



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 03:19 PM BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

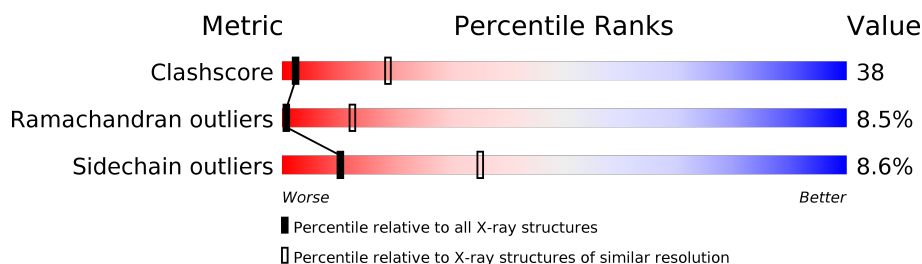
1 Overall quality at a glance

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	141614	1000 (6.16-3.82)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)

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 ≥ 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 $\leq 5\%$.

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	
2	H	397	

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Mol	Chain	Length	Quality of chain
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			

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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.

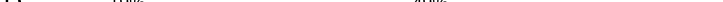
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	W	975	Total	C	N	O	S	0	0	0
			7905	5081	1308	1482	34			

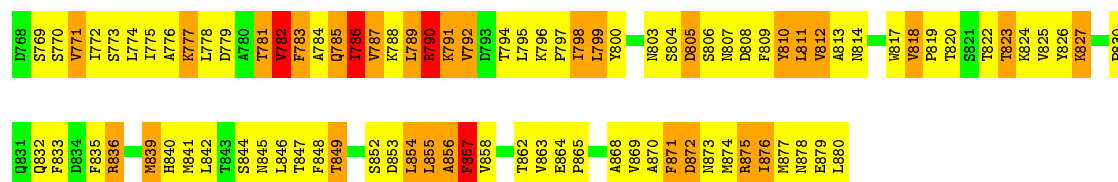
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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		



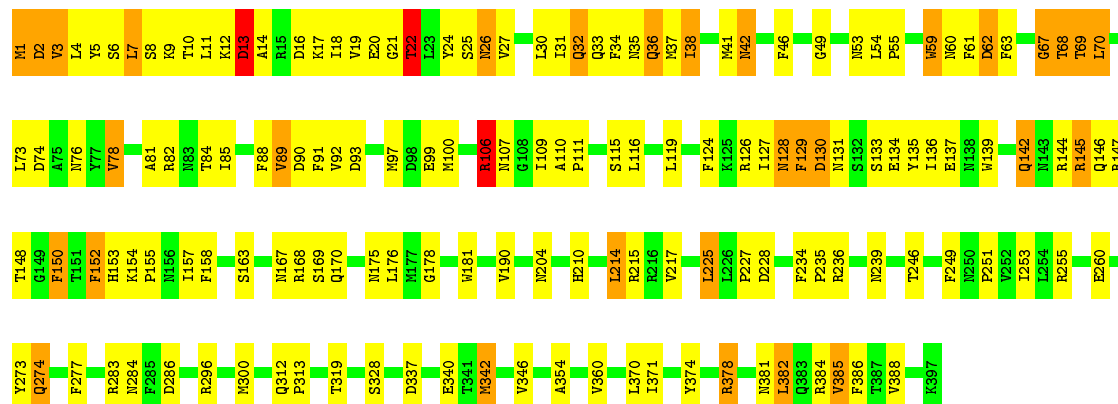


Chain B: 



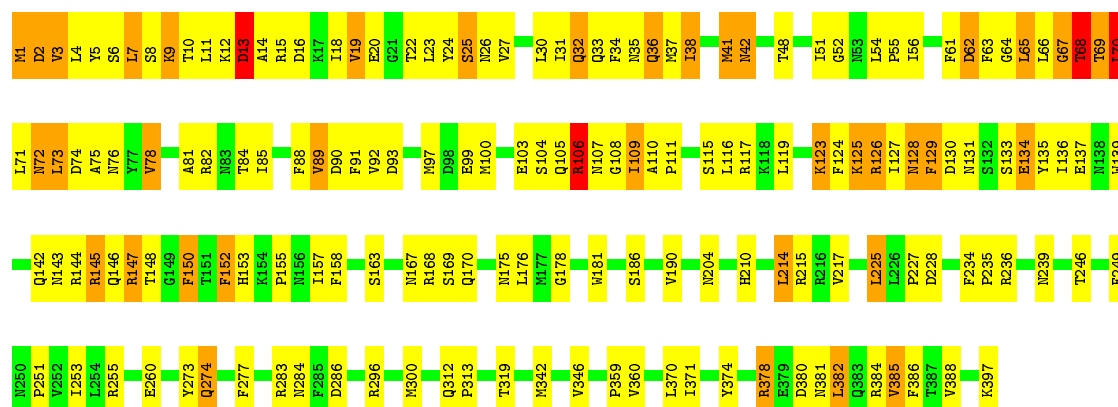
• Molecule 2: Intermediate capsid protein VP6

Chain C: 60% 31% 8%



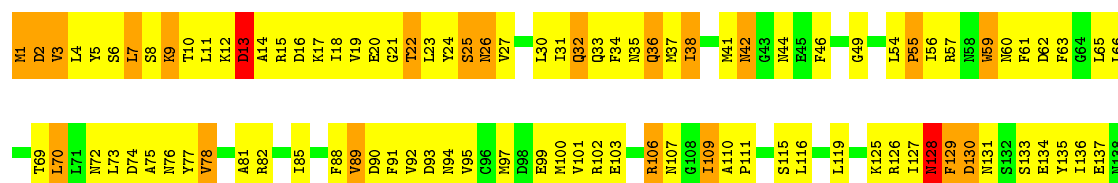
• Molecule 2: Intermediate capsid protein VP6

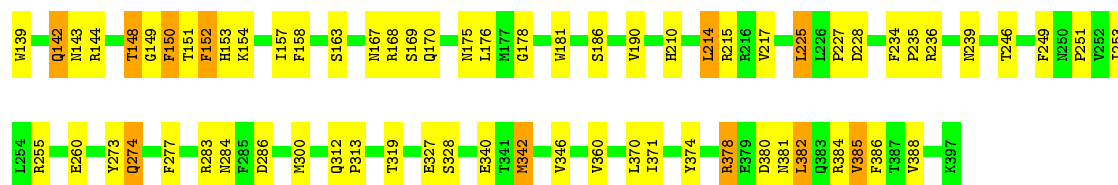
Chain D: 57% 32% 9%



• Molecule 2: Intermediate capsid protein VP6

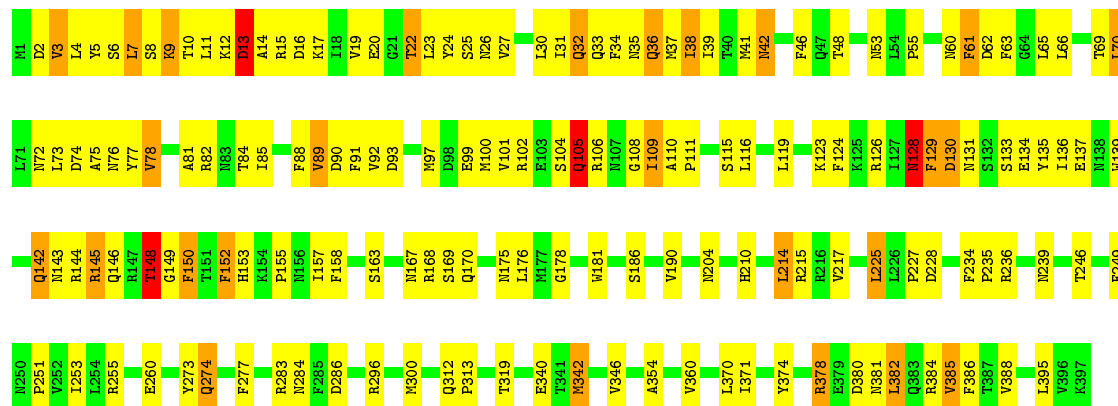
Chain E: 58% 33% 8%





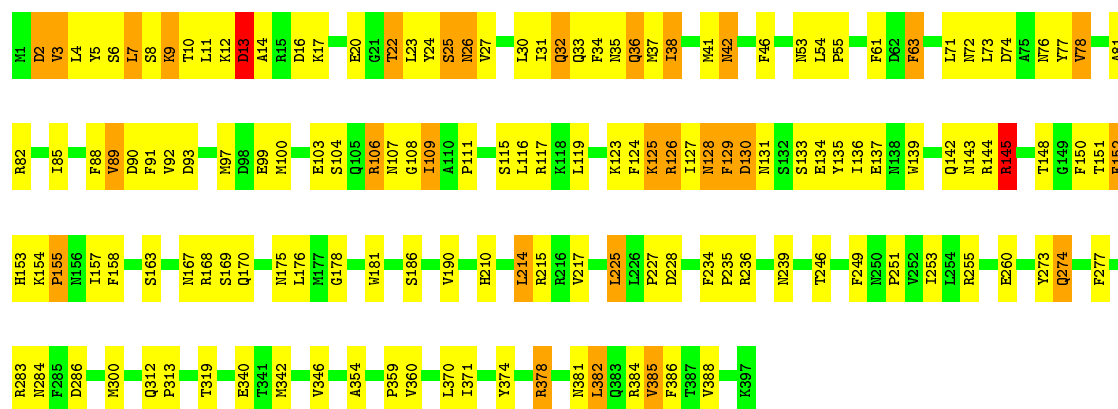
• Molecule 2: Intermediate capsid protein VP6

Chain F: 59% 34% 7%



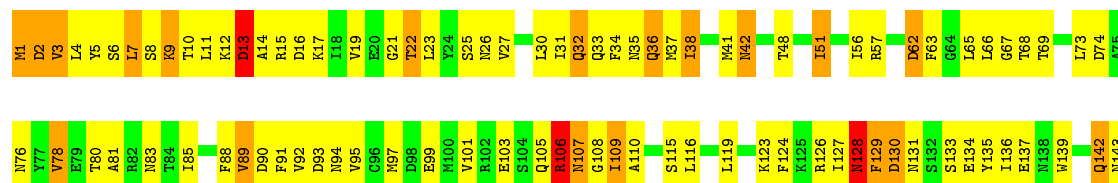
• Molecule 2: Intermediate capsid protein VP6

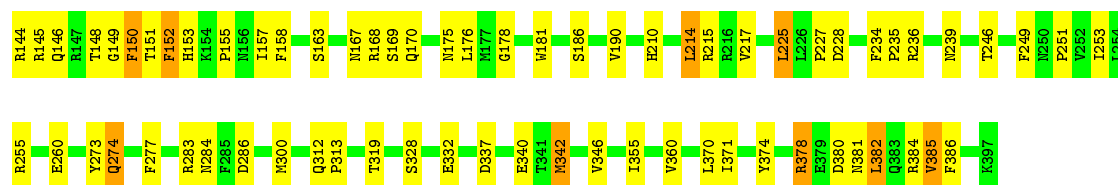
Chain G: 62% 30% 7%



• Molecule 2: Intermediate capsid protein VP6

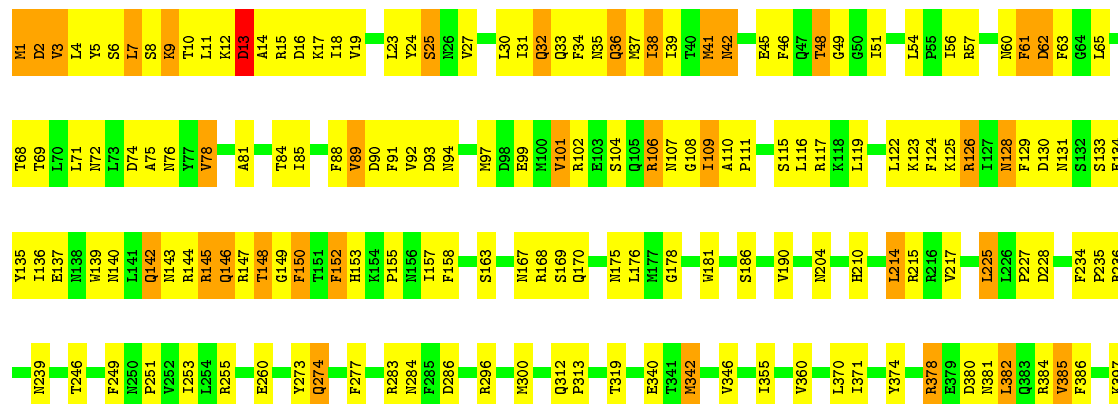
Chain H: 60% 32% 7%





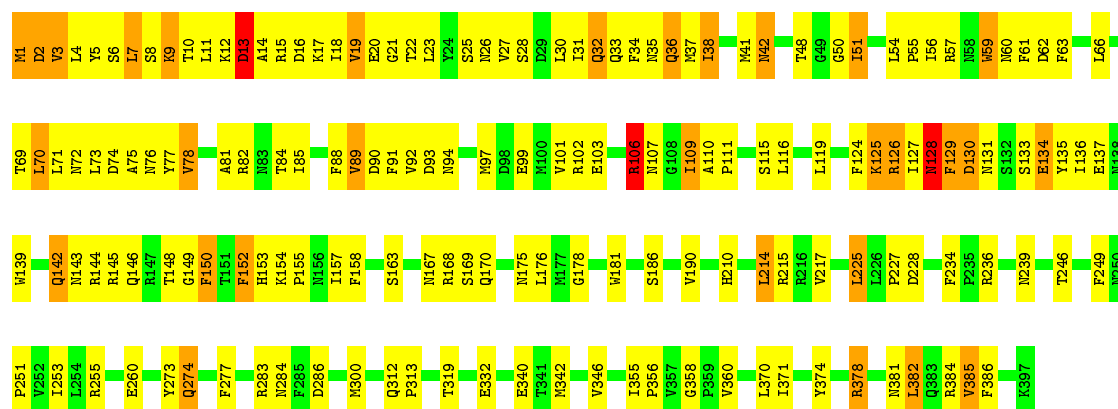
• Molecule 2: Intermediate capsid protein VP6

Chain I: 58% 33% 9%



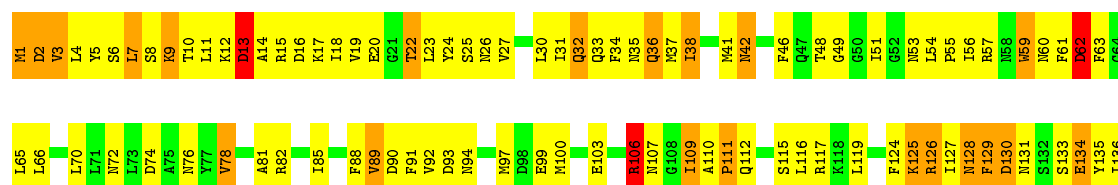
• Molecule 2: Intermediate capsid protein VP6

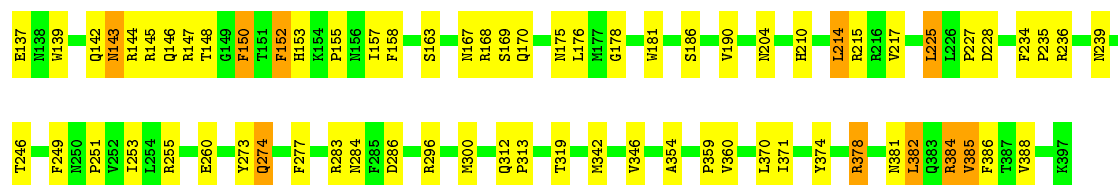
Chain J: 58% 34% 8%



• Molecule 2: Intermediate capsid protein VP6

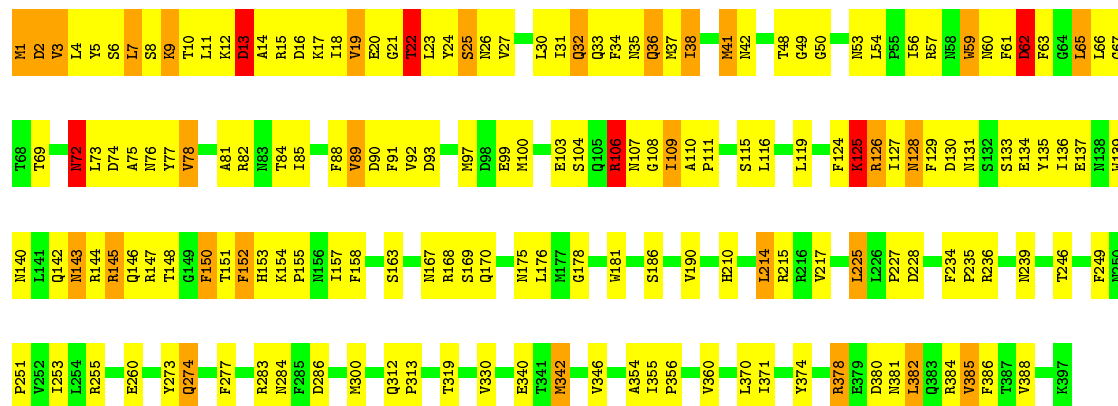
Chain K: 59% 33% 8%





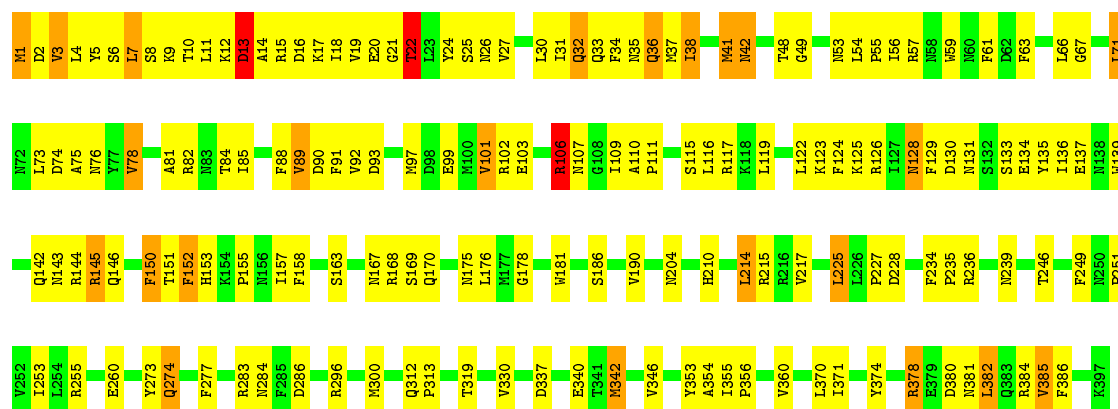
• Molecule 2: Intermediate capsid protein VP6

Chain L: 57% 35% 7% •



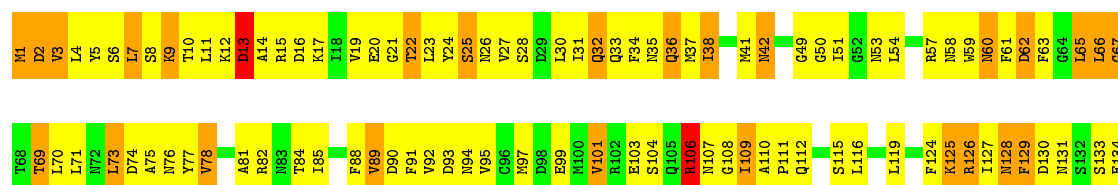
• Molecule 2: Intermediate capsid protein VP6

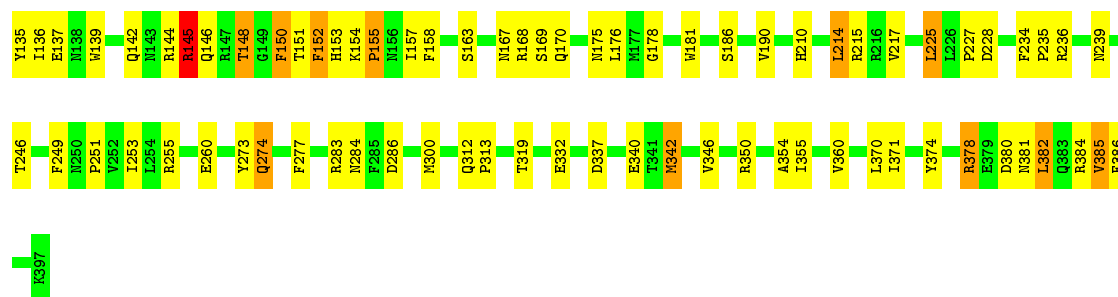
Chain M: 58% 35% 6% •



• Molecule 2: Intermediate capsid protein VP6

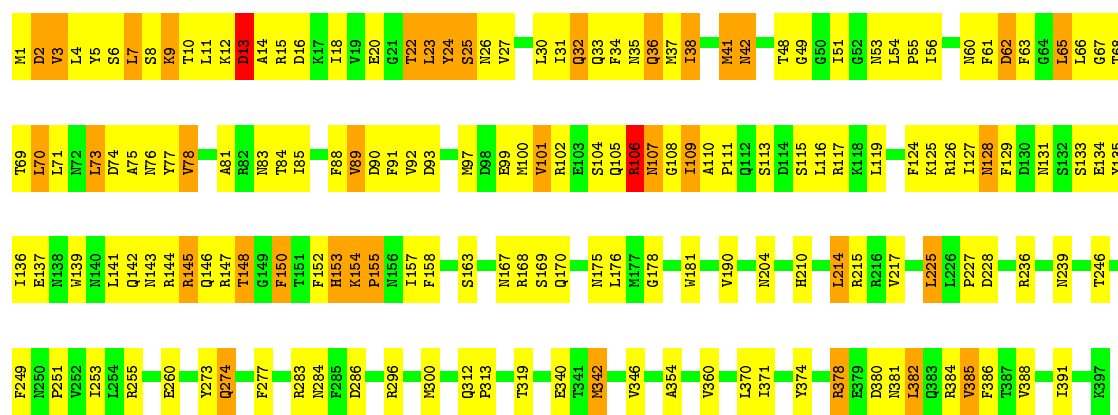
Chain N: 56% 34% 9% •





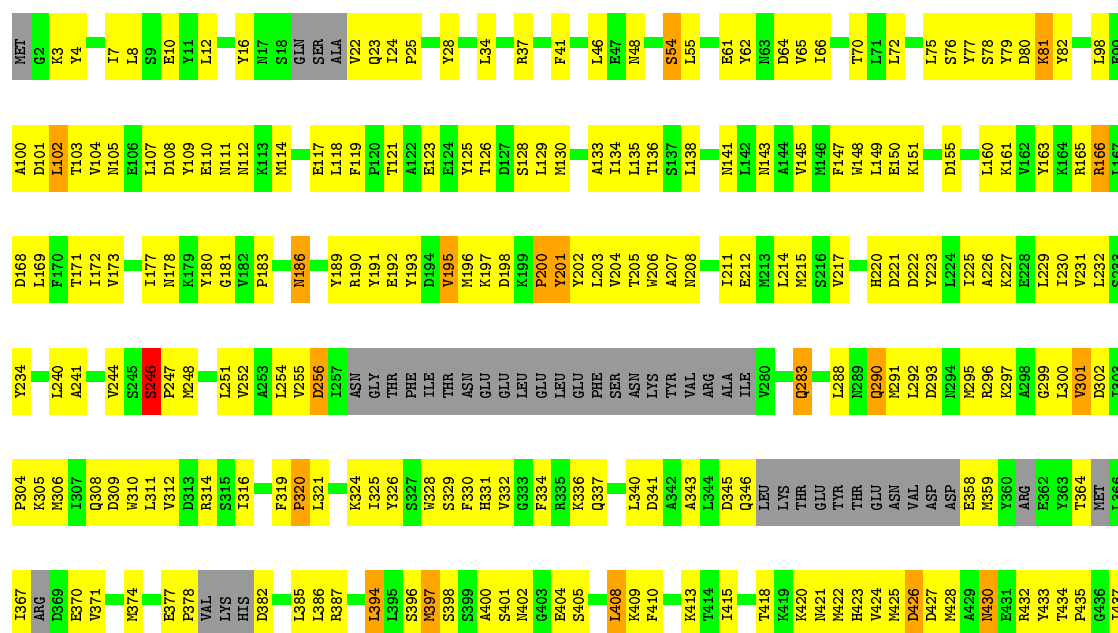
• Molecule 2: Intermediate capsid protein VP6

Chain O: 57% 33% 9%



• Molecule 3: RNA-directed RNA polymerase

Chain W: 40% 44% 5% 10%



LYS	ILE	PRO	ALA	VAL	THR	F1031	H1034	A1037	I1042	M1043	K1047	M1048	G1049	S1050	W1051	I1052	S1053	L1054	Y1058	P1059	M1063	K1068	K1069	H1070	W1071	M1072	I1073	T1074	R1077	S1078	P1079	Y1080	T1081	H1082	A1083	R1084	F1085	F1086	GLN	GLU	PRO																
GLN	LEU	Y961	L962	ILE	S964	L965	G966	PRO	LYS	ILE	ASP	ALA	ASP	TYR	VAL	GLY	SER	LYS	ILE	Y981	S982	ARG	D984	K985	Y986	R987	I988	S991	Y992	L996	I999	H1000	Y1001	G1002	C1003	I934	S985	LYS	TYR	S938	V939	Y940	I944	E945	Y948	I951	S952	L953	H954	E957	I958						
F884	F885	T886	V887	ILE	S964	L965	G966	PRO	LYS	ILE	ASP	ALA	ASP	TYR	VAL	GLY	SER	LYS	ILE	Y981	S982	ARG	D984	K985	Y986	R987	I988	S991	Y992	L996	I999	H1000	Y1001	G1002	C1003	I934	S985	LYS	TYR	S938	V939	Y940	I944	E945	Y948	I951	S952	L953	H954	E957	I958						
T813	R814	L815	S816	L819	L820	K823	N824	N825	R826	V827	S828	R829	G830	I831	A832	E835	K836	A837	K838	L839	N840	A843	P844	I845	S846	L847	E848	Q853	S854	L857	L858	L861	Q862	K863	P864	V865	T866	F867	R868	S869	S870	K871	I872	T873	I874	N875	R879	D880	I881	K882	P883						
I736	M737	T740	S741	I744	T745	G746	S747	L748	N750	R751	E754	T758	T759	M760	S761	T762	F766	E769	D770	F771	I772	T777	T778	V779	D780	E781	V782	Y783	I784	Q785	R786	S790	L791	K795	S796	G797	I798	B801	I802	A803	A804	T807	R808	K809	N810	Y811	T734	K735									
I648	Q649	D650	V651	D654	V655	Y659	N663	V666	K667	S671	THR	T673	V673	I674	R675	R680	K686	I687	F688	F689	R690	A691	G692	L695	L696	N697	N698	R701	G702	Q703	S704	T705	D708	Q709	I712	Y717	I718	R721	L722	R723	T807	R808	K809	N810	Y811	T734	K735										
V580	I581	R582	K583	I584	Q585	Y586	A588	V589	A590	S591	G592	E593	K594	Q595	T596	R597	A598	A599	M600	I602	L605	A606	L607	L612	SER	ARG	ILE	ALA	ASN	MET	THR	LYS	H619	SER	PHE	A622	T623	K624	I625	I626	R627	V628	D629	N633	L637	GLN	PHE	ASN	THR	GLU	VAL	THR	LYS	MET			
ASN	THR	MET	V516	L517	Y518	T519	D520	V521	W524	S527	Q528	E529	N530	T531	Q532	P533	F534	R535	K536	G537	I538	I539	M540	G541	L542	ASP	ILE	LEU	ALA	ASN	MET	THR	LYS	H619	SER	ASP	ALA	R488	E489	Y490	A491	Q496	S497	N498	Q499	L500	L501	S502	Y503	V506	THR	ARG	F509	LEU	SER	GLN	ASN
T438	P439	P440	V441	D444	F445	P446	I447	L448	G450	R451	R452	R458	T459	R460	I461	F462	F463	I464	L465	P466	Y467	E468	Y469	F470	I471	A472	Q473	H474	A475	V476	V477	A478	ASU	K479	ASP	ALA	R488	E489	Y490	A491	Q496	S497	N498	Q499	L500	L501	S502	Y503	V506	THR	ARG	F509	LEU	SER	GLN	ASN	

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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.49 (at 3.78Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.293 , 0.296	Depositor
Wilson B-factor (Å ²)	167.1	Xtriage
Anisotropy	0.043	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	62014	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [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 ⓘ

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	2
1	B	808/880 (92%)	458 (57%)	204 (25%)	146 (18%)	0	2
2	C	395/397 (100%)	318 (80%)	54 (14%)	23 (6%)	1	20
2	D	395/397 (100%)	315 (80%)	50 (13%)	30 (8%)	1	15
2	E	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	20
2	F	395/397 (100%)	324 (82%)	47 (12%)	24 (6%)	1	18
2	G	395/397 (100%)	323 (82%)	49 (12%)	23 (6%)	1	20
2	H	395/397 (100%)	323 (82%)	50 (13%)	22 (6%)	2	20
2	I	395/397 (100%)	320 (81%)	51 (13%)	24 (6%)	1	18
2	J	395/397 (100%)	320 (81%)	53 (13%)	22 (6%)	2	20
2	K	395/397 (100%)	318 (80%)	52 (13%)	25 (6%)	1	18
2	L	395/397 (100%)	322 (82%)	47 (12%)	26 (7%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	M	395/397 (100%)	322 (82%)	52 (13%)	21 (5%)	2	21
2	N	395/397 (100%)	317 (80%)	50 (13%)	28 (7%)	1	16
2	O	395/397 (100%)	317 (80%)	47 (12%)	31 (8%)	1	14
3	W	933/1089 (86%)	807 (86%)	93 (10%)	33 (4%)	3	28
All	All	7655/8010 (96%)	5858 (76%)	1147 (15%)	650 (8%)	1	12

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%)	2	15
1	B	744/809 (92%)	635 (85%)	109 (15%)	3	16
2	C	350/350 (100%)	325 (93%)	25 (7%)	14	41
2	D	350/350 (100%)	322 (92%)	28 (8%)	12	37
2	E	350/350 (100%)	325 (93%)	25 (7%)	14	41
2	F	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	G	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	H	350/350 (100%)	329 (94%)	21 (6%)	19	46
2	I	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	J	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	K	350/350 (100%)	327 (93%)	23 (7%)	16	43
2	L	350/350 (100%)	321 (92%)	29 (8%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	350/350 (100%)	325 (93%)	25 (7%)	14	41
2	N	350/350 (100%)	324 (93%)	26 (7%)	13	40
2	O	350/350 (100%)	329 (94%)	21 (6%)	19	46
3	W	885/990 (89%)	828 (94%)	57 (6%)	17	44
All	All	6894/7158 (96%)	6301 (91%)	593 (9%)	10	35

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 monosaccharides 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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