



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 17, 2017 – 10:09 AM EDT

PDB ID : 4C10
EMDB ID: : EMD-2436
Title : Cryo-EM reconstruction of empty enterovirus 71 in complex with a neutralizing antibody E19
Authors : Plevka, P.; Perera, R.; Cardoso, J.; Suksatu, A.; Kuhn, R.J.; Rossmann, M.G.
Deposited on : unknown
Resolution : 13.00 Å(reported)
Based on PDB ID : 3ZFE

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

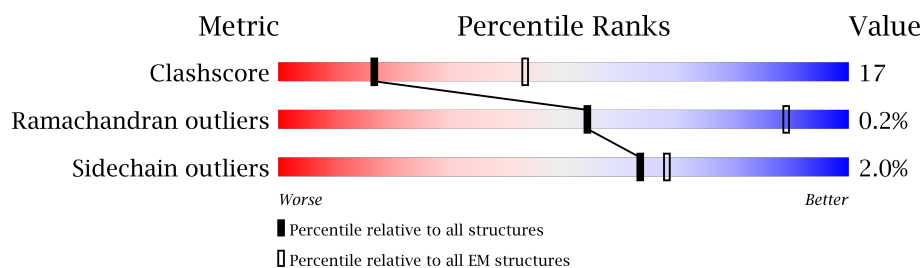
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 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	4	217	
2	5	220	
3	A	298	
4	B	254	
5	C	242	
6	D	69	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9058 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 EV19 5 C1-6 F1 C11.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	4	217	Total	C	N	O	0	0
			1265	831	217	217		

- Molecule 2 is a protein called EV19 5 C1-6 F1 C11.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	5	220	Total	C	N	O	0	0
			1264	824	220	220		

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	297	Total	C	N	O	S	0	1
			2299	1447	395	444	13		

- Molecule 4 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	244	Total	C	N	O	S	0	0
			1893	1212	313	359	9		

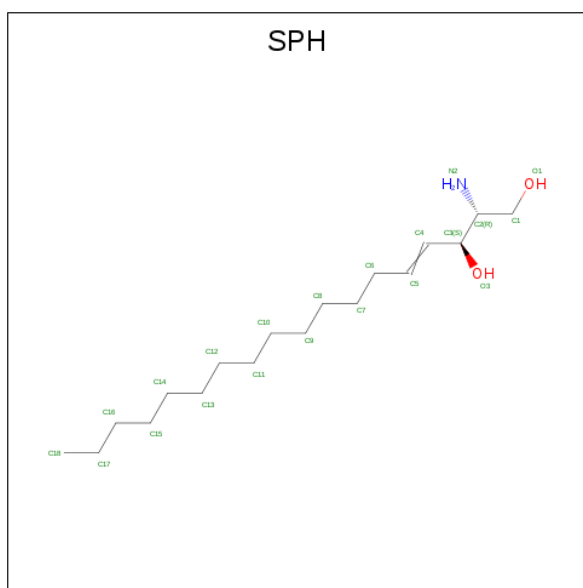
- Molecule 5 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	242	Total	C	N	O	S	0	0
			1866	1198	311	345	12		

- Molecule 6 is a protein called VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	57	Total	C	N	O	S	0	0
			443	276	72	94	1		

- Molecule 7 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Na	0
			1	1	
8	A	4	Total	Na	0
			4	4	
8	C	1	Total	Na	0
			1	1	

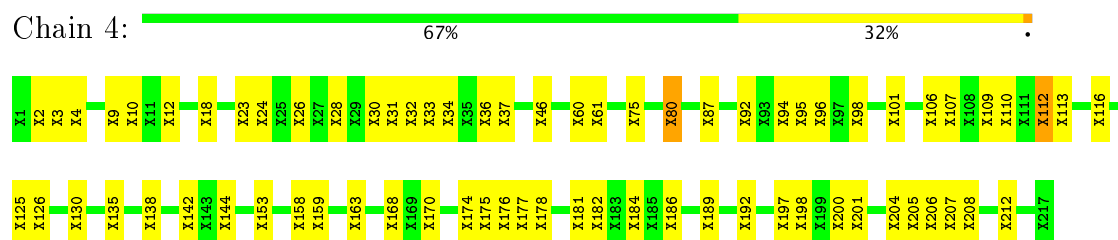
- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
9	C	1	Total	Cl	0
			1	1	

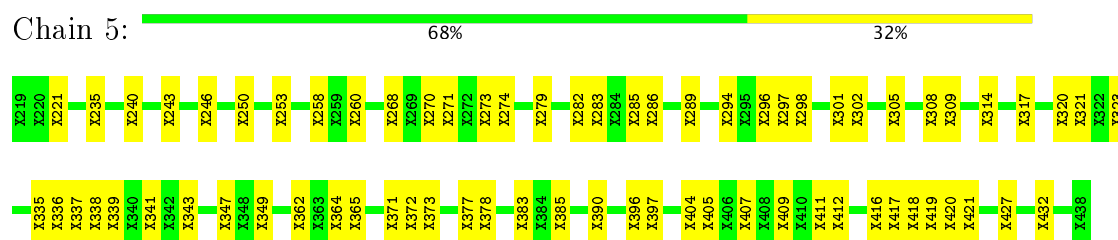
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

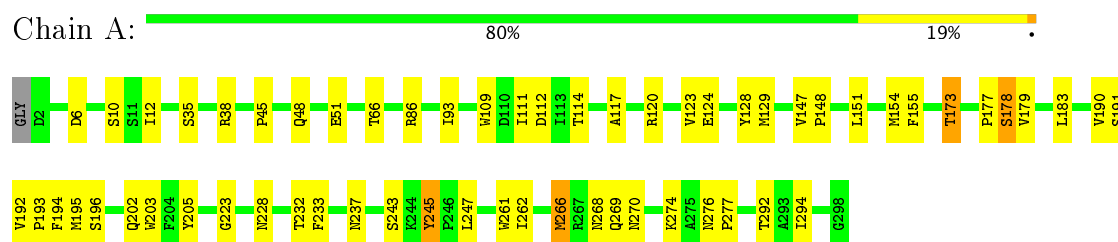
- Molecule 1: EV19 5 C1-6 F1 C11



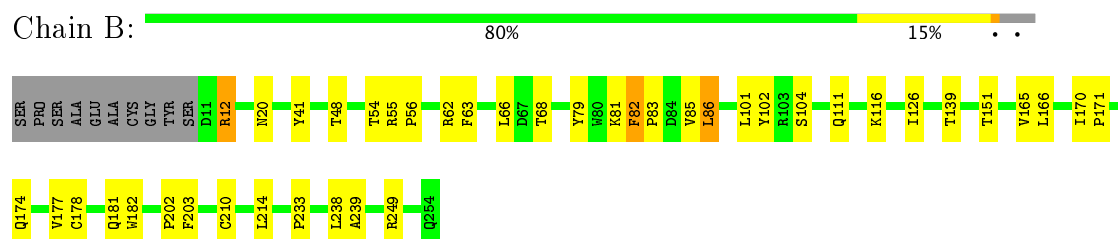
- Molecule 2: EV19 5 C1-6 F1 C11



- Molecule 3: VP1



- Molecule 4: VP3



- Molecule 5: VP2

I133	G1	G9	Q12	F13	I14	I15	I16	D17	S21	I24	L25	I34	H35	E39	V49	M56	M57	V58	P59	T60	N61	G62	T63	S64	S65	L66	M66	E67	R68	L69	R70	F71	P72	D89	P90	Q103	Q110	F111	S112	G113	S114	L115	E116	M126	A127	T128	G129	K130
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Chain D: 71% 12% 17%

MET	GLY	SER	GLN	VAL	SER	THR	GLN	ARG	SER	GLY	SER	H13	S23	T24	I25	N26	Y27	Y37	T62	E63	M64	P67	L68	K69
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	10833	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF DETERMINED FOR ALL PARTICLES FROM ONE FILM, PHASE FLIP	Depositor
Microscope	FEI/PHILIPS CM200FEG/ST	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	49500	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SPH, NA, CL

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	$\# Z > 2$
3	A	0.32	0/2358	0.59	0/3215
4	B	0.32	0/1948	0.63	1/2670 (0.0%)
5	C	0.32	0/1920	0.59	0/2626
6	D	0.32	0/452	0.54	0/611
All	All	0.32	0/6678	0.60	1/9122 (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	4	0	4
2	5	0	2
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	82	PHE	N-CA-C	6.65	128.95	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	112	UNK	Mainchain
1	4	46	UNK	Peptide
1	4	80	UNK	Peptide

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Mol	Chain	Res	Type	Group
1	4	98	UNK	Peptide
2	5	338	UNK	Mainchain

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	4	1265	0	1179	101	0
2	5	1264	0	1131	97	0
3	A	2299	0	2231	56	0
4	B	1893	0	1827	41	0
5	C	1866	0	1834	61	0
6	D	443	0	420	9	0
7	A	21	0	37	7	0
8	A	4	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	C	1	0	0	0	0
All	All	9058	0	8659	309	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 17.

The worst 5 of 309 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)
1:4:138:UNK:CG	1:4:138:UNK:CB	1.78	1.62
1:4:198:UNK:CG	1:4:198:UNK:CB	1.79	1.61
2:5:365:UNK:CG	2:5:365:UNK:CB	1.78	1.58
2:5:240:UNK:CG	2:5:314:UNK:HG1	1.16	1.57
2:5:314:UNK:CG	2:5:314:UNK:CB	1.77	1.57

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	
3	A	295/298 (99%)	280 (95%)	14 (5%)	1 (0%)	44	81
4	B	242/254 (95%)	224 (93%)	18 (7%)	0	100	100
5	C	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	38	77
6	D	55/69 (80%)	51 (93%)	4 (7%)	0	100	100
All	All	832/863 (96%)	783 (94%)	47 (6%)	2 (0%)	54	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	58	VAL
3	A	262	ILE

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	
3	A	253/253 (100%)	248 (98%)	5 (2%)	60	82
4	B	208/215 (97%)	202 (97%)	6 (3%)	48	73
5	C	203/203 (100%)	200 (98%)	3 (2%)	70	85
6	D	48/58 (83%)	48 (100%)	0	100	100
All	All	712/729 (98%)	698 (98%)	14 (2%)	63	82

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	48	THR
4	B	86	LEU
5	C	70	ARG
4	B	12	ARG
4	B	111	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	270	ASN
5	C	237	GLN
3	A	282	ASN
3	A	268	ASN
4	B	109	HIS

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](#)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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
7	SPH	A	301	-	19,20,20	0.66	1 (5%)	18,21,21	1.08	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
7	SPH	A	301	-	-	0/21/21/21	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	301	SPH	C3-C4	2.40	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	301	SPH	C10-C9-C8	-2.22	103.04	114.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	301	SPH	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	112:UNK	C	113:UNK	N	0.93