



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 2, 2016 – 01:32 PM EDT

PDB ID : 5KC2  
EMDB ID: : EMD-8235  
Title : Negative stain structure of Vps15/Vps34 complex  
Authors : Kirsten, M.L.; Zhang, L.; Ohashi, Y.; Perisic, O.; Williams, R.L.; Sachse, C.  
Deposited on : 2016-06-04  
Resolution : 28.00 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Mogul : unknown  
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

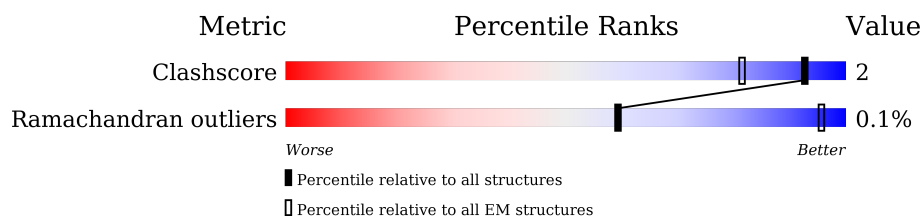
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 28.00 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

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  $\geq 3$ , 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	C	875	
2	B	1454	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9967 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 Phosphatidylinositol 3-kinase VPS34.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	783	Total	C	N	O	0	0
			3888	2322	783	783		

- Molecule 2 is a protein called Serine/threonine-protein kinase VPS15.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	1224	Total	C	N	O	0	0
			6079	3631	1224	1224		



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	14172	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	120	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	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  >2	RMSZ	# Z  >2
1	C	0.20	0/3885	0.47	0/5418
2	B	0.19	0/6069	0.41	0/8456
All	All	0.19	0/9954	0.43	0/13874

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

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	C	3888	0	1633	14	0
2	B	6079	0	2576	13	0
All	All	9967	0	4209	26	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 2.

All (26) 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:C:6:ILE:HA	1:C:212:GLU:HA	1.68	0.75
1:C:130:PHE:HA	1:C:136:THR:HA	1.68	0.74

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:LYS:H	1:C:105:SER:HA	1.60	0.67
1:C:23:LYS:HA	1:C:89:ASP:H	1.61	0.64
1:C:140:GLY:HA2	1:C:209:PRO:HA	1.83	0.61
1:C:115:ASN:H	1:C:120:ILE:HA	1.67	0.58
1:C:592:VAL:HA	1:C:611:PHE:HA	1.87	0.55
1:C:54:SER:HA	1:C:115:ASN:HA	1.86	0.55
2:B:1277:ILE:HA	2:B:1295:GLY:HA3	1.89	0.55
2:B:1071:LEU:HA	2:B:1453:PHE:HA	1.89	0.55
1:C:25:LEU:HA	1:C:204:LEU:HA	1.88	0.55
2:B:1258:TRP:HA	2:B:1266:ILE:H	1.72	0.54
2:B:1132:THR:H	2:B:1147:SER:HA	1.73	0.54
2:B:1290:SER:HA	2:B:1306:ASN:HA	1.88	0.54
2:B:1305:TRP:HA	2:B:1312:CYS:HA	1.90	0.52
2:B:1155:LEU:HA	2:B:1173:CYS:HA	1.94	0.49
1:C:45:LEU:O	1:C:49:ASN:N	2.33	0.48
2:B:1395:PRO:HA	2:B:1405:LEU:HA	1.96	0.46
1:C:219:GLU:H	2:B:439:THR:CB	2.30	0.45
1:C:17:PRO:HA	1:C:97:ARG:HA	1.98	0.45
1:C:141:PHE:HA	1:C:207:GLU:HA	2.00	0.44
1:C:11:SER:CB	1:C:217:PHE:H	2.30	0.43
2:B:1201:LEU:HA	2:B:1216:ILE:H	1.84	0.43
2:B:1273:ASP:H	2:B:1297:SER:HA	1.86	0.41
2:B:1154:VAL:O	2:B:1174:ILE:N	2.50	0.40
2:B:1427:ILE:HA	2:B:1445:ASP:HA	2.04	0.40

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	C	777/875 (89%)	721 (93%)	54 (7%)	2 (0%)	46 83

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1204/1454 (83%)	1109 (92%)	95 (8%)	0	100	100
All	All	1981/2329 (85%)	1830 (92%)	149 (8%)	2 (0%)	59	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	29	LYS
1	C	753	ILE

### 5.3.2 Protein sidechains [i](#)

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

### 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.