wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:57 PM BST

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.; Cardosa, J.; Suksatu, A.; Kuhn, R.J.; Rossmann, M.G.
Deposited on	:	2013-08-08
Resolution	:	13.00 Å(reported)
Based on PDB ID	:	3ZFE

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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

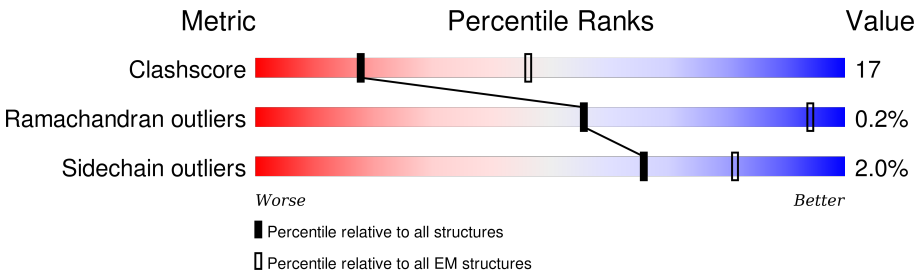
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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	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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	4	217	67% 32% •
2	5	220	68% 32%
3	A	298	80% 19% •
4	B	254	80% 15% • •
5	C	242	78% 21% •
6	D	69	71% 12% 17%

2 Entry composition (i)

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
			Total	C	N	O		
1	4	217	1265	831	217	217	0	0

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

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

- Molecule 3 is a protein called VP1.

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

- Molecule 4 is a protein called VP3.

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

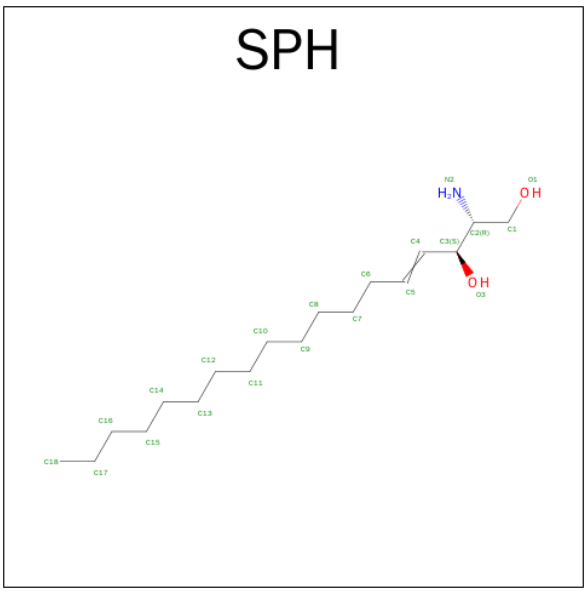
- Molecule 5 is a protein called VP2.

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

- Molecule 6 is a protein called VP4.

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

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



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

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

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

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

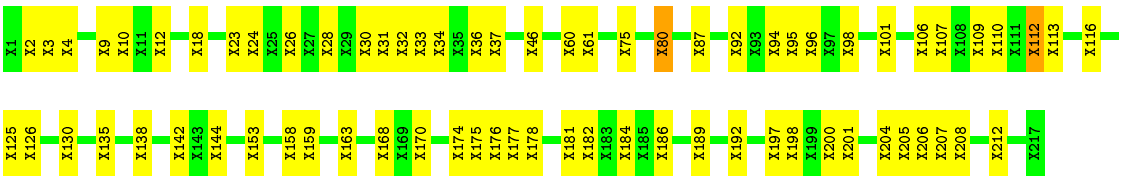
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
9	C	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

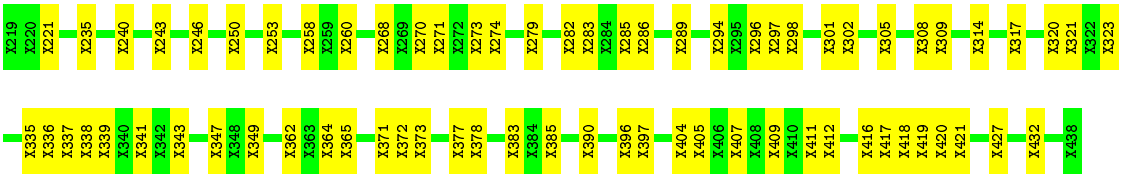
- Molecule 1: EV19 5 C1-6 F1 C11

Chain 4:



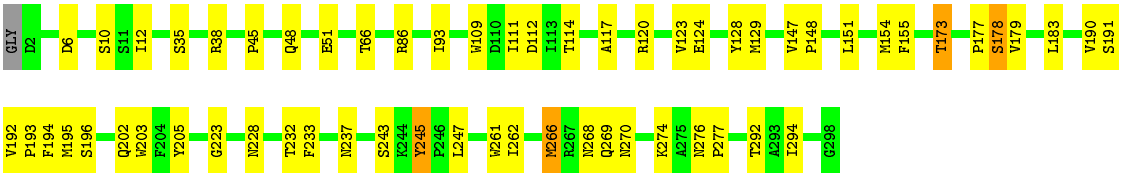
- Molecule 2: EV19 5 C1-6 F1 C11

Chain 5:



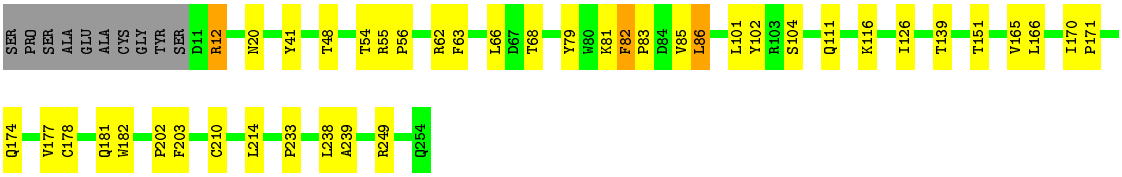
- Molecule 3: VP1

Chain A:



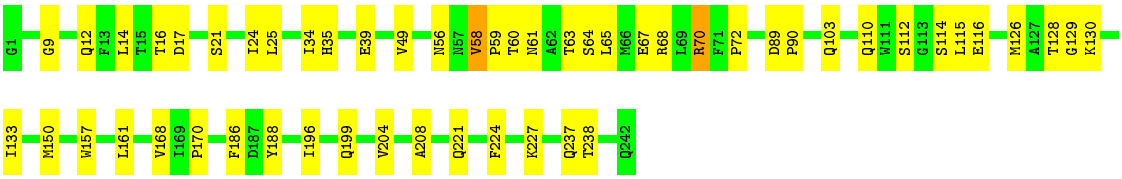
- Molecule 4: VP3

Chain B:



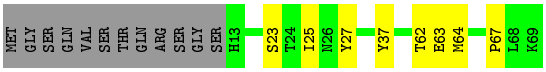
- Molecule 5: VP2

Chain C:



- Molecule 6: VP4

Chain D:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of images	Not provided	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 ($e^-/Å^2$)	18	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO163 FILM	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: 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(^{o})	Ideal(^{o})
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 (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	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%)	46	83
4	B	242/254 (95%)	224 (93%)	18 (7%)	0	100	100
5	C	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	39	80
6	D	55/69 (80%)	51 (93%)	4 (7%)	0	100	100
All	All	832/863 (96%)	783 (94%)	47 (6%)	2 (0%)	56	86

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%)	63	85
4	B	208/215 (97%)	202 (97%)	6 (3%)	50	78
5	C	203/203 (100%)	200 (98%)	3 (2%)	72	88
6	D	48/58 (83%)	48 (100%)	0	100	100
All	All	712/729 (98%)	698 (98%)	14 (2%)	66	85

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	0.64	1 (5%)	16,21,21	1.08	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
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	2.27	1.54	1.49

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	301	SPH	C10-C9-C8	-2.21	103.04	114.54

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)

There are no chain breaks in this entry.