



wwPDB EM Map/Model Validation Report ⓘ

Jun 23, 2016 – 07:37 PM EDT

PDB ID : 5FZ2
EMDB ID: : EMD-3362
Title : Natively membrane-anchored full-length Herpes simplex virus 1 glycoprotein B
Authors : Zeev-Ben-Mordehai, T.; Vasishtan, D.; Duran, A.H.; Vollmer, B.; White, P.; Pandurangan, A.P.; Siebert, C.A.; Topf, M.; Grunewald, K.
Deposited on : 2016-03-10
Resolution : 23.00 Å(reported)
Based on PDB ID : 2GUM

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) : rb-20027790

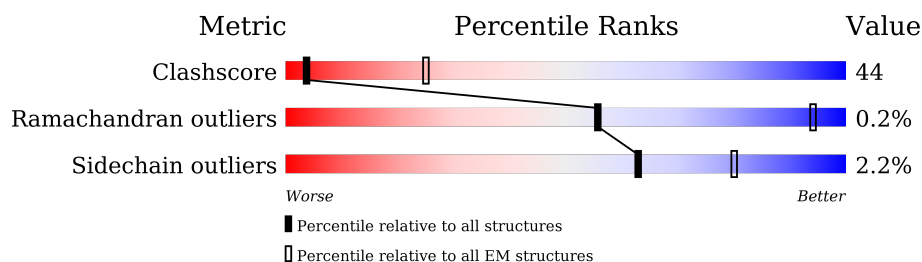
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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
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	1-A	904	18% 18% . 63%
1	1-B	904	18% 18% . 63%
1	1-C	904	18% 18% . 63%
1	2-A	904	18% 18% . 63%
1	2-B	904	18% 18% . 63%
1	2-C	904	18% 18% . 63%
1	3-A	904	18% 19% . 63%
1	3-B	904	18% 19% . 63%
1	3-C	904	18% 19% . 63%

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Mol	Chain	Length	Quality of chain
1	4-A	904	<div><div></div><div></div><div></div><div></div></div>
1	4-B	904	<div><div></div><div></div><div></div><div></div></div>
1	4-C	904	<div><div></div><div></div><div></div><div></div></div>

2 Entry composition

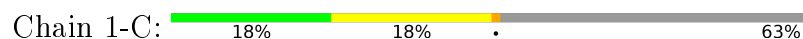
There is only 1 type of molecule in this entry. The entry contains 32768 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ENVELOPE GLYCOPROTEIN B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	2-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	3-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	4-A	336	Total	C	N	O	S	0	1
			2728	1729	475	513	11		
1	1-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	2-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	3-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	4-B	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	1-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	2-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	3-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		
1	4-C	336	Total	C	N	O	S	0	1
			2732	1733	475	513	11		

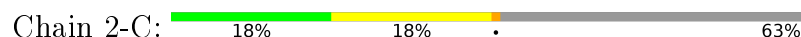
Chain 1-B: 18% 18% . 63%

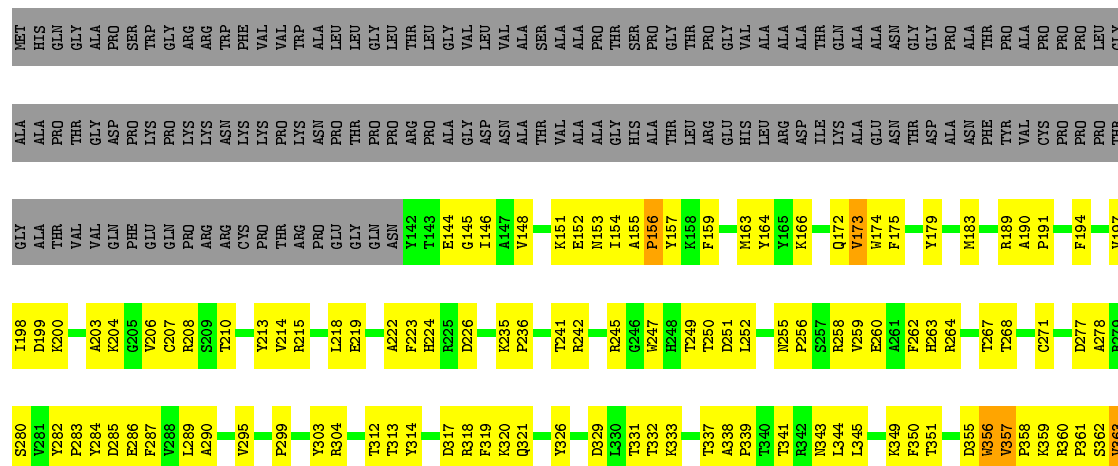


- Molecule 1: ENVELOPE GLYCOPROTEIN B

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM







SER	THR	THR	VAL	GLU	CYS
ALA	THR	THR	MET	ILE	VAL
LYS	THR	LYS	GLY	LYS	THR
VAL	GLU	GLU	ILE	ASP	VAL
THR	LEU	LEU	VAL	SER	ALA
ASP	LYS	LYS	GLY	GLY	ALA
MET	ASN	ASN	GLY	LEU	ASP
VAL	PRO	PRO	VAL	LEU	ASN
MET	THR	THR	VAL	ASP	VAL
MET	ASN	ASN	SER	THR	ILE
ARG	PRO	PRO	ALA	THR	VAL
LYS	PRO	PRO	ALA	THR	VAL
ARG	ASP	ASP	VAL	GLU	GLN
ARG	ALA	ALA	SER	VAL	ASN
ASN	SER	SER	GLY	GLN	SER
THR	GLY	GLY	VAL	ARG	MET
ASN	GLU	GLU	SER	ARG	THR
THR	GLY	GLY	SER	ASN	ILE
THR	GLU	GLU	PHE	ASN	VAL
GLN	GLU	GLU	MET	LEU	GLN
VAL	GLY	GLY	SER	HIS	SER
PRO	GLY	GLY	ASN	ASP	ARG
ASN	ASN	ASN	PRO	LEU	PRO
LYS	PHE	PHE	PHE	ARG	ALA
ASP	ASP	ASP	GLY	PHE	CYS
GLY	GLU	GLU	ALA	ALA	TYR
ASP	ALA	ALA	LEU	ASP	SER
ALA	LYS	LYS	ALA	ILE	ARG
ASP	LEU	LEU	VAL	ASP	PRO
GLU	ALA	ALA	GLY	THR	LEU
ASP	GLU	GLU	LEU	VAL	VAL
ASP	ALA	ALA	LEU	ILE	SER
LEU	ARG	ARG	VAL	HIS	PHE
	GLU	GLU	LEU	ALA	ARG
	MET	MET	ALA	ASP	TYR
	ILE	ILE	ALA	VAL	GLU
	ARG	ARG	GLY	ASN	ASP
	TYR	TYR	LEU	THR	GLN
	MET	MET	PHE	PHE	GLY
	ALA	ALA	ALA	ILE	PRO
	LEU	LEU	PHE	ASP	LEU
	VAL	VAL	ALA	LEU	VAL
	SER	SER	ALA	GLY	GLY
	ALA	ALA	PHE	LEU	GLN
	GLU	GLU	ARG	GLY	LEU
	ARG	ARG	TYR	ALA	GLY
	THR	THR	VAL	PHE	GLU
	GLU	GLU	VAL	THR	THR
	LYS	LYS	ASN	LEU	ARG
	LYS	LYS	PRO	GLY	LEU
	LYS	LYS	MET	GLY	THR
	GLY	GLY	LYS	ARG	ASP
	THR	THR	ALA	VAL	ALA
	SER	SER	LEU	VAL	ILE
	ALA	ALA	TYR	GLY	GLU
	LEU	LEU	PRO	LYS	ARG
			LEU	VAL	PRO

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of tilted images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE-FLIPPED TILT SERIES PRIOR TO TOMOGRAPHIC RECONSTRUCTION	Depositor
Microscope	OTHER	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	3000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	95000	Depositor
Image detector	GATAN K2 SUMMIT	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	1-A	0.97	0/2800	1.07	1/3800 (0.0%)
1	1-B	0.97	0/2806	1.07	1/3810 (0.0%)
1	1-C	0.97	0/2806	1.07	1/3810 (0.0%)
1	2-A	0.98	0/2800	1.07	1/3800 (0.0%)
1	2-B	0.98	0/2806	1.07	1/3810 (0.0%)
1	2-C	0.98	0/2806	1.07	1/3810 (0.0%)
1	3-A	0.98	0/2800	1.07	1/3800 (0.0%)
1	3-B	0.98	0/2806	1.07	1/3810 (0.0%)
1	3-C	0.98	0/2806	1.07	1/3810 (0.0%)
1	4-A	0.98	0/2800	1.08	1/3800 (0.0%)
1	4-B	0.98	0/2806	1.07	1/3810 (0.0%)
1	4-C	0.98	0/2806	1.07	1/3810 (0.0%)
All	All	0.98	0/33648	1.07	12/45680 (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
1	1-A	0	4
1	1-B	0	4
1	1-C	0	4
1	2-A	0	3
1	2-B	0	3
1	2-C	0	3
1	3-A	0	2
1	3-B	0	2
1	3-C	0	2
1	4-A	0	2
1	4-B	0	2
1	4-C	0	2
All	All	0	33

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	4-B	409	LEU	C-N-CA	5.22	133.26	122.30
1	4-A	409	LEU	C-N-CA	5.21	133.25	122.30
1	2-A	409	LEU	C-N-CA	5.20	133.23	122.30
1	2-B	409	LEU	C-N-CA	5.20	133.23	122.30
1	2-C	409	LEU	C-N-CA	5.20	133.23	122.30

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-A	154	ILE	Peptide
1	1-A	156	PRO	Peptide
1	1-A	355	ASP	Peptide
1	1-A	363	VAL	Peptide
1	1-B	154	ILE	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	1-A	2728	0	2613	239	0
1	1-B	2732	0	2618	236	0
1	1-C	2732	0	2618	233	0
1	2-A	2728	0	2613	240	0
1	2-B	2732	0	2618	241	0
1	2-C	2732	0	2618	234	0
1	3-A	2728	0	2613	237	0
1	3-B	2732	0	2618	238	0
1	3-C	2732	0	2618	237	0
1	4-A	2728	0	2613	240	0
1	4-B	2732	0	2618	233	0
1	4-C	2732	0	2618	236	0
All	All	32768	0	31396	2844	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 44.

The worst 5 of 2844 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:304:ARG:HB2	1:B:356:TRP:HZ3	1.12	1.13
1:C:304:ARG:HB2	1:C:356:TRP:HZ3	1.12	1.11
1:B:363:VAL:HB	1:B:364:CYS:HA	1.35	1.07
1:A:304:ARG:HB2	1:A:356:TRP:HZ3	1.12	1.06
1:A:363:VAL:HB	1:A:364:CYS:HA	1.38	1.06

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	1-A	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	46	83
1	1-B	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	46	83
1	1-C	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	46	83
1	2-A	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	46	83
1	2-B	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	46	83
1	2-C	334/904 (37%)	327 (98%)	6 (2%)	1 (0%)	46	83
1	3-A	334/904 (37%)	327 (98%)	7 (2%)	0	100	100
1	3-B	334/904 (37%)	327 (98%)	7 (2%)	0	100	100
1	3-C	334/904 (37%)	327 (98%)	7 (2%)	0	100	100
1	4-A	334/904 (37%)	326 (98%)	7 (2%)	1 (0%)	46	83
1	4-B	334/904 (37%)	326 (98%)	7 (2%)	1 (0%)	46	83
1	4-C	334/904 (37%)	326 (98%)	7 (2%)	1 (0%)	46	83
All	All	4008/10848 (37%)	3921 (98%)	78 (2%)	9 (0%)	56	86

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	357	VAL
1	2-B	357	VAL
1	2-C	357	VAL
1	4-A	363	VAL
1	4-B	363	VAL

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	1-A	289/747 (39%)	282 (98%)	7 (2%)	57	82
1	1-B	290/747 (39%)	283 (98%)	7 (2%)	57	82
1	1-C	290/747 (39%)	283 (98%)	7 (2%)	57	82
1	2-A	289/747 (39%)	282 (98%)	7 (2%)	57	82
1	2-B	290/747 (39%)	283 (98%)	7 (2%)	57	82
1	2-C	290/747 (39%)	283 (98%)	7 (2%)	57	82
1	3-A	289/747 (39%)	283 (98%)	6 (2%)	61	84
1	3-B	290/747 (39%)	284 (98%)	6 (2%)	61	84
1	3-C	290/747 (39%)	284 (98%)	6 (2%)	61	84
1	4-A	289/747 (39%)	284 (98%)	5 (2%)	68	87
1	4-B	290/747 (39%)	285 (98%)	5 (2%)	68	87
1	4-C	290/747 (39%)	285 (98%)	5 (2%)	68	87
All	All	3476/8964 (39%)	3401 (98%)	75 (2%)	63	83

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2-B	364	CYS
1	2-C	430	ASN
1	4-B	430	ASN
1	2-B	430	ASN

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Mol	Chain	Res	Type
1	2-C	356	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	2-C	443	GLN
1	3-A	443	GLN
1	4-C	430	ASN
1	3-A	153	ASN
1	3-A	430	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.