



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jan 3, 2017 – 02:16 PM EST

PDB ID : 5KP9
EMDB ID: : EMD-8278
Title : Structure of Nanoparticle Released from Enveloped Protein Nanoparticle
Authors : Votteler, J.; Ogohara, C.; Yi, S.; Hsia, Y.; Natterman, U.; Belnap, D.M.; King, N.P.; Sundquist, W.I.
Deposited on : 2016-07-02
Resolution : 5.70 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

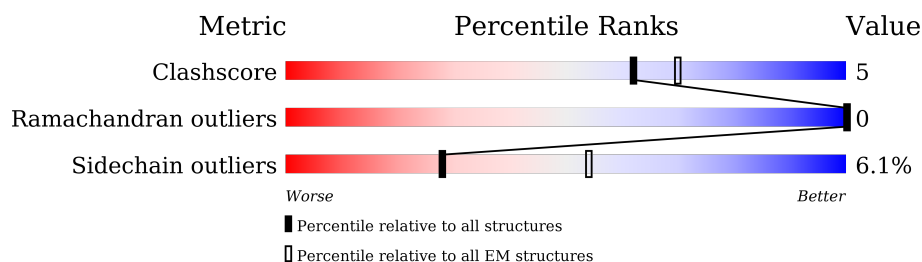
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 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	B	282	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1518 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 EPN-01*.

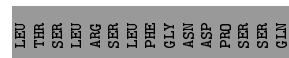
Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	202	Total	C	N	O	S	0	0
			1518	987	249	273	9		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	LYS	GLU	conflict	UNP Q9WXS1
B	31	LEU	GLU	conflict	UNP Q9WXS1
B	59	MET	LYS	conflict	UNP Q9WXS1
B	185	VAL	ASP	conflict	UNP Q9WXS1
B	188	ALA	ARG	conflict	UNP Q9WXS1
B	204	GLN	-	linker	UNP Q9WXS1
B	205	LYS	-	linker	UNP Q9WXS1
B	206	LEU	-	linker	UNP Q9WXS1
B	207	ILE	-	linker	UNP Q9WXS1
B	208	SER	-	linker	UNP Q9WXS1
B	209	GLU	-	linker	UNP Q9WXS1
B	210	GLU	-	linker	UNP Q9WXS1
B	211	ASP	-	linker	UNP Q9WXS1

- Molecule 1: EPN-01*

28%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	8573	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	41911	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	B	0.74	0/1547	0.75	2/2086 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	VAL	CG1-CB-CG2	8.22	124.05	110.90
1	B	134	VAL	CG1-CB-CG2	5.41	119.55	110.90

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	B	1518	0	1583	17	0
All	All	1518	0	1583	17	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 5.

All (17) 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:B:115:LEU:HD13	1:B:142:MET:CE	1.80	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD13	1:B:142:MET:HE3	1.21	1.09
1:B:115:LEU:CD1	1:B:142:MET:HE3	1.86	1.03
1:B:29:VAL:HG13	1:B:34:VAL:HB	1.62	0.80
1:B:0:LYS:N	1:B:3:GLU:OE1	2.15	0.79
1:B:115:LEU:CD1	1:B:142:MET:CE	2.54	0.76
1:B:5:PHE:HE2	1:B:11:VAL:HG21	1.50	0.76
1:B:0:LYS:CA	1:B:3:GLU:OE1	2.37	0.73
1:B:47:ASP:OD1	1:B:76:LYS:HB3	1.97	0.63
1:B:5:PHE:HE2	1:B:11:VAL:CG2	2.12	0.62
1:B:126:LEU:HD23	1:B:149:VAL:HG13	1.84	0.59
1:B:88:PRO:HA	1:B:127:LYS:HE2	1.95	0.49
1:B:17:ASN:N	1:B:21:GLU:OE2	2.38	0.44
1:B:130:PRO:HG2	1:B:133:VAL:CG2	2.49	0.43
1:B:67:THR:HA	1:B:88:PRO:HD3	2.01	0.42
1:B:134:VAL:HG13	1:B:138:PHE:CB	2.50	0.42
1:B:25:LYS:HD3	1:B:180:VAL:HG13	2.01	0.41

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	B	200/282 (71%)	195 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	163/235 (69%)	153 (94%)	10 (6%)	23	60

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	GLU
1	B	6	LYS
1	B	14	LEU
1	B	29	VAL
1	B	47	ASP
1	B	109	VAL
1	B	134	VAL
1	B	150	LYS
1	B	171	LEU
1	B	179	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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.