



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 07:59 PM BST

PDB ID : 6ESC
Title : Crystal structure of Pseudorabies virus glycoprotein B
Authors : Backovic, M.; Vaney, M.C.; Rey, F.A.; Haouz, A.
Deposited on : 2017-10-20
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

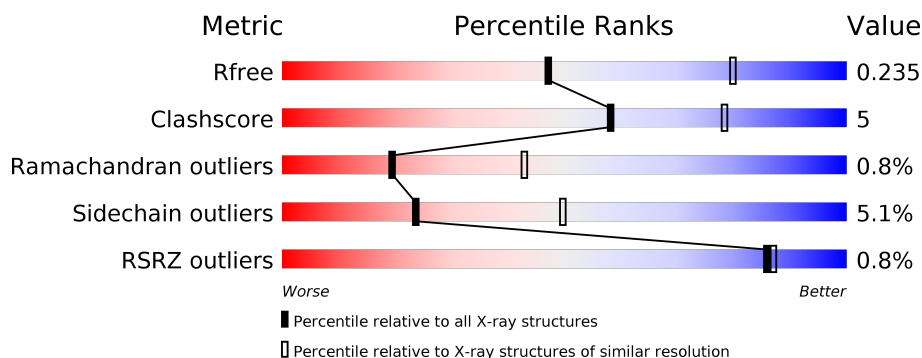
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	739	<div> <div></div> <div>68%</div> <div>11%</div> <div>20%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4875 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	594	4763	2987	865	893	18	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

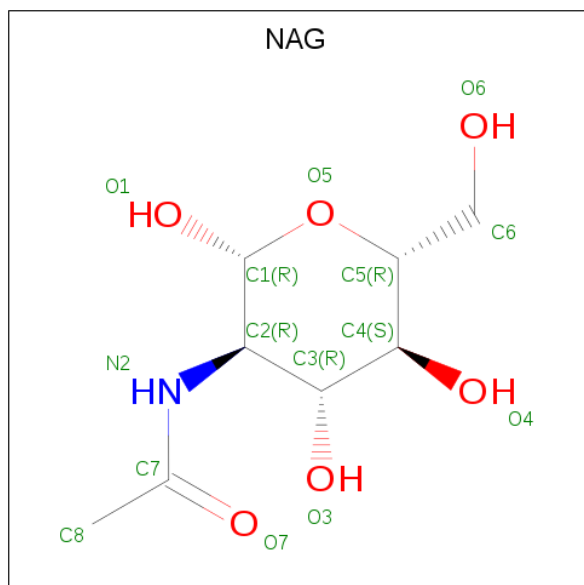
Chain	Residue	Modelled	Actual	Comment	Reference
A	757	SER	-	expression tag	UNP G3G8X1
A	758	ARG	-	expression tag	UNP G3G8X1
A	759	PHE	-	expression tag	UNP G3G8X1
A	760	GLU	-	expression tag	UNP G3G8X1
A	761	SER	-	expression tag	UNP G3G8X1
A	762	ASP	-	expression tag	UNP G3G8X1
A	763	ASP	-	expression tag	UNP G3G8X1
A	764	ASP	-	expression tag	UNP G3G8X1
A	765	ASP	-	expression tag	UNP G3G8X1
A	766	LYS	-	expression tag	UNP G3G8X1
A	767	ALA	-	expression tag	UNP G3G8X1
A	768	GLY	-	expression tag	UNP G3G8X1
A	769	TRP	-	expression tag	UNP G3G8X1
A	770	SER	-	expression tag	UNP G3G8X1
A	771	HIS	-	expression tag	UNP G3G8X1
A	772	PRO	-	expression tag	UNP G3G8X1
A	773	GLN	-	expression tag	UNP G3G8X1
A	774	PHE	-	expression tag	UNP G3G8X1
A	775	GLU	-	expression tag	UNP G3G8X1
A	776	LYS	-	expression tag	UNP G3G8X1
A	777	GLY	-	expression tag	UNP G3G8X1
A	778	GLY	-	expression tag	UNP G3G8X1
A	779	GLY	-	expression tag	UNP G3G8X1
A	780	SER	-	expression tag	UNP G3G8X1
A	781	GLY	-	expression tag	UNP G3G8X1
A	782	GLY	-	expression tag	UNP G3G8X1
A	783	GLY	-	expression tag	UNP G3G8X1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	784	SER	-	expression tag	UNP G3G8X1
A	785	GLY	-	expression tag	UNP G3G8X1
A	786	GLY	-	expression tag	UNP G3G8X1
A	787	GLY	-	expression tag	UNP G3G8X1
A	788	SER	-	expression tag	UNP G3G8X1
A	789	TRP	-	expression tag	UNP G3G8X1
A	790	SER	-	expression tag	UNP G3G8X1
A	791	HIS	-	expression tag	UNP G3G8X1
A	792	PRO	-	expression tag	UNP G3G8X1
A	793	GLN	-	expression tag	UNP G3G8X1
A	794	PHE	-	expression tag	UNP G3G8X1
A	795	GLU	-	expression tag	UNP G3G8X1
A	796	LYS	-	expression tag	UNP G3G8X1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	99.89 Å 99.89 Å 272.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.15 – 2.70 46.15 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.15-2.70) 99.8 (46.15-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.69 Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.193 , 0.236 0.191 , 0.235	Depositor DCC
R_{free} test set	1385 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.3	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4875	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/4869	0.75	1/6608 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	SER	N-CA-C	-5.15	97.10	111.00

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	A	4763	0	4629	45	0
2	A	14	0	13	0	0
3	A	6	0	8	0	0
4	A	92	0	0	1	0
All	All	4875	0	4650	45	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 (45) 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:653:ILE:CD1	1:A:653:ILE:CG1	1.74	1.64
1:A:310:MET:CE	1:A:358:LEU:HD13	2.24	0.67
1:A:547:VAL:O	1:A:551:LEU:HG	1.95	0.66
1:A:310:MET:HE1	1:A:358:LEU:HD13	1.83	0.59
1:A:128:VAL:HG23	1:A:606:VAL:HG22	1.84	0.59
1:A:587:GLN:NE2	1:A:602:ARG:HH11	2.00	0.58
1:A:203:VAL:HG11	1:A:224:ALA:HB1	1.86	0.57
1:A:138:VAL:HG22	1:A:600:ILE:HD13	1.86	0.57
1:A:577:PRO:HG3	1:A:593:MET:HG2	1.87	0.56
1:A:606:VAL:HG21	1:A:651:LEU:HD12	1.89	0.55
1:A:587:GLN:HE21	1:A:602:ARG:HH11	1.55	0.55
1:A:128:VAL:CG2	1:A:606:VAL:HG22	2.36	0.54
1:A:634:GLU:HG3	1:A:639:GLY:O	2.07	0.54
1:A:417:ASP:H	1:A:420:ARG:HH21	1.56	0.53
1:A:269:LYS:HB3	1:A:277:HIS:HB3	1.89	0.53
1:A:128:VAL:HG23	1:A:606:VAL:CG2	2.38	0.53
1:A:297:TYR:CE2	1:A:376:VAL:HG11	2.44	0.53
1:A:611:TYR:HB2	1:A:632:THR:HG22	1.91	0.52
1:A:665:HIS:CD2	1:A:681:TYR:H	2.29	0.50
1:A:175:HIS:CD2	1:A:355:ARG:HH22	2.29	0.50
1:A:628:ARG:HD2	1:A:657:LEU:HD13	1.94	0.50
1:A:679:GLU:HB2	1:A:684:VAL:HG21	1.94	0.49
1:A:214:ILE:HG12	1:A:247:LEU:HD11	1.97	0.47
1:A:204:PRO:HD3	1:A:361:PRO:O	2.16	0.46
1:A:685:ARG:HB2	1:A:685:ARG:HE	1.61	0.46
1:A:610:VAL:HG13	1:A:633:PHE:HB3	1.98	0.46
1:A:159:ILE:HD12	1:A:449:LEU:HD21	1.97	0.46
1:A:138:VAL:HG22	1:A:600:ILE:CD1	2.46	0.46
1:A:175:HIS:HD2	1:A:355:ARG:HH22	1.62	0.45
1:A:261:HIS:HD2	1:A:263:THR:O	1.99	0.44
1:A:271:GLY:HA3	1:A:277:HIS:CE1	2.52	0.44
1:A:128:VAL:CG2	1:A:606:VAL:CG2	2.95	0.44
1:A:342:ASP:HB3	1:A:345:SER:O	2.17	0.43
1:A:631:VAL:HG21	1:A:651:LEU:HD22	2.00	0.43
1:A:122:GLU:O	1:A:123:ARG:HB2	2.18	0.43
1:A:667:ARG:HB3	1:A:669:PHE:CE2	2.54	0.43
1:A:665:HIS:HB3	1:A:680:ASP:HA	2.00	0.43
1:A:727:ASP:HB3	1:A:730:GLU:HB2	2.01	0.42
1:A:147:PRO:HB2	1:A:149:TYR:CE2	2.54	0.42
1:A:269:LYS:HE2	1:A:278:THR:O	2.21	0.41
1:A:318:GLU:HA	1:A:321:HIS:CE1	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:ARG:NH2	1:A:650:GLU:HB2	2.36	0.41
1:A:174:ALA:HB3	1:A:289:VAL:HG12	2.01	0.40
1:A:139:ARG:HD2	4:A:1110:HOH:O	2.21	0.40
1:A:420:ARG:HD2	1:A:524:LEU:HD12	2.02	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 X-ray entries followed by that with respect to entries of similar resolution.

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	590/739 (80%)	554 (94%)	31 (5%)	5 (1%)	19	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	150	SER
1	A	427	VAL
1	A	318	GLU
1	A	452	ASP

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 X-ray entries followed by that with respect to entries of similar resolution.

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	509/612 (83%)	483 (95%)	26 (5%)	24	50

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	LEU
1	A	167	ILE
1	A	176	ILE
1	A	266	THR
1	A	270	ILE
1	A	289	VAL
1	A	323	GLU
1	A	336	GLU
1	A	374	ARG
1	A	375	ARG
1	A	401	THR
1	A	408	SER
1	A	412	ASP
1	A	452	ASP
1	A	453	ARG
1	A	458	LEU
1	A	524	LEU
1	A	532	GLU
1	A	575	LEU
1	A	627	SER
1	A	632	THR
1	A	658	ILE
1	A	679	GLU
1	A	693	ILE
1	A	707	ARG
1	A	745	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	241	ASN
1	A	261	HIS
1	A	333	GLN
1	A	447	HIS
1	A	587	GLN
1	A	635	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	665	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1001	1	14,14,15	0.34	0	17,19,21	1.11	1 (5%)
3	GOL	A	1002	-	5,5,5	0.23	0	5,5,5	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
3	GOL	A	1002	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1001	NAG	C1-O5-C5	4.26	117.97	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GOL	C1-C2-C3-O3
3	A	1002	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	594/739 (80%)	-0.09	5 (0%) 86 87	45, 69, 110, 147	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	123	ARG	3.1
1	A	477	GLN	2.8
1	A	113	ARG	2.5
1	A	270	ILE	2.4
1	A	592	ARG	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	1001	14/15	0.94	0.13	76,83,90,92	0
3	GOL	A	1002	6/6	0.94	0.20	59,68,72,75	0

6.5 Other polymers

There are no such residues in this entry.