



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Sep 3, 2017 – 08:52 AM EDT

PDB ID : 5IRE
EMDB ID: : EMD-8116
Title : The cryo-EM structure of Zika Virus
Authors : Sirohi, D.; Chen, Z.; Sun, L.; Klose, T.; Pierson, T.; Rossmann, M.; Kuhn, R.
Deposited on : unknown
Resolution : 3.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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) : rb-20029824

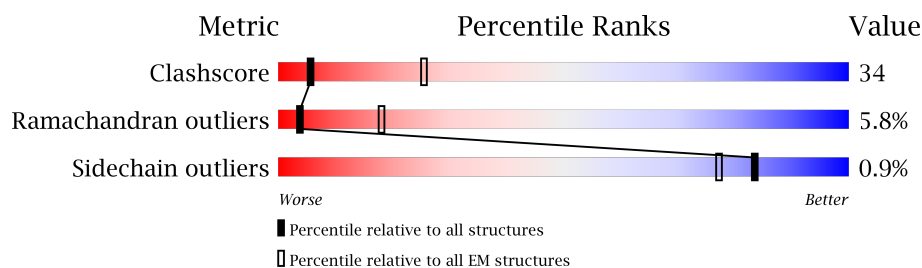
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	504	66% 28% . .
1	C	504	62% 32% 6% .
1	E	504	67% 27% 5% .
2	B	75	80% 19% .
2	D	75	73% 24% .
2	F	75	73% 23% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	600	-	-	X	-
3	NAG	E	600	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11024 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.

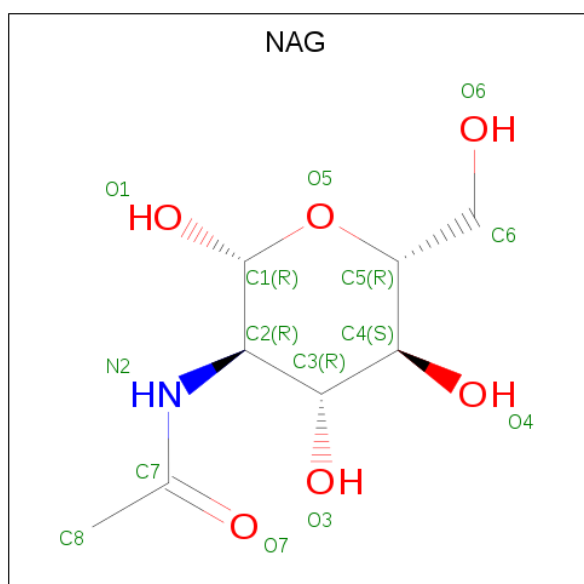
- Molecule 1 is a protein called E protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	501	Total	C	N	O	S	0	0
			3167	1993	576	582	16		
1	C	501	Total	C	N	O	S	0	0
			3225	2035	589	586	15		
1	E	501	Total	C	N	O	S	0	0
			3186	2003	581	585	17		

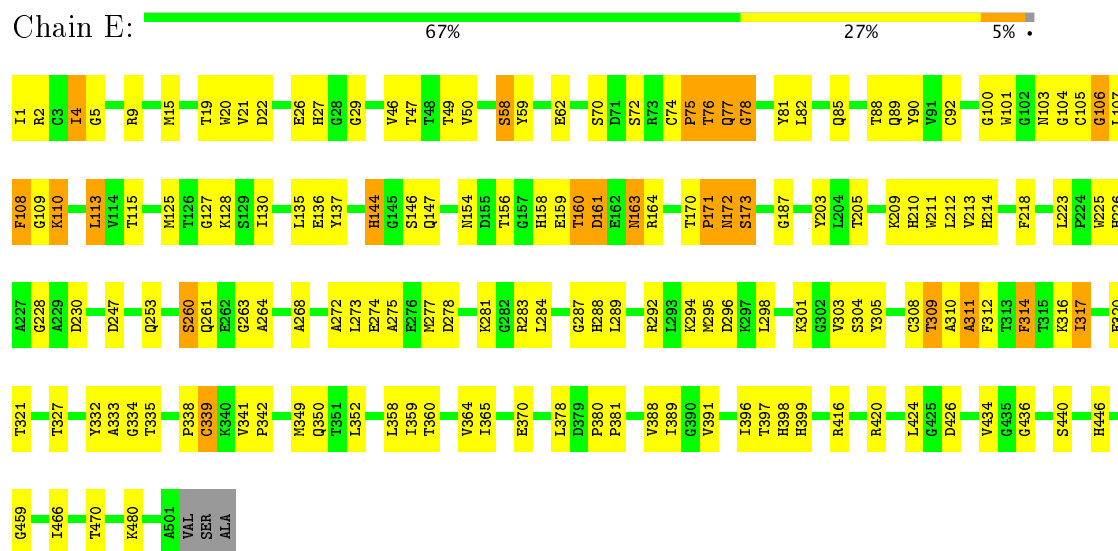
- Molecule 2 is a protein called M protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	75	Total	C	N	O	0	0
			456	285	85	86		
2	D	75	Total	C	N	O	0	0
			456	285	85	86		
2	F	75	Total	C	N	O	0	0
			450	282	82	86		

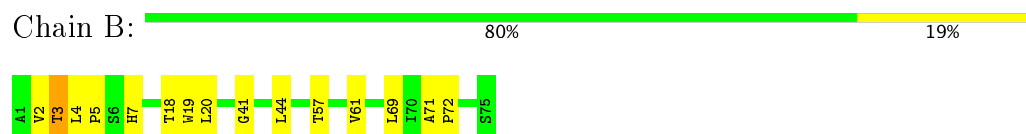
- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



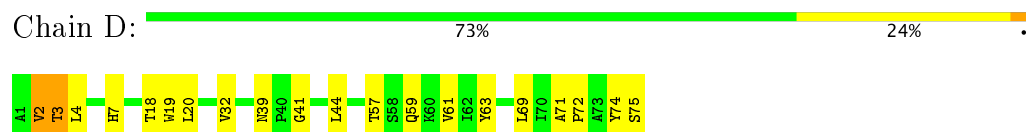
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total 28	C 16	N 2	O 10	0
3	A	1	Total 28	C 16	N 2	O 10	0
3	C	1	Total 28	C 16	N 2	O 10	0
3	C	1	Total 28	C 16	N 2	O 10	0
3	E	1	Total 28	C 16	N 2	O 10	0
3	E	1	Total 28	C 16	N 2	O 10	0



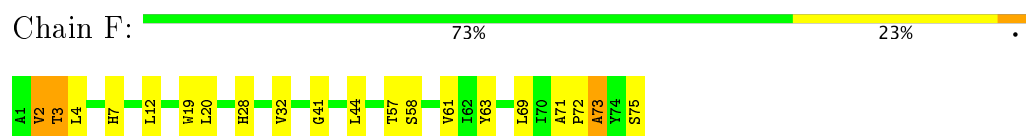
- Molecule 2: M protein



- Molecule 2: M protein



- Molecule 2: M protein



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, 1	Depositor
Number of particles used	11842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY; Phase flipping was performed during 3D reconstruction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	23	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	14000	Depositor
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 >2	RMSZ	# Z >2
1	A	0.56	2/3228 (0.1%)	0.64	3/4439 (0.1%)
1	C	0.60	2/3289 (0.1%)	0.62	3/4514 (0.1%)
1	E	0.53	0/3247	0.60	1/4460 (0.0%)
2	B	0.41	0/466	0.48	0/650
2	D	0.47	0/466	0.54	1/650 (0.2%)
2	F	0.42	0/460	0.48	0/643
All	All	0.55	4/11156 (0.0%)	0.60	8/15356 (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
1	C	0	1
1	E	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	ARG	NE-CZ	-7.87	1.22	1.33
1	C	73	ARG	CZ-NH1	-7.82	1.22	1.33
1	A	164	ARG	CZ-NH1	-7.61	1.23	1.33
1	A	164	ARG	NE-CZ	-7.48	1.23	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	CYS	C-N-CD	-13.49	90.92	120.60
1	C	73	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	A	113	LEU	CA-CB-CG	5.36	127.64	115.30
1	C	113	LEU	CA-CB-CG	5.35	127.61	115.30
1	E	113	LEU	CA-CB-CG	5.25	127.37	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ILE	Peptide
1	C	359	ILE	Peptide
1	E	359	ILE	Peptide

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	3167	0	2593	176	0
1	C	3225	0	2708	307	0
1	E	3186	0	2621	223	0
2	B	456	0	329	16	0
2	D	456	0	329	24	0
2	F	450	0	318	24	0
3	A	28	0	25	1	0
3	C	28	0	25	9	0
3	E	28	0	24	1	0
All	All	11024	0	8972	677	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 34.

The worst 5 of 677 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:138:ARG:HD3	1:C:166:LYS:CE	1.23	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:PHE:CE2	1:C:405:SER:HA	1.41	1.56
1:A:222:PRO:HG3	2:B:3:THR:CB	1.38	1.53
1:C:27:HIS:CE1	1:C:45:LEU:HD21	1.44	1.52
1:C:465:GLN:HE21	1:C:494:VAL:CG1	1.26	1.49

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	499/504 (99%)	407 (82%)	61 (12%)	31 (6%)	2	25
1	C	499/504 (99%)	394 (79%)	71 (14%)	34 (7%)	1	23
1	E	499/504 (99%)	407 (82%)	65 (13%)	27 (5%)	2	28
2	B	73/75 (97%)	63 (86%)	7 (10%)	3 (4%)	3	34
2	D	73/75 (97%)	63 (86%)	8 (11%)	2 (3%)	6	43
2	F	73/75 (97%)	61 (84%)	9 (12%)	3 (4%)	3	34
All	All	1716/1737 (99%)	1395 (81%)	221 (13%)	100 (6%)	4	27

5 of 100 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	MET
1	A	17	GLY
1	A	75	PRO
1	A	78	GLY
1	A	79	GLU

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 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	221/410 (54%)	220 (100%)	1 (0%)	91	96
1	C	235/410 (57%)	232 (99%)	3 (1%)	73	88
1	E	225/410 (55%)	222 (99%)	3 (1%)	73	88
2	B	25/64 (39%)	25 (100%)	0	100	100
2	D	25/64 (39%)	25 (100%)	0	100	100
2	F	24/64 (38%)	24 (100%)	0	100	100
All	All	755/1422 (53%)	748 (99%)	7 (1%)	83	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	382	PHE
1	E	339	CYS
1	E	108	PHE
1	C	57	ARG
1	E	154	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	399	HIS
1	C	465	GLN
1	E	147	GLN
1	C	154	ASN
1	E	398	HIS

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 ⓘ

6 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	$\# Z > 2$
3	NAG	A	600	1,3	14,14,15	0.54	0	15,19,21	1.08	1 (6%)
3	NAG	A	601	3	14,14,15	0.55	0	15,19,21	0.79	1 (6%)
3	NAG	C	600	1,3	14,14,15	0.59	0	15,19,21	0.76	0
3	NAG	C	601	3	14,14,15	0.56	0	15,19,21	0.64	0
3	NAG	E	600	1,3	14,14,15	0.79	0	15,19,21	1.02	2 (13%)
3	NAG	E	601	3	14,14,15	0.85	1 (7%)	15,19,21	0.98	1 (6%)

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
3	NAG	A	600	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	601	3	-	0/6/23/26	0/1/1/1
3	NAG	C	600	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	601	3	-	0/6/23/26	0/1/1/1
3	NAG	E	600	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	E	601	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	NAG	C1-C2	2.01	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	600	NAG	O5-C1-C2	-2.70	107.72	111.47
3	A	601	NAG	C2-N2-C7	-2.20	119.73	122.94
3	E	601	NAG	C2-N2-C7	-2.01	120.01	122.94
3	E	600	NAG	C2-N2-C7	-2.01	120.02	122.94
3	A	600	NAG	C4-C3-C2	2.08	114.07	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	600	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	601	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	NAG	1	0
3	C	600	NAG	9	0
3	C	601	NAG	2	0
3	E	600	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.