



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:10 PM BST

PDB ID : 5A22
EMDB ID: : EMD-6337
Title : Structure of the L protein of vesicular stomatitis virus from electron cryomicroscopy
Authors : Liang, B.; Li, Z.; Jenni, S.; Rameh, A.A.; Morin, B.M.; Grant, T.; Grigorieff, N.; Harrison, S.C.; Whelan, S.P.J.
Deposited on : 2015-05-06
Resolution : 3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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) : trunk27241

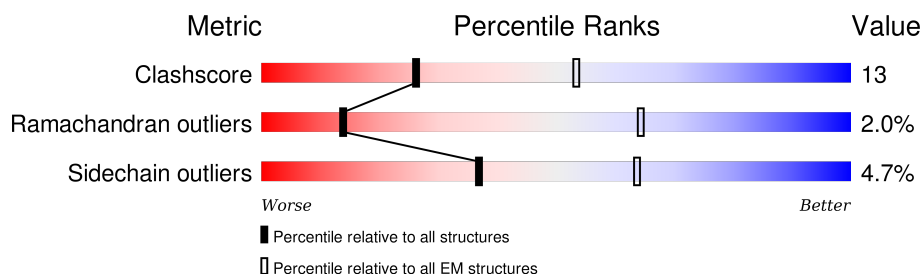
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	2109	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32187 atoms, of which 16110 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 VESICULAR STOMATITIS VIRUS L POLYMERASE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	2002	32185	10249	16110	2803	2934	89	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ARG	PRO	CONFLICT	UNP P03523
A	467	ASP	HIS	CONFLICT	UNP P03523
A	548	LEU	PHE	CONFLICT	UNP P03523
A	549	ARG	PRO	CONFLICT	UNP P03523
A	670	ARG	PRO	CONFLICT	UNP P03523
A	910	PHE	SER	CONFLICT	UNP P03523
A	1026	ALA	PRO	CONFLICT	UNP P03523
A	1348	GLY	ALA	CONFLICT	UNP P03523
A	1589	ALA	PRO	CONFLICT	UNP P03523

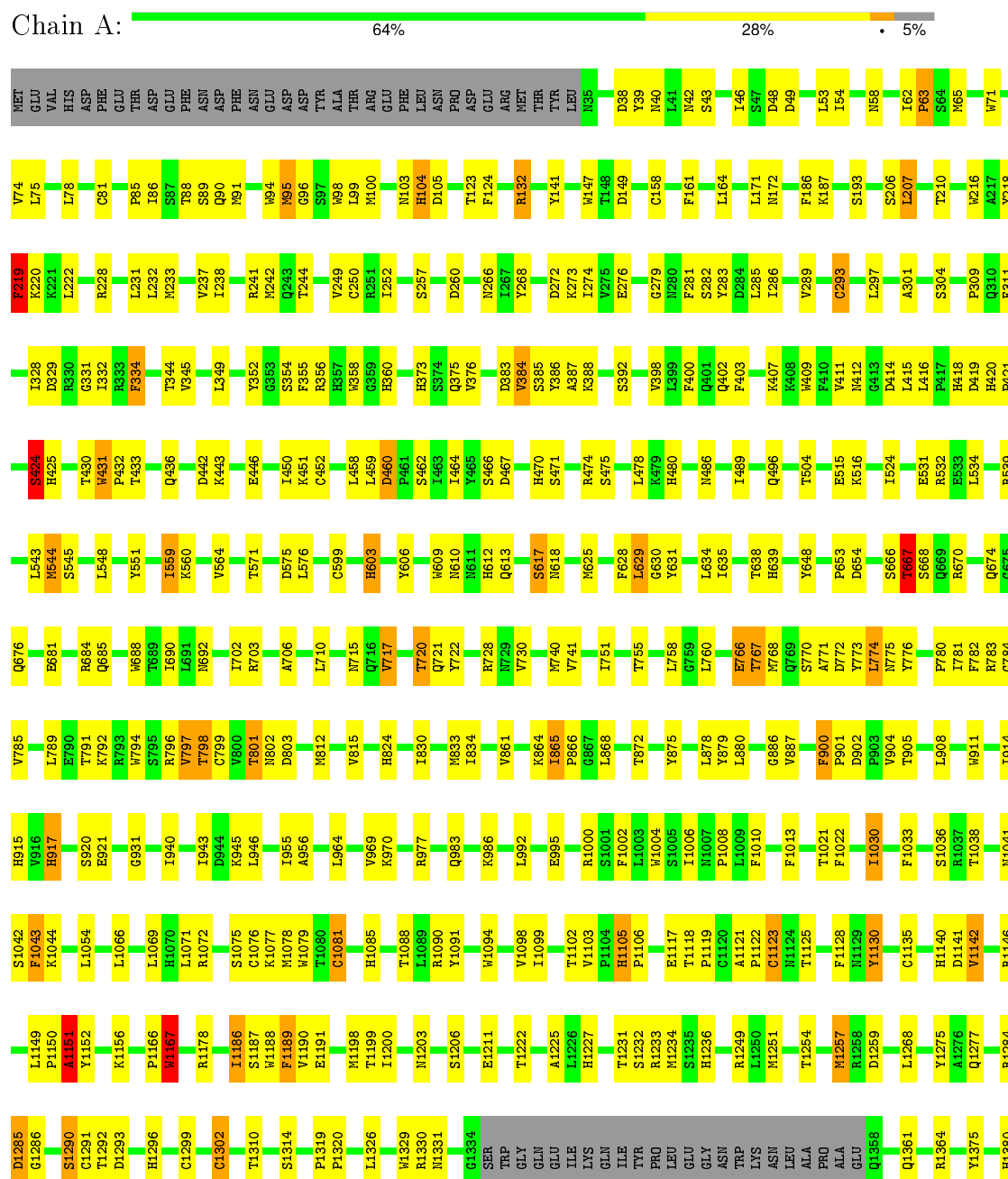
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	2	Total	Zn	0
			2	2	

3 Residue-property plots

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: VESICULAR STOMATITIS VIRUS L POLYMERASE



R0086	K2010	D1922	C1838	Y1732	ASP		A1381
I2087	Q2011	R1923	K1839	P1733	MET	S1502	H503
M2096	K2012	P1924	GLY	D1734	SER	Y1504	S1384
L2097	W2013	A1925	LEU	D1735	Y1598		F1387
		D1926	LYS	L1736	P1599	I1519	P1388
	R2016	I1930	LYS		P1600	F1522	L1389
	G2017		LEU	P1739	W1601	L1529	S1390
	D2018	Y1934	ILE	R1740	Y1615		I1391
		Y1937	ASP	T1741		Y1533	R1396
	K2022	I1937	GLU	W1742	Y1621		G1397
	D2023		PRO				
	T2024	I1943	ASN	L1754	M1627	L1537	L1401
	R2025	H1944	D1850	Q1755	P1628	S1538	
	I2026	H1945	W1852	I1756			L1408
	S2027	H1946					M1409
	D2028	I1946	W1859	I1759	L1635		
	S2029	G1949	K1860	V1760	L1636	A1549	
	L2030	P1950	M1761	M1761	S1637	N1550	
	A2031	I1951	M1861	D1762	G1638	L1551	C1413
	P2032	P1952	L1862		I1639		C1414
		P1953	Y1863	V1765	R1640	L1555	Q1415
	W2036	P1954	A1864		L1641	R1556	V1416
	I2037	N1954	F1865	S1771	G1642	S1557	I1417
	R2038	P1955			Q1643	GLY	H1418
	S2039	P1956	F1872	V1778	L1644	GLU	R1419
	L2040	S1957	A1873	R1779	P1645	GLY	
	E2041	D1958	R1874	M1780	T1646	TRP	L1425
	L2042	G1959	A1875	Y1781	G1647	GLU	
	V2043	I1960	K1876	V1782	ASP	ASP	L1436
		A1961	K1877	H1783	Y1650	ILE	I1437
	V2047	Q1962	V1878	R1784	K1651	HIS	
	R2048	N1963		I1785	I1652	VAL	I1440
	L2049	V1964	Y1881			LYS	
	F2052	I1966	F1882	Q1789	L1656	PHE	L1443
		A1967	T1883			THR	
			L1884	G1798	Y1663	LYS	P1447
			T1885		R1664	ASP	P1448
			G1886	C1802	D1665	ASP	F1449
			I1887	E1803	F1666	ILE	L1450
			P1888	S1804	L1667	LEU	
				E1805	S1668	LEU	T1453
					G1669	CYS	R1454
			F1891	T1810	G1670	PRO	
			I1892	I1811	D1671	GLU	D1460
			P1893	L1812		GLU	E1461
			D1894	G1813		ILE	L1462
			P1895		G1674	ARG	E1463
			F1896			HIS	H1467
			V1897	D1820		ALA	K1468
			M1898	L1821		CYS	
			I1899	V1822		PHE	Y1473
			E1900	Q1823		GLY	
			T1901	T1824		ILE	S1476
			I1905	F1825		ALA	
			F1906	S1827		LYS	M1480
						ASP	
			V1912	V1834		ASN	Y1487
			A1916	Y1835		LYS	
				M1836		ASP	
				V1837		ASN	Y1495
						LYS	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	29000	Depositor
Image detector	K2 DIRECT DETECTION CAMERA	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.46	0/16456	0.67	0/22270

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
1	A	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1071	LEU	Peptide
1	A	1125	THR	Peptide
1	A	431	TRP	Peptide
1	A	63	PRO	Peptide
1	A	766	GLU	Peptide

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	A	16075	16110	16109	427	0
2	A	2	0	0	0	0
All	All	16077	16110	16109	427	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 13.

The worst 5 of 427 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:100:MET:SD	1:A:241:ARG:NH1	2.51	0.84
1:A:88:THR:O	1:A:91:MET:N	2.21	0.73
1:A:767:THR:OG1	1:A:768:MET:N	2.22	0.72
1:A:977:ARG:O	1:A:986:LYS:NZ	2.22	0.72
1:A:419:ASP:HB2	1:A:421:PRO:HD2	1.71	0.71

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	1994/2109 (94%)	1678 (84%)	277 (14%)	39 (2%)	9 54

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	355	PHE
1	A	730	VAL
1	A	1381	ALA
1	A	2066	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	1794/1890 (95%)	1709 (95%)	85 (5%)	32 72

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	801	THR
1	A	1088	THR
1	A	1973	PHE
1	A	865	ILE
1	A	1000	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	HIS
1	A	496	GLN
1	A	1277	GLN

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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.