



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Jan 18, 2017 – 04:27 PM EST

PDB ID : 5LK8
EMDB ID: : EMD-4064
Title : single particle reconstruction of slow bee paralysis virus empty particle
Authors : Kalynych, S.; Fuzik, T.; Plevka, P.
Deposited on : 2016-07-21
Resolution : 3.42 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
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)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

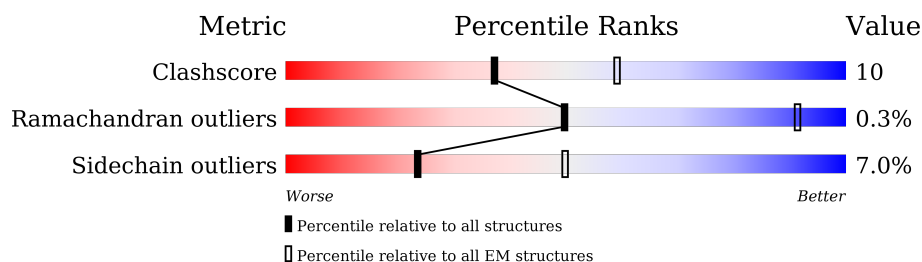
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.42 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	266	
2	B	261	
3	C	430	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5461 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 VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	223	Total	C	N	O	S	0	0
			1781	1149	312	313	7		

- Molecule 2 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	215	Total	C	N	O	S	0	0
			1725	1128	285	299	13		

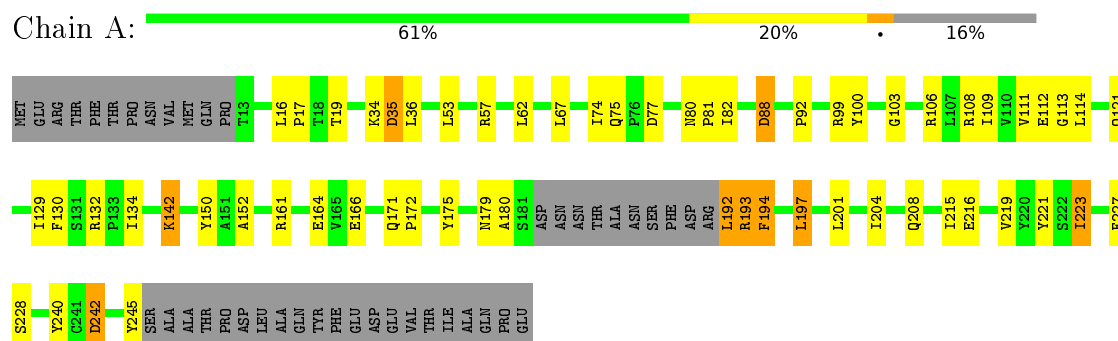
- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	255	Total	C	N	O	S	0	0
			1955	1265	329	354	7		

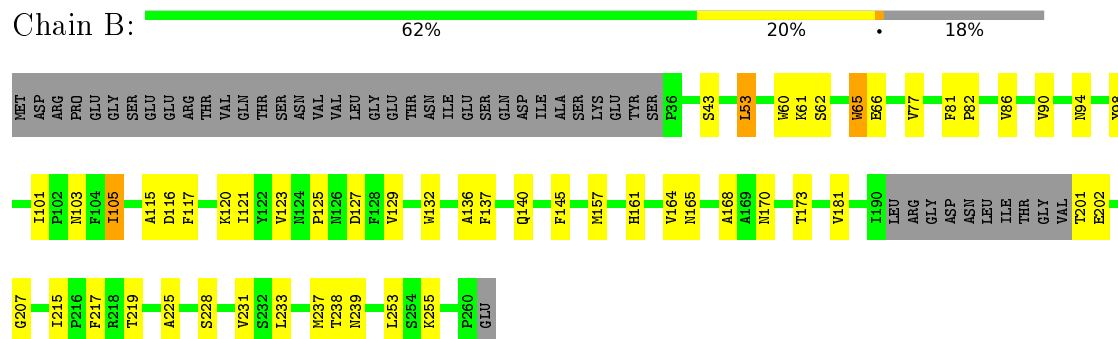
3 Residue-property plots [i](#)

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.

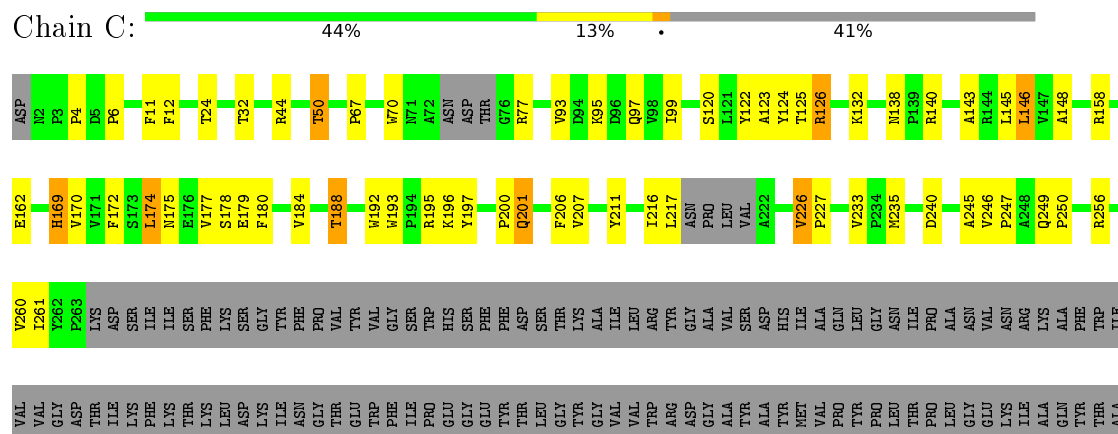
• Molecule 1: VP1



• Molecule 2: VP2



• Molecule 3: VP3



SER	LEU	LEU	ALA	SER	ASN	THR	ALA	ILE	SER	GLN	ILE	ARG	PRO	TYR	ILE	PRO	ASP	TYR	ILE	VAL	ASP	SER	ALA	ALA	SER	LYS	ASP	ASN	ILE	LEU	TRP	SER	PRO	ILE	GLU	ASP	ARG	LEU	ARG	ALA	GLN	THR	GLU	TRP	VAL	MET	ALA	GLU	PRO	GLU
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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	10350	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)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	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	0.32	0/1831	0.61	1/2494 (0.0%)
2	B	0.31	0/1775	0.56	0/2414
3	C	0.32	0/2013	0.60	0/2756
All	All	0.32	0/5619	0.59	1/7664 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	LEU	CA-CB-CG	6.70	130.70	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	201	GLN	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	1781	0	1736	43	0
2	B	1725	0	1715	35	0
3	C	1955	0	1918	45	0
All	All	5461	0	5369	107	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 10.

All (107) 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:192:LEU:HD12	1:A:194:PHE:HB2	1.56	0.86
3:C:143:ALA:HB3	3:C:174:LEU:HD13	1.65	0.78
3:C:124:TYR:HB3	3:C:192:TRP:HB3	1.70	0.72
2:B:123:VAL:HG23	2:B:231:VAL:HG22	1.72	0.71
2:B:101:ILE:HG22	2:B:103:ASN:H	1.59	0.68
1:A:62:LEU:HD21	1:A:215:ILE:HD11	1.74	0.66
2:B:125:PRO:HB3	2:B:170:ASN:HD21	1.60	0.66
3:C:11:PHE:O	3:C:12:PHE:HD1	1.79	0.65
3:C:67:PRO:HD3	3:C:99:ILE:HD11	1.81	0.63
1:A:223:ILE:HG13	1:A:227:PHE:CD1	2.35	0.62
3:C:177:VAL:HG12	3:C:179:GLU:H	1.64	0.62
1:A:240:TYR:CD2	3:C:95:LYS:HE2	2.36	0.61
2:B:165:ASN:HB2	2:B:168:ALA:O	2.00	0.61
1:A:121:GLN:HG2	1:A:152:ALA:HB2	1.83	0.60
1:A:103:GLY:HA3	1:A:227:PHE:HA	1.83	0.59
2:B:60:TRP:CD1	2:B:61:LYS:HG3	2.37	0.59
1:A:88:ASP:N	1:A:88:ASP:OD1	2.35	0.59
1:A:166:GLU:HB3	3:C:32:THR:HG22	1.85	0.57
3:C:67:PRO:HB3	3:C:233:VAL:HG22	1.87	0.56
2:B:116:ASP:HB2	2:B:238:THR:HB	1.87	0.56
1:A:114:LEU:HD21	1:A:204:ILE:HG22	1.88	0.56
1:A:17:PRO:O	3:C:126:ARG:NH2	2.39	0.56
1:A:223:ILE:HG23	1:A:227:PHE:HB3	1.87	0.56
1:A:242:ASP:N	1:A:242:ASP:OD1	2.39	0.55
2:B:145:PHE:CE1	3:C:256:ARG:HG3	2.42	0.55
1:A:34:LYS:NZ	3:C:50:THR:HG21	2.20	0.55
1:A:100:TYR:HB3	1:A:175:TYR:HB3	1.89	0.54
3:C:138:ASN:O	3:C:140:ARG:N	2.42	0.53
1:A:36:LEU:HD13	3:C:247:PRO:HB3	1.90	0.52
2:B:127:ASP:HB3	3:C:140:ARG:HH22	1.75	0.52
3:C:188:THR:HG21	3:C:193:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:TYR:CZ	2:B:253:LEU:HD21	2.46	0.51
1:A:228:SER:HB2	3:C:50:THR:HG23	1.92	0.51
2:B:157:MET:O	2:B:157:MET:HG3	2.11	0.51
2:B:53:LEU:O	2:B:103:ASN:HA	2.10	0.51
3:C:132:LYS:HB3	3:C:235:MET:HB2	1.93	0.51
3:C:226:VAL:HG12	3:C:227:PRO:HD2	1.93	0.51
3:C:196:LYS:HG3	3:C:206:PHE:CG	2.47	0.50
3:C:216:ILE:O	3:C:217:LEU:HB2	2.11	0.50
1:A:109:ILE:HG13	1:A:219:VAL:HG13	1.94	0.50
3:C:177:VAL:HG12	3:C:178:SER:N	2.27	0.49
2:B:120:LYS:HB2	2:B:173:THR:HG22	1.95	0.49
1:A:62:LEU:HD21	1:A:215:ILE:CD1	2.43	0.49
2:B:77:VAL:HG21	2:B:233:LEU:HD11	1.95	0.49
2:B:137:PHE:CZ	2:B:207:GLY:HA3	2.47	0.49
3:C:95:LYS:HE3	3:C:197:TYR:CE1	2.47	0.49
2:B:82:PRO:HG3	2:B:117:PHE:CZ	2.47	0.48
2:B:140:GLN:OE1	2:B:181:VAL:HG13	2.13	0.48
1:A:180:ALA:O	2:B:145:PHE:HD2	1.97	0.48
3:C:170:VAL:HG11	3:C:180:PHE:HZ	1.79	0.48
2:B:66:GLU:OE1	2:B:228:SER:HB3	2.14	0.48
3:C:148:ALA:HB2	3:C:169:HIS:HB3	1.96	0.48
2:B:81:PHE:CD1	2:B:82:PRO:HA	2.48	0.47
3:C:177:VAL:HG12	3:C:179:GLU:N	2.29	0.47
2:B:121:ILE:HG23	2:B:164:VAL:HG21	1.97	0.47
1:A:35:ASP:OD2	3:C:24:THR:HB	2.15	0.47
3:C:93:VAL:HG12	3:C:97:GLN:HB2	1.96	0.47
2:B:86:VAL:HG12	2:B:98:TYR:CE1	2.51	0.46
3:C:120:SER:O	3:C:250:PRO:HA	2.15	0.46
1:A:130:PHE:CD2	1:A:134:ILE:HD11	2.51	0.46
3:C:260:VAL:O	3:C:261:ILE:HD13	2.16	0.45
2:B:115:ALA:HA	2:B:239:ASN:O	2.15	0.45
1:A:179:ASN:HA	2:B:145:PHE:CE2	2.51	0.45
2:B:132:TRP:CD1	2:B:215:ILE:HD12	2.52	0.45
1:A:75:GLN:HE21	1:A:77:ASP:HB3	1.81	0.45
2:B:125:PRO:CB	2:B:170:ASN:HD21	2.27	0.45
1:A:112:GLU:HG3	1:A:113:GLY:N	2.32	0.44
1:A:121:GLN:NE2	1:A:150:TYR:HB2	2.32	0.44
1:A:142:LYS:CE	1:A:142:LYS:HA	2.47	0.44
1:A:132:ARG:HA	1:A:132:ARG:HD2	1.66	0.44
1:A:99:ARG:HA	1:A:99:ARG:HD2	1.73	0.44
2:B:65:TRP:CZ3	2:B:217:PHE:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:TYR:HB2	3:C:245:ALA:HB3	1.98	0.44
3:C:70:TRP:HZ3	3:C:174:LEU:HD11	1.82	0.44
2:B:136:ALA:HB2	2:B:161:HIS:HB3	1.98	0.44
2:B:105:ILE:HA	2:B:105:ILE:HD12	1.86	0.44
1:A:106:ARG:O	1:A:221:TYR:HA	2.17	0.44
1:A:130:PHE:CE2	1:A:134:ILE:HD11	2.52	0.43
3:C:70:TRP:CZ3	3:C:174:LEU:HD11	2.54	0.43
1:A:74:ILE:HG13	1:A:74:ILE:O	2.18	0.43
1:A:19:THR:HG23	3:C:126:ARG:NH2	2.34	0.43
1:A:16:LEU:HD12	1:A:17:PRO:HD2	2.00	0.43
3:C:70:TRP:CZ3	3:C:145:LEU:HD21	2.54	0.43
2:B:219:THR:OG1	2:B:225:ALA:HB1	2.18	0.43
2:B:127:ASP:C	3:C:140:ARG:HH12	2.21	0.42
1:A:108:ARG:HE	1:A:164:GLU:HG2	1.83	0.42
3:C:193:TRP:HZ2	3:C:207:VAL:O	2.03	0.42
3:C:123:ALA:N	3:C:246:VAL:O	2.52	0.42
1:A:62:LEU:HD13	1:A:204:ILE:HG23	2.01	0.42
1:A:88:ASP:HB2	1:A:92:PRO:HG2	2.02	0.42
1:A:228:SER:HB3	3:C:44:ARG:NH2	2.34	0.42
2:B:94:ASN:HB3	2:B:255:LYS:HG3	2.02	0.42
1:A:80:ASN:HA	1:A:81:PRO:HD3	1.83	0.42
3:C:122:TYR:O	3:C:195:ARG:HD3	2.20	0.42
3:C:123:ALA:HB3	3:C:246:VAL:HB	2.02	0.41
2:B:86:VAL:HG12	2:B:98:TYR:HE1	1.85	0.41
1:A:179:ASN:HA	2:B:145:PHE:HE2	1.84	0.41
2:B:129:VAL:HG12	2:B:219:THR:HA	2.03	0.41
3:C:146:LEU:HD11	3:C:169:HIS:ND1	2.35	0.41
1:A:67:LEU:HB2	1:A:197:LEU:O	2.21	0.41
2:B:117:PHE:CE1	2:B:237:MET:HG2	2.56	0.41
1:A:34:LYS:HZ1	3:C:50:THR:HG21	1.84	0.40
3:C:172:PHE:CE2	3:C:174:LEU:HA	2.56	0.40
3:C:249:GLN:NE2	3:C:250:PRO:O	2.51	0.40
1:A:171:GLN:HA	1:A:172:PRO:HD3	1.93	0.40
1:A:192:LEU:HG	1:A:193:ARG:H	1.85	0.40
3:C:4:PRO:O	3:C:6:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	219/266 (82%)	200 (91%)	19 (9%)	0	100	100
2	B	211/261 (81%)	202 (96%)	8 (4%)	1 (0%)	34	75
3	C	249/430 (58%)	229 (92%)	19 (8%)	1 (0%)	39	79
All	All	679/957 (71%)	631 (93%)	46 (7%)	2 (0%)	50	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	202	GLU
3	C	200	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	187/230 (81%)	169 (90%)	18 (10%)	10	42
2	B	188/234 (80%)	181 (96%)	7 (4%)	41	77
3	C	211/366 (58%)	195 (92%)	16 (8%)	16	55
All	All	586/830 (71%)	545 (93%)	41 (7%)	23	59

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	82	ILE
1	A	88	ASP
1	A	111	VAL
1	A	129	ILE
1	A	142	LYS
1	A	161	ARG
1	A	192	LEU
1	A	193	ARG
1	A	194	PHE
1	A	197	LEU
1	A	201	LEU
1	A	208	GLN
1	A	216	GLU
1	A	223	ILE
1	A	242	ASP
1	A	245	TYR
2	B	43	SER
2	B	53	LEU
2	B	62	SER
2	B	65	TRP
2	B	90	VAL
2	B	105	ILE
2	B	201	THR
3	C	50	THR
3	C	77	ARG
3	C	125	THR
3	C	126	ARG
3	C	146	LEU
3	C	158	ARG
3	C	162	GLU
3	C	169	HIS
3	C	174	LEU
3	C	175	ASN
3	C	184	VAL
3	C	188	THR
3	C	201	GLN
3	C	211	TYR
3	C	226	VAL
3	C	240	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	170	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](#)

There are no chain breaks in this entry.