



wwPDB EM Map/Model Validation Report ⓘ

Oct 13, 2016 – 11:26 AM EDT

PDB ID : 5K0U
EMDB ID: : EMD-8189
Title : CryoEM structure of the full virion of a human rhinovirus C
Authors : Liu, Y.; Hill, M.G.; Klose, T.; Chen, Z.; Watters, K.E.; Jiang, W.; Palmenberg, A.C.; Rossmann, M.G.
Deposited on : 2016-05-17
Resolution : 2.79 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

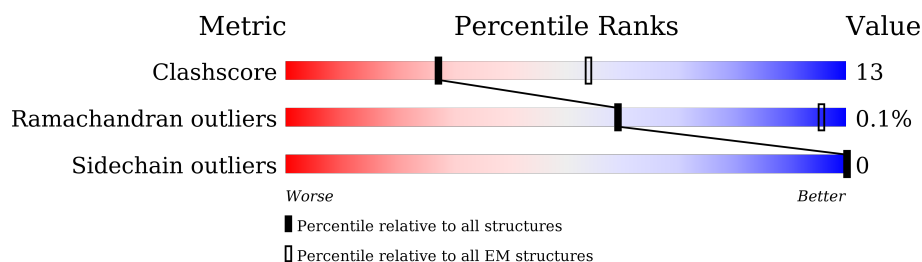
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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	279	
2	B	235	
3	C	265	
4	D	66	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6281 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	263	Total	C	N	O	S	0	0
			2115	1352	361	394	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	LYS	THR	engineered mutation	UNP E5D8F2

- Molecule 2 is a protein called Capsid protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	235	Total	C	N	O	S	0	0
			1816	1163	300	336	17		

- Molecule 3 is a protein called Capsid protein VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	255	Total	C	N	O	S	0	0
			1978	1249	345	375	9		

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	39	Total	C	N	O	0	0
			312	198	51	63		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		AltConf
5	A	24	Total	O	0
			24	24	
5	B	16	Total	O	0
			16	16	

Continued on next page...

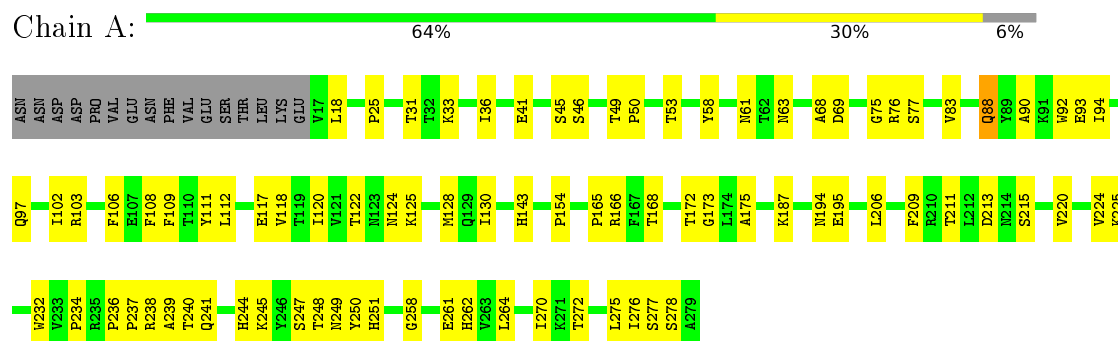
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
5	C	18	Total 18	O 18	0
5	D	2	Total 2	O 2	0

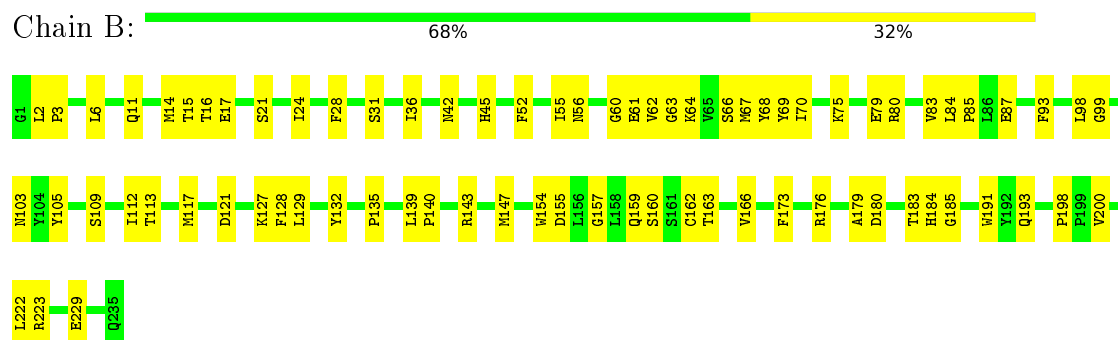
3 Residue-property plots

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.

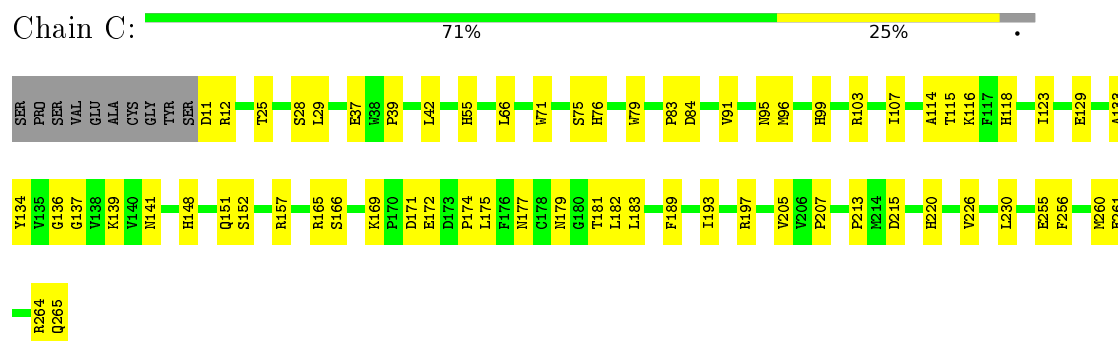
• Molecule 1: Capsid protein VP1



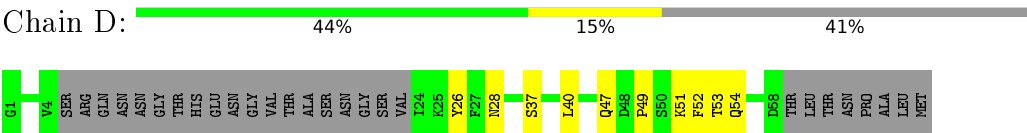
• Molecule 2: Capsid protein VP3



• Molecule 3: Capsid protein VP2



• Molecule 4: Capsid protein VP4



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8973	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	14000	Depositor
Image detector	Not provided	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	0.49	0/2181	0.58	0/2966
2	B	0.48	0/1862	0.59	0/2532
3	C	0.49	0/2032	0.60	0/2774
4	D	0.41	0/318	0.54	0/427
All	All	0.48	0/6393	0.59	0/8699

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	2115	0	2043	78	0
2	B	1816	0	1821	65	0
3	C	1978	0	1920	52	0
4	D	312	0	296	9	0
5	A	24	0	0	0	0
5	B	16	0	0	0	0
5	C	18	0	0	1	0
5	D	2	0	0	1	0
All	All	6281	0	6080	159	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 13.

The worst 5 of 159 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:A:122:THR:HG22	1:A:124:ASN:H	1.40	0.86
2:B:157:GLY:HA2	3:C:197:ARG:HH11	1.40	0.83
1:A:97:GLN:HB3	1:A:245:LYS:HB2	1.61	0.81
2:B:121:ASP:O	3:C:197:ARG:NH2	2.14	0.80
2:B:87:GLU:HG2	2:B:179:ALA:HB2	1.63	0.80

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	261/279 (94%)	241 (92%)	19 (7%)	1 (0%)	39	74
2	B	233/235 (99%)	227 (97%)	6 (3%)	0	100	100
3	C	253/265 (96%)	235 (93%)	18 (7%)	0	100	100
4	D	35/66 (53%)	27 (77%)	8 (23%)	0	100	100
All	All	782/845 (92%)	730 (93%)	51 (6%)	1 (0%)	59	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	GLN

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	232/248 (94%)	232 (100%)	0	100	100
2	B	206/206 (100%)	206 (100%)	0	100	100
3	C	222/230 (96%)	222 (100%)	0	100	100
4	D	35/57 (61%)	35 (100%)	0	100	100
All	All	695/741 (94%)	695 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
2	B	45	HIS
4	D	47	GLN
3	C	141	ASN
1	A	244	HIS
3	C	163	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.