wwPDB EM Map/Model Validation Report (i)

Aug 23, 2016 – 03:08 PM EDT

PDB ID	:	5A8F
EMDB ID:	:	EMD-3097
Title	:	Structure and genome release mechanism of human cardiovirus Saffold virus-3
Authors	:	Mullapudi, E.; Novacek, J.; Palkova, L.; Kulich, P.; Lindberg, M.; vanKuppeveld, F.J.M.; Plevka, P.
Deposited on	:	2015-07-15
Resolution	:	10.60 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

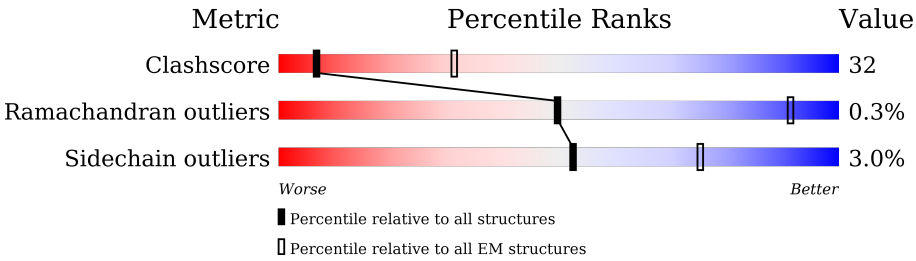
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 10.60 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	219	67% 32% •
2	B	189	74% 24% •
3	C	258	69% 28% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5243 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 HUMAN SAFFOLD VIRUS-3 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	219	1749	1124	289	329	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	PHE	VAL	CONFLICT	UNP C0MHL9

- Molecule 2 is a protein called GENOME POLYPHUMAN SAFFOLD VIRUS-3 VP3 PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	189	1471	952	236	275	8	0	0

- Molecule 3 is a protein called HUMAN SAFFOLD VIRUS-3 VP2.

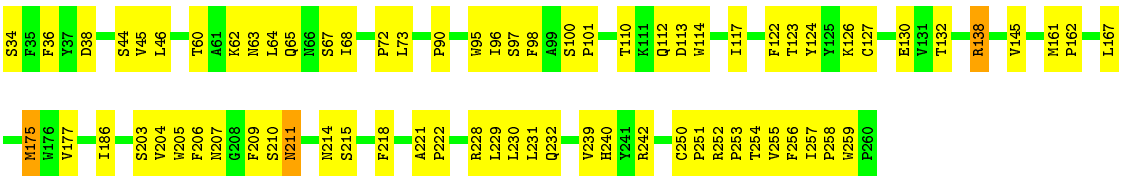
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	258	2023	1274	364	378	7	0	0

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.

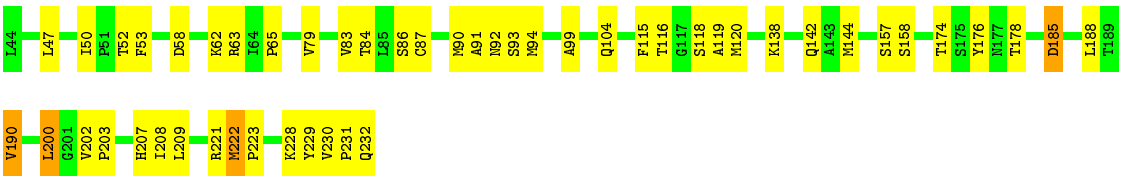
- Molecule 1: HUMAN SAFFOLD VIRUS-3 VP1

Chain A:



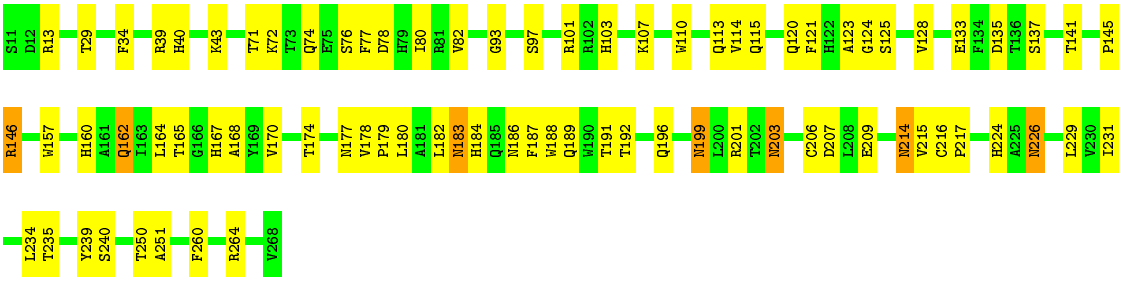
- Molecule 2: GENOME POLYPHUMAN SAFFOLD VIRUS-3 VP3 PROTEIN

Chain B:



- Molecule 3: HUMAN SAFFOLD VIRUS-3 VP2

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	2330	Depositor
Maximum defocus (nm)	3950	Depositor
Magnification	55000	Depositor
Image detector	FEI EAGLE (4K X 4K)	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	0.32	0/1805	0.62	0/2468
2	B	0.34	0/1514	0.63	0/2075
3	C	0.31	0/2078	0.63	0/2843
All	All	0.32	0/5397	0.62	0/7386

There are no bond length outliers.

There are no bond angle outliers.

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	1749	0	1699	160	0
2	B	1471	0	1455	173	0
3	C	2023	0	1959	195	0
All	All	5243	0	5113	326	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 32.

The worst 5 of 326 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:120:MET:HG3	3:C:121:PHE:CZ	1.30	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:HA	2:B:229:TYR:CE1	1.37	1.54
1:A:257:ILE:HG13	2:B:229:TYR:CD2	1.41	1.52
1:A:258:PRO:HD2	2:B:229:TYR:CD1	1.50	1.45
1:A:257:ILE:HG13	2:B:229:TYR:CE2	1.41	1.44

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	217/219 (99%)	204 (94%)	12 (6%)	1 (0%)	34 77
2	B	187/189 (99%)	180 (96%)	6 (3%)	1 (0%)	34 77
3	C	256/258 (99%)	243 (95%)	13 (5%)	0	100 100
All	All	660/666 (99%)	627 (95%)	31 (5%)	2 (0%)	50 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	CYS
2	B	222	MET

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	205/205 (100%)	202 (98%)	3 (2%)	72	88
2	B	167/167 (100%)	160 (96%)	7 (4%)	36	70
3	C	222/222 (100%)	214 (96%)	8 (4%)	42	74
All	All	594/594 (100%)	576 (97%)	18 (3%)	52	77

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	190	VAL
2	B	200	LEU
3	C	199	ASN
2	B	178	THR
2	B	185	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	74	GLN
3	C	160	HIS
3	C	226	ASN
3	C	86	HIS
3	C	113	GLN

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.