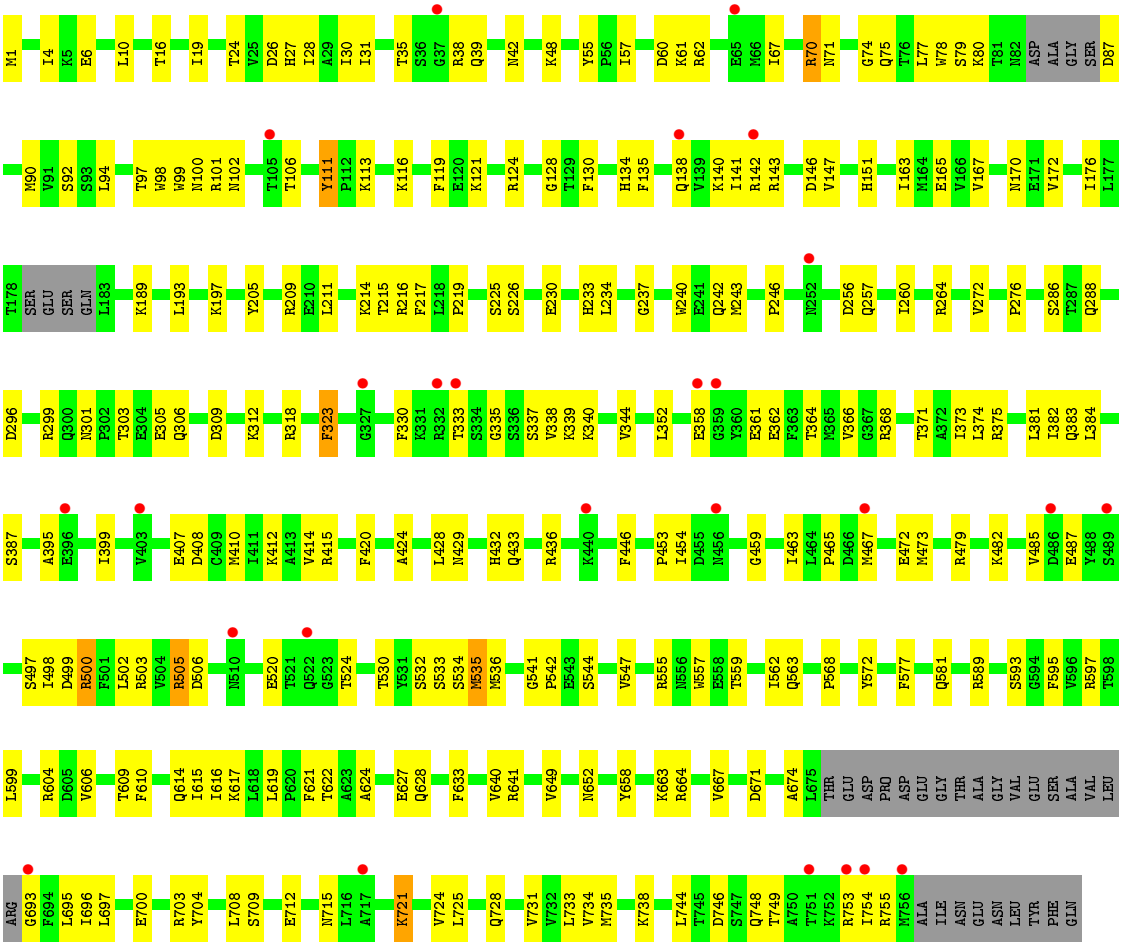
• Molecule 3: Polymerase basic protein 2

Chain C:



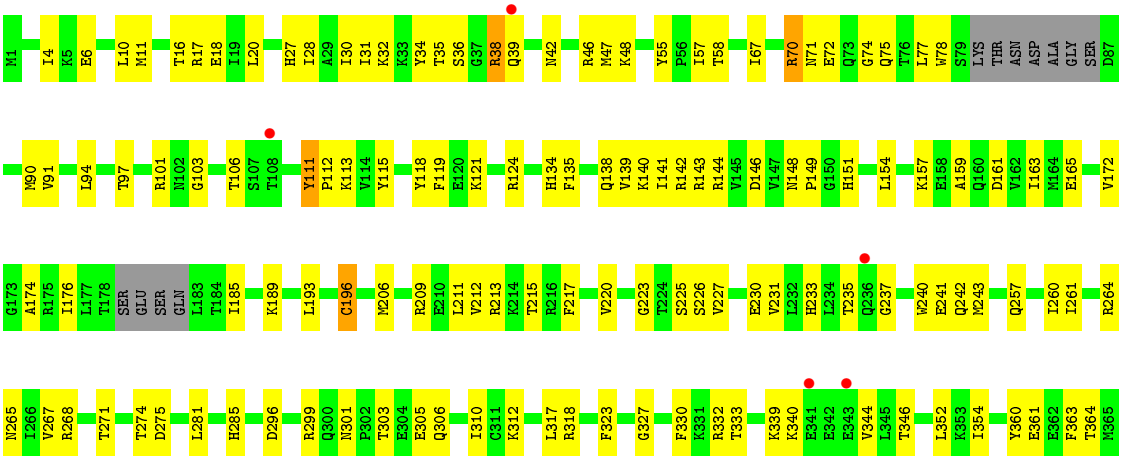
• Molecule 3: Polymerase basic protein 2

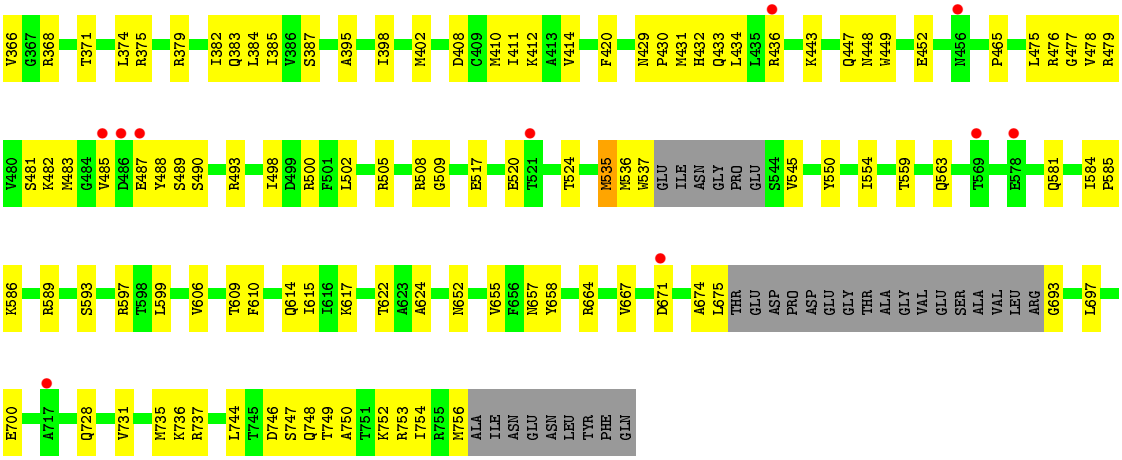
Chain F:



• Molecule 3: Polymerase basic protein 2

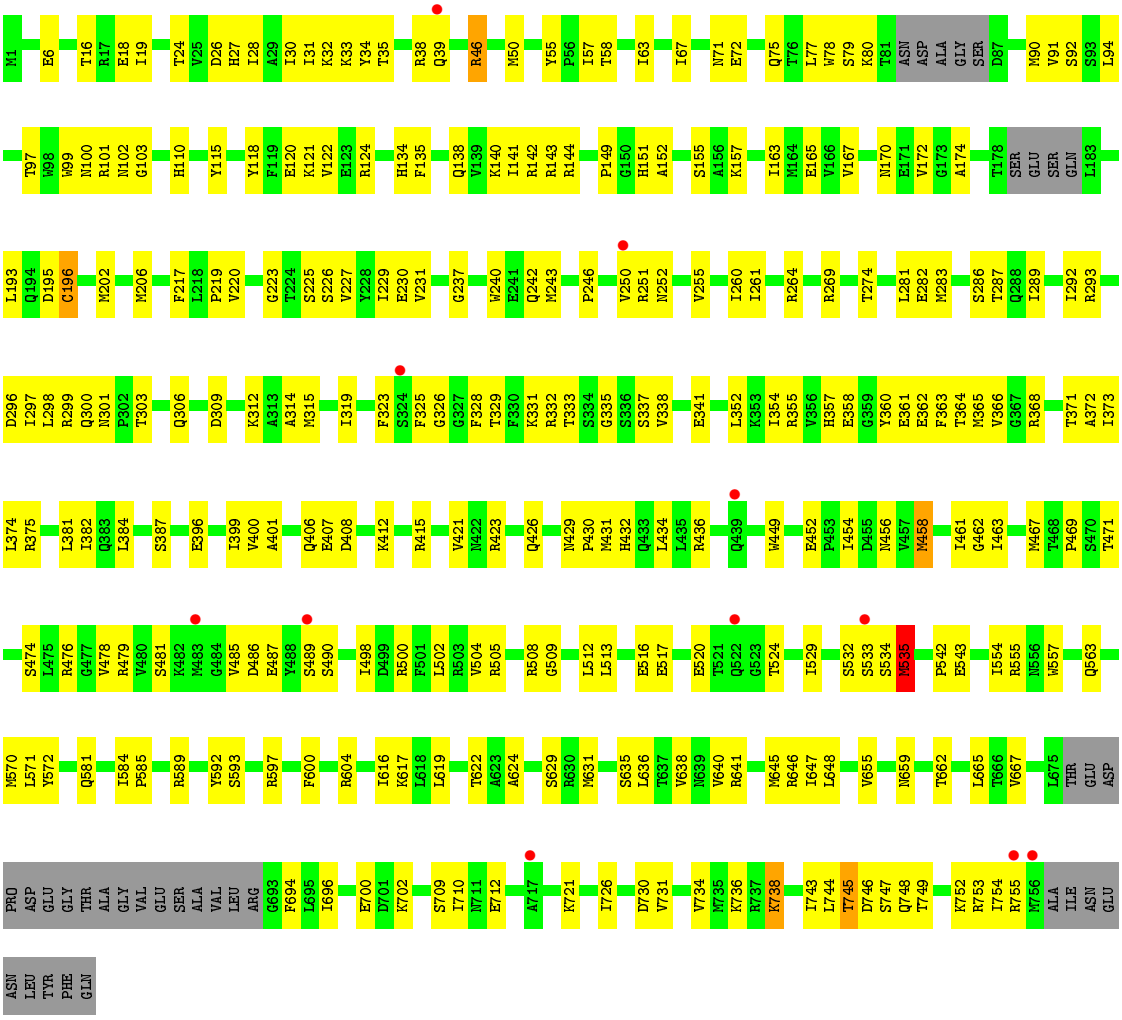
Chain I:





• Molecule 3: Polymerase basic protein 2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	337.12Å 192.86Å 235.69Å 90.00° 91.46° 90.00°	Depositor
Resolution (Å)	235.61 – 3.63 235.61 – 3.63	Depositor EDS
% Data completeness (in resolution range)	48.0 (235.61-3.63) 48.0 (235.61-3.63)	Depositor EDS
R_{merge}	0.48	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.68Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.277 , 0.323 0.277 , 0.323	Depositor DCC
R_{free} test set	4059 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	76.8	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 85.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.023 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.027 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.026 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.035 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.035 for -h,-k,l	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	67760	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.59% 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

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	0.27	0/5921	0.47	0/7981
1	D	0.26	0/5921	0.46	0/7981
1	G	0.27	0/5921	0.48	1/7981 (0.0%)
1	J	0.26	0/5874	0.46	0/7915
2	B	0.27	0/5580	0.47	0/7527
2	E	0.26	0/5386	0.45	0/7270
2	H	0.27	0/5493	0.47	0/7409
2	K	0.26	0/5394	0.46	0/7278
3	C	0.26	0/5883	0.48	0/7928
3	F	0.25	0/5917	0.48	0/7974
3	I	0.26	0/5846	0.49	0/7876
3	L	0.26	0/5909	0.49	0/7963
All	All	0.26	0/69045	0.47	1/93083 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	257	ILE	C-N-CA	-5.14	108.84	121.70

There are no chirality outliers.

There are no planarity outliers.

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	5796	0	5734	206	0
1	D	5796	0	5734	173	0
1	G	5796	0	5734	196	0
1	J	5751	0	5689	209	0
2	B	5474	0	5423	206	0
2	E	5283	0	5219	208	0
2	H	5389	0	5338	219	0
2	K	5290	0	5246	226	0
3	C	5790	0	5939	200	0
3	F	5824	0	5969	181	1
3	I	5755	0	5903	205	1
3	L	5816	0	5963	216	0
All	All	67760	0	67891	2181	1

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 16.

The worst 5 of 2181 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)
3:I:318:ARG:HD3	3:I:493:ARG:HB3	1.54	0.90
1:G:321:ASN:HB3	1:G:544:GLU:HB3	1.52	0.89
1:G:68:PRO:HB3	1:G:72:LEU:HG	1.56	0.87
1:J:7:GLN:NE2	1:J:8:CYS:SG	2.48	0.87
2:H:485:ASN:ND2	2:H:489:THR:O	2.08	0.86

All (1) 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)
3:F:415:ARG:NH2	3:I:448:ASN:OD1[4_545]	2.19	0.01

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	714/716 (100%)	654 (92%)	60 (8%)	0	100	100
1	D	714/716 (100%)	652 (91%)	62 (9%)	0	100	100
1	G	714/716 (100%)	648 (91%)	66 (9%)	0	100	100
1	J	706/716 (99%)	647 (92%)	57 (8%)	2 (0%)	41	74
2	B	671/757 (89%)	611 (91%)	60 (9%)	0	100	100
2	E	647/757 (86%)	594 (92%)	53 (8%)	0	100	100
2	H	659/757 (87%)	599 (91%)	59 (9%)	1 (0%)	47	79
2	K	648/757 (86%)	600 (93%)	48 (7%)	0	100	100
3	C	719/765 (94%)	649 (90%)	69 (10%)	1 (0%)	51	83
3	F	723/765 (94%)	645 (89%)	77 (11%)	1 (0%)	51	83
3	I	712/765 (93%)	643 (90%)	69 (10%)	0	100	100
3	L	722/765 (94%)	652 (90%)	68 (9%)	2 (0%)	41	74
All	All	8349/8952 (93%)	7594 (91%)	748 (9%)	7 (0%)	51	83

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	536	MET
3	F	535	MET
2	H	429	LYS
3	L	535	MET
3	L	745	THR

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	640/640 (100%)	625 (98%)	15 (2%)	50	75
1	D	640/640 (100%)	622 (97%)	18 (3%)	43	71
1	G	640/640 (100%)	626 (98%)	14 (2%)	52	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	635/640 (99%)	620 (98%)	15 (2%)	49	74
2	B	605/668 (91%)	593 (98%)	12 (2%)	55	78
2	E	587/668 (88%)	577 (98%)	10 (2%)	60	81
2	H	597/668 (89%)	587 (98%)	10 (2%)	60	81
2	K	585/668 (88%)	574 (98%)	11 (2%)	57	79
3	C	643/674 (95%)	637 (99%)	6 (1%)	78	89
3	F	647/674 (96%)	637 (98%)	10 (2%)	65	83
3	I	639/674 (95%)	630 (99%)	9 (1%)	67	84
3	L	646/674 (96%)	632 (98%)	14 (2%)	52	76
All	All	7504/7928 (95%)	7360 (98%)	144 (2%)	57	79

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	205	TYR
1	G	427	GLU
3	L	134	HIS
3	F	323	PHE
1	G	48	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	591	GLN
2	E	605	HIS
1	J	7	GLN
2	E	312	ASN
1	G	144	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

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, 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	716/716 (100%)	-0.02	4 (0%)	89	81	39, 83, 142, 203	0
1	D	716/716 (100%)	0.19	19 (2%)	54	38	56, 106, 163, 212	0
1	G	716/716 (100%)	0.06	5 (0%)	87	79	42, 82, 147, 205	0
1	J	710/716 (99%)	0.08	13 (1%)	68	53	59, 101, 145, 200	0
2	B	685/757 (90%)	0.15	12 (1%)	68	53	49, 85, 137, 215	0
2	E	661/757 (87%)	0.21	12 (1%)	68	53	64, 108, 152, 240	0
2	H	673/757 (88%)	0.11	7 (1%)	82	71	39, 88, 138, 185	0
2	K	662/757 (87%)	0.18	5 (0%)	86	76	44, 98, 142, 202	0
3	C	727/765 (95%)	0.14	18 (2%)	57	41	55, 103, 163, 227	0
3	F	731/765 (95%)	0.31	26 (3%)	42	29	64, 119, 176, 210	0
3	I	722/765 (94%)	0.16	15 (2%)	63	48	46, 99, 151, 179	0
3	L	730/765 (95%)	0.16	11 (1%)	73	60	55, 100, 160, 232	0
All	All	8449/8952 (94%)	0.14	147 (1%)	70	56	39, 97, 155, 240	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	665	SER	7.8
3	F	717	ALA	7.3
3	F	510	ASN	6.0
3	I	456	ASN	5.2
1	D	68	PRO	5.2

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.