



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 16, 2017 – 09:13 am GMT

PDB ID : 4F5X  
Title : Location of the dsRNA-dependent polymerase, VP1, in rotavirus particles  
Authors : Estrozi, L.F.; Settembre, E.C.; Goret, G.; McClain, B.; Zhang, X.; Chen, J.Z.; Grigorieff, N.; Harrison, S.C.  
Deposited on : 2012-05-13  
Resolution : 5.00 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.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : **FAILED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28986

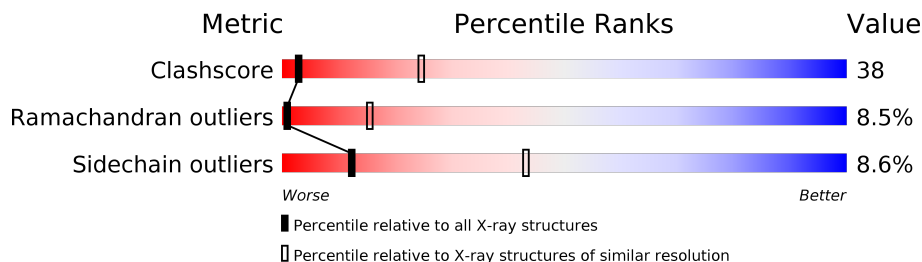
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.00 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))
Clashscore	112137	1094 (6.30-3.70)
Ramachandran outliers	110173	1027 (6.30-3.70)
Sidechain outliers	110143	1004 (6.30-3.70)










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  $\geq 3$ , 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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	880	
1	B	880	
2	C	397	
2	D	397	
2	E	397	
2	F	397	
2	G	397	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	H	397	 60% 32% 7% .
2	I	397	 58% 33% 9%
2	J	397	 58% 34% 8% .
2	K	397	 59% 33% 8% .
2	L	397	 57% 35% 7% .
2	M	397	 58% 35% 6% .
2	N	397	 56% 34% 9% .
2	O	397	 57% 33% 9% .
3	W	1089	 40% 44% 5% 10%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 62014 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 VP2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6374	4049	1099	1190	36			
1	B	810	Total	C	N	O	S	0	0	0
			6624	4211	1138	1239	36			

- Molecule 2 is a protein called Intermediate capsid protein VP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	D	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	E	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	F	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	G	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	H	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	I	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	J	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	K	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	L	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	M	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			
2	N	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	397	Total	C	N	O	S	0	0	0
			3162	2001	550	596	15			

- Molecule 3 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	975	Total	C	N	O	S	0	0	0
			7905	5081	1308	1482	34			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		



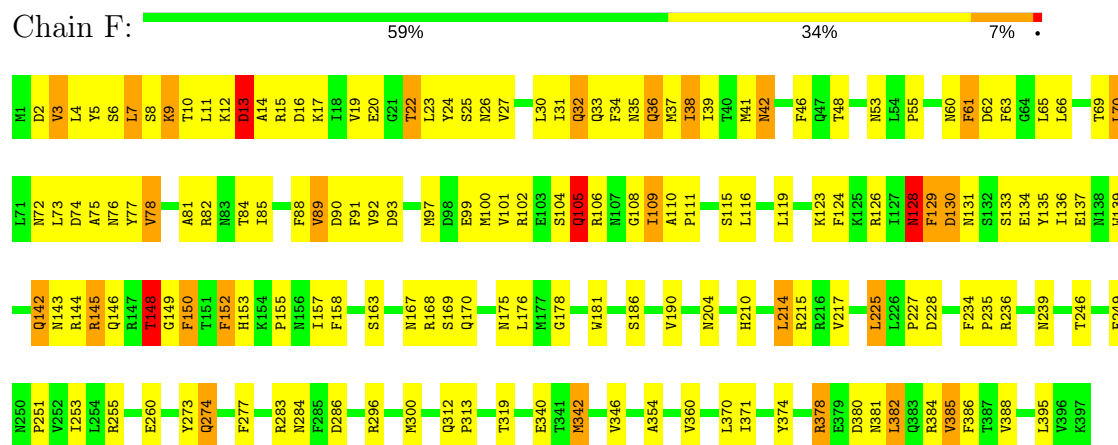


Chain B:  19% 49% 22% 8%

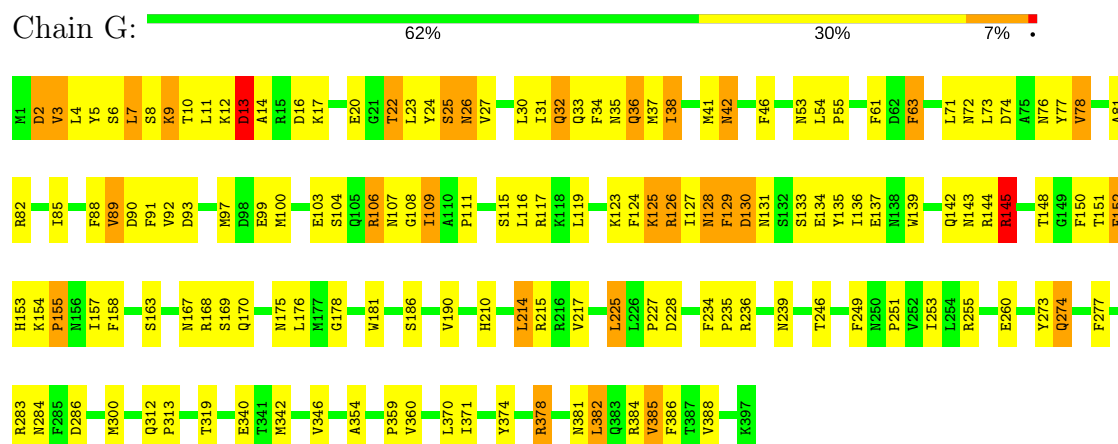




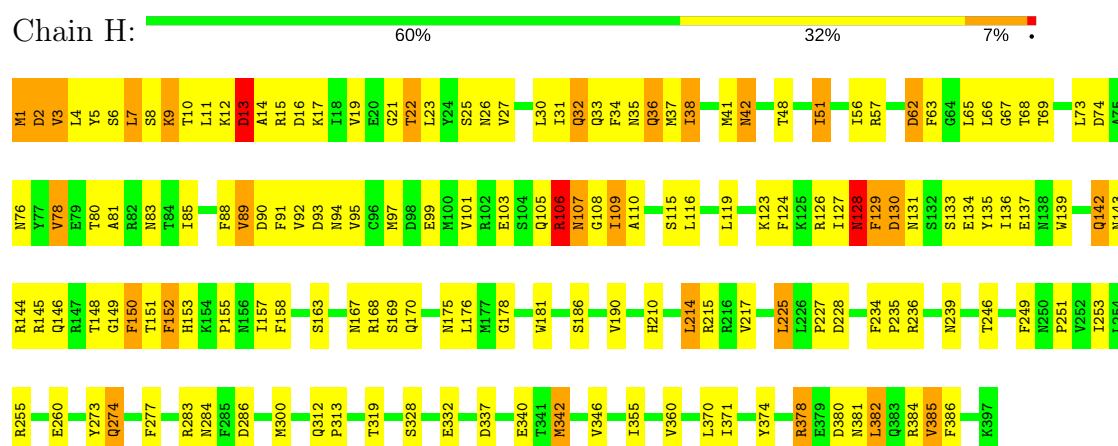




• Molecule 2: Intermediate capsid protein VP6

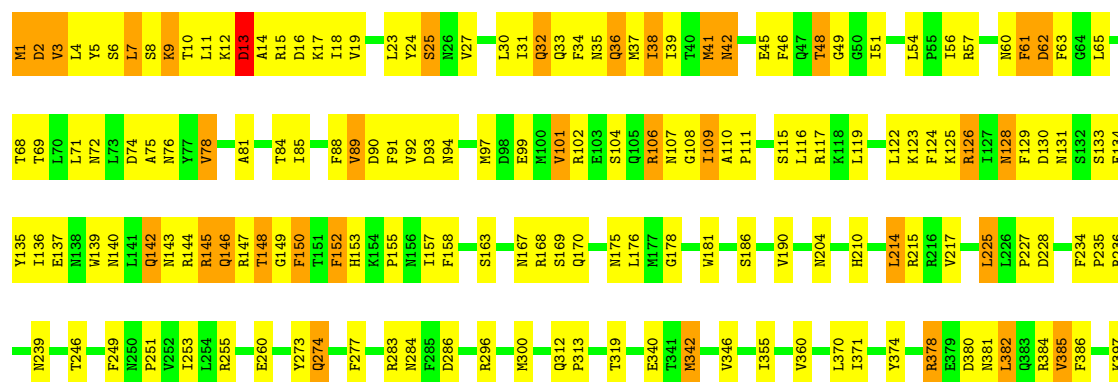


• Molecule 2: Intermediate capsid protein VP6

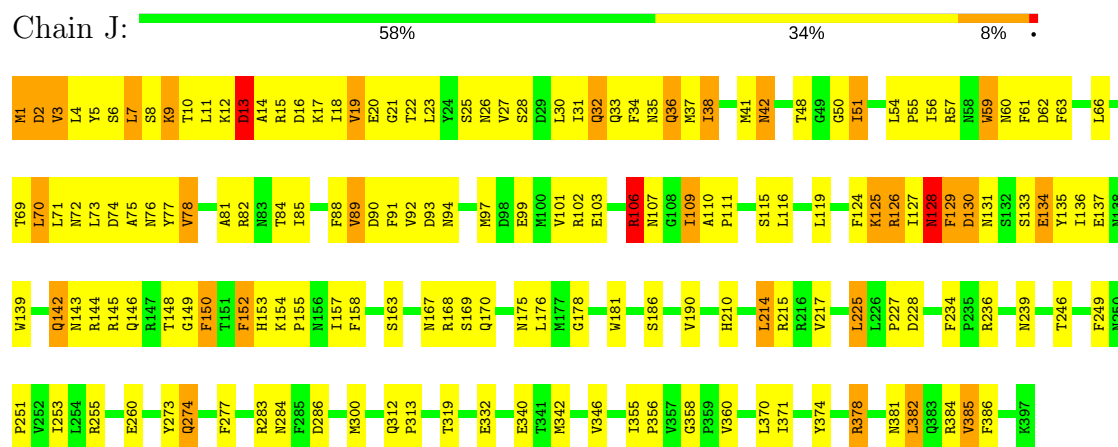


• Molecule 2: Intermediate capsid protein VP6

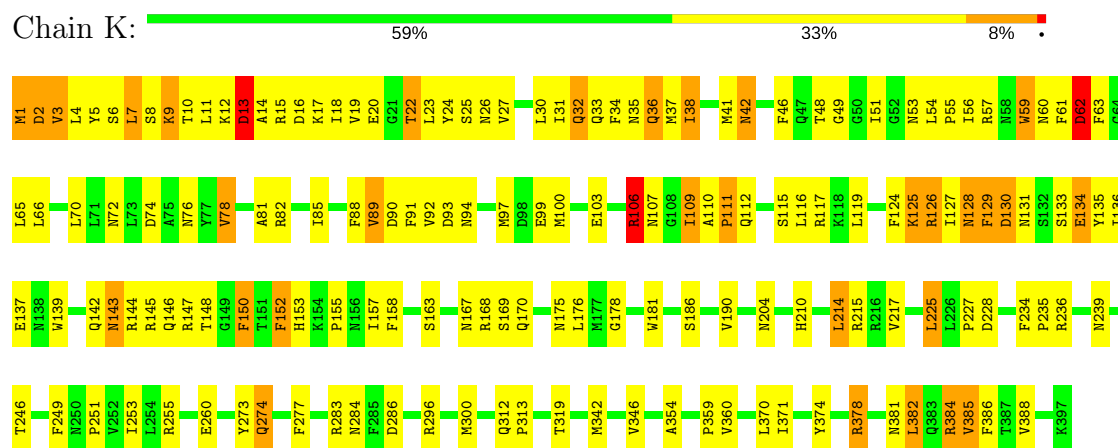




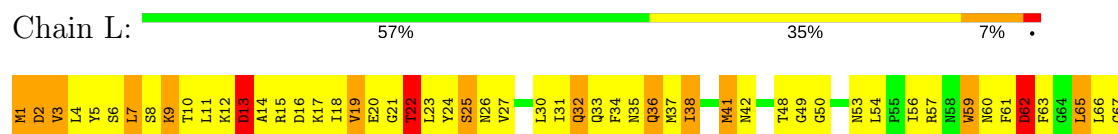
• Molecule 2: Intermediate capsid protein VP6

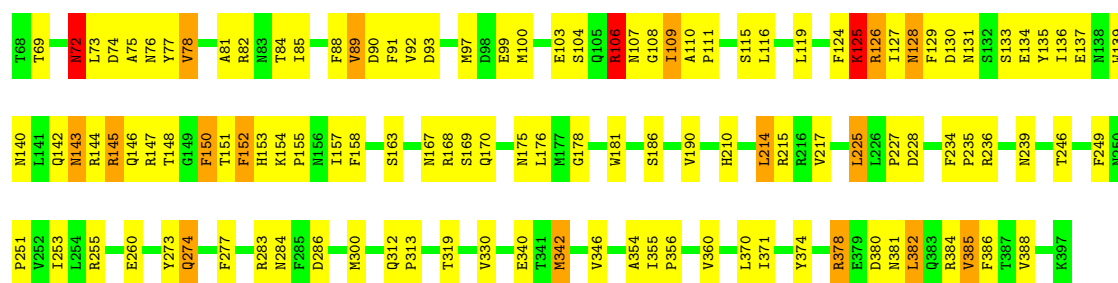


• Molecule 2: Intermediate capsid protein VP6



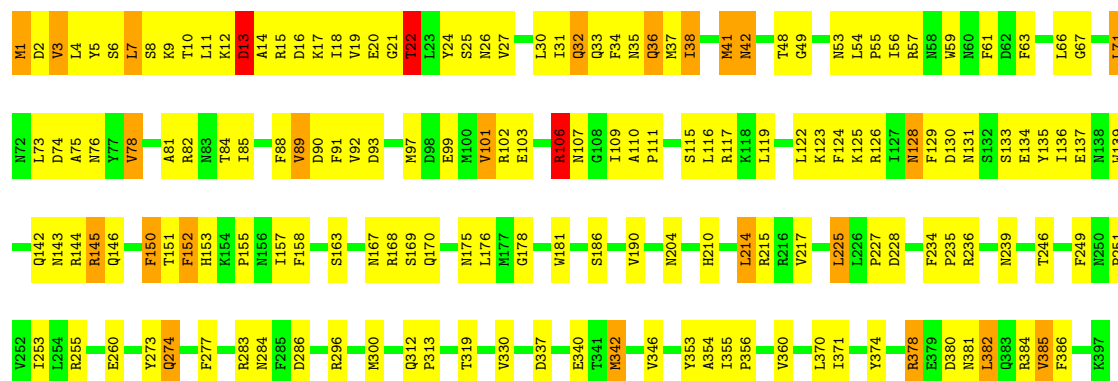
• Molecule 2: Intermediate capsid protein VP6





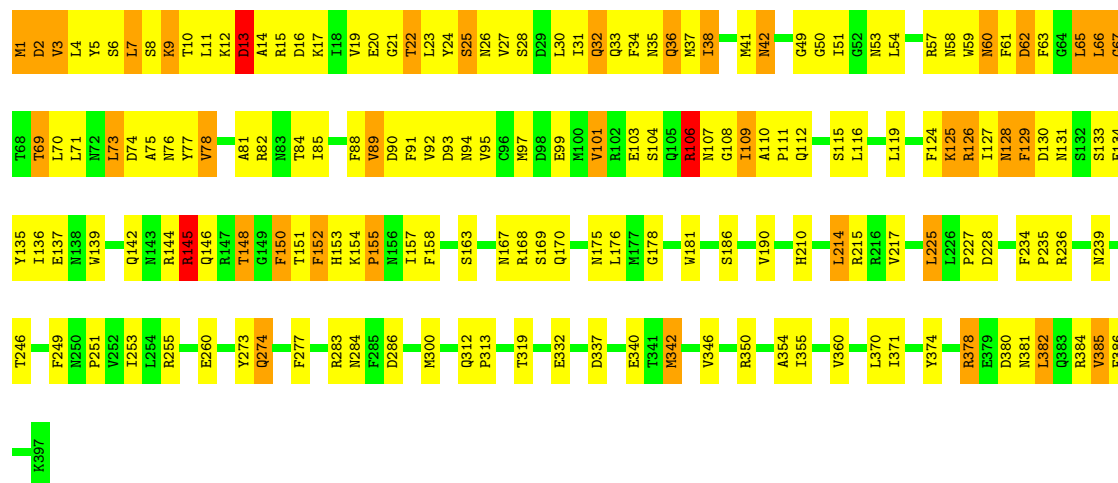
• Molecule 2: Intermediate capsid protein VP6

Chain M: 58% 35% 6%



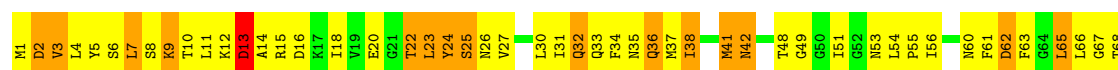
• Molecule 2: Intermediate capsid protein VP6

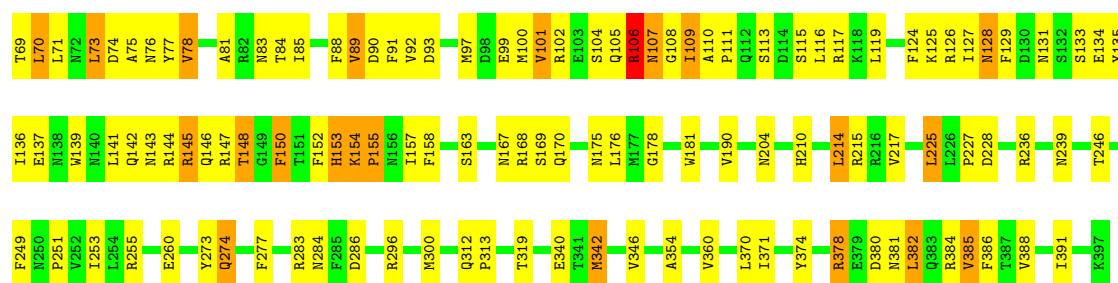
Chain N: 56% 34% 9%



• Molecule 2: Intermediate capsid protein VP6

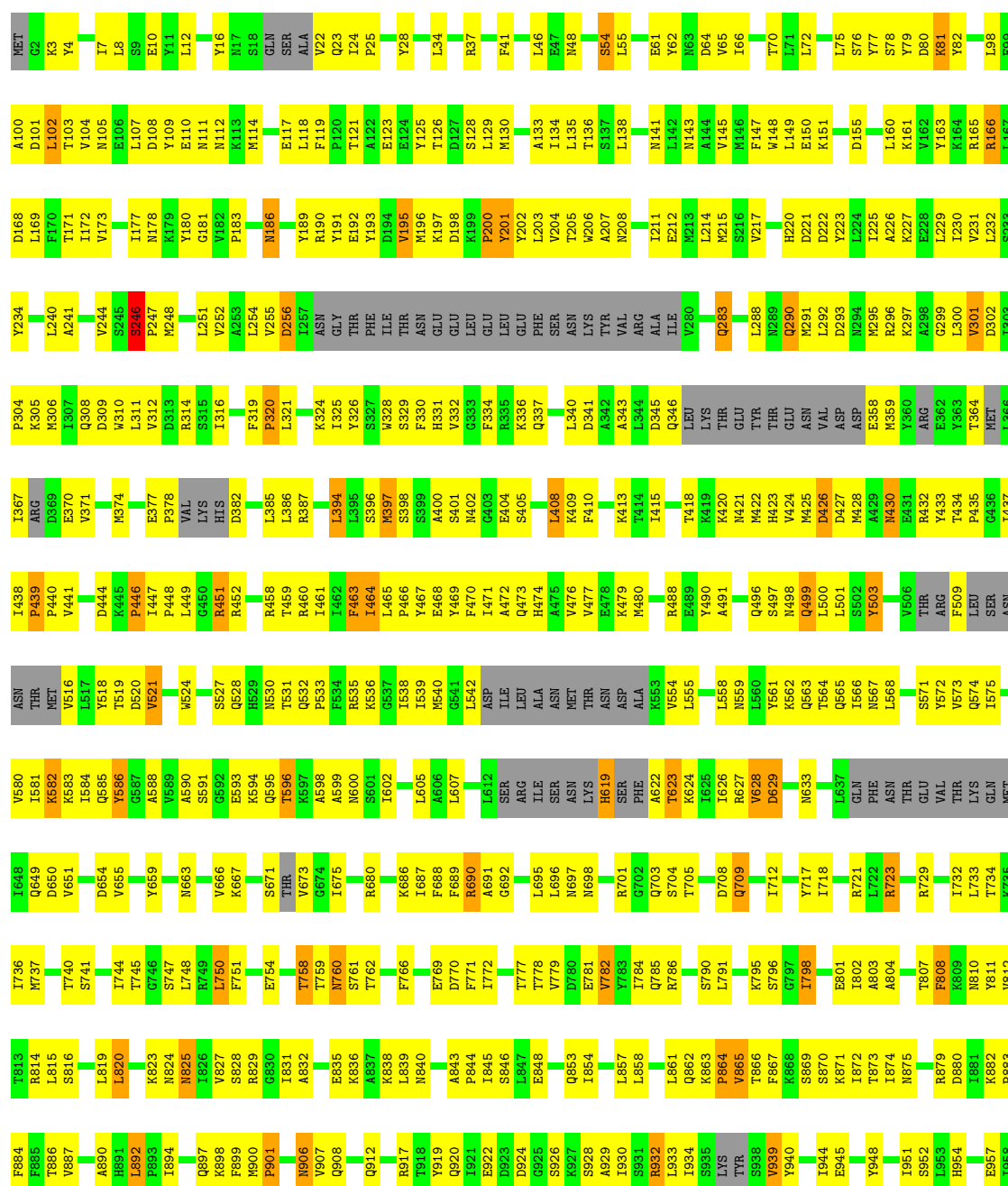
Chain O: 57% 33% 9%





• Molecule 3: RNA-directed RNA polymerase

Chain W:  40%  44%  5%  10%





## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	740.75Å 1198.07Å 1345.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 5.00	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-5.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.293 , 0.296	Depositor
Wilson B-factor (Å <sup>2</sup> )	167.1	Xtriage
Anisotropy	0.043	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	62014	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	146.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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

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	0.48	0/6491	0.84	9/8806 (0.1%)
1	B	0.50	0/6745	0.82	10/9149 (0.1%)
2	C	0.51	0/3232	0.78	5/4397 (0.1%)
2	D	0.51	0/3232	0.78	5/4397 (0.1%)
2	E	0.51	0/3232	0.77	5/4397 (0.1%)
2	F	0.50	0/3232	0.76	5/4397 (0.1%)
2	G	0.50	0/3232	0.77	5/4397 (0.1%)
2	H	0.50	0/3232	0.76	5/4397 (0.1%)
2	I	0.50	0/3232	0.77	5/4397 (0.1%)
2	J	0.51	0/3232	0.78	5/4397 (0.1%)
2	K	0.51	0/3232	0.77	5/4397 (0.1%)
2	L	0.51	0/3232	0.77	5/4397 (0.1%)
2	M	0.51	0/3232	0.77	5/4397 (0.1%)
2	N	0.51	0/3232	0.77	5/4397 (0.1%)
2	O	0.52	0/3232	0.79	7/4397 (0.2%)
3	W	0.41	0/8045	0.62	3/10847 (0.0%)
All	All	0.49	0/63297	0.77	89/85963 (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

There are no bond length outliers.

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	TYR	CB-CG-CD2	10.70	127.42	121.00
1	A	273	TYR	CB-CG-CD1	-9.86	115.08	121.00
1	A	273	TYR	CA-CB-CG	9.85	132.12	113.40
1	B	273	TYR	CB-CG-CD1	9.85	126.91	121.00
1	B	273	TYR	CB-CG-CD2	-9.21	115.48	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

## 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	6374	0	6394	1006	0
1	B	6624	0	6652	1133	0
2	C	3162	0	3101	170	0
2	D	3162	0	3101	179	0
2	E	3162	0	3101	164	0
2	F	3162	0	3101	160	0
2	G	3162	0	3101	149	0
2	H	3162	0	3101	175	0
2	I	3162	0	3101	215	0
2	J	3162	0	3101	187	0
2	K	3162	0	3101	166	0
2	L	3162	0	3101	178	0
2	M	3162	0	3101	173	0
2	N	3162	0	3101	191	0
2	O	3162	0	3101	163	0
3	W	7905	0	7966	543	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	O	1	0	0	0	0
All	All	62014	0	61325	4691	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 38.

The worst 5 of 4691 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:B:75:VAL:HG22	3:W:673:VAL:CG1	1.63	1.28
1:B:771:VAL:HB	1:B:809:PHE:HB3	1.23	1.18
1:B:75:VAL:CG2	3:W:673:VAL:HG12	1.72	1.18
1:A:333:VAL:HG11	1:A:380:LYS:HA	1.27	1.15
1:A:428:GLN:OE1	1:A:456:PHE:HB2	1.46	1.13

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	779/880 (88%)	431 (55%)	199 (26%)	149 (19%)	0	3
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0	3
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	2	24
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1	18
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2	24
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	2	23
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	2	24
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	2	25
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	2	23
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	2	25
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	1	22
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1	21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	2	26
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1	19
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1	18
3	W	933/1089 (86%)	807 (86%)	93 (10%)	33 (4%)	4	35
All	All	7655/8010 (96%)	5858 (76%)	1147 (15%)	650 (8%)	1	15

5 of 650 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	LYS
1	A	130	GLN
1	A	193	SER
1	A	198	LYS
1	A	220	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	715/809 (88%)	603 (84%)	112 (16%)	3	19
1	B	744/809 (92%)	635 (85%)	109 (15%)	3	21
2	C	350/350 (100%)	325 (93%)	25 (7%)	17	50
2	D	350/350 (100%)	322 (92%)	28 (8%)	14	46
2	E	350/350 (100%)	325 (93%)	25 (7%)	17	50
2	F	350/350 (100%)	327 (93%)	23 (7%)	19	52
2	G	350/350 (100%)	327 (93%)	23 (7%)	19	52
2	H	350/350 (100%)	329 (94%)	21 (6%)	22	56
2	I	350/350 (100%)	327 (93%)	23 (7%)	19	52
2	J	350/350 (100%)	327 (93%)	23 (7%)	19	52
2	K	350/350 (100%)	327 (93%)	23 (7%)	19	52
2	L	350/350 (100%)	321 (92%)	29 (8%)	13	45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	350/350 (100%)	325 (93%)	25 (7%)	17	50
2	N	350/350 (100%)	324 (93%)	26 (7%)	16	49
2	O	350/350 (100%)	329 (94%)	21 (6%)	22	56
3	W	885/990 (89%)	828 (94%)	57 (6%)	20	53
All	All	6894/7158 (96%)	6301 (91%)	593 (9%)	12	43

5 of 593 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	284	ASN
2	G	143	ASN
3	W	198	ASP
2	E	13	ASP
2	F	60	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 253 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	53	ASN
2	I	131	ASN
3	W	499	GLN
2	G	142	GLN
2	H	128	ASN

### 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 5 ligands modelled in this entry, 5 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

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 [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.