wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 01:11 AM EST

PDB ID	:	6NK7
EMDB ID	:	EMD-9395
Title	:	Electron Cryo-Microscopy of Chikungunya 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	:	4.99 Å(reported)
Based on initial models	:	6NK3, 3N42, 3J0C, 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:

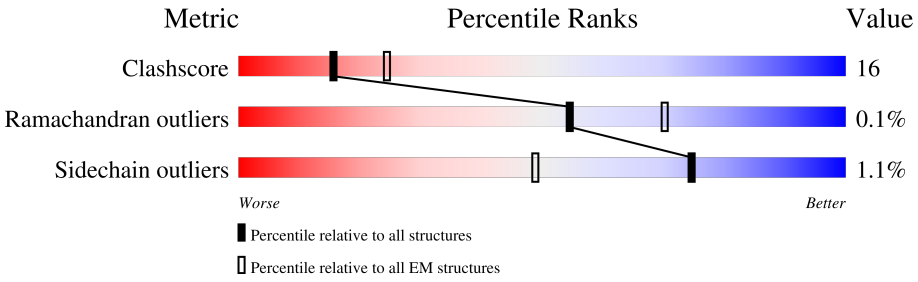
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 4.99 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	A	439	70% 29% .
1	B	439	68% 32%
1	C	439	68% 31%
1	D	439	61% 38%
2	E	419	60% 39%
2	F	419	61% 38% .
2	G	419	59% 40% .
2	H	419	65% 35%
3	I	151	58% 42%

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Mol	Chain	Length	Quality of chain
3	J	151	59% 40%
3	K	151	52% 47%
3	L	151	60% 39%
4	U	60	63% 35%
4	V	60	58% 42%
4	W	60	55% 45%
4	X	60	57% 43%
5	N	261	67% 31%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35205 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 E1 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	439	Total	C	N	O	S	0	0
			3326	2106	556	637	27		
1	B	439	Total	C	N	O	S	0	0
			3326	2106	556	637	27		
1	C	439	Total	C	N	O	S	0	0
			3326	2106	556	637	27		
1	D	439	Total	C	N	O	S	0	0
			3326	2106	556	637	27		

- Molecule 2 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	419	Total	C	N	O	S	0	0
			3295	2067	592	608	28		
2	F	419	Total	C	N	O	S	0	0
			3295	2067	592	608	28		
2	G	419	Total	C	N	O	S	0	0
			3295	2067	592	608	28		
2	H	419	Total	C	N	O	S	0	0
			3295	2067	592	608	28		

- Molecule 3 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
3	J	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
3	K	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		
3	L	151	Total	C	N	O	S	0	0
			1156	730	204	217	5		

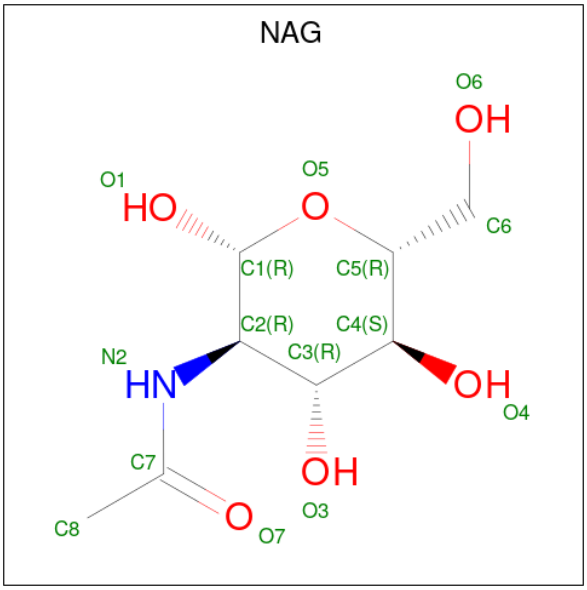
- Molecule 4 is a protein called E3 glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	U	60	Total	C	N	O	S	0	0
			479	297	84	89	9		
4	V	60	Total	C	N	O	S	0	0
			479	297	84	89	9		
4	W	60	Total	C	N	O	S	0	0
			479	297	84	89	9		
4	X	60	Total	C	N	O	S	0	0
			479	297	84	89	9		

- Molecule 5 is a protein called Matrix remodeling-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	261	Total	C	N	O	S	0	0
			2111	1306	408	388	9		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	
6	D	1	Total	C	N	O	0
			14	8	1	5	

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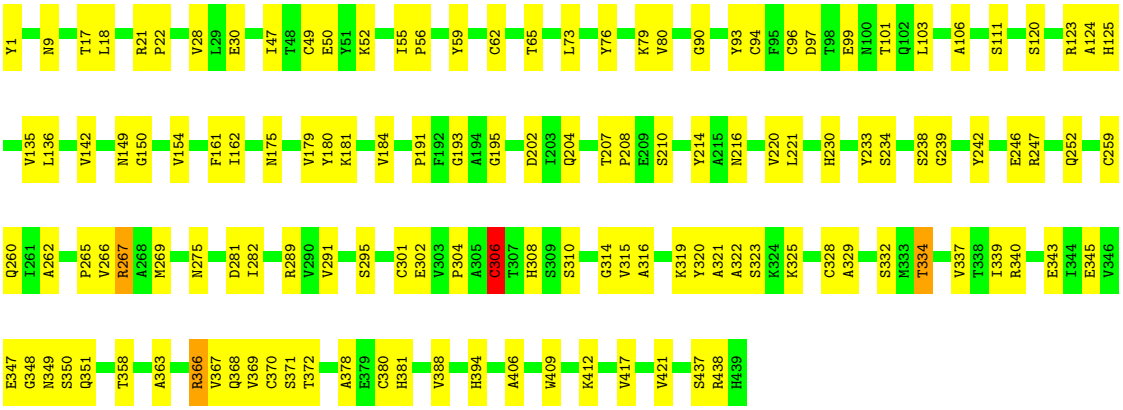
Mol	Chain	Residues	Atoms				AltConf
6	N	1	Total	C	N	O	0
			14	8	1	5	

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.

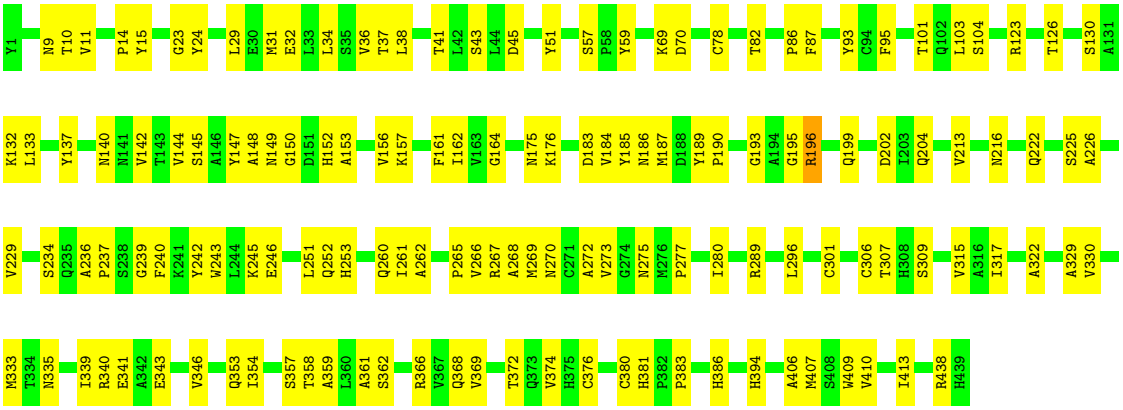
• Molecule 1: E1 glycoprotein

Chain A:



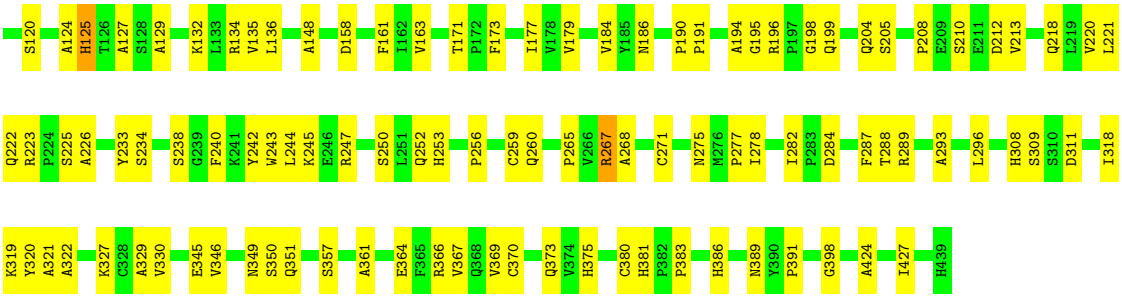
• Molecule 1: E1 glycoprotein

Chain B:



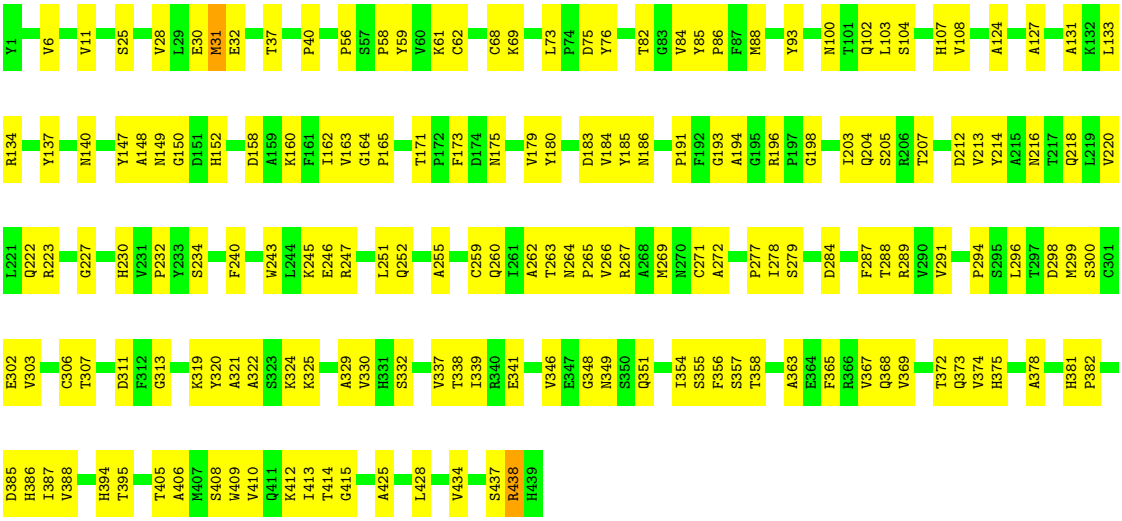
• Molecule 1: E1 glycoprotein

Chain C:



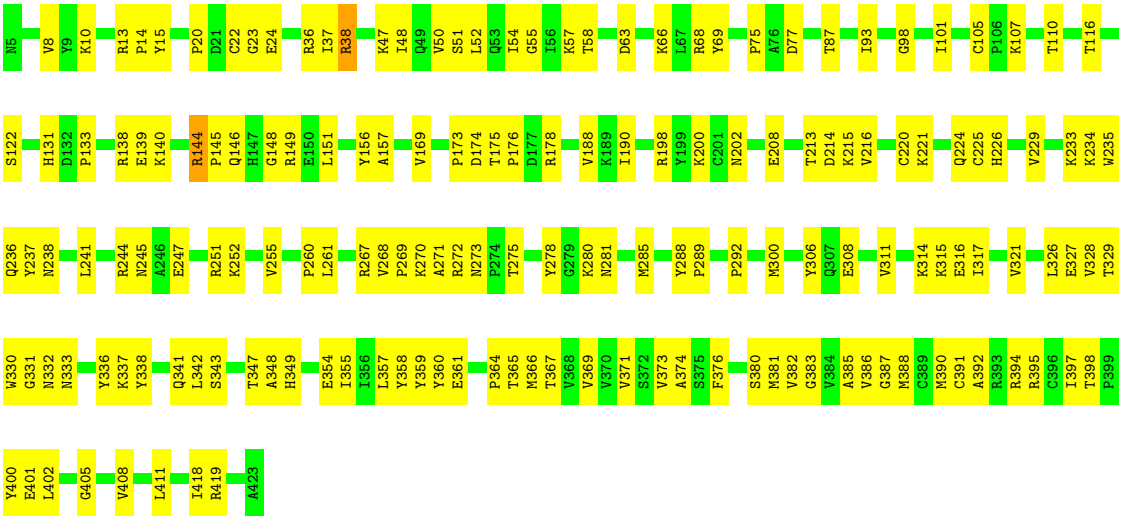
• Molecule 1: E1 glycoprotein

Chain D:



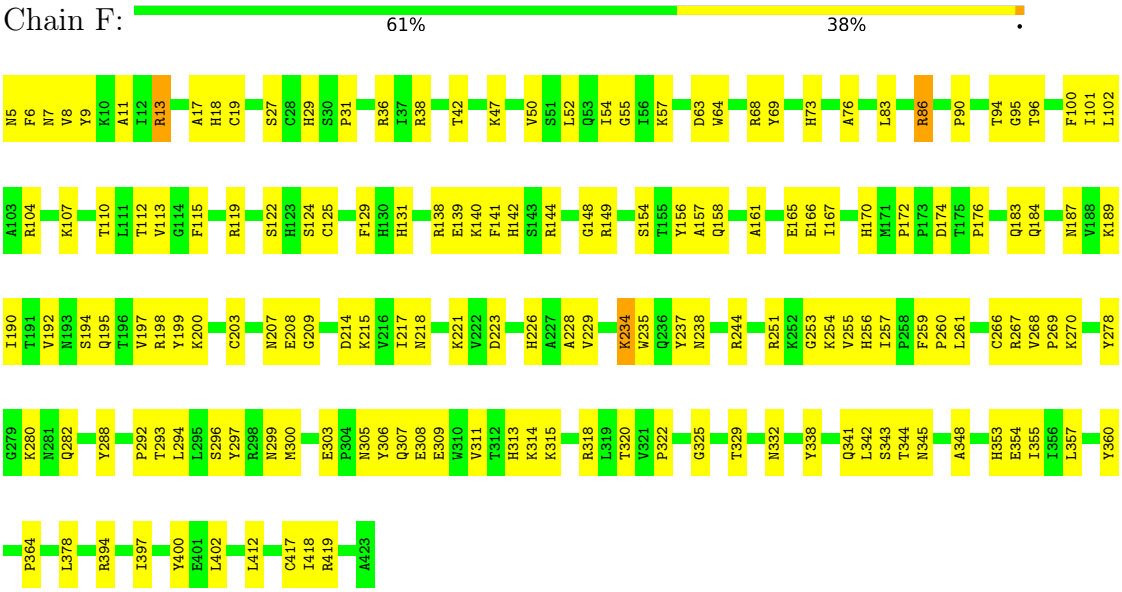
• Molecule 2: E2 glycoprotein

Chain E:



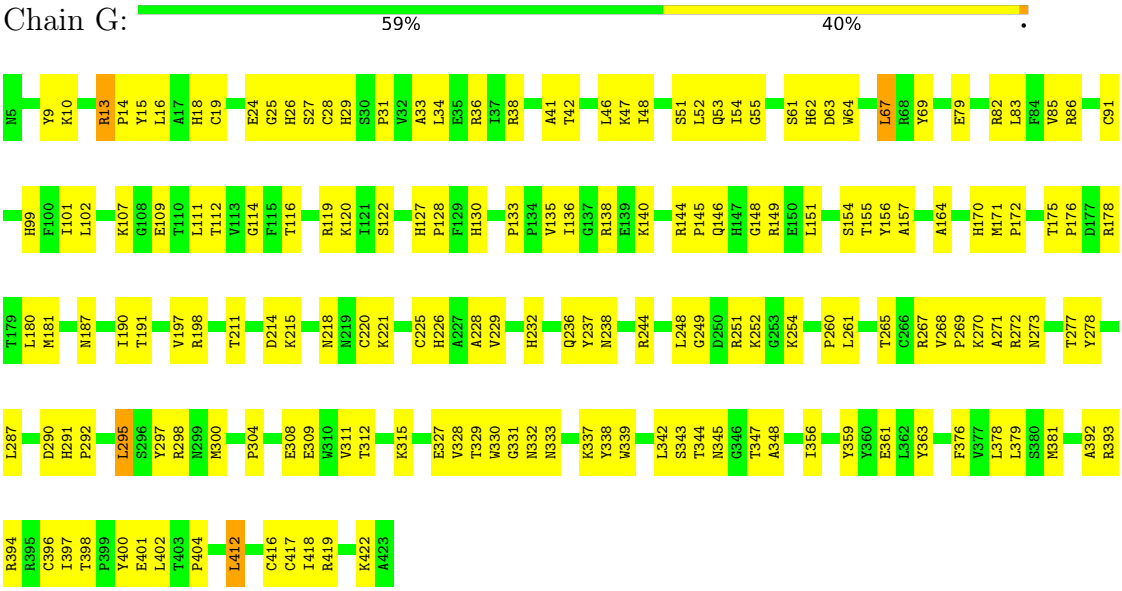
• Molecule 2: E2 glycoprotein

Chain F:



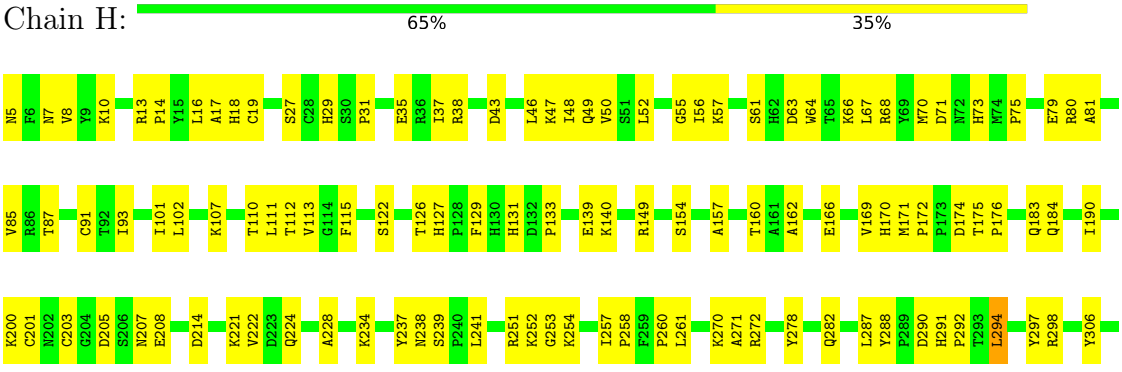
• Molecule 2: E2 glycoprotein

Chain G:



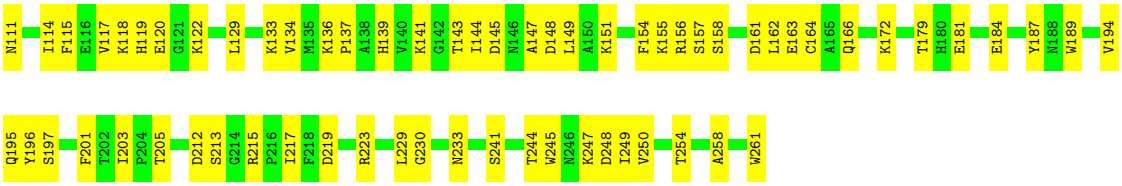
• Molecule 2: E2 glycoprotein

Chain H:



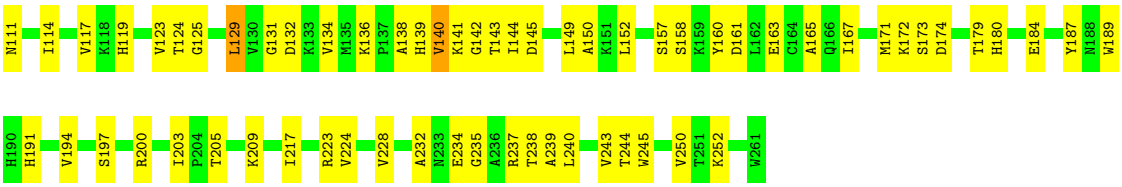
• Molecule 3: Capsid protein

Chain I:



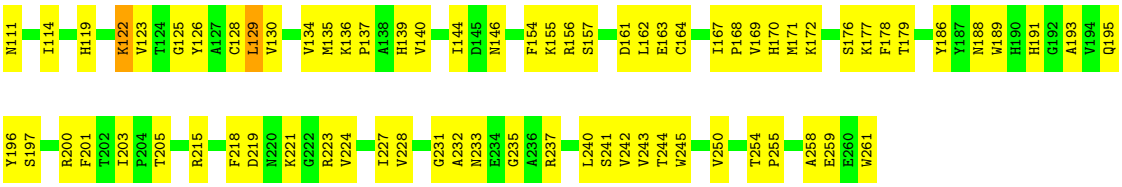
• Molecule 3: Capsid protein

Chain J:



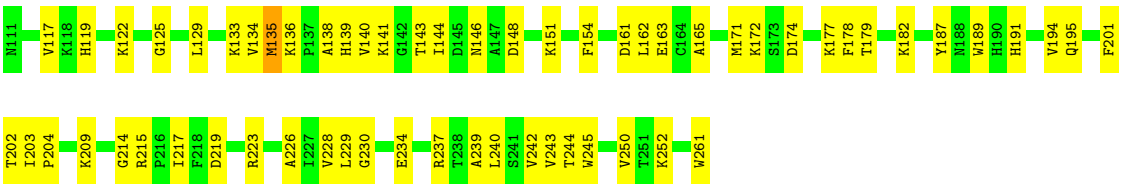
• Molecule 3: Capsid protein

Chain K:



• Molecule 3: Capsid protein

Chain L:

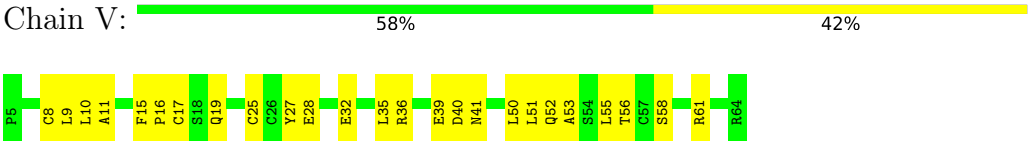


• Molecule 4: E3 glycoprotein

Chain U:

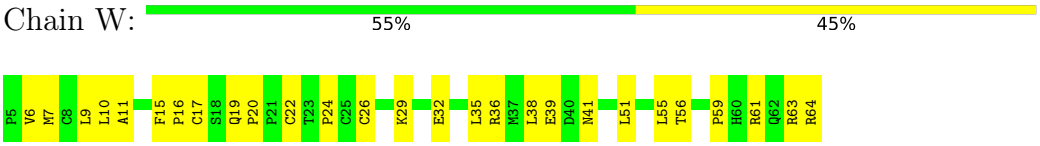
• Molecule 4: E3 glycoprotein

Chain V:



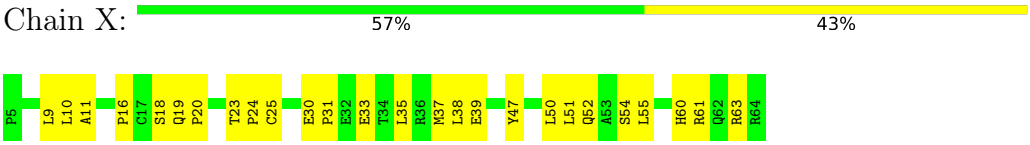
• Molecule 4: E3 glycoprotein

Chain W:



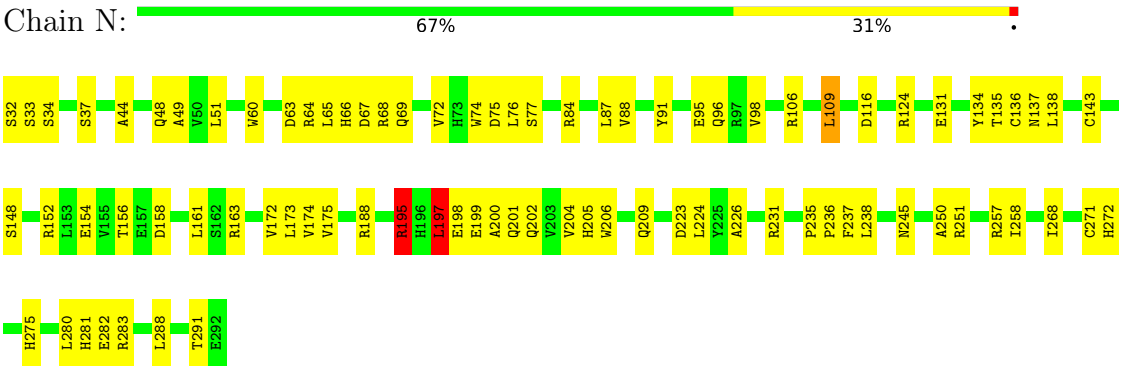
• Molecule 4: E3 glycoprotein

Chain X:



• Molecule 5: Matrix remodeling-associated protein 8

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8357	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 (i)

5.1 Standard geometry (i)

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	A	0.38	0/3408	0.62	1/4651 (0.0%)
1	B	0.37	0/3408	0.61	0/4651
1	C	0.34	0/3408	0.63	3/4651 (0.1%)
1	D	0.34	0/3408	0.61	1/4651 (0.0%)
2	E	0.36	0/3382	0.65	0/4606
2	F	0.37	0/3382	0.67	3/4606 (0.1%)
2	G	0.35	0/3382	0.64	3/4606 (0.1%)
2	H	0.37	0/3382	0.66	1/4606 (0.0%)
3	I	0.38	0/1184	0.65	0/1599
3	J	0.38	0/1184	0.64	1/1599 (0.1%)
3	K	0.38	0/1184	0.63	1/1599 (0.1%)
3	L	0.38	0/1184	0.63	1/1599 (0.1%)
4	U	0.29	0/491	0.58	1/667 (0.1%)
4	V	0.27	0/491	0.57	0/667
4	W	0.34	0/491	0.52	0/667
4	X	0.31	0/491	0.60	1/667 (0.1%)
5	N	0.34	0/2162	0.70	2/2932 (0.1%)
All	All	0.36	0/36022	0.64	19/49024 (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
1	D	0	2
2	E	0	2
2	F	0	2
2	G	0	3
2	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
All	All	0	14

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	158	ASP	CB-CG-OD1	9.24	126.62	118.30
2	H	205	ASP	CB-CG-OD1	8.66	126.10	118.30
1	C	389	ASN	C-N-CA	8.46	142.86	121.70
3	L	129	LEU	CA-CB-CG	7.13	131.69	115.30
2	F	238	ASN	C-N-CA	6.33	137.52	121.70

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	125	HIS	Peptide
1	D	180	TYR	Peptide
1	D	415	GLY	Peptide
2	E	342	LEU	Peptide
2	E	348	ALA	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	3326	0	3252	89	0
1	B	3326	0	3254	113	0
1	C	3326	0	3252	107	0
1	D	3326	0	3250	116	0
2	E	3295	0	3241	115	0
2	F	3295	0	3241	116	0
2	G	3295	0	3241	150	0
2	H	3295	0	3241	110	0
3	I	1156	0	1135	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1156	0	1135	40	0
3	K	1156	0	1135	56	0
3	L	1156	0	1135	38	0
4	U	479	0	468	20	0
4	V	479	0	468	19	0
4	W	479	0	468	20	0
4	X	479	0	468	15	0
5	N	2111	0	2011	103	0
6	A	14	0	12	0	0
6	B	14	0	12	0	0
6	C	14	0	12	1	0
6	D	14	0	12	0	0
6	N	14	0	13	0	0
All	All	35205	0	34456	1135	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 1135 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:145:SER:CB	5:N:236:PRO:HB2	1.20	1.61
2:G:27:SER:CB	5:N:65:LEU:HD12	1.09	1.57
2:G:180:LEU:CD2	5:N:84:ARG:HH22	1.18	1.52
2:G:180:LEU:HD22	5:N:84:ARG:NH2	1.30	1.43
1:C:87:PHE:CE2	5:N:65:LEU:HD22	1.53	1.41

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	437/439 (100%)	394 (90%)	43 (10%)	0	100	100
1	B	437/439 (100%)	405 (93%)	32 (7%)	0	100	100
1	C	437/439 (100%)	392 (90%)	44 (10%)	1 (0%)	47	81
1	D	437/439 (100%)	407 (93%)	30 (7%)	0	100	100
2	E	417/419 (100%)	366 (88%)	51 (12%)	0	100	100
2	F	417/419 (100%)	350 (84%)	67 (16%)	0	100	100
2	G	417/419 (100%)	348 (84%)	68 (16%)	1 (0%)	47	81
2	H	417/419 (100%)	345 (83%)	72 (17%)	0	100	100
3	I	149/151 (99%)	135 (91%)	14 (9%)	0	100	100
3	J	149/151 (99%)	135 (91%)	14 (9%)	0	100	100
3	K	149/151 (99%)	132 (89%)	17 (11%)	0	100	100
3	L	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
4	U	58/60 (97%)	51 (88%)	7 (12%)	0	100	100
4	V	58/60 (97%)	47 (81%)	11 (19%)	0	100	100
4	W	58/60 (97%)	46 (79%)	12 (21%)	0	100	100
4	X	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
5	N	259/261 (99%)	242 (93%)	15 (6%)	2 (1%)	19	60
All	All	4503/4537 (99%)	3980 (88%)	519 (12%)	4 (0%)	54	86

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	401	GLU
5	N	195	ARG
1	C	370	CYS
5	N	197	LEU

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	369/369 (100%)	365 (99%)	4 (1%)	73 85
1	B	369/369 (100%)	366 (99%)	3 (1%)	81 89
1	C	369/369 (100%)	368 (100%)	1 (0%)	92 95
1	D	369/369 (100%)	366 (99%)	3 (1%)	81 89
2	E	369/369 (100%)	365 (99%)	4 (1%)	73 85
2	F	369/369 (100%)	363 (98%)	6 (2%)	62 79
2	G	369/369 (100%)	367 (100%)	2 (0%)	88 93
2	H	369/369 (100%)	367 (100%)	2 (0%)	88 93
3	I	120/120 (100%)	118 (98%)	2 (2%)	60 78
3	J	120/120 (100%)	115 (96%)	5 (4%)	30 54
3	K	120/120 (100%)	119 (99%)	1 (1%)	81 89
3	L	120/120 (100%)	117 (98%)	3 (2%)	47 68
4	U	57/57 (100%)	57 (100%)	0	100 100
4	V	57/57 (100%)	56 (98%)	1 (2%)	59 77
4	W	57/57 (100%)	56 (98%)	1 (2%)	59 77
4	X	57/57 (100%)	55 (96%)	2 (4%)	36 59
5	N	226/226 (100%)	223 (99%)	3 (1%)	69 82
All	All	3886/3886 (100%)	3843 (99%)	43 (1%)	74 85

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	141	LYS
3	L	209	LYS
3	J	171	MET
3	K	122	LYS
4	W	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	29	HIS
2	H	332	ASN
2	G	147	HIS
2	G	307	GLN
3	J	195	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)

5 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	$\#\|Z\| > 2$
6	NAG	C	501	1	14,14,15	0.31	0	17,19,21	0.45	0
6	NAG	D	501	1	14,14,15	0.57	0	17,19,21	0.65	0
6	NAG	A	501	1	14,14,15	0.45	0	17,19,21	0.47	0
6	NAG	N	301	5	14,14,15	0.36	0	17,19,21	0.65	1 (5%)
6	NAG	B	501	1	14,14,15	0.59	0	17,19,21	0.57	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
6	NAG	C	501	1	-	2/6/23/26	0/1/1/1
6	NAG	D	501	1	-	2/6/23/26	0/1/1/1
6	NAG	A	501	1	-	0/6/23/26	0/1/1/1
6	NAG	N	301	5	-	1/6/23/26	0/1/1/1
6	NAG	B	501	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	301	NAG	C1-O5-C5	2.26	115.26	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	501	NAG	O5-C5-C6-O6
6	D	501	NAG	O5-C5-C6-O6
6	D	501	NAG	C4-C5-C6-O6
6	C	501	NAG	C4-C5-C6-O6
6	N	301	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
6	C	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-9395. 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

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

9 Map-model fit

This section was not generated.