



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jul 26, 2019 – 09:07 AM EDT

PDB ID : 6CVB
EMDB ID: : EMD-7638
Title : CryoEM structure of human enterovirus D68 in complex with 6'-sialyl-N-acetyl
lactosamine
Authors : Liu, Y.; Rossmann, M.G.
Deposited on : 2018-03-27
Resolution : 2.43 Å(reported)

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

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
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) : 2.4

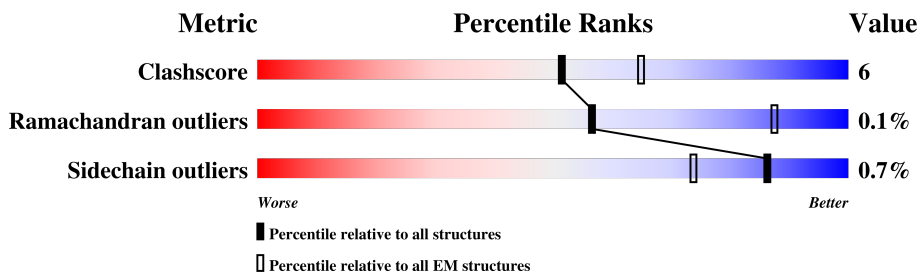
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.43 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. 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	297	87% 11% .
2	B	247	84% 15% .
3	C	248	75% 20% .
4	D	68	40% . 56%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6660 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 viral protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	290	Total	C	N	O	S	0	0
			2273	1448	392	424	9		

- Molecule 2 is a protein called viral protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	247	Total	C	N	O	S	0	0
			1900	1201	313	368	18		

- Molecule 3 is a protein called viral protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	237	Total	C	N	O	S	0	0
			1864	1188	326	337	13		

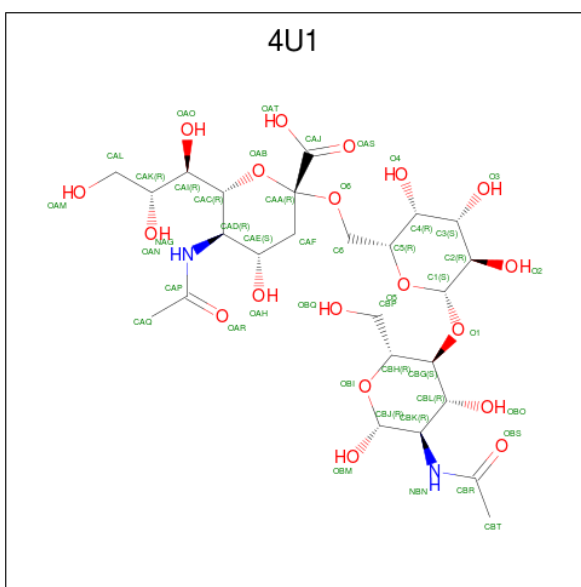
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	116	ARG	LYS	conflict	UNP A0A097ZN88

- Molecule 4 is a protein called viral protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	30	Total	C	N	O	0	0
			240	153	36	51		

- Molecule 5 is (6R)-5-(acetylamino)-3,5-dideoxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]-beta-L-threo-hex-2-ulopyranonosyl-(2->6)-beta-D-galactopyranosyl-(1->4)-2-(acetylamino)-2-deoxy-beta-D-glucopyranose (three-letter code: 4U1) (formula: C₂₅H₄₂N₂O₁₉).



Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			46	25	2	19	

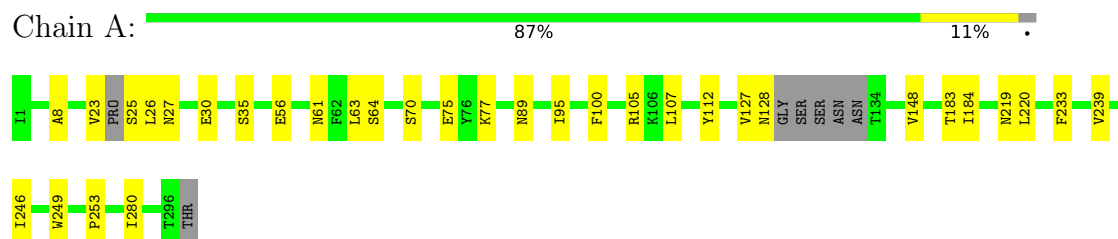
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	128	Total O 128 128	0
6	B	92	Total O 92 92	0
6	C	101	Total O 101 101	0
6	D	16	Total O 16 16	0

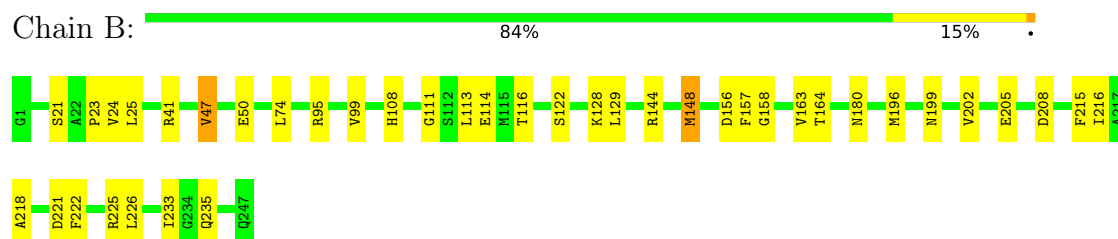
3 Residue-property plots [i](#)

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

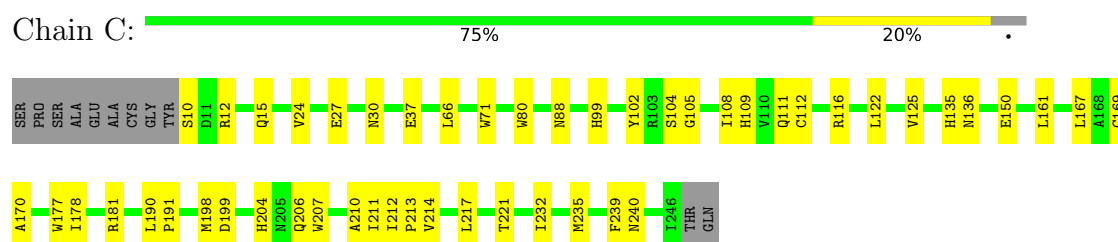
- Molecule 1: viral protein 1



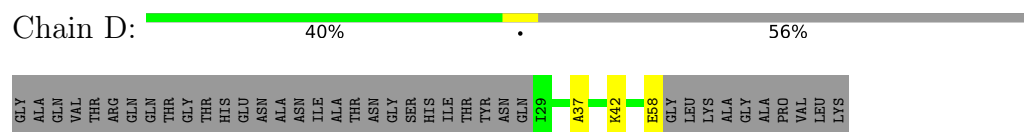
- Molecule 2: viral protein 3



- Molecule 3: viral protein 2



- Molecule 4: viral protein 4



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	5938	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; On-the-fly CTF correction during 2D alignment and 3D reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4U1

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	0/2323	0.60	0/3155
2	B	0.52	0/1945	0.67	0/2649
3	C	0.53	0/1922	0.63	0/2630
4	D	0.47	0/246	0.55	0/332
All	All	0.51	0/6436	0.63	0/8766

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	2273	0	2279	32	0
2	B	1900	0	1850	29	0
3	C	1864	0	1793	32	0
4	D	240	0	219	3	0
5	B	46	0	41	2	0
6	A	128	0	0	0	0
6	B	92	0	0	1	0
6	C	101	0	0	1	0
6	D	16	0	0	0	0
All	All	6660	0	6182	79	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 6.

The worst 5 of 79 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:23:VAL:HG11	1:A:26:LEU:HG	1.21	1.11
1:A:27:ASN:HD22	1:A:35:SER:HA	1.26	1.01
1:A:23:VAL:HG21	1:A:26:LEU:HD11	1.40	1.00
1:A:23:VAL:CG1	1:A:26:LEU:HG	2.06	0.82
1:A:26:LEU:O	1:A:26:LEU:HD12	1.85	0.76

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	284/297 (96%)	272 (96%)	12 (4%)	0	100	100
2	B	245/247 (99%)	236 (96%)	9 (4%)	0	100	100
3	C	235/248 (95%)	223 (95%)	11 (5%)	1 (0%)	36	45
4	D	28/68 (41%)	25 (89%)	3 (11%)	0	100	100
All	All	792/860 (92%)	756 (96%)	35 (4%)	1 (0%)	56	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	30	ASN

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	251/257 (98%)	251 (100%)	0	100	100
2	B	216/216 (100%)	212 (98%)	4 (2%)	60	72
3	C	200/208 (96%)	199 (100%)	1 (0%)	90	94
4	D	27/55 (49%)	27 (100%)	0	100	100
All	All	694/736 (94%)	689 (99%)	5 (1%)	86	91

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	41	ARG
2	B	47	VAL
2	B	148	MET
2	B	226	LEU
3	C	88	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	96	ASN
2	B	180	ASN
3	C	15	GLN
2	B	79	GLN
2	B	240	HIS

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
5	4U1	B	301	-	44,48,48	0.57	0	63,71,71	1.03	4 (6%)

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
5	4U1	B	301	-	-	6/30/94/94	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	4U1	C1-O1-CBG	-3.64	108.89	117.97
5	B	301	4U1	CAF-CAA-CAJ	-2.38	110.41	113.58
5	B	301	4U1	CAK-CAI-CAC	-2.27	108.68	113.03
5	B	301	4U1	CBJ-CBK-NBN	-2.02	108.39	110.73

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	4U1	C5-C6-O6-CAA
5	B	301	4U1	OBI-CBH-CBP-OBQ

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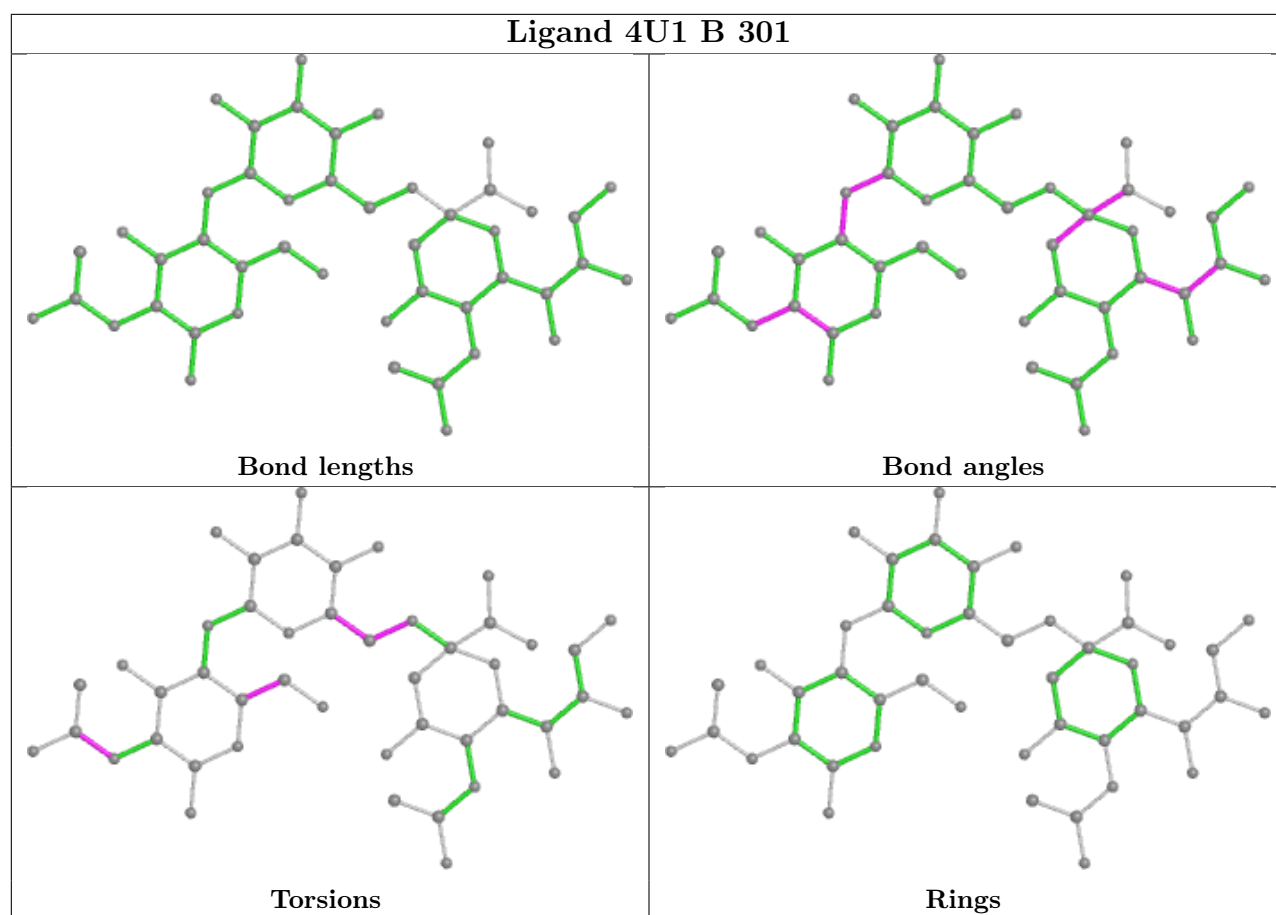
Mol	Chain	Res	Type	Atoms
5	B	301	4U1	CBT-CBR-NBN-CBK
5	B	301	4U1	OBS-CBR-NBN-CBK
5	B	301	4U1	CBG-CBH-CBP-OBQ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	4U1	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.