



wwPDB EM Model Validation Summary Report ⓘ

Mar 2, 2020 – 03:51 PM EST

PDB ID : 6PSF
EMDB ID : EMD-20458
Title : Rhinovirus C15 complexed with domains I and II of receptor CDHR3
Authors : Sun, Y.; Watters, K.; Klose, T.; Palmenberg, A.C.
Deposited on : 2019-07-12
Resolution : 3.50 Å (reported)
Based on initial model : 5K0U

This is a wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

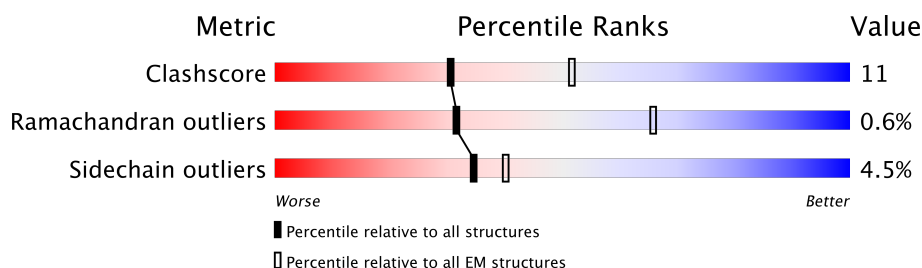
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. 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 respectively. 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	73% 20% 6%
2	B	235	73% 26% .
3	C	265	70% 23% . 5%
4	D	66	23% 14% . 62%
5	U	239	26% 17% . . 55%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6899 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	261	Total	C	N	O	S	0	0
			2100	1341	359	392	8		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	LYS	THR	variant	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	253	Total	C	N	O	S	0	0
			1959	1239	340	371	9		

- Molecule 4 is a protein called Capsid protein VP4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	25	Total	C	N	O	0	0
			196	123	33	40		

- Molecule 5 is a protein called Cadherin-related family member 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	U	108	Total	C	N	O	S	0	0
			828	534	131	162	1		

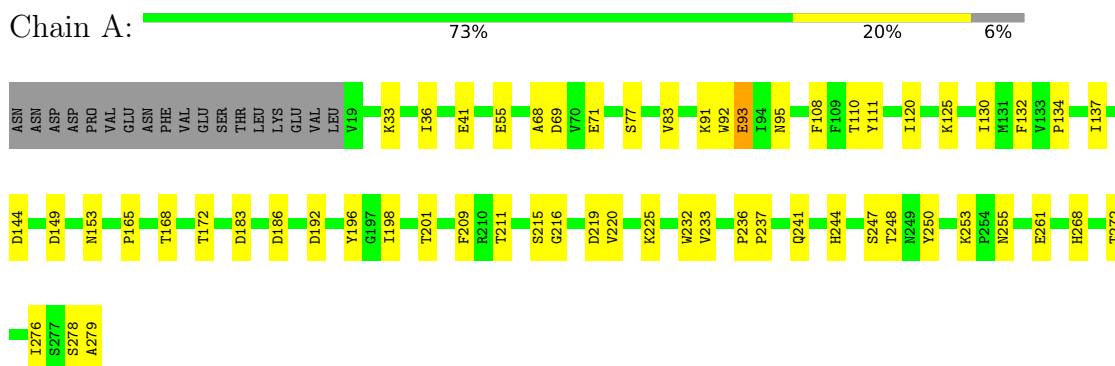
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	9	MET	-	expression tag	UNP Q6ZTQ4
U	10	ALA	-	expression tag	UNP Q6ZTQ4
U	11	SER	-	expression tag	UNP Q6ZTQ4
U	12	ASP	-	expression tag	UNP Q6ZTQ4
U	13	TYR	-	expression tag	UNP Q6ZTQ4
U	14	LYS	-	expression tag	UNP Q6ZTQ4
U	15	ASP	-	expression tag	UNP Q6ZTQ4
U	16	ASP	-	expression tag	UNP Q6ZTQ4
U	17	ASP	-	expression tag	UNP Q6ZTQ4
U	18	ASP	-	expression tag	UNP Q6ZTQ4
U	19	LYS	-	expression tag	UNP Q6ZTQ4
U	238	GLY	-	expression tag	UNP Q6ZTQ4
U	239	GLY	-	expression tag	UNP Q6ZTQ4
U	240	THR	-	expression tag	UNP Q6ZTQ4
U	241	LYS	-	expression tag	UNP Q6ZTQ4
U	242	HIS	-	expression tag	UNP Q6ZTQ4
U	243	HIS	-	expression tag	UNP Q6ZTQ4
U	244	HIS	-	expression tag	UNP Q6ZTQ4
U	245	HIS	-	expression tag	UNP Q6ZTQ4
U	246	HIS	-	expression tag	UNP Q6ZTQ4
U	247	HIS	-	expression tag	UNP Q6ZTQ4

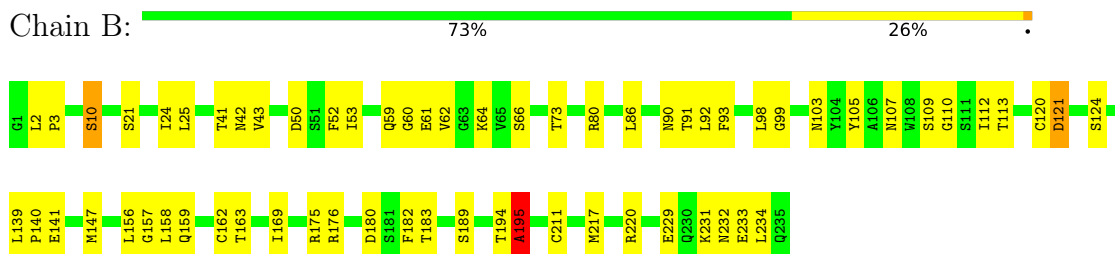
3 Residue-property plots [i](#)

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

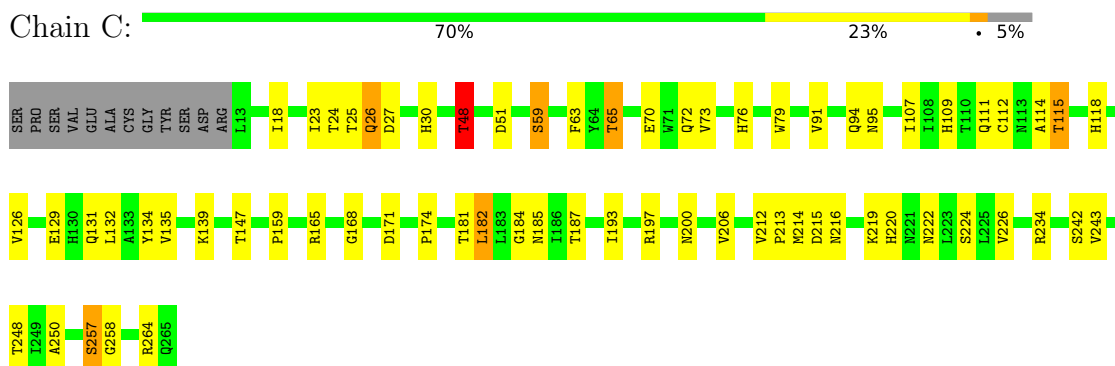
- Molecule 1: Capsid protein VP1



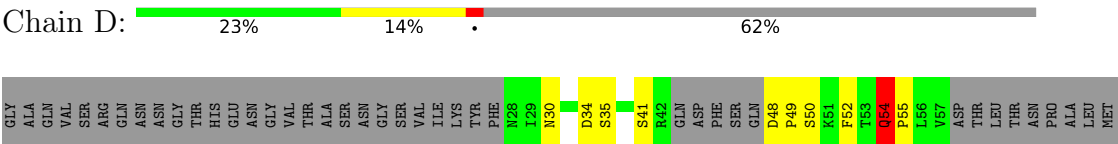
- Molecule 2: Capsid protein VP3



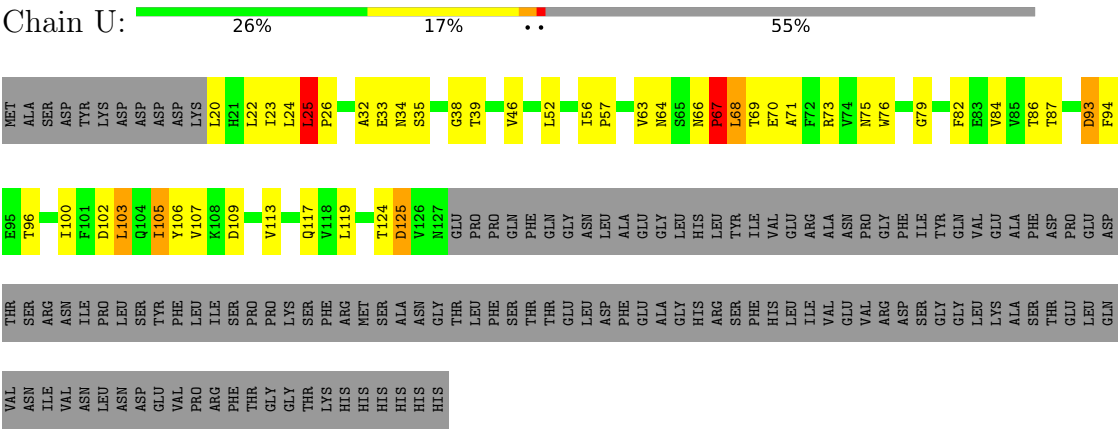
- Molecule 3: Capsid protein VP2



- Molecule 4: Capsid protein VP4



● Molecule 5: Cadherin-related family member 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	9607	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/2166	0.54	1/2945 (0.0%)
2	B	0.56	1/1862 (0.1%)	0.63	4/2532 (0.2%)
3	C	0.52	0/2013	0.59	3/2749 (0.1%)
4	D	0.50	0/199	0.57	1/267 (0.4%)
5	U	0.58	1/847 (0.1%)	0.94	8/1163 (0.7%)
All	All	0.54	2/7087 (0.0%)	0.64	17/9656 (0.2%)

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
2	B	0	1
5	U	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	U	67	PRO	C-N	-13.66	1.02	1.34
2	B	10	SER	C-N	7.06	1.50	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	67	PRO	O-C-N	-14.13	100.10	122.70
5	U	93	ASP	N-CA-C	-9.95	84.14	111.00
5	U	67	PRO	CA-C-N	9.41	137.89	117.20
5	U	106	TYR	N-CA-C	-9.04	86.59	111.00
2	B	195	ALA	CB-CA-C	8.47	122.81	110.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	10	SER	Mainchain
5	U	25	LEU	Peptide
5	U	67	PRO	Peptide

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	2100	0	2023	48	0
2	B	1816	0	1821	41	0
3	C	1959	0	1903	42	0
4	D	196	0	188	6	0
5	U	828	0	822	33	0
All	All	6899	0	6757	146	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 11.

The worst 5 of 146 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)
5:U:71:ALA:HA	5:U:87:THR:HG22	1.54	0.89
5:U:66:ASN:HB3	5:U:67:PRO:HD3	1.62	0.82
2:B:176:ARG:NH2	2:B:180:ASP:OD2	2.19	0.74
3:C:216:ASN:HD22	3:C:219:LYS:HD3	1.52	0.74
3:C:91:VAL:O	3:C:95:ASN:ND2	2.25	0.70

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	259/279 (93%)	233 (90%)	26 (10%)	0	100	100
2	B	233/235 (99%)	218 (94%)	14 (6%)	1 (0%)	36	75
3	C	251/265 (95%)	229 (91%)	22 (9%)	0	100	100
4	D	21/66 (32%)	18 (86%)	2 (10%)	1 (5%)	2	22
5	U	106/239 (44%)	97 (92%)	6 (6%)	3 (3%)	5	35
All	All	870/1084 (80%)	795 (91%)	70 (8%)	5 (1%)	31	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	55	PRO
5	U	26	PRO
5	U	68	LEU
2	B	195	ALA
5	U	67	PRO

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	230/248 (93%)	226 (98%)	4 (2%)	63	84
2	B	206/206 (100%)	196 (95%)	10 (5%)	27	62
3	C	220/230 (96%)	207 (94%)	13 (6%)	21	57
4	D	23/57 (40%)	21 (91%)	2 (9%)	11	41
5	U	97/212 (46%)	91 (94%)	6 (6%)	20	55
All	All	776/953 (81%)	741 (96%)	35 (4%)	34	65

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	25	THR
3	C	48	THR
5	U	105	ILE
3	C	26	GLN
3	C	27	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	107	ASN
2	B	151	HIS
3	C	163	ASN
2	B	90	ASN
3	C	216	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	U	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	67:PRO	C	68:LEU	N	1.02