



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:54 AM UTC

PDB ID : 6F5P / pdb_00006f5p
Title : A mechanism for the activation of the influenza virus transcriptase
Authors : Serna Martin, I.; Grimes, J.M.
Deposited on : 2017-12-02
Resolution : 4.14 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

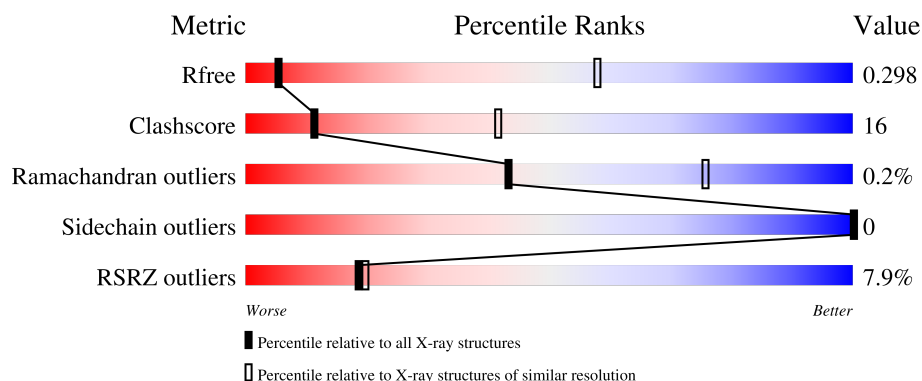
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.14 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.



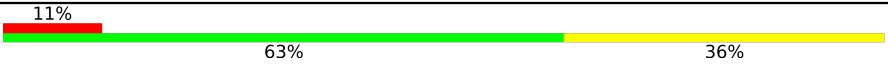
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1004 (4.46-3.82)
Clashscore	190562	1004 (4.44-3.84)
Ramachandran outliers	187476	1224 (4.48-3.80)
Sidechain outliers	187428	1211 (4.48-3.80)
RSRZ outliers	180081	1001 (4.46-3.82)

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 of 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 $\leq 5\%$. 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	709	6% 64% 35% .
1	D	709	7% 66% 33% .
2	B	754	5% 66% 28% 6%
2	C	754	5% 66% 29% .
3	E	774	13% 64% 35%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	774	
4	G	28	
5	H	10	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35282 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	708	Total	C	N	O	S	0	0	0
			5736	3654	972	1065	45			
1	D	708	Total	C	N	O	S	0	0	0
			5736	3654	972	1065	45			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	710	Total	C	N	O	S	0	0	0
			5643	3584	948	1057	54			
2	C	721	Total	C	N	O	S	0	0	0
			5736	3638	971	1073	54			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	771	Total	C	N	O	S	0	0	0
			6140	3883	1079	1141	37			
3	F	771	Total	C	N	O	S	0	0	0
			6140	3883	1079	1141	37			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	12	Total	C	N	O	P	0	0	0
			97	56	12	27	2			

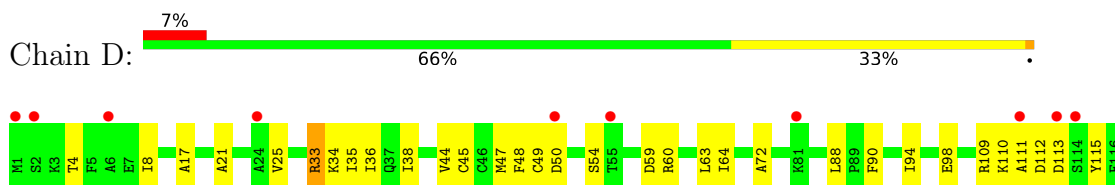
- Molecule 5 is a protein called ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA.

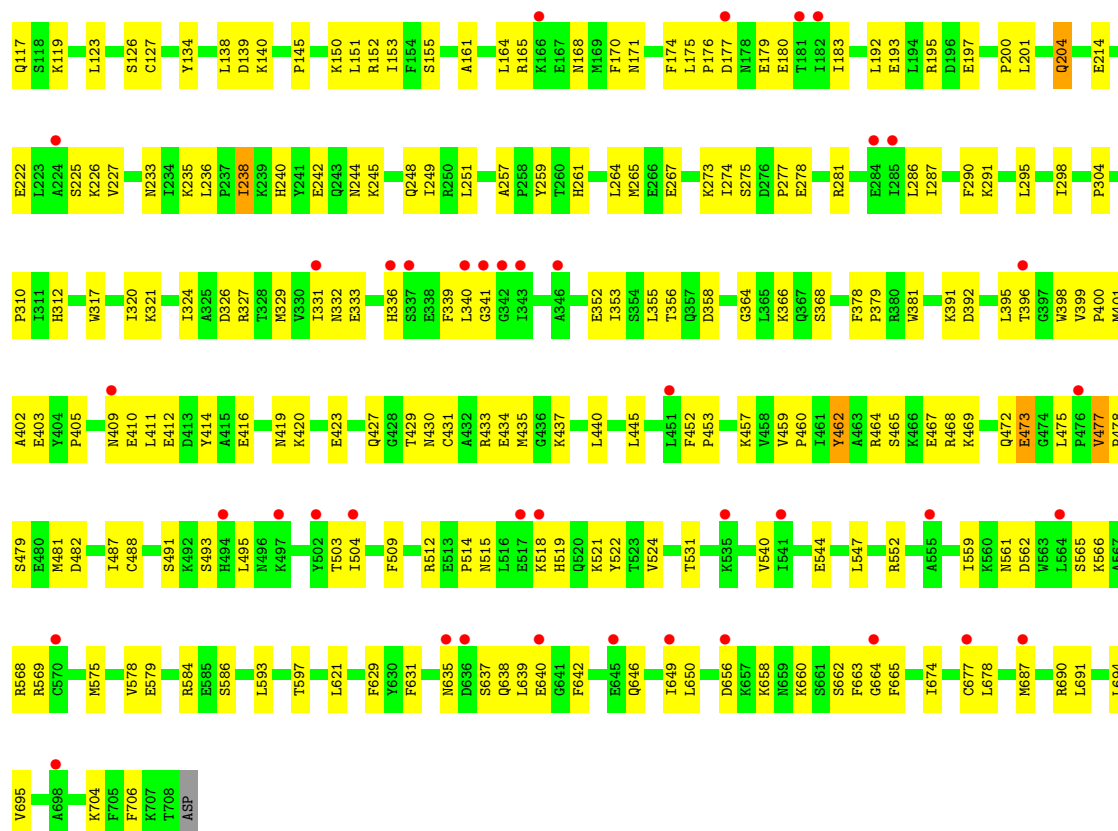
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	10	Total	C	N	O	50	0	0
			50	30	10	10			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

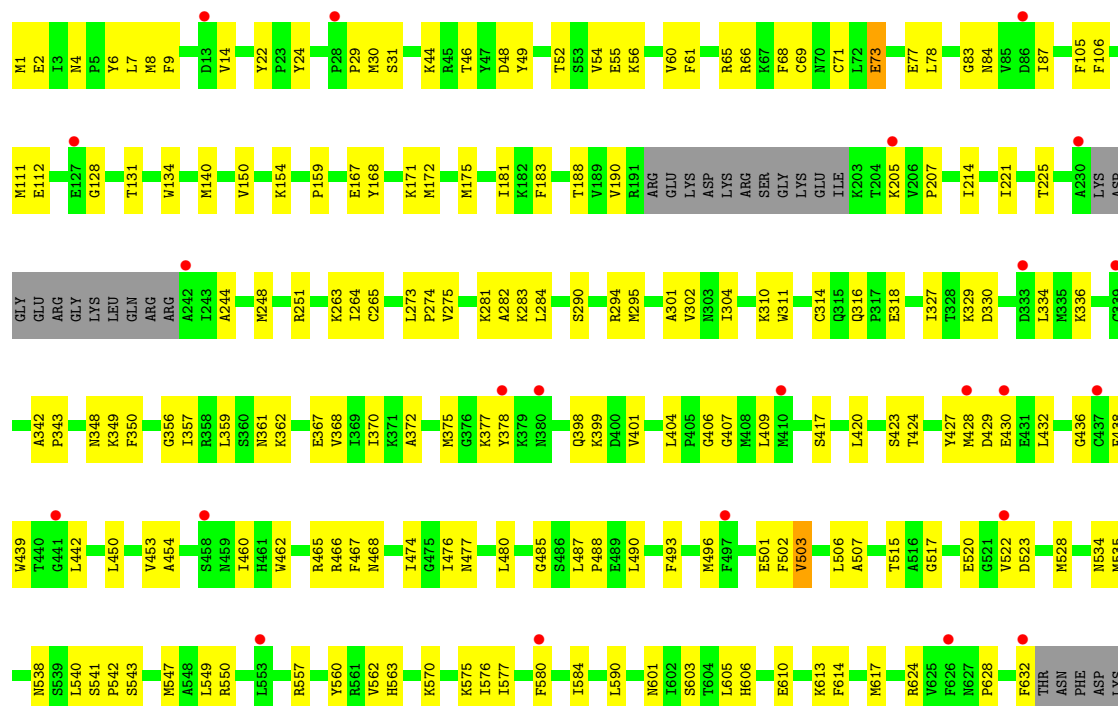
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Mg 2	0	0
6	D	2	Total 2	Mg 2	0	0

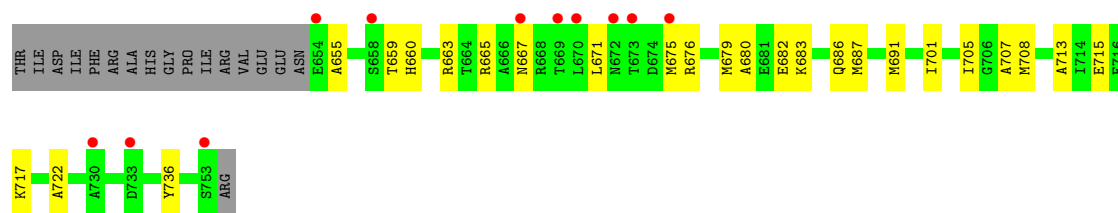
- Molecule 1: Polymerase acidic protein



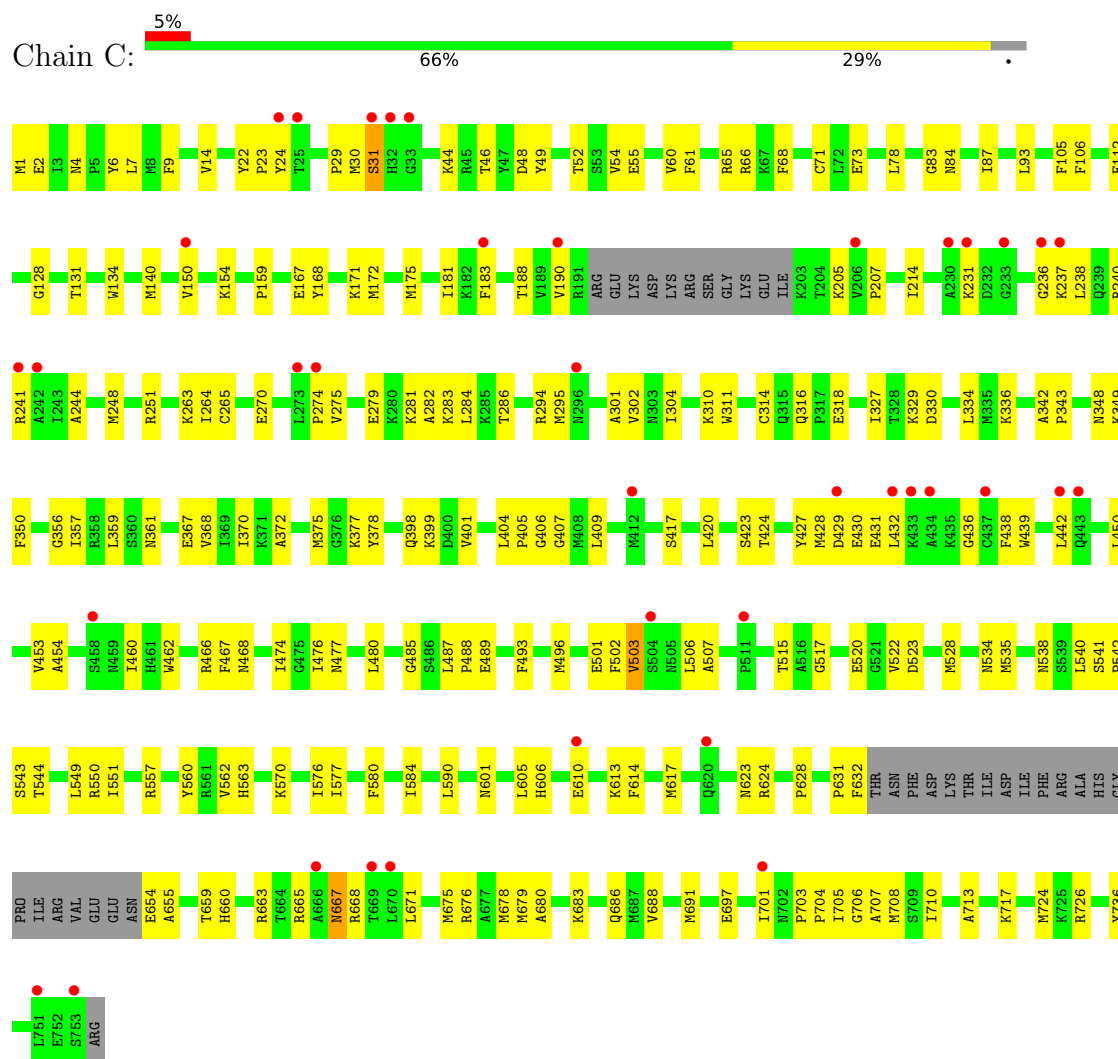


● Molecule 2: RNA-directed RNA polymerase catalytic subunit

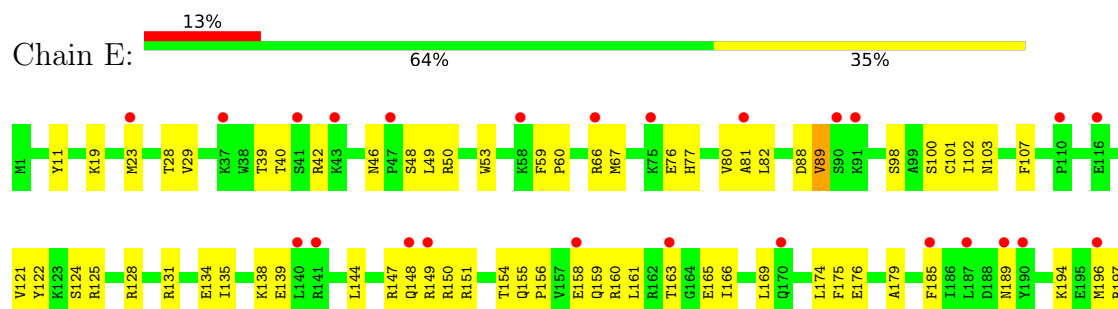


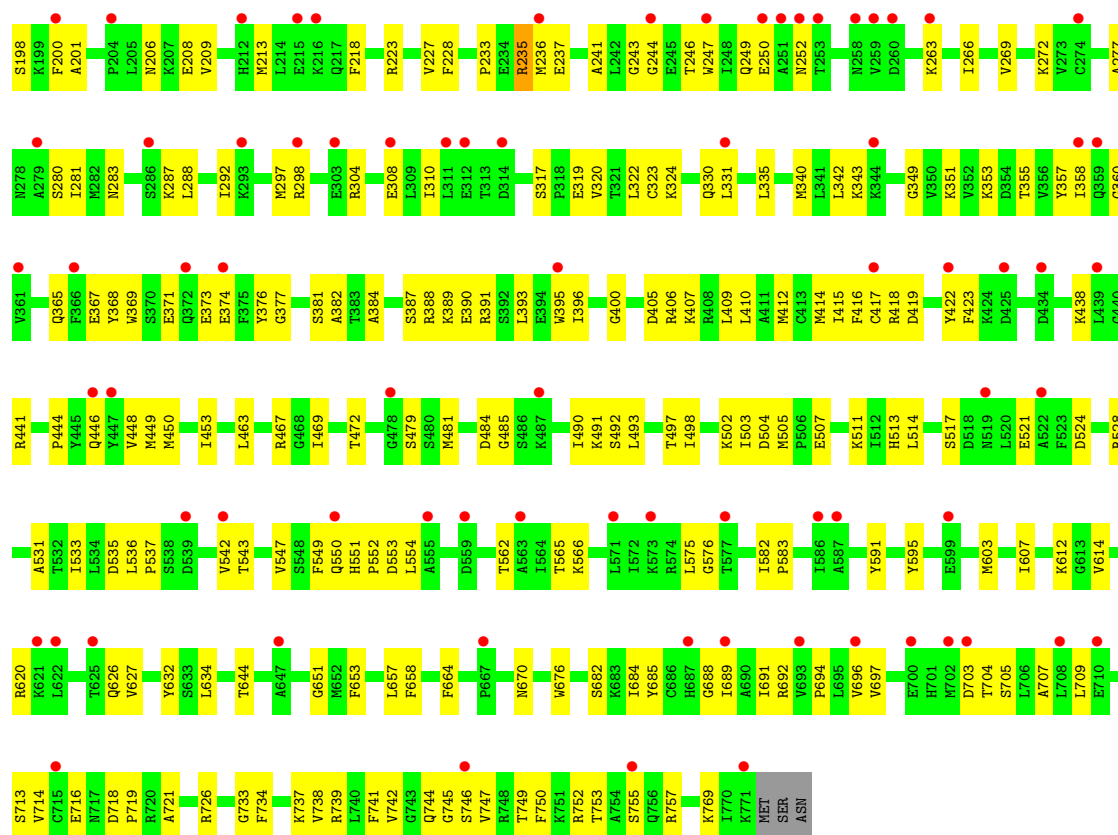


• Molecule 2: RNA-directed RNA polymerase catalytic subunit

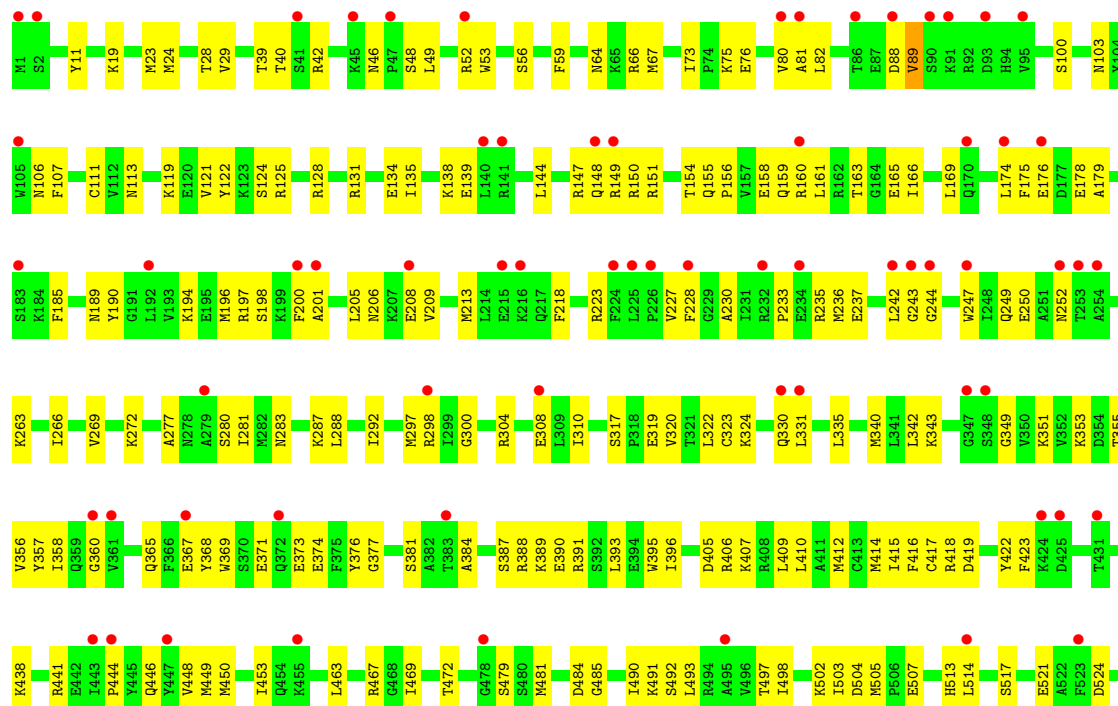


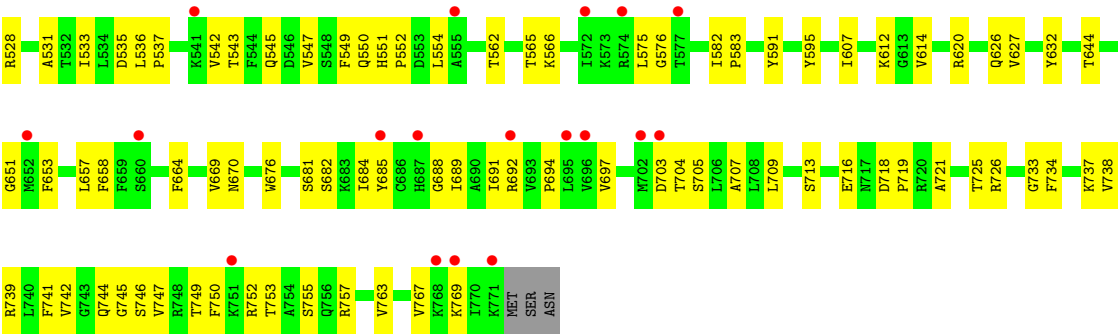
• Molecule 3: Polymerase basic protein 2



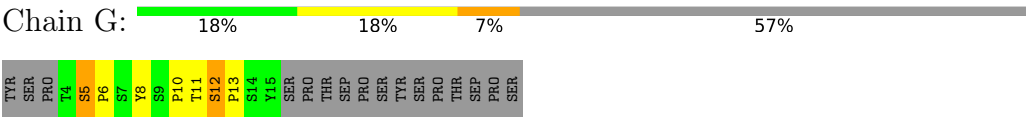


● Molecule 3: Polymerase basic protein 2





● Molecule 4: DNA-directed RNA polymerase subunit



● Molecule 5: ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA-ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	185.70Å 185.70Å 597.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	131.31 – 4.14 131.31 – 4.14	Depositor EDS
% Data completeness (in resolution range)	68.9 (131.31-4.14) 68.9 (131.31-4.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 4.15Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.260 , 0.296 0.262 , 0.298	Depositor DCC
R_{free} test set	2819 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	105.8	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 145.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	35282	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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, 0.333 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: MG, SEP

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	0.24	1/5855 (0.0%)	0.54	12/7866 (0.2%)
1	D	0.24	2/5855 (0.0%)	0.54	9/7866 (0.1%)
2	B	0.20	0/5741	0.45	3/7716 (0.0%)
2	C	0.25	1/5835 (0.0%)	0.47	4/7839 (0.1%)
3	E	0.20	2/6251 (0.0%)	0.46	2/8415 (0.0%)
3	F	0.20	2/6251 (0.0%)	0.45	0/8415
4	G	0.30	0/79	0.60	0/105
5	H	0.54	0/49	2.90	8/67 (11.9%)
All	All	0.22	8/35916 (0.0%)	0.50	38/48289 (0.1%)

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	D	0	4
2	B	0	1
2	C	0	1
All	All	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	30	MET	SD-CE	-8.09	1.59	1.79
3	F	249	GLN	CD-NE2	-7.50	1.17	1.33
3	E	249	GLN	CD-NE2	-7.42	1.17	1.33
1	A	238	ILE	CG1-CD1	-7.29	1.23	1.51
1	D	238	ILE	CG1-CD1	-7.16	1.23	1.51

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	3	ALA	CB-CA-C	-10.83	95.31	111.77
5	H	7	ALA	N-CA-CB	-9.24	94.96	109.19
1	D	33	ARG	NE-CZ-NH2	9.08	127.37	119.20
5	H	3	ALA	N-CA-C	8.43	126.79	107.48
1	D	33	ARG	NE-CZ-NH1	-8.27	113.23	121.50

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	GLN	Sidechain
1	D	204	GLN	Sidechain
1	D	472	GLN	Peptide
1	D	473	GLU	Peptide
1	D	664	GLY	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	5736	0	5749	235	0
1	D	5736	0	5749	224	0
2	B	5643	0	5736	195	0
2	C	5736	0	5837	214	0
3	E	6140	0	6250	220	0
3	F	6140	0	6250	236	0
4	G	97	0	73	11	0
5	H	50	0	52	0	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
All	All	35282	0	35696	1145	0

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 1145 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:410:GLU:OE1	1:D:411:LEU:N	1.59	1.34
1:A:410:GLU:OE1	1:A:411:LEU:N	1.59	1.34
3:E:367:GLU:O	3:E:418:ARG:NH1	1.87	1.08
3:F:367:GLU:O	3:F:418:ARG:NH1	1.87	1.07
1:A:410:GLU:OE1	1:A:411:LEU:HB2	1.57	1.05

There are no symmetry-related clashes.

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	706/709 (100%)	674 (96%)	31 (4%)	1 (0%)	48	81
1	D	706/709 (100%)	678 (96%)	27 (4%)	1 (0%)	48	81
2	B	702/754 (93%)	678 (97%)	23 (3%)	1 (0%)	48	81
2	C	715/754 (95%)	691 (97%)	23 (3%)	1 (0%)	48	81
3	E	769/774 (99%)	732 (95%)	35 (5%)	2 (0%)	36	70
3	F	769/774 (99%)	731 (95%)	36 (5%)	2 (0%)	36	70
4	G	8/28 (29%)	6 (75%)	1 (12%)	1 (12%)	0	4
5	H	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
All	All	4383/4512 (97%)	4196 (96%)	178 (4%)	9 (0%)	43	76

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	13	PRO
3	E	89	VAL
3	E	533	ILE
3	F	89	VAL
3	F	533	ILE

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	630/631 (100%)	630 (100%)	0	100	100
1	D	630/631 (100%)	630 (100%)	0	100	100
2	B	630/669 (94%)	630 (100%)	0	100	100
2	C	639/669 (96%)	639 (100%)	0	100	100
3	E	676/679 (100%)	676 (100%)	0	100	100
3	F	676/679 (100%)	676 (100%)	0	100	100
4	G	10/24 (42%)	10 (100%)	0	100	100
All	All	3891/3982 (98%)	3891 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	534	ASN
3	E	454	GLN
3	F	626	GLN
2	C	563	HIS
3	E	78	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
4	SEP	G	12	4	8,9,10	1.48	1 (12%)	7,12,14	2.32	2 (28%)
4	SEP	G	5	4	8,9,10	1.62	1 (12%)	7,12,14	1.14	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
4	SEP	G	12	4	-	6/6/8/10	-
4	SEP	G	5	4	-	6/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	SEP	P-O1P	3.55	1.61	1.50
4	G	12	SEP	P-O1P	3.10	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	12	SEP	OG-CB-CA	5.12	113.13	108.14
4	G	12	SEP	O3P-P-OG	2.73	113.79	106.67

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	5	SEP	N-CA-CB-OG
4	G	5	SEP	C-CA-CB-OG
4	G	5	SEP	CB-OG-P-O2P
4	G	5	SEP	CB-OG-P-O3P
4	G	12	SEP	N-CA-CB-OG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	12	SEP	2	0
4	G	5	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	708/709 (99%)	0.67	40 (5%) 30 27	65, 123, 199, 259	0
1	D	708/709 (99%)	0.71	50 (7%) 22 22	67, 140, 219, 293	0
2	B	710/754 (94%)	0.60	34 (4%) 35 31	63, 115, 202, 293	0
2	C	721/754 (95%)	0.57	38 (5%) 32 28	75, 135, 203, 265	0
3	E	771/774 (99%)	1.01	101 (13%) 7 10	71, 161, 254, 321	0
3	F	771/774 (99%)	0.92	84 (10%) 10 13	82, 161, 229, 299	0
4	G	10/28 (35%)	0.88	0 100 100	167, 181, 197, 197	0
5	H	0/10	-	-	-	-
All	All	4399/4512 (97%)	0.75	347 (7%) 18 20	63, 139, 226, 321	0

The worst 5 of 347 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	242	ALA	6.5
3	E	200	PHE	5.7
1	D	341	GLY	5.5
1	A	497	LYS	5.2
1	A	340	LEU	5.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å ²)	Q<0.9
4	SEP	G	12	10/11	0.51	0.14	191,224,246,253	0
4	SEP	G	5	10/11	0.77	0.15	184,191,200,207	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	D	801	1/1	0.03	0.33	145,145,145,145	0
6	MG	A	801	1/1	0.26	0.24	103,103,103,103	0
6	MG	D	800	1/1	0.65	0.17	193,193,193,193	0
6	MG	A	800	1/1	0.85	0.15	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.