



## wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 02:43 PM EDT

PDB ID : 3JCX  
EMDB ID: : EMD-6629  
Title : Canine Parvovirus complexed with Fab E  
Authors : Organtini, L.J.; Iketani, S.; Huang, K.; Ashley, R.E.; Makhov, A.M.; Conway, J.F.; Parrish, C.R.; Hafenstein, S.  
Deposited on : 2016-03-21  
Resolution : 4.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

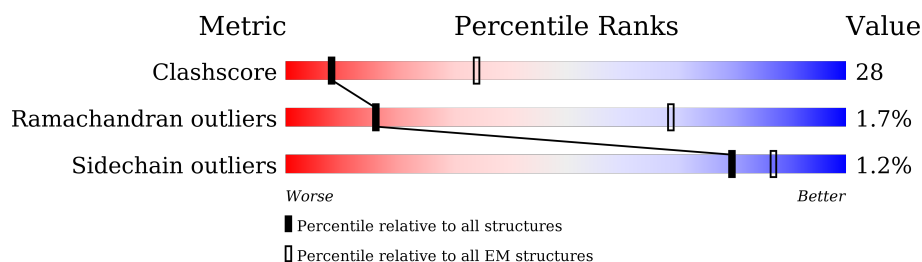
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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  $\geq 3$ , 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	584	
2	H	115	
3	L	107	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6072 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 Capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	548	Total	C	N	O	S	0	0
			4353	2765	742	830	16		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	TYR	GLU	CONFLICT	UNP B2ZG07
A	104	GLU	GLN	CONFLICT	UNP B2ZG07
A	300	ASP	ALA	CONFLICT	UNP B2ZG07
A	509	GLN	GLU	CONFLICT	UNP B2ZG07

- Molecule 2 is a protein called Fab E heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	115	Total	C	N	O	S	0	0
			899	575	148	172	4		

- Molecule 3 is a protein called Fab E light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			820	507	139	167	7		



M76	Q77	A78	E79	D80	L81	A82	V83	Y84	Y85	C86	M87	O88	S89	T90	S91	Y92	P93	L94	T95	S98	G99	T100	K101	L102	A107
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	47563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND4	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	FEI Falcon II (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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.51	0/4483	0.65	2/6133 (0.0%)
2	H	3.45	18/927 (1.9%)	1.91	26/1266 (2.1%)
3	L	0.79	4/834 (0.5%)	0.89	5/1127 (0.4%)
All	All	1.43	22/6244 (0.4%)	0.97	33/8526 (0.4%)

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	13
2	H	0	10
3	L	0	2
All	All	0	25

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	153	TRP	CB-CG	88.39	3.09	1.50
2	H	153	TRP	CG-CD1	26.65	1.74	1.36
2	H	206	TYR	CD1-CE1	-21.78	1.06	1.39
2	H	153	TRP	CA-CB	19.93	1.97	1.53
2	H	206	TYR	CD2-CE2	-15.23	1.16	1.39

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	153	TRP	N-CA-CB	21.15	148.68	110.60
2	H	153	TRP	CA-CB-CG	21.06	153.72	113.70
2	H	153	TRP	CD1-CG-CD2	-19.65	90.58	106.30
2	H	153	TRP	N-CA-C	-17.26	64.40	111.00
2	H	152	MET	CB-CG-SD	12.82	150.87	112.40

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	188	ALA	Peptide
1	A	189	ALA	Peptide
1	A	255	LEU	Peptide
1	A	257	THR	Peptide
1	A	87	MET	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	4353	0	4144	146	0
2	H	899	0	861	143	0
3	L	820	0	798	69	0
All	All	6072	0	5803	338	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 28.

The worst 5 of 338 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)
2:H:153:TRP:CA	2:H:153:TRP:CB	1.97	1.40
2:H:153:TRP:HA	2:H:153:TRP:CB	1.77	1.11
1:A:87:MET:O	2:H:206:TYR:CE1	2.13	1.01
3:L:1:LEU:HD22	3:L:88:GLN:HE22	1.30	0.96
1:A:81:ARG:NH2	2:H:155:ASP:OD1	2.04	0.91

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	A	546/584 (94%)	472 (86%)	66 (12%)	8 (2%)	13	58
2	H	113/115 (98%)	80 (71%)	28 (25%)	5 (4%)	3	35
3	L	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
All	All	764/806 (95%)	641 (84%)	110 (14%)	13 (2%)	16	56

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	152	MET
2	H	212	TYR
2	H	153	TRP
1	A	199	PRO
1	A	451	TYR

### 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	477/496 (96%)	470 (98%)	7 (2%)	72	89
2	H	101/101 (100%)	100 (99%)	1 (1%)	82	91
3	L	93/93 (100%)	93 (100%)	0	100	100
All	All	671/690 (97%)	663 (99%)	8 (1%)	79	90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	234	HIS
2	H	136	HIS
1	A	403	HIS
1	A	137	HIS
1	A	277	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	114	GLN
2	H	134	HIS
3	L	35	GLN
1	A	509	GLN
3	L	26	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 carbohydrates 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.