wwPDB/EMDataBank EM Map/Model Validation Summary Report (i)

Nov 3, 2016 – 05:53 PM EDT

PDB ID	:	3IYP
EMDB ID:	:	EMD-5179
Title	:	The Interaction of Decay-accelerating Factor with Echovirus 7
Authors	:	Plevka, P.; Hafenstein, S.; Zhang, Y.; Harris, K.G.; Cifuente, J.O.; Bowman, V.D.; Chipman, P.R.; Lin, F.; Medof, D.E.; Bator, C.M.; Rossmann, M.G.
Deposited on	:	2010-04-07
Resolution	:	7.20 Å(reported)
Based on PDB ID	:	2X5I, 1OJY

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 (i) symbol.

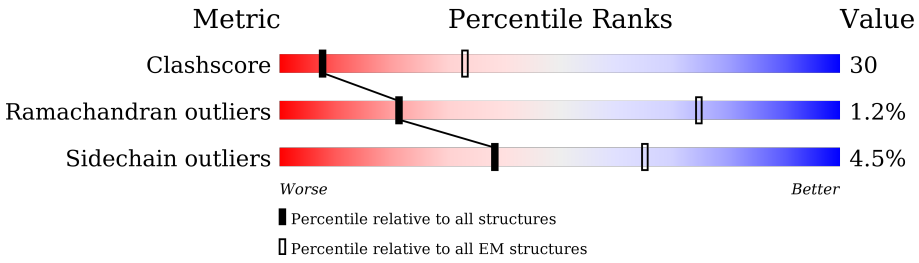
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis	:	NOT EXECUTED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 7.20 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	A	292	58% 36% • 5%
2	B	238	63% 36% •
3	C	260	53% 41% • •
4	D	70	56% 31% 13%
5	F	381	33% 28% 5% 34%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8495 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	277	2235	1414	391	419	11	0	0

- Molecule 2 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	238	1836	1169	303	346	18	0	0

- Molecule 3 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	252	1979	1251	336	374	18	0	0

- Molecule 4 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	61	476	296	82	95	3	0	0

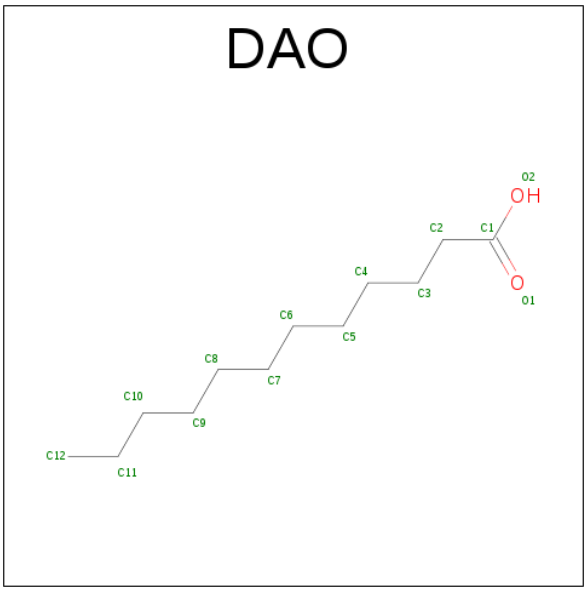
- Molecule 5 is a protein called Complement decay-accelerating factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	252	1955	1226	328	384	17	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	GLN	GLY	CONFLICT	UNP P08174

- Molecule 6 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



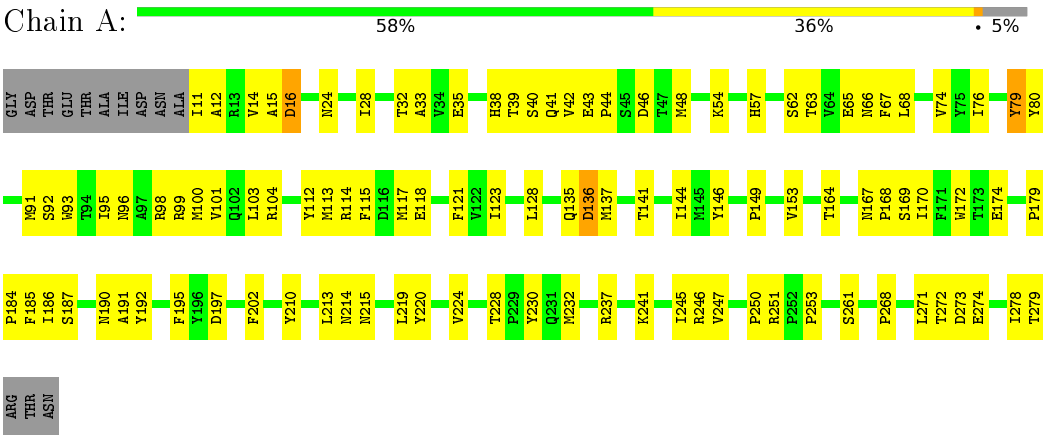
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
6	A	1	14	12	2	0

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.

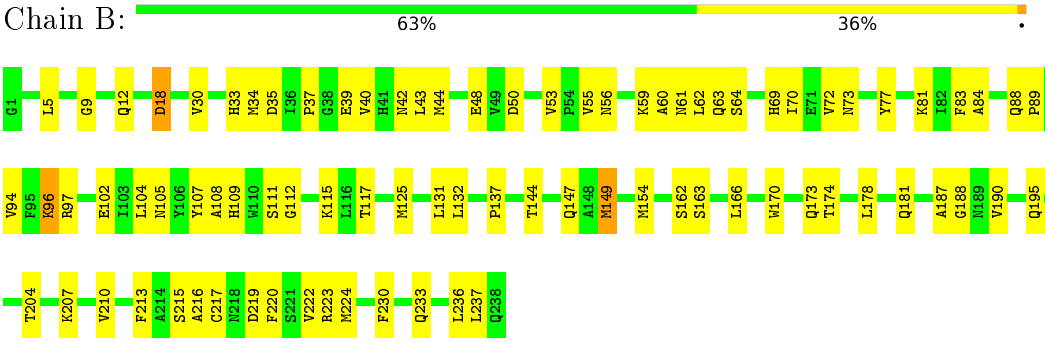
- Molecule 1: Capsid protein

Chain A:



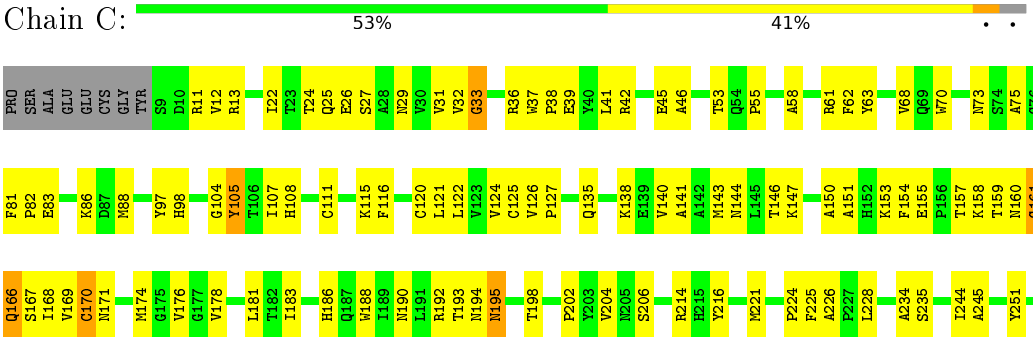
- Molecule 2: Polyprotein

Chain B:



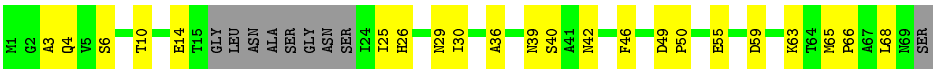
- Molecule 3: Polyprotein

Chain C:



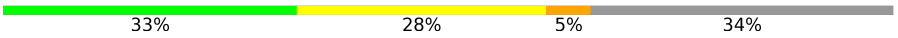
- Molecule 4: Polyprotein

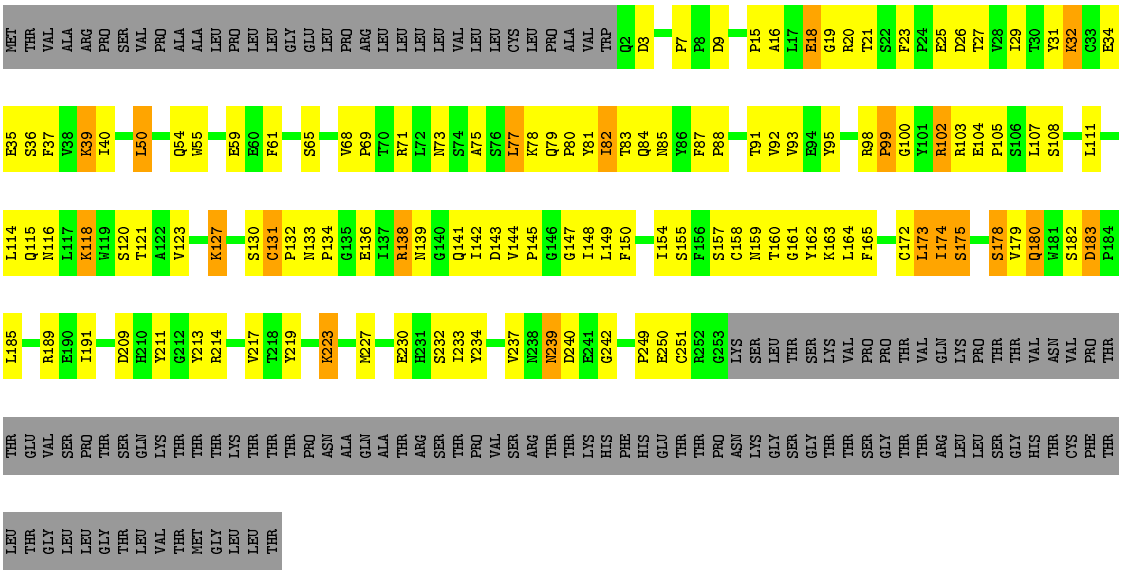
Chain D:



- Molecule 5: Complement decay-accelerating factor

Chain F:





4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	11430	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1120	Depositor
Maximum defocus (nm)	3670	Depositor
Magnification	Not provided	Depositor
Image detector	Kodak SO163 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: DAO

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	0.31	0/2302	0.50	0/3142
2	B	0.35	0/1884	0.52	0/2568
3	C	0.36	0/2031	0.50	0/2769
4	D	0.58	0/484	0.54	0/653
5	F	0.37	1/2008 (0.0%)	0.51	0/2731
All	All	0.36	1/8709 (0.0%)	0.51	0/11863

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	242	GLY	C-O	-5.07	1.15	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2235	0	2158	111	0
2	B	1836	0	1789	103	0
3	C	1979	0	1891	230	0
4	D	476	0	463	20	0
5	F	1955	0	1845	228	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	14	0	23	2	0
All	All	8495	0	8169	493	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 30.

The worst 5 of 493 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:C:141:ALA:CB	5:F:145:PRO:HA	1.13	1.54
3:C:141:ALA:CB	5:F:145:PRO:CA	1.89	1.51
3:C:141:ALA:HB2	5:F:145:PRO:CA	1.41	1.50
3:C:158:LYS:N	5:F:160:THR:H	1.16	1.42
3:C:161:GLY:N	5:F:157:SER:HB3	1.29	1.41

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	275/292 (94%)	244 (89%)	28 (10%)	3 (1%)	17 63
2	B	236/238 (99%)	214 (91%)	20 (8%)	2 (1%)	24 69
3	C	250/260 (96%)	222 (89%)	21 (8%)	7 (3%)	6 44
4	D	57/70 (81%)	48 (84%)	9 (16%)	0	100 100
5	F	250/381 (66%)	227 (91%)	22 (9%)	1 (0%)	39 80
All	All	1068/1241 (86%)	955 (89%)	100 (9%)	13 (1%)	21 61

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
3	C	195	ASN
1	A	24	ASN
2	B	96	LYS
3	C	33	GLY

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
1	A	253/265 (96%)	250 (99%)	3 (1%)	78 90
2	B	205/205 (100%)	204 (100%)	1 (0%)	92 96
3	C	213/219 (97%)	211 (99%)	2 (1%)	84 93
4	D	52/58 (90%)	52 (100%)	0	100 100
5	F	223/338 (66%)	186 (83%)	37 (17%)	3 19
All	All	946/1085 (87%)	903 (96%)	43 (4%)	38 69

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	79	GLN
5	F	114	LEU
5	F	227	MET
5	F	82	ILE
5	F	85	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	79	GLN
5	F	239	ASN
5	F	85	ASN
3	C	163	HIS
5	F	222	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

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
6	DAO	A	1289	-	10,13,13	0.32	0	10,13,13	0.89	0

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
6	DAO	A	1289	-	-	0/9/11/11	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1289	DAO	2	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.