



## wwPDB EM Validation Summary Report ⓘ

Jul 21, 2025 – 06:27 PM EDT

PDB ID : 9CU7 / pdb\_00009cu7  
EMDB ID : EMD-45930  
Title : Structure of 16.ND.92 Fab in complex with A/Solomon Islands/3/2006(H1N1) influenza virus Hemagglutinin  
Authors : Ouyang, W.O.; Pholcharee, T.; Wu, N.C.  
Deposited on : 2024-07-25  
Resolution : 2.82 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
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

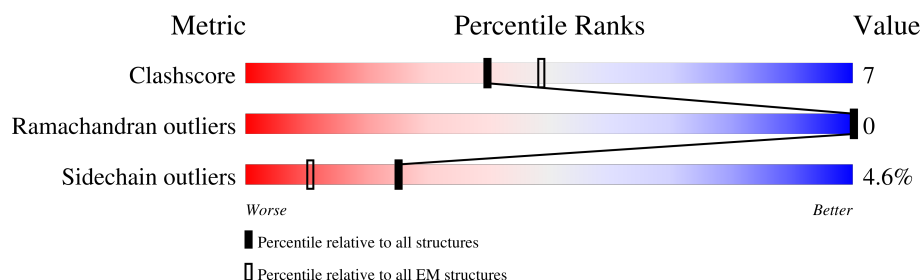
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.82 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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	H	127	80% 17% .
1	I	127	69% 27% .
1	J	127	74% 22% .
2	L	107	81% 18% .
2	M	107	84% 15% .
2	N	107	82% 15% .
3	A	321	83% 15% .
3	C	321	82% 17% .
3	E	321	80% 19% .

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Mol	Chain	Length	Quality of chain
4	B	169	 85% 14% •
4	D	169	 85% 13% •
4	F	169	 83% 17% •

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16913 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 Variable Heavy Chain of 16.ND.92 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	127	Total	C	N	O	S	0	0
			950	599	162	184	5		
1	I	127	Total	C	N	O	S	0	0
			957	603	163	186	5		
1	J	127	Total	C	N	O	S	0	0
			957	603	163	186	5		

- Molecule 2 is a protein called Variable Light Chain of 16.ND.92 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total	C	N	O	S	0	0
			831	528	140	160	3		
2	M	107	Total	C	N	O	S	0	0
			831	528	140	160	3		
2	N	107	Total	C	N	O	S	0	0
			831	528	140	160	3		

- Molecule 3 is a protein called Hemagglutinin HA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	321	Total	C	N	O	S	0	0
			2505	1582	441	471	11		
3	C	321	Total	C	N	O	S	0	0
			2505	1582	441	471	11		
3	E	321	Total	C	N	O	S	0	0
			2505	1582	441	471	11		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ARG	LEU	conflict	UNP A0A0G2RTI0
C	53	ARG	LEU	conflict	UNP A0A0G2RTI0
E	53	ARG	LEU	conflict	UNP A0A0G2RTI0

- Molecule 4 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	169	Total	C	N	O	S	0	0
			1347	844	231	265	7		
4	D	169	Total	C	N	O	S	0	0
			1347	844	231	265	7		
4	F	169	Total	C	N	O	S	0	0
			1347	844	231	265	7		

### 3 Residue-property plots


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.

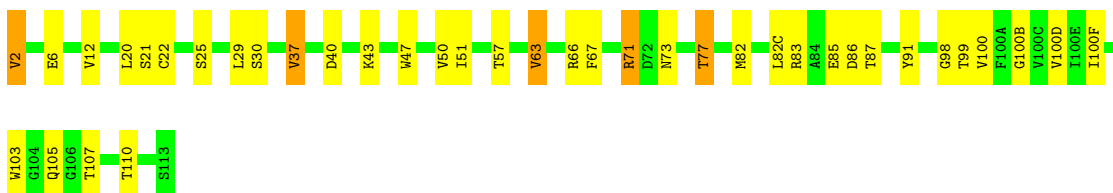
- Molecule 1: Variable Heavy Chain of 16.ND.92 Fab

Chain H: 



- Molecule 1: Variable Heavy Chain of 16.ND.92 Fab

Chain I: 




- Molecule 1: Variable Heavy Chain of 16.ND.92 Fab

Chain J: 




- Molecule 2: Variable Light Chain of 16.ND.92 Fab

Chain L: 




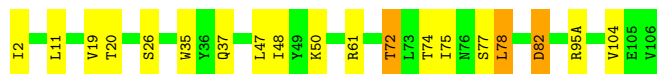
- Molecule 2: Variable Light Chain of 16.ND.92 Fab

Chain M: 




- Molecule 2: Variable Light Chain of 16.ND.92 Fab

Chain N:  82% 15%




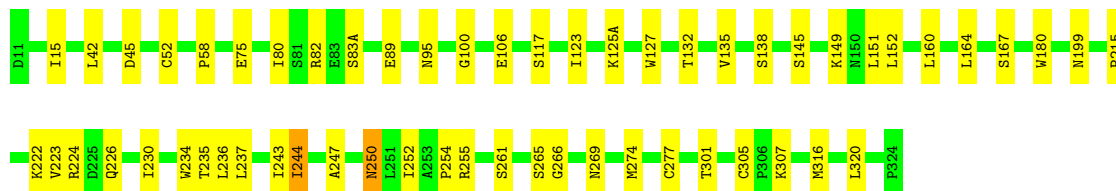
- Molecule 3: Hemagglutinin HA1

Chain A:  83% 15%




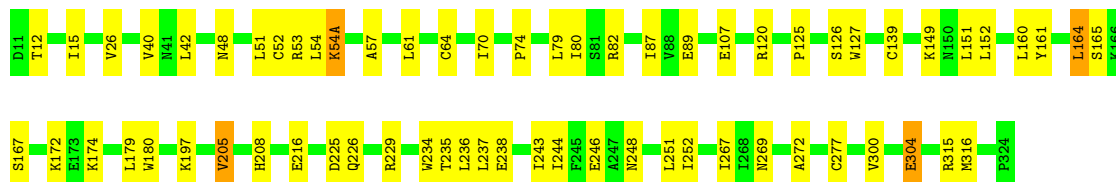
- Molecule 3: Hemagglutinin HA1

Chain C:  82% 17%




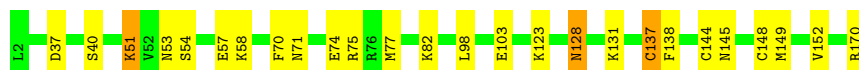
- Molecule 3: Hemagglutinin HA1

Chain E:  80% 19%




- Molecule 4: Hemagglutinin HA2

Chain B:  85% 14%

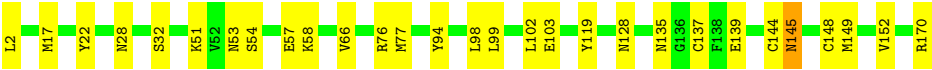
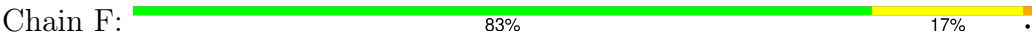


- Molecule 4: Hemagglutinin HA2

Chain D:  85% 13%



● Molecule 4: Hemagglutinin HA2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	152449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	57.35	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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	H	0.36	0/971	0.44	0/1321
1	I	0.36	0/978	0.44	0/1329
1	J	0.32	0/978	0.39	0/1329
2	L	0.35	0/853	0.53	1/1161 (0.1%)
2	M	0.40	0/853	0.57	0/1161
2	N	0.25	0/853	0.32	0/1161
3	A	0.23	0/2571	0.30	0/3499
3	C	0.22	0/2571	0.31	0/3499
3	E	0.23	0/2571	0.32	0/3499
4	B	0.27	0/1373	0.38	1/1846 (0.1%)
4	D	0.25	0/1373	0.28	0/1846
4	F	0.24	0/1373	0.27	0/1846
All	All	0.28	0/17318	0.36	2/23497 (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	I	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	137	CYS	CB-CA-C	-5.57	99.99	113.19
2	L	71	PHE	CA-CB-CG	5.12	118.92	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	71	ARG	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	H	950	0	899	16	0
1	I	957	0	912	22	0
1	J	957	0	912	21	0
2	L	831	0	806	8	0
2	M	831	0	806	8	0
2	N	831	0	806	11	0
3	A	2505	0	2421	29	0
3	C	2505	0	2421	38	0
3	E	2505	0	2421	38	0
4	B	1347	0	1263	17	0
4	D	1347	0	1263	18	0
4	F	1347	0	1263	19	0
All	All	16913	0	16193	228	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 7.

The worst 5 of 228 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:A:42:LEU:HD11	3:A:316:MET:HE2	1.65	0.77
1:I:98:GLY:HA2	1:I:100(D):VAL:HG22	1.69	0.74
1:J:100(I):ASP:OD2	2:N:50:LYS:NZ	2.23	0.72
1:H:22:CYS:HB2	1:H:78:VAL:HG13	1.71	0.71
4:D:17:MET:HE1	4:D:23:GLY:HA3	1.72	0.70

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	H	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
1	I	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
1	J	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
2	L	105/107 (98%)	96 (91%)	9 (9%)	0	100	100
2	M	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
2	N	105/107 (98%)	94 (90%)	11 (10%)	0	100	100
3	A	319/321 (99%)	307 (96%)	12 (4%)	0	100	100
3	C	319/321 (99%)	306 (96%)	13 (4%)	0	100	100
3	E	319/321 (99%)	307 (96%)	12 (4%)	0	100	100
4	B	167/169 (99%)	160 (96%)	7 (4%)	0	100	100
4	D	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
4	F	167/169 (99%)	161 (96%)	6 (4%)	0	100	100
All	All	2148/2172 (99%)	2054 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	H	99/102 (97%)	93 (94%)	6 (6%)	15	41
1	I	101/102 (99%)	95 (94%)	6 (6%)	16	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	101/102 (99%)	95 (94%)	6 (6%)	16	43
2	L	92/92 (100%)	84 (91%)	8 (9%)	8	25
2	M	92/92 (100%)	87 (95%)	5 (5%)	18	46
2	N	92/92 (100%)	86 (94%)	6 (6%)	14	38
3	A	276/281 (98%)	263 (95%)	13 (5%)	22	52
3	C	276/281 (98%)	270 (98%)	6 (2%)	47	78
3	E	276/281 (98%)	261 (95%)	15 (5%)	18	46
4	B	141/146 (97%)	138 (98%)	3 (2%)	48	79
4	D	141/146 (97%)	135 (96%)	6 (4%)	25	56
4	F	141/146 (97%)	137 (97%)	4 (3%)	38	71
All	All	1828/1863 (98%)	1744 (95%)	84 (5%)	25	53

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	54	LEU
4	B	51	LYS
3	E	79	LEU
3	E	205	VAL
4	D	17	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	25	HIS
3	E	271	ASN
3	A	95	ASN
3	E	171	ASN
3	A	73	ASN

### 5.3.3 RNA ⓘ

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](#)

There are no chain breaks in this entry.

## 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45930. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 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 standard-deviation projections (False-color)

This section was not generated.

### 6.5 Orthogonal surface views

This section was not generated.

### 6.6 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.