wwPDB EM Validation Summary Report

Jun 26, 2025 – 12:29 AM JST

PDB ID	:	8X9W / pdb_00008x9w
EMDB ID	:	EMD-38186
Title	:	portal vertex capsomer of the VZV C-Capsid
Authors	:	Nan, W.; Lei, C.; Jiangxi, W.
Deposited on	:	2023-12-01
Resolution	:	4.50 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
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:

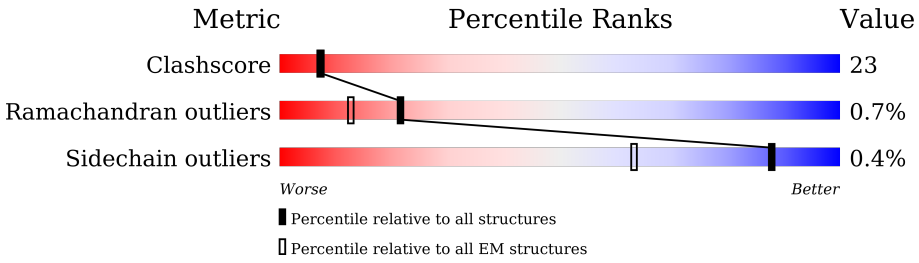
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	1387	56% 41% ·
1	C	1387	49% 43% · 7%
2	B	87	98% ·
2	H	87	98% ·
2	I	87	98% ·
2	J	87	98% ·
2	K	87	74% 14% 13%
2	L	87	76% 11% 13%
2	Q	87	74% 14% 13%

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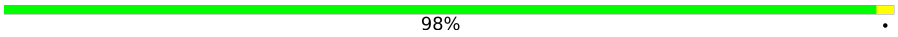
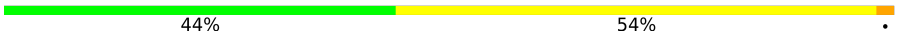
Mol	Chain	Length	Quality of chain
2	R	87	
2	S	87	
2	T	87	
3	F	297	
4	O	307	
5	X	289	
6	k	550	
7	l	94	
7	m	94	
8	n	47	
8	o	47	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 37344 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1347	Total 10392	C 6579	N 1822	O 1927	S 64	0	0
1	C	1287	Total 9888	C 6258	N 1737	O 1829	S 64	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	ALA	-	expression tag	UNP P09245
A	9	ALA	-	expression tag	UNP P09245
A	10	ALA	-	expression tag	UNP P09245
A	11	ALA	-	expression tag	UNP P09245
A	12	ALA	-	expression tag	UNP P09245
A	13	ALA	-	expression tag	UNP P09245
A	22	ILE	LEU	conflict	UNP P09245
A	327	ASN	GLN	conflict	UNP P09245
A	329	ALA	THR	conflict	UNP P09245
A	343	SER	GLY	conflict	UNP P09245
A	344	LEU	MET	conflict	UNP P09245
A	348	GLY	ALA	conflict	UNP P09245
A	814	ALA	GLY	conflict	UNP P09245
C	8	ALA	-	expression tag	UNP P09245
C	9	ALA	-	expression tag	UNP P09245
C	10	ALA	-	expression tag	UNP P09245
C	11	ALA	-	expression tag	UNP P09245
C	12	ALA	-	expression tag	UNP P09245
C	13	ALA	-	expression tag	UNP P09245
C	22	ILE	LEU	conflict	UNP P09245
C	323	ASN	GLN	conflict	UNP P09245
C	325	ALA	THR	conflict	UNP P09245
C	339	SER	GLY	conflict	UNP P09245
C	340	LEU	MET	conflict	UNP P09245
C	344	GLY	ALA	conflict	UNP P09245
C	814	ALA	GLY	conflict	UNP P09245

- Molecule 2 is a protein called coiled-coil domain of portal.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	87	Total 435	C 261	N 87	O 87	0	0
2	H	87	Total 435	C 261	N 87	O 87	0	0
2	I	87	Total 435	C 261	N 87	O 87	0	0
2	J	87	Total 435	C 261	N 87	O 87	0	0
2	K	76	Total 380	C 228	N 76	O 76	0	0
2	L	76	Total 380	C 228	N 76	O 76	0	0
2	Q	76	Total 380	C 228	N 76	O 76	0	0
2	R	76	Total 380	C 228	N 76	O 76	0	0
2	S	76	Total 380	C 228	N 76	O 76	0	0
2	T	87	Total 435	C 261	N 87	O 87	0	0

- Molecule 3 is a protein called Tri2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	297	Total 2124	C 1367	N 365	O 383	S 9	0	0

- Molecule 4 is a protein called Tri2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	307	Total 2279	C 1456	N 399	O 413	S 11	0	0

- Molecule 5 is a protein called Tri1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	289	Total 2198	C 1392	N 397	O 395	S 14	0	0

- Molecule 6 is a protein called CVC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	k	550	Total	C	N	O	S	0	0
			4206	2674	764	747	21		

- Molecule 7 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	94	Total	C	N	O	S	0	0
			766	486	138	138	4		
7	m	80	Total	C	N	O	S	0	0
			648	410	121	115	2		

- Molecule 8 is a protein called Large tegument protein deneddylase.

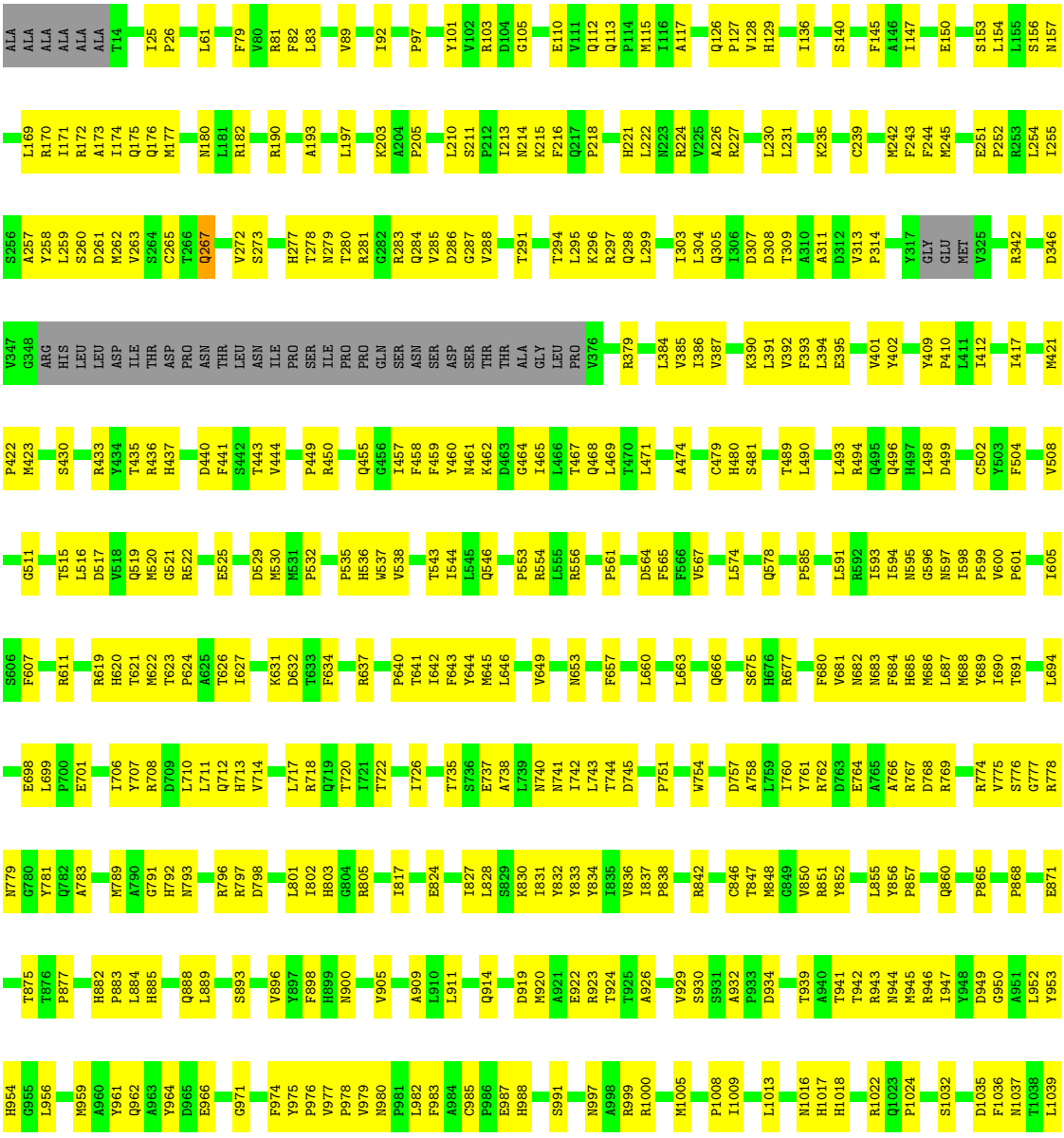
Mol	Chain	Residues	Atoms					AltConf	Trace
8	n	47	Total	C	N	O	S	0	0
			384	237	84	61	2		
8	o	47	Total	C	N	O	S	0	0
			384	237	84	61	2		

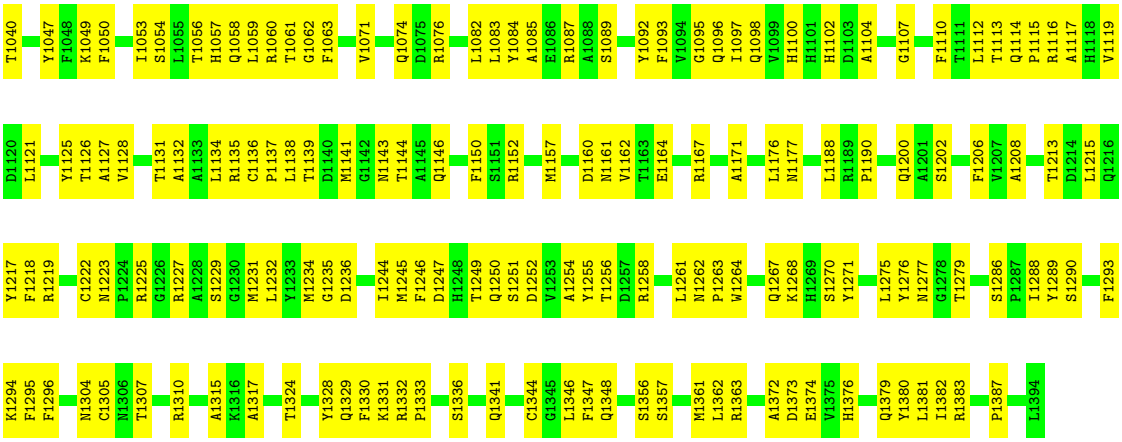
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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: Major capsid protein

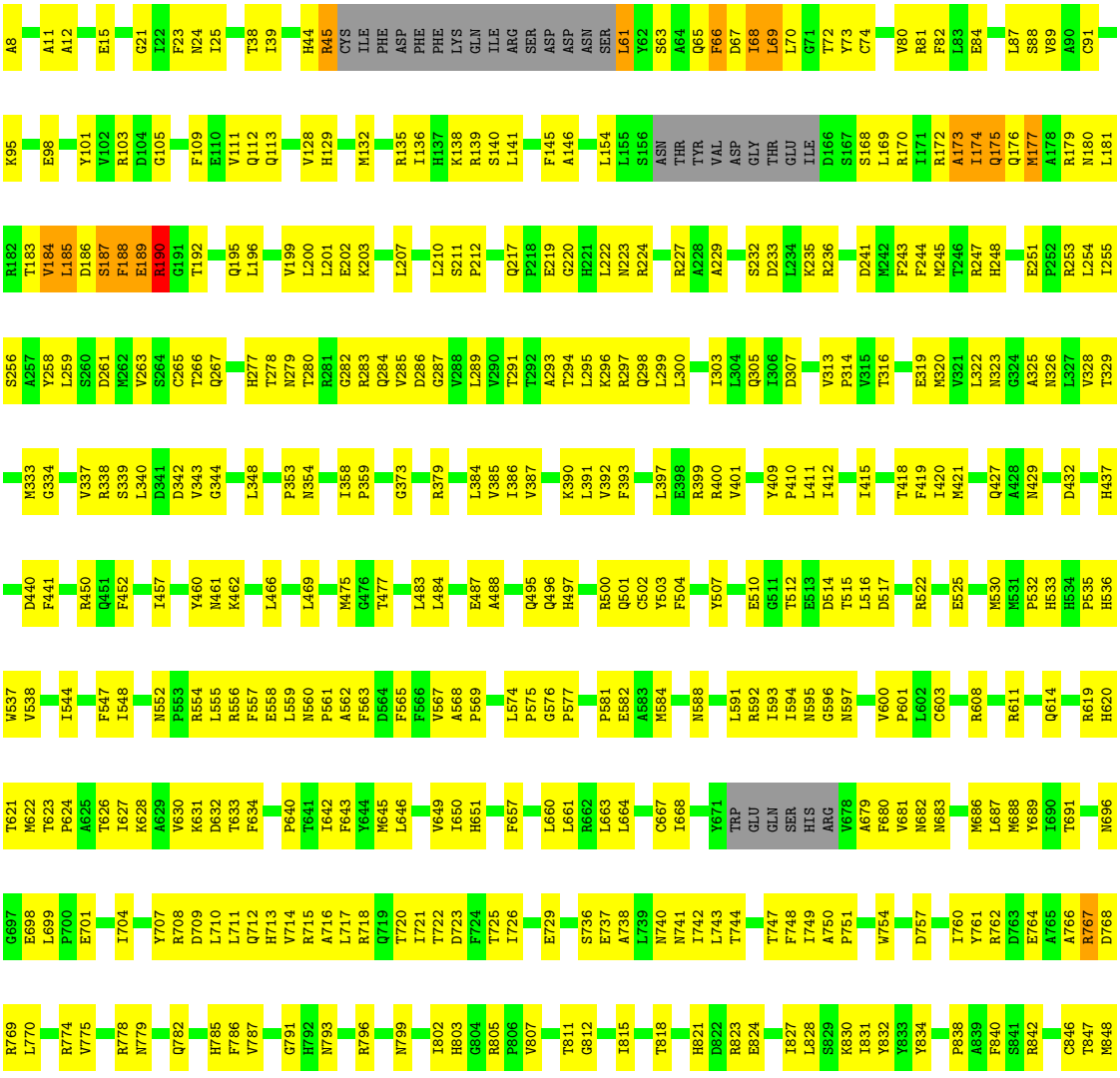
Chain A:

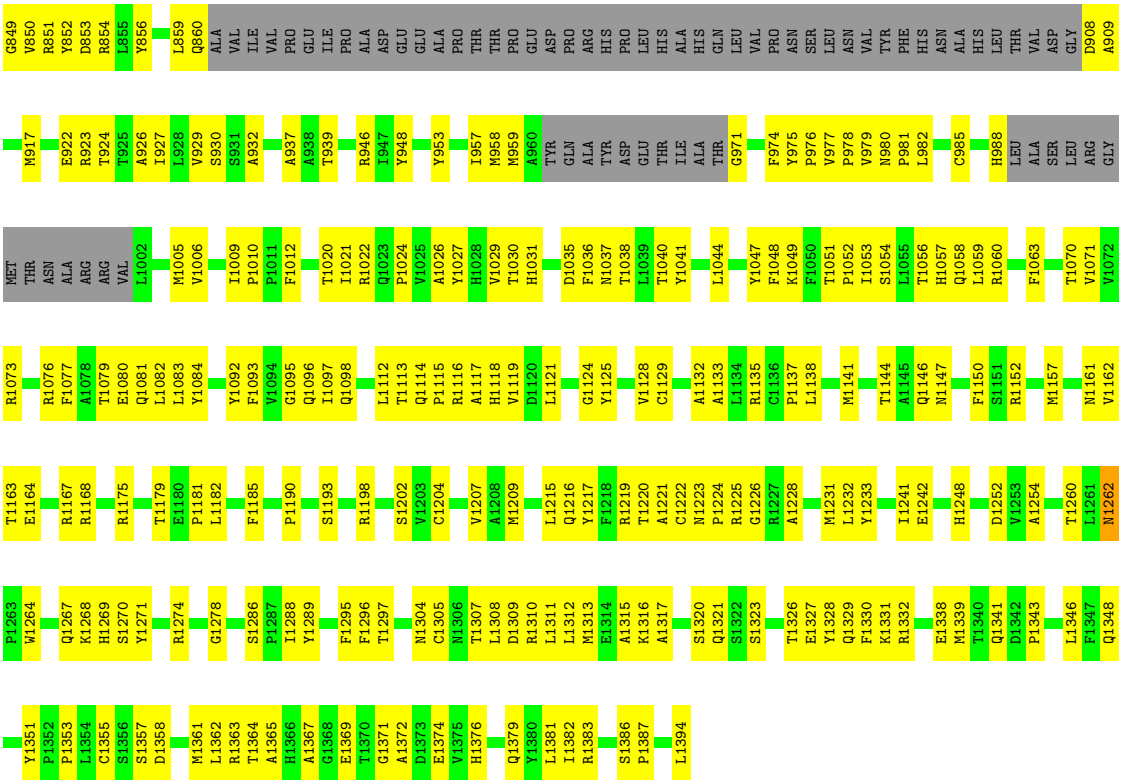




• Molecule 1: Major capsid protein

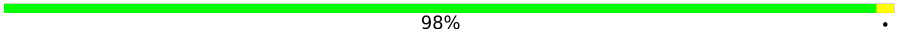
Chain C:

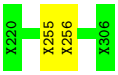




• Molecule 2: coiled-coil domain of portal

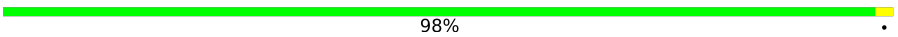
Chain B:

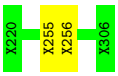




• Molecule 2: coiled-coil domain of portal

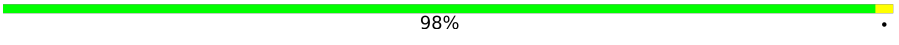
Chain H:

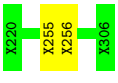




• Molecule 2: coiled-coil domain of portal

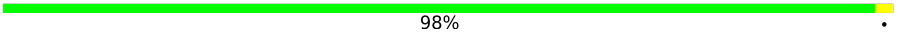
Chain I:

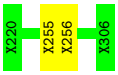




• Molecule 2: coiled-coil domain of portal

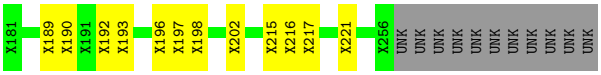
Chain J:





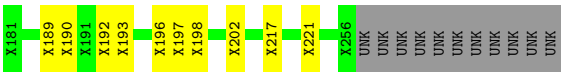
• Molecule 2: coiled-coil domain of portal

Chain K:



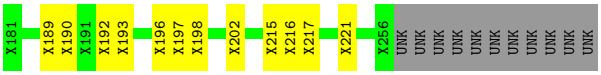
• Molecule 2: coiled-coil domain of portal

Chain L:



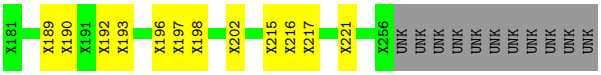
• Molecule 2: coiled-coil domain of portal

Chain Q:



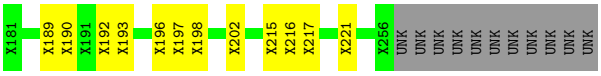
• Molecule 2: coiled-coil domain of portal

Chain R:



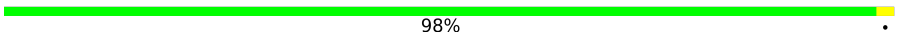
• Molecule 2: coiled-coil domain of portal

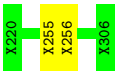
Chain S:



• Molecule 2: coiled-coil domain of portal

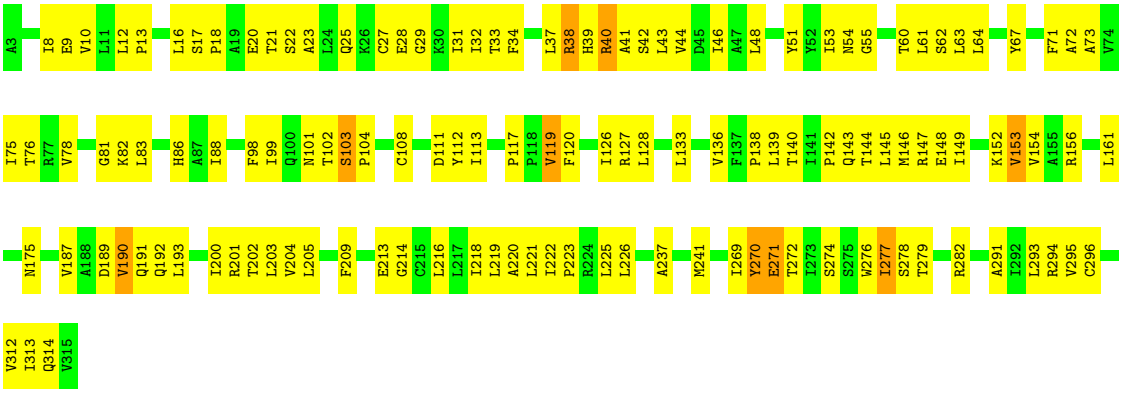
Chain T:





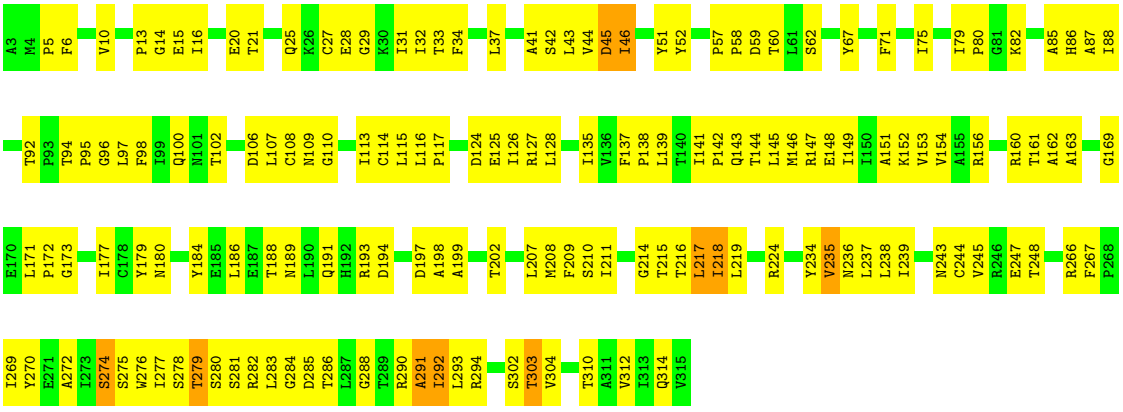
• Molecule 3: Tri2A

Chain F:



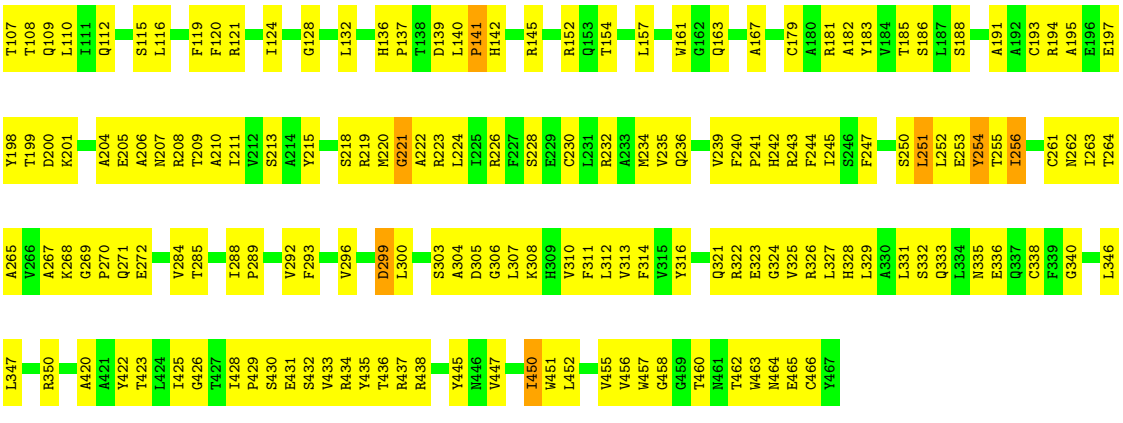
- Molecule 4: Tri2B

Chain O:



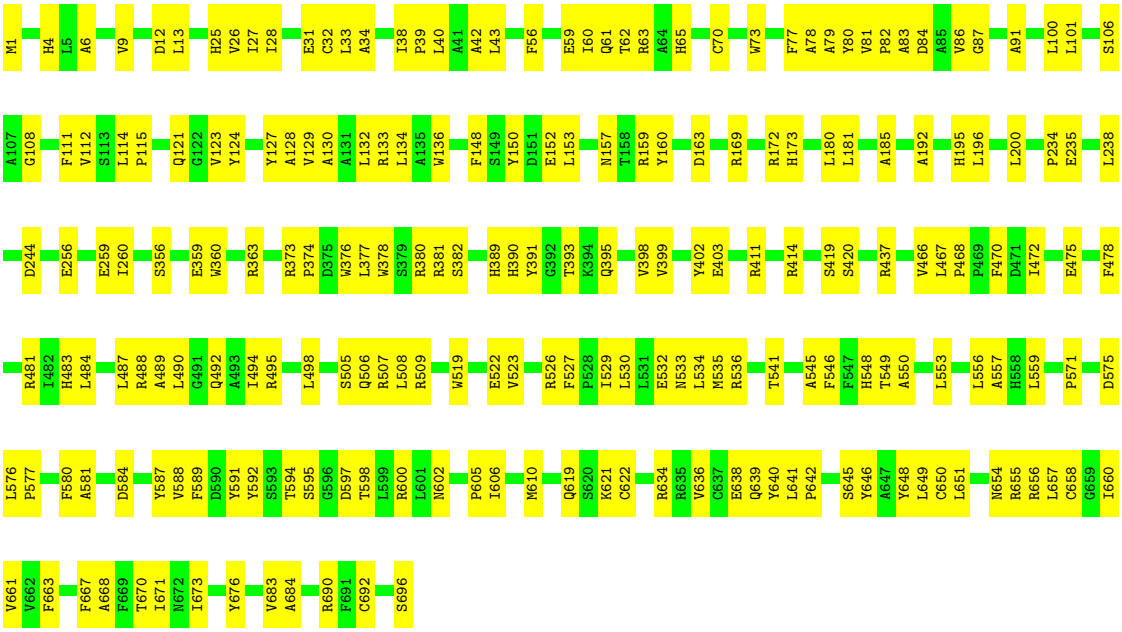
- Molecule 5: Tri1

Chain X:



- Molecule 6: CVC1

Chain k:

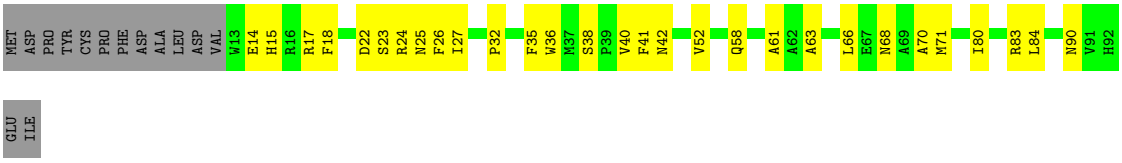


• Molecule 7: Capsid vertex component 2

Chain l:

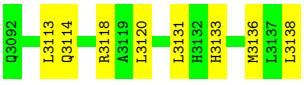
• Molecule 7: Capsid vertex component 2

Chain m:



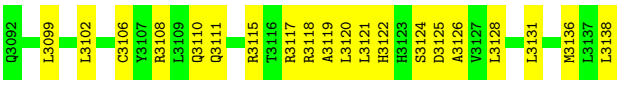
• Molecule 8: Large tegument protein deneddylase

Chain n:



• Molecule 8: Large tegument protein deneddylase

Chain o:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor

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	0.23	0/10642	0.46	0/14510
1	C	0.27	0/10114	0.51	4/13779 (0.0%)
3	F	0.22	0/2158	0.68	4/2951 (0.1%)
4	O	0.23	0/2320	0.73	8/3165 (0.3%)
5	X	0.22	0/2244	0.64	6/3050 (0.2%)
6	k	0.15	0/4307	0.38	0/5866
7	l	0.18	0/786	0.40	1/1072 (0.1%)
7	m	0.17	0/664	0.41	0/905
8	n	0.09	0/388	0.31	0/521
8	o	0.12	0/388	0.35	0/521
All	All	0.23	0/34011	0.51	23/46340 (0.0%)

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	C	0	1
3	F	0	1
4	O	0	2
All	All	0	4

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	217	LEU	CA-C-N	9.70	139.16	121.70
4	O	217	LEU	C-N-CA	9.70	139.16	121.70
3	F	277	ILE	CA-C-N	8.20	136.47	121.70
3	F	277	ILE	C-N-CA	8.20	136.47	121.70
5	X	221	GLY	CA-C-N	6.39	133.20	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	45	ARG	Sidechain
3	F	271	GLU	Peptide
4	O	218	ILE	Peptide
4	O	86	HIS	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	10392	0	10096	480	0
1	C	9888	0	9673	529	0
2	B	435	0	90	1	0
2	H	435	0	90	1	0
2	I	435	0	90	1	0
2	J	435	0	90	1	0
2	K	380	0	80	6	0
2	L	380	0	80	5	0
2	Q	380	0	80	6	0
2	R	380	0	80	6	0
2	S	380	0	80	6	0
2	T	435	0	90	1	0
3	F	2124	0	2111	116	0
4	O	2279	0	2316	143	0
5	X	2198	0	2124	166	0
6	k	4206	0	4190	178	0
7	l	766	0	745	26	0
7	m	648	0	631	33	0
8	n	384	0	410	7	0
8	o	384	0	410	19	0
All	All	37344	0	33556	1644	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 23.

The worst 5 of 1644 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:C:337:VAL:CG2	1:C:340:LEU:HD21	1.31	1.58
1:C:337:VAL:CG2	1:C:340:LEU:CD2	1.82	1.55
1:C:337:VAL:HG22	1:C:340:LEU:CD2	1.58	1.17
1:C:337:VAL:HG21	1:C:340:LEU:CD2	1.80	1.07
1:C:337:VAL:CG2	1:C:340:LEU:HD23	1.66	1.06

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 PDB entries followed by that with respect to all EM entries.

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	1341/1387 (97%)	1196 (89%)	144 (11%)	1 (0%)	48 83
1	C	1273/1387 (92%)	1142 (90%)	126 (10%)	5 (0%)	30 68
3	F	287/297 (97%)	222 (77%)	56 (20%)	9 (3%)	3 22
4	O	299/307 (97%)	247 (83%)	44 (15%)	8 (3%)	4 26
5	X	283/289 (98%)	237 (84%)	41 (14%)	5 (2%)	7 34
6	k	534/550 (97%)	508 (95%)	26 (5%)	0	100 100
7	l	92/94 (98%)	86 (94%)	6 (6%)	0	100 100
7	m	78/94 (83%)	75 (96%)	3 (4%)	0	100 100
8	n	45/47 (96%)	44 (98%)	1 (2%)	0	100 100
8	o	45/47 (96%)	42 (93%)	3 (7%)	0	100 100
All	All	4277/4499 (95%)	3799 (89%)	450 (10%)	28 (1%)	21 56

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	66	PHE
3	F	38	ARG
3	F	103	SER

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Mol	Chain	Res	Type
3	F	119	VAL
3	F	190	VAL

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 PDB entries followed by that with respect to all EM entries.

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	1101/1168 (94%)	1101 (100%)	0	100 100
1	C	1050/1168 (90%)	1035 (99%)	15 (1%)	62 75
3	F	212/252 (84%)	212 (100%)	0	100 100
4	O	242/258 (94%)	242 (100%)	0	100 100
5	X	220/240 (92%)	220 (100%)	0	100 100
6	k	429/429 (100%)	429 (100%)	0	100 100
7	l	80/80 (100%)	80 (100%)	0	100 100
7	m	66/80 (82%)	66 (100%)	0	100 100
8	n	41/41 (100%)	41 (100%)	0	100 100
8	o	41/41 (100%)	41 (100%)	0	100 100
All	All	3482/3757 (93%)	3467 (100%)	15 (0%)	88 90

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	177	MET
1	C	190	ARG
1	C	184	VAL
1	C	1262	ASN
1	C	187	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1146	GLN

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Mol	Chain	Res	Type
6	k	548	HIS
1	C	1321	GLN
5	X	328	HIS
7	l	90	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)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	k	7
3	F	4
4	O	3
5	X	2

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	k	266:ARG	C	355:ARG	N	36.83
1	O	250:GLN	C	256:PRO	N	16.00
1	k	200:LEU	C	230:PRO	N	14.76
1	X	351:ILE	C	417:CYS	N	12.96
1	F	260:MET	C	265:ARG	N	11.08