wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 01:14 AM EST

PDB ID	:	6NK6
EMDB ID	:	EMD-9394
Title	:	Electron Cryo-Microscopy Of Chikungunya VLP in complex with mouse Mxra8 receptor
Authors	:	Basore, K.; Kim, A.S.; Nelson, C.A.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2019-01-04
Resolution	:	4.06 Å(reported)
Based on initial models	:	3J0C, 3N42, 6NK3, 5H23

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 (i) 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 (i)) were used in the production of this report:

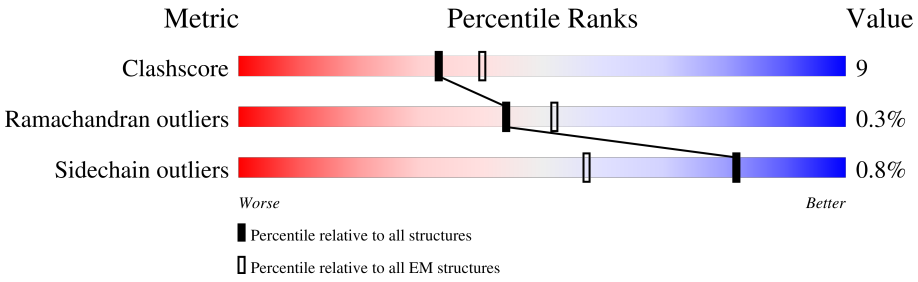
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.06 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	M	269	75% 25%
1	N	269	69% 27%
1	O	269	71% 29%
1	P	269	74% 25%
2	A	439	84% 15%
2	B	439	80% 20%
2	C	439	80% 20%
2	D	439	78% 22%
3	E	419	71% 28%

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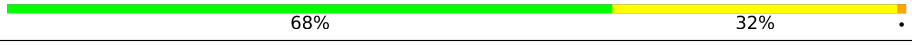
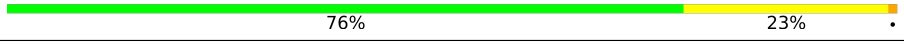
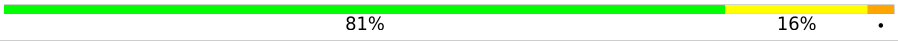
Mol	Chain	Length	Quality of chain
3	F	419	
3	G	419	
3	H	419	
4	I	151	
4	J	151	
4	K	151	
4	L	151	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39805 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 Matrix remodeling-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	269	Total	C	N	O	S	0	0
			2169	1344	416	400	9		
1	N	261	Total	C	N	O	S	0	0
			2111	1306	408	388	9		
1	O	269	Total	C	N	O	S	0	0
			2168	1344	416	399	9		
1	P	269	Total	C	N	O	S	0	0
			2169	1344	416	400	9		

- Molecule 2 is a protein called E1 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		
2	B	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		
2	C	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		
2	D	439	Total	C	N	O	S	0	0
			3318	2102	558	633	25		

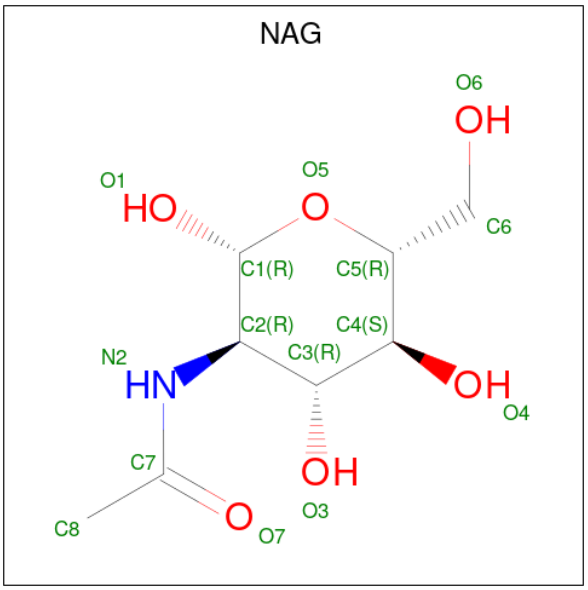
- Molecule 3 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		
3	F	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		
3	G	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		
3	H	419	Total	C	N	O	S	0	0
			3280	2055	587	611	27		

- Molecule 4 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		
4	J	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		
4	K	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		
4	L	151	Total	C	N	O	S	0	0
			1157	731	204	216	6		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
5	M	1	Total	C	N	O	0
			14	8	1	5	
5	N	1	Total	C	N	O	0
			14	8	1	5	
5	O	1	Total	C	N	O	0
			14	8	1	5	
5	P	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	E	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	

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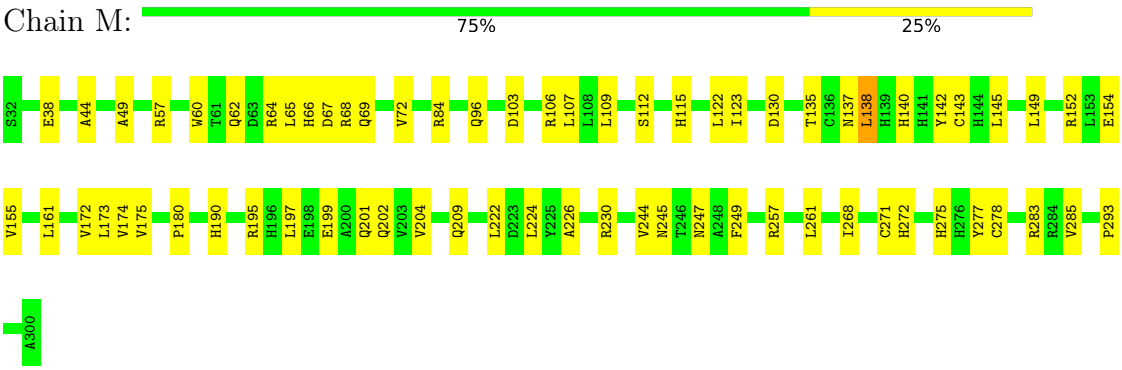
Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	

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.

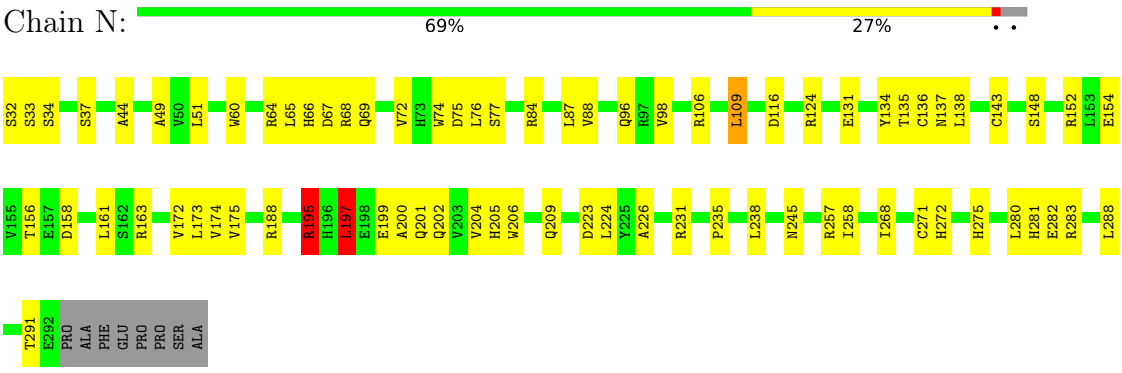
• Molecule 1: Matrix remodeling-associated protein 8

Chain M:



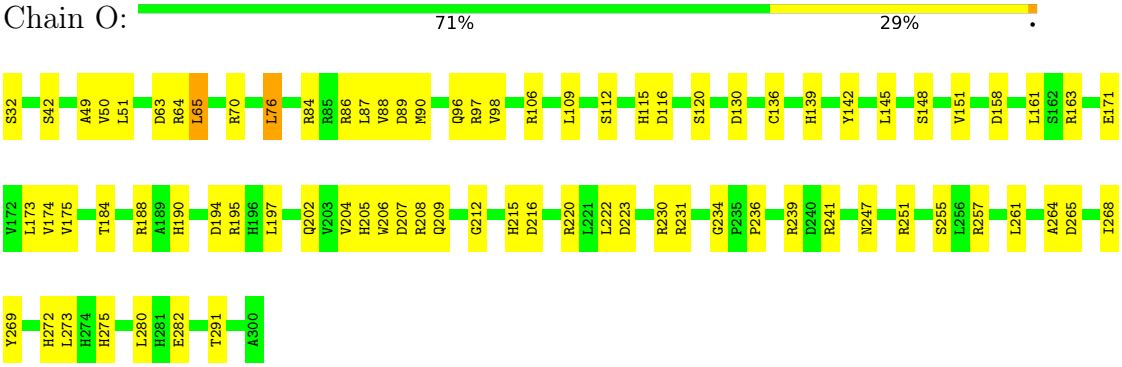
• Molecule 1: Matrix remodeling-associated protein 8

Chain N:



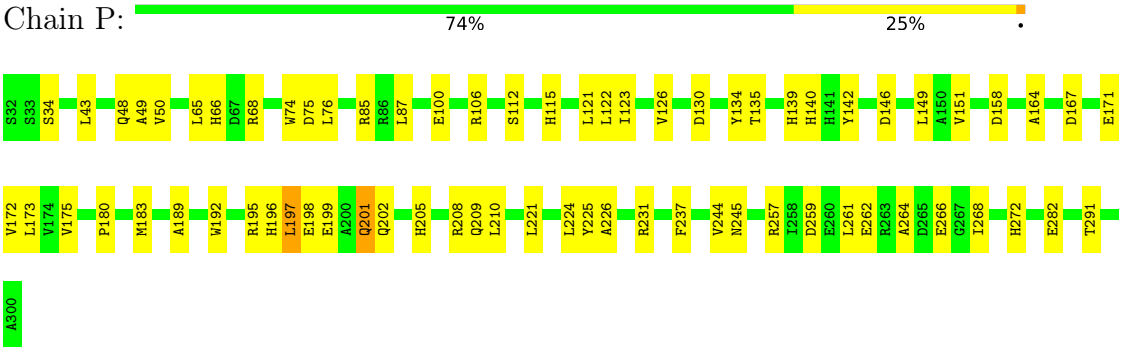
• Molecule 1: Matrix remodeling-associated protein 8

Chain O:



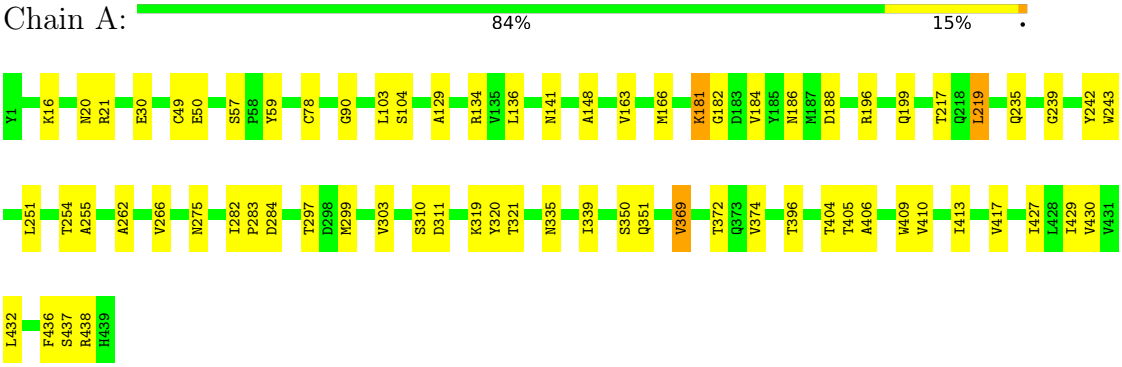
• Molecule 1: Matrix remodeling-associated protein 8

Chain P:



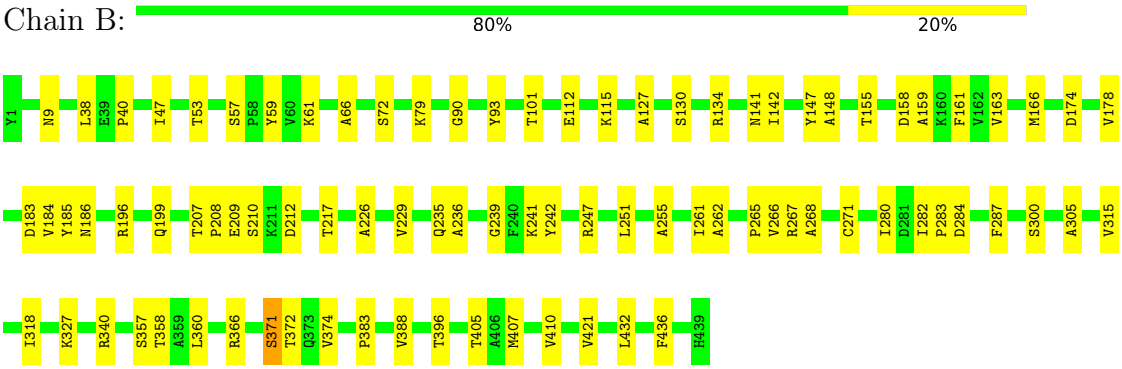
• Molecule 2: E1 glycoprotein

Chain A:



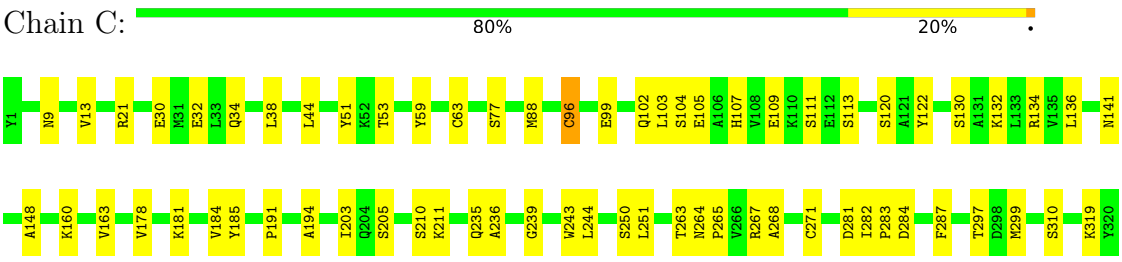
• Molecule 2: E1 glycoprotein

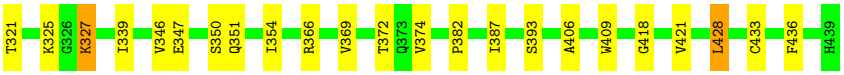
Chain B:



• Molecule 2: E1 glycoprotein

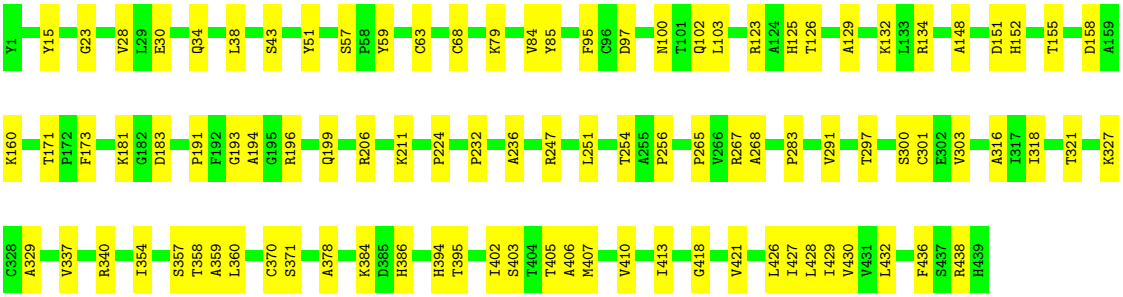
Chain C:





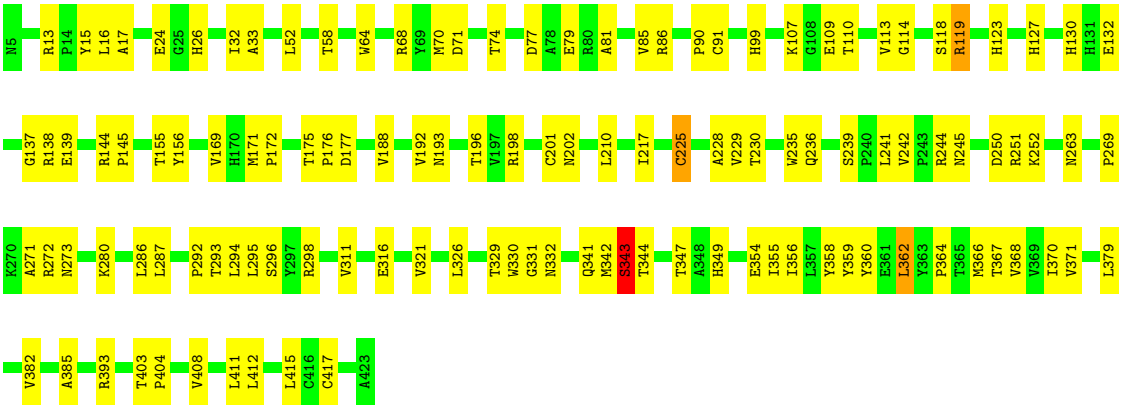
• Molecule 2: E1 glycoprotein

Chain D:



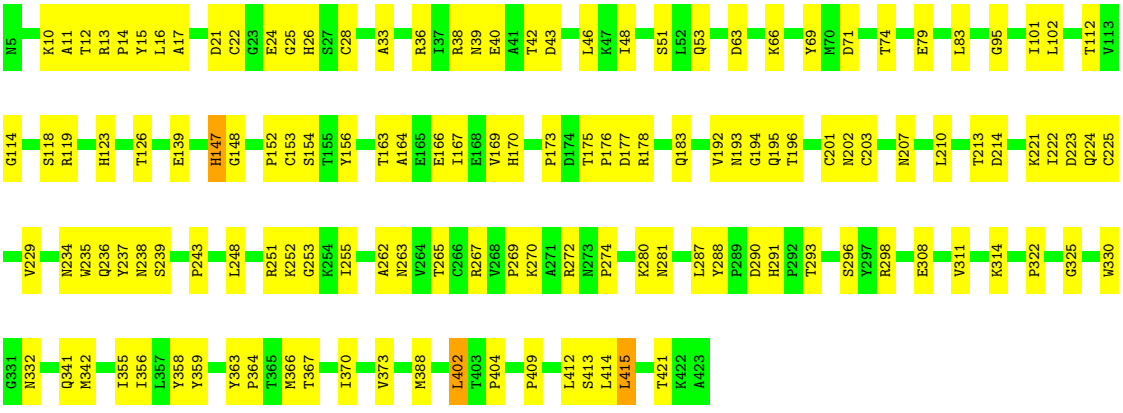
• Molecule 3: E2 glycoprotein

Chain E:



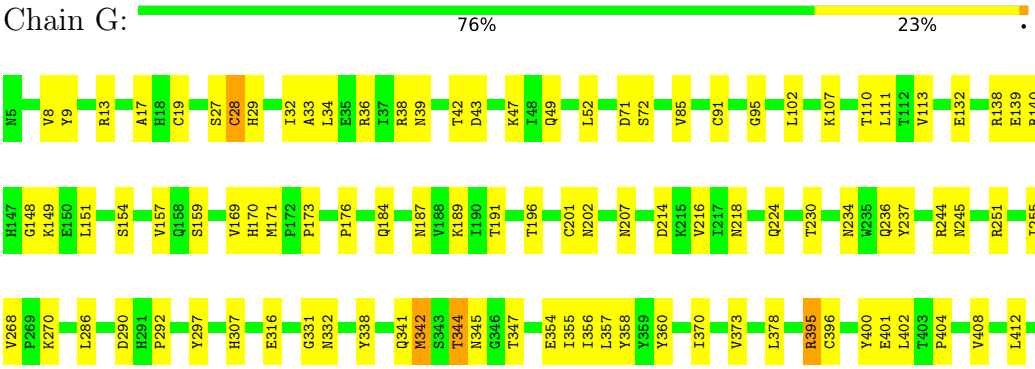
• Molecule 3: E2 glycoprotein

Chain F:



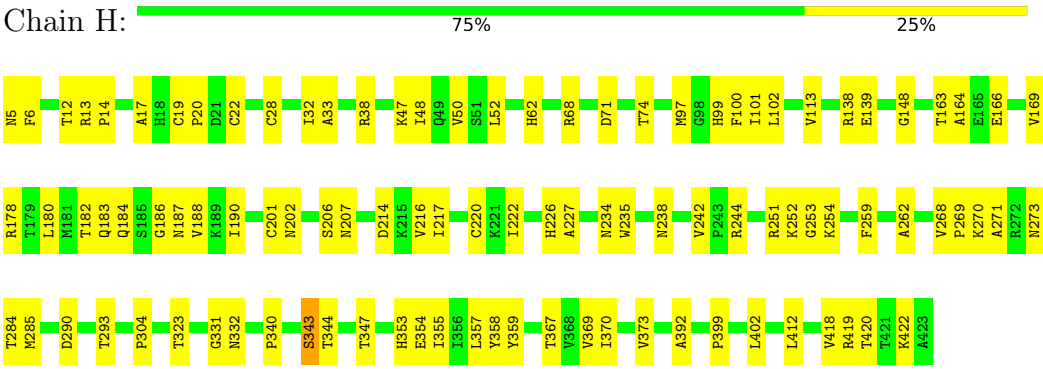
• Molecule 3: E2 glycoprotein

Chain G:



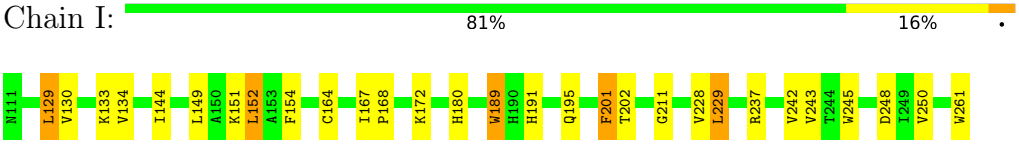
• Molecule 3: E2 glycoprotein

Chain H:



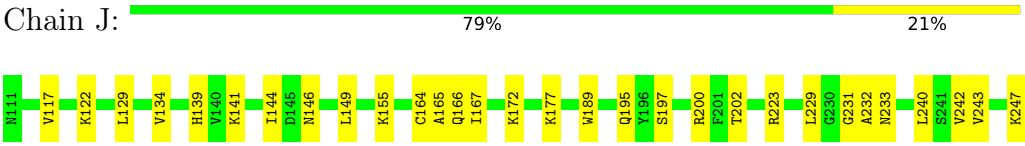
• Molecule 4: Capsid protein

Chain I:



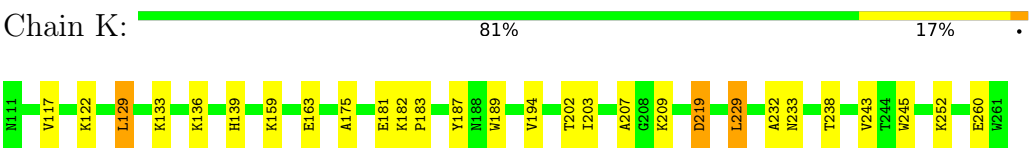
• Molecule 4: Capsid protein

Chain J:



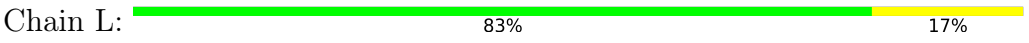
• Molecule 4: Capsid protein

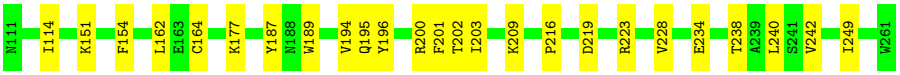
Chain K:



• Molecule 4: Capsid protein

Chain L:




N111
I114
K151
F154
L162
E163
C164
K177
Y187
N188
W189
V194
Q195
Y196
R200
F201
T202
I203
K209
P216
D219
R223
V228
E234
T238
A239
L240
S241
V242
I249
W261

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	22486	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	M	0.36	0/2224	0.76	7/3020 (0.2%)
1	N	0.34	0/2162	0.70	2/2932 (0.1%)
1	O	0.36	0/2223	0.78	3/3018 (0.1%)
1	P	0.36	0/2224	0.78	3/3020 (0.1%)
2	A	0.39	0/3400	0.67	2/4643 (0.0%)
2	B	0.39	0/3400	0.67	0/4643
2	C	0.40	0/3400	0.71	4/4643 (0.1%)
2	D	0.41	0/3400	0.70	2/4643 (0.0%)
3	E	0.39	0/3367	0.71	3/4592 (0.1%)
3	F	0.34	0/3367	0.68	3/4592 (0.1%)
3	G	0.37	0/3367	0.67	1/4592 (0.0%)
3	H	0.37	0/3367	0.68	2/4592 (0.0%)
4	I	0.38	0/1185	0.73	3/1599 (0.2%)
4	J	0.35	0/1185	0.74	1/1599 (0.1%)
4	K	0.45	1/1185 (0.1%)	0.83	5/1599 (0.3%)
4	L	0.37	0/1185	0.69	0/1599
All	All	0.38	1/40641 (0.0%)	0.71	41/55326 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	233	ASN	CA-C	6.60	1.70	1.52

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	362	LEU	CA-CB-CG	8.11	133.96	115.30
2	C	96	CYS	CA-CB-SG	7.75	127.95	114.00
2	D	370	CYS	CA-CB-SG	-7.68	100.17	114.00
4	K	233	ASN	O-C-N	-7.50	110.70	122.70
3	E	225	CYS	CA-CB-SG	7.09	126.76	114.00

There are no chirality outliers.

There are no planarity outliers.

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	M	2169	0	2062	40	0
1	N	2111	0	2011	45	0
1	O	2168	0	2062	52	0
1	P	2169	0	2062	44	0
2	A	3318	0	3246	47	0
2	B	3318	0	3246	56	0
2	C	3318	0	3246	57	0
2	D	3318	0	3246	62	0
3	E	3280	0	3210	85	0
3	F	3280	0	3210	89	0
3	G	3280	0	3210	64	0
3	H	3280	0	3210	73	0
4	I	1157	0	1137	17	0
4	J	1157	0	1137	20	0
4	K	1157	0	1137	15	0
4	L	1157	0	1137	17	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
5	E	14	0	13	0	0
5	F	14	0	13	0	0
5	G	14	0	13	0	0
5	H	14	0	13	1	0
5	M	14	0	13	0	0
5	N	14	0	13	0	0
5	O	14	0	13	0	0
5	P	14	0	13	0	0
All	All	39805	0	38725	721	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 9.

The worst 5 of 721 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:F:169:VAL:O	3:F:253:GLY:HA3	1.59	1.02
3:E:355:ILE:O	3:E:358:TYR:HB2	1.72	0.90
3:F:356:ILE:O	3:F:359:TYR:HB3	1.72	0.90
3:H:148:GLY:HA3	3:H:268:VAL:O	1.74	0.87
2:C:299:MET:HA	2:C:319:LYS:O	1.79	0.83

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	M	267/269 (99%)	251 (94%)	16 (6%)	0	100	100
1	N	259/269 (96%)	242 (93%)	15 (6%)	2 (1%)	19	58
1	O	267/269 (99%)	250 (94%)	17 (6%)	0	100	100
1	P	267/269 (99%)	250 (94%)	16 (6%)	1 (0%)	34	71
2	A	437/439 (100%)	413 (94%)	23 (5%)	1 (0%)	47	80
2	B	437/439 (100%)	413 (94%)	23 (5%)	1 (0%)	47	80
2	C	437/439 (100%)	410 (94%)	26 (6%)	1 (0%)	47	80
2	D	437/439 (100%)	417 (95%)	19 (4%)	1 (0%)	47	80
3	E	417/419 (100%)	360 (86%)	56 (13%)	1 (0%)	47	80
3	F	417/419 (100%)	363 (87%)	51 (12%)	3 (1%)	22	61
3	G	417/419 (100%)	361 (87%)	54 (13%)	2 (0%)	29	67
3	H	417/419 (100%)	361 (87%)	55 (13%)	1 (0%)	47	80
4	I	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
4	J	149/151 (99%)	146 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	K	149/151 (99%)	145 (97%)	4 (3%)	0	100	100
4	L	149/151 (99%)	147 (99%)	2 (1%)	0	100	100
All	All	5072/5112 (99%)	4674 (92%)	384 (8%)	14 (0%)	44	75

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	181	LYS
3	F	402	LEU
2	C	181	LYS
3	G	342	MET
3	G	344	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 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	M	232/232 (100%)	232 (100%)	0	100	100
1	N	226/232 (97%)	223 (99%)	3 (1%)	69	82
1	O	232/232 (100%)	232 (100%)	0	100	100
1	P	232/232 (100%)	230 (99%)	2 (1%)	78	88
2	A	366/366 (100%)	363 (99%)	3 (1%)	81	89
2	B	366/366 (100%)	361 (99%)	5 (1%)	67	80
2	C	366/366 (100%)	364 (100%)	2 (0%)	88	93
2	D	366/366 (100%)	365 (100%)	1 (0%)	92	95
3	E	369/369 (100%)	366 (99%)	3 (1%)	81	89
3	F	369/369 (100%)	367 (100%)	2 (0%)	88	93
3	G	369/369 (100%)	361 (98%)	8 (2%)	52	71
3	H	369/369 (100%)	369 (100%)	0	100	100
4	I	120/120 (100%)	117 (98%)	3 (2%)	47	68
4	J	120/120 (100%)	119 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	120/120 (100%)	118 (98%)	2 (2%)	60 78
4	L	120/120 (100%)	119 (99%)	1 (1%)	81 89
All	All	4342/4348 (100%)	4306 (99%)	36 (1%)	82 89

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	237	TYR
4	L	189	TRP
3	G	342	MET
4	K	189	TRP
4	I	189	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	236	GLN
3	G	53	GLN
3	H	234	ASN
3	F	341	GLN
2	C	102	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands 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	$\#\|Z\| > 2$
5	NAG	B	501	2	14,14,15	0.29	0	17,19,21	0.69	1 (5%)
5	NAG	C	501	2	14,14,15	0.27	0	17,19,21	0.68	1 (5%)
5	NAG	N	401	1	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
5	NAG	A	501	2	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
5	NAG	D	501	2	14,14,15	0.25	0	17,19,21	0.58	0
5	NAG	H	501	3	14,14,15	0.22	0	17,19,21	0.66	1 (5%)
5	NAG	G	501	3	14,14,15	0.45	0	17,19,21	0.66	1 (5%)
5	NAG	F	501	3	14,14,15	0.52	0	17,19,21	0.60	0
5	NAG	M	501	1	14,14,15	0.47	0	17,19,21	0.49	0
5	NAG	O	501	1	14,14,15	0.34	0	17,19,21	0.59	1 (5%)
5	NAG	E	501	3	14,14,15	0.37	0	17,19,21	0.55	0
5	NAG	P	501	1	14,14,15	0.46	0	17,19,21	0.71	1 (5%)

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
5	NAG	B	501	2	-	2/6/23/26	0/1/1/1
5	NAG	C	501	2	-	1/6/23/26	0/1/1/1
5	NAG	N	401	1	-	1/6/23/26	0/1/1/1
5	NAG	A	501	2	-	0/6/23/26	0/1/1/1
5	NAG	D	501	2	-	2/6/23/26	0/1/1/1
5	NAG	H	501	3	-	2/6/23/26	0/1/1/1
5	NAG	G	501	3	-	2/6/23/26	0/1/1/1
5	NAG	F	501	3	-	2/6/23/26	0/1/1/1
5	NAG	M	501	1	-	2/6/23/26	0/1/1/1
5	NAG	O	501	1	-	0/6/23/26	0/1/1/1
5	NAG	E	501	3	-	0/6/23/26	0/1/1/1
5	NAG	P	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	NAG	C1-O5-C5	2.65	115.78	112.19
5	P	501	NAG	C1-O5-C5	2.52	115.61	112.19
5	B	501	NAG	C1-O5-C5	2.43	115.49	112.19
5	N	401	NAG	C1-O5-C5	2.32	115.33	112.19
5	C	501	NAG	C1-O5-C5	2.25	115.24	112.19

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	501	NAG	C4-C5-C6-O6
5	M	501	NAG	C4-C5-C6-O6
5	D	501	NAG	O5-C5-C6-O6
5	M	501	NAG	O5-C5-C6-O6
5	H	501	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	501	NAG	1	0

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-9394. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.