



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:36 PM BST

PDB ID : 1UPN
EMDB ID: : EMD-1057
Title : COMPLEX OF ECHOVIRUS TYPE 12 WITH DOMAINS 3 AND 4 OF ITS RECEPTOR DECAY ACCELERATING FACTOR (CD55) BY CRYO ELECTRON MICROSCOPY AT 16 Å
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Deposited on : 2003-10-08
Resolution : 16.00 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

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

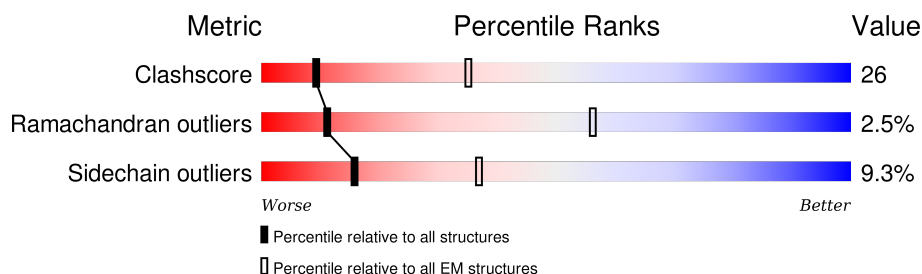
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 16.00 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	292	
2	B	262	
3	C	238	
4	D	69	
5	E	129	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7463 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 ECHOVIRUS 11 COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	289	Total	C	N	O	S	0	0
			2283	1439	398	435	11		

- Molecule 2 is a protein called ECHOVIRUS 11 COAT PROTEIN VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	252	Total	C	N	O	S	0	0
			1963	1240	331	376	16		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	226	PHE	SER	CONFLICT	UNP Q8JKE8

- Molecule 3 is a protein called ECHOVIRUS 11 COAT PROTEIN VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	238	Total	C	N	O	S	0	0
			1818	1161	299	345	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	63	GLU	GLN	CONFLICT	UNP Q8JKE8

- Molecule 4 is a protein called ECHOVIRUS 11 COAT PROTEIN VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	60	Total	C	N	O	S	0	0
			466	289	81	95	1		

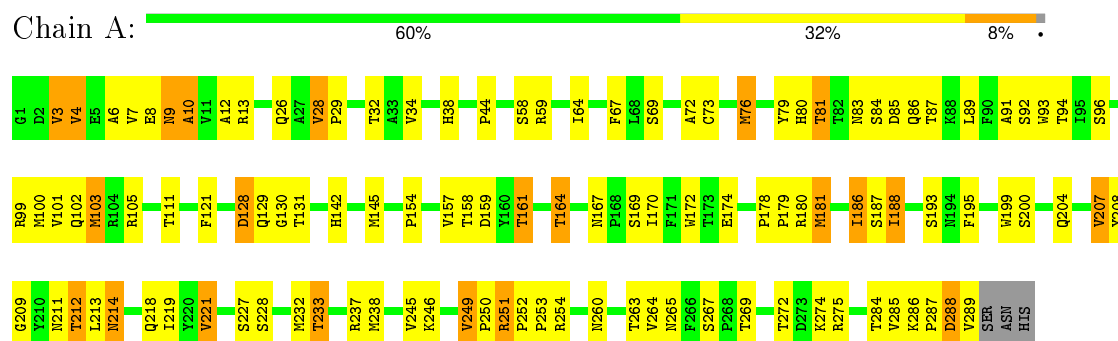
- Molecule 5 is a protein called COMPLEMENT DECAY-ACCELERATING FACTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	125	Total	C	N	O	S	0	0
			933	583	159	182	9		

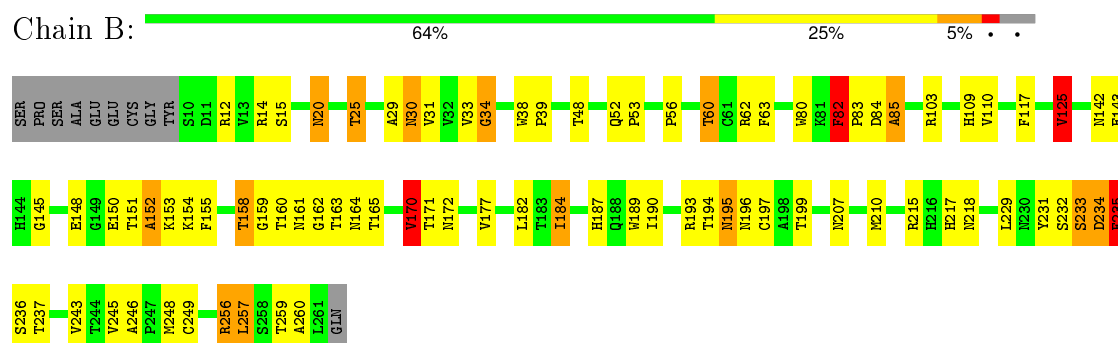
3 Residue-property plots

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

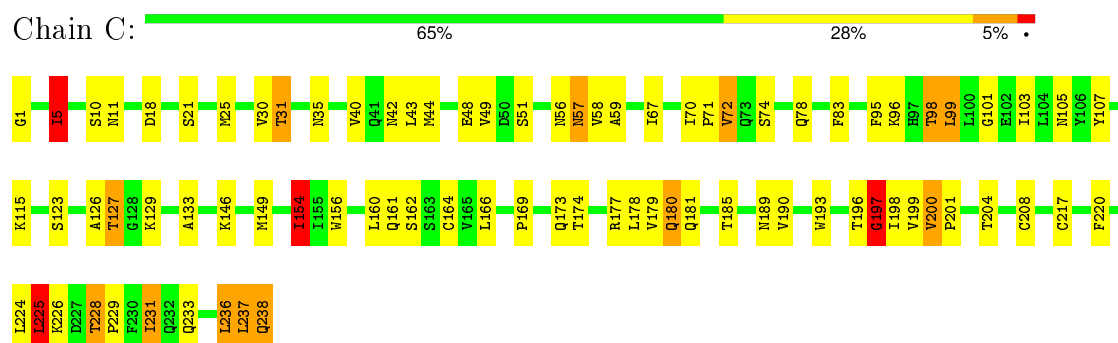
• Molecule 1: ECHOVIRUS 11 COAT PROTEIN VP1



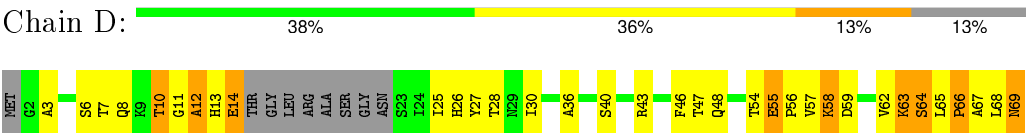
• Molecule 2: ECHOVIRUS 11 COAT PROTEIN VP2



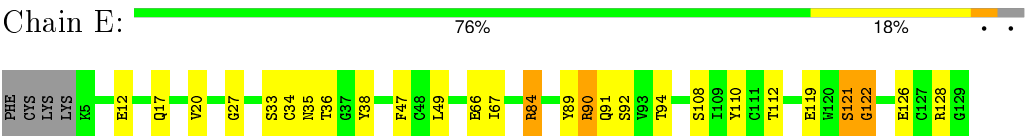
• Molecule 3: ECHOVIRUS 11 COAT PROTEIN VP3



• Molecule 4: ECHOVIRUS 11 COAT PROTEIN VP4



• Molecule 5: COMPLEMENT DECAY-ACCELERATING FACTOR



4 Experimental information

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	Not provided	Depositor
Microscope	JEOL 1200 EX II	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	30000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.77	2/2348 (0.1%)	0.95	3/3206 (0.1%)
2	B	0.76	0/2015	1.05	8/2753 (0.3%)
3	C	0.77	1/1865 (0.1%)	0.99	6/2549 (0.2%)
4	D	0.87	0/474	1.04	3/639 (0.5%)
5	E	0.64	0/959	0.81	2/1299 (0.2%)
All	All	0.76	3/7661 (0.0%)	0.98	22/10446 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	76	MET	SD-CE	6.53	2.14	1.77
3	C	1	GLY	N-CA	6.17	1.55	1.46
1	A	3	VAL	CA-CB	5.00	1.65	1.54

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	ASN	N-CA-CB	-8.59	95.15	110.60
2	B	82	PHE	N-CA-C	8.56	134.11	111.00
3	C	237	LEU	CB-CG-CD1	-7.95	97.49	111.00
3	C	197	GLY	N-CA-C	7.88	132.81	113.10
1	A	237	ARG	NE-CZ-NH2	-7.41	116.59	120.30

There are no chirality outliers.

There are no planarity outliers.

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	A	2283	0	2212	148	0
2	B	1963	0	1872	131	0
3	C	1818	0	1775	114	0
4	D	466	0	447	47	0
5	E	933	0	852	87	0
All	All	7463	0	7158	387	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 26.

The worst 5 of 387 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:B:160:THR:HA	5:E:35:ASN:CB	1.34	1.48
5:E:66:GLU:C	5:E:67:ILE:HG13	1.21	1.48
2:B:165:THR:CG2	5:E:17:GLN:HB3	1.41	1.47
2:B:165:THR:CB	5:E:17:GLN:OE1	1.72	1.37
1:A:76:MET:SD	1:A:76:MET:CE	2.14	1.35

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	287/292 (98%)	258 (90%)	20 (7%)	9 (3%)	5	42
2	B	250/262 (95%)	220 (88%)	23 (9%)	7 (3%)	6	44
3	C	236/238 (99%)	224 (95%)	10 (4%)	2 (1%)	24	69
4	D	56/69 (81%)	43 (77%)	9 (16%)	4 (7%)	1	22
5	E	121/129 (94%)	117 (97%)	2 (2%)	2 (2%)	11	55
All	All	950/990 (96%)	862 (91%)	64 (7%)	24 (2%)	11	46

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	9	ASN
1	A	214	ASN
1	A	228	SER
2	B	152	ALA

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	259/262 (99%)	236 (91%)	23 (9%)	12	44
2	B	217/225 (96%)	199 (92%)	18 (8%)	14	49
3	C	204/204 (100%)	176 (86%)	28 (14%)	4	27
4	D	51/57 (90%)	45 (88%)	6 (12%)	6	32
5	E	101/110 (92%)	99 (98%)	2 (2%)	63	85
All	All	832/858 (97%)	755 (91%)	77 (9%)	16	42

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	184	ILE
3	C	30	VAL
4	D	25	ILE
2	B	229	LEU
2	B	256	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	GLN
2	B	195	ASN
4	D	44	GLN
2	B	142	ASN

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Mol	Chain	Res	Type
2	B	172	ASN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.