Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:28 AM JST

PDB ID	:	5YS6
Title	:	Structure of the ectodomain of pseudorabies virus glycoproten B
Authors	:	Hu, X.L.; Yang, F.L.
Deposited on	:	2017-11-13
Resolution	:	3.10 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

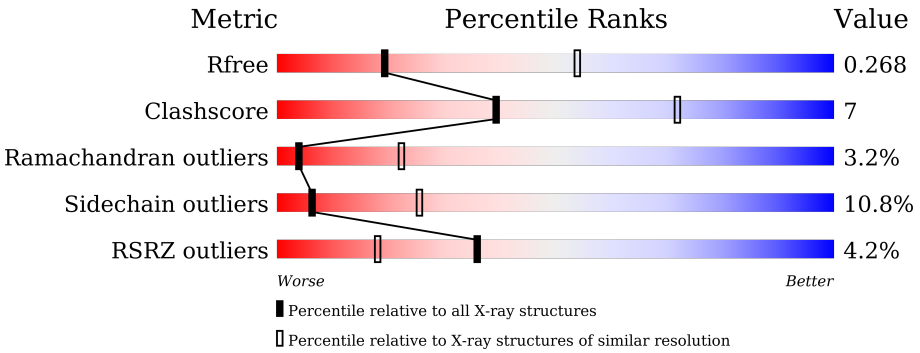
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of 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 <=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	702	3% 61% 17% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4582 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 PRV glycoproten B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	572	4582	2875	830	859	18	0	0	0

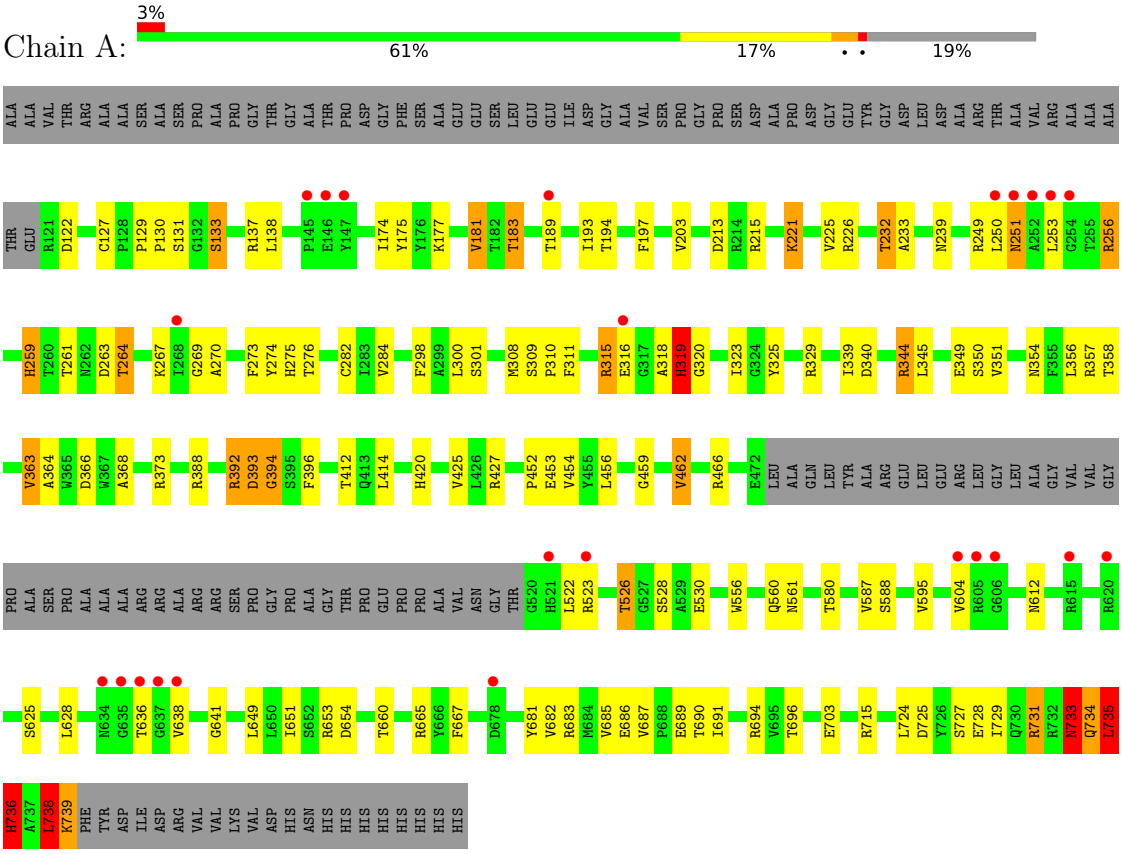
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	753	HIS	-	expression tag	UNP A0A1Q0AKY3
A	754	HIS	-	expression tag	UNP A0A1Q0AKY3
A	755	HIS	-	expression tag	UNP A0A1Q0AKY3
A	756	HIS	-	expression tag	UNP A0A1Q0AKY3
A	757	HIS	-	expression tag	UNP A0A1Q0AKY3
A	758	HIS	-	expression tag	UNP A0A1Q0AKY3
A	759	HIS	-	expression tag	UNP A0A1Q0AKY3
A	760	HIS	-	expression tag	UNP A0A1Q0AKY3

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: PRV glycoproten B



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	100.29Å 100.29Å 272.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.57 – 3.10 35.57 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.57-3.10) 99.7 (35.57-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.227 , 0.267 0.231 , 0.268	Depositor DCC
R_{free} test set	958 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	80.6	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4582	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.35	0/4686	0.53	1/6359 (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	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	735	LEU	CA-CB-CG	-5.72	102.15	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	250	LEU	Peptide
1	A	736	HIS	Peptide
1	A	738	LEU	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	4582	0	4446	67	1
All	All	4582	0	4446	67	1

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 7.

All (67) 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:318:ALA:O	1:A:320:GLY:N	2.10	0.85
1:A:580:THR:HG22	1:A:587:VAL:H	1.44	0.82
1:A:368:ALA:HB3	1:A:373:ARG:HD2	1.68	0.76
1:A:323:ILE:HG22	1:A:325:TYR:H	1.53	0.73
1:A:724:LEU:HD22	1:A:729:ILE:HD11	1.75	0.68
1:A:452:PRO:HD3	1:A:466:ARG:HH21	1.58	0.67
1:A:420:HIS:H	1:A:522:LEU:HD21	1.63	0.64
1:A:735:LEU:O	1:A:738:LEU:HB2	1.98	0.64
1:A:738:LEU:HB3	1:A:739:LYS:HG3	1.82	0.62
1:A:318:ALA:C	1:A:320:GLY:H	2.04	0.61
1:A:462:VAL:HG22	1:A:523:ARG:HH11	1.67	0.60
1:A:308:MET:HG3	1:A:323:ILE:HG12	1.84	0.60
1:A:311:PHE:HE2	1:A:373:ARG:HD3	1.66	0.59
1:A:654:ASP:OD2	1:A:654:ASP:N	2.36	0.59
1:A:298:PHE:CD2	1:A:310:PRO:HG3	2.39	0.57
1:A:628:LEU:HD22	1:A:653:ARG:HD3	1.86	0.57
1:A:388:ARG:NH2	1:A:453:GLU:OE1	2.37	0.57
1:A:308:MET:HE1	1:A:356:LEU:HD13	1.86	0.56
1:A:392:ARG:O	1:A:394:GLY:N	2.40	0.55
1:A:183:THR:HB	1:A:276:THR:HG22	1.90	0.54
1:A:183:THR:OG1	1:A:194:THR:OG1	2.26	0.53
1:A:177:LYS:HE3	1:A:203:VAL:HG22	1.90	0.53
1:A:452:PRO:HD3	1:A:466:ARG:NH2	2.25	0.52
1:A:175:TYR:HD2	1:A:284:VAL:HG22	1.75	0.51
1:A:267:LYS:HB2	1:A:275:HIS:HB2	1.93	0.51
1:A:213:ASP:HA	1:A:339:ILE:HG21	1.93	0.51
1:A:392:ARG:HG3	1:A:393:ASP:N	2.26	0.50
1:A:414:LEU:HB3	1:A:454:VAL:HG12	1.94	0.50
1:A:354:ASN:O	1:A:364:ALA:HA	2.12	0.49
1:A:356:LEU:HB3	1:A:363:VAL:HG23	1.95	0.49
1:A:727:SER:O	1:A:731:ARG:HB2	2.13	0.49
1:A:604:VAL:HG21	1:A:649:LEU:HD12	1.94	0.49
1:A:215:ARG:C	1:A:344:ARG:HH22	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ASP:OD1	1:A:264:THR:N	2.40	0.48
1:A:725:ASP:HB3	1:A:728:GLU:HB2	1.95	0.48
1:A:174:ILE:HD11	1:A:300:LEU:HD13	1.95	0.47
1:A:318:ALA:C	1:A:320:GLY:N	2.60	0.47
1:A:556:TRP:O	1:A:560:GLN:HG2	2.15	0.47
1:A:612:ASN:HA	1:A:681:TYR:HB2	1.95	0.47
1:A:129:PRO:HA	1:A:130:PRO:HD3	1.79	0.46
1:A:259:HIS:HA	1:A:282:CYS:O	2.16	0.46
1:A:526:THR:C	1:A:528:SER:H	2.20	0.45
1:A:213:ASP:O	1:A:339:ILE:HD13	2.16	0.45
1:A:127:CYS:HB3	1:A:588:SER:HB2	1.99	0.45
1:A:739:LYS:HG3	1:A:739:LYS:H	1.31	0.45
1:A:351:VAL:HG11	1:A:366:ASP:CG	2.38	0.44
1:A:459:GLY:O	1:A:526:THR:HG22	2.17	0.44
1:A:329:ARG:NH1	1:A:357:ARG:O	2.43	0.44
1:A:641:GLY:HA2	1:A:651:ILE:O	2.18	0.44
1:A:665:ARG:HB3	1:A:667:PHE:CE1	2.52	0.44
1:A:131:SER:HG	1:A:133:SER:HG	1.62	0.43
1:A:308:MET:HG2	1:A:309:SER:N	2.33	0.43
1:A:232:THR:HG22	1:A:233:ALA:H	1.83	0.43
1:A:215:ARG:O	1:A:344:ARG:NH2	2.49	0.43
1:A:194:THR:HG21	1:A:274:TYR:CE1	2.54	0.43
1:A:733:ASN:OD1	1:A:733:ASN:N	2.50	0.43
1:A:181:VAL:HG13	1:A:197:PHE:HB3	2.01	0.42
1:A:682:VAL:HG12	1:A:683:ARG:HG3	2.00	0.42
1:A:177:LYS:NZ	1:A:221:LYS:O	2.52	0.42
1:A:340:ASP:O	1:A:344:ARG:HA	2.20	0.42
1:A:452:PRO:HA	1:A:466:ARG:HG3	2.02	0.42
1:A:523:ARG:H	1:A:523:ARG:HG2	1.64	0.41
1:A:612:ASN:HA	1:A:681:TYR:CB	2.50	0.41
1:A:256:ARG:HA	1:A:256:ARG:HD2	1.69	0.41
1:A:456:LEU:HD23	1:A:523:ARG:NH1	2.36	0.40
1:A:388:ARG:HD3	1:A:396:PHE:CE1	2.56	0.40
1:A:318:ALA:O	1:A:319:HIS:C	2.58	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ASN:OD1	1:A:694:ARG:NH2[3_775]	2.15	0.05

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	568/702 (81%)	499 (88%)	51 (9%)	18 (3%)	4 22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	HIS
1	A	393	ASP
1	A	736	HIS
1	A	249	ARG
1	A	251	ASN
1	A	269	GLY
1	A	316	GLU
1	A	427	ARG
1	A	733	ASN
1	A	734	GLN
1	A	735	LEU
1	A	394	GLY
1	A	738	LEU
1	A	270	ALA
1	A	315	ARG
1	A	349	GLU
1	A	345	LEU
1	A	425	VAL

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	490/582 (84%)	437 (89%)	53 (11%)	6 25

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	133	SER
1	A	137	ARG
1	A	138	LEU
1	A	181	VAL
1	A	183	THR
1	A	189	THR
1	A	193	ILE
1	A	221	LYS
1	A	225	VAL
1	A	226	ARG
1	A	232	THR
1	A	239	ASN
1	A	251	ASN
1	A	253	LEU
1	A	256	ARG
1	A	259	HIS
1	A	261	THR
1	A	264	THR
1	A	273	PHE
1	A	301	SER
1	A	315	ARG
1	A	319	HIS
1	A	344	ARG
1	A	350	SER
1	A	358	THR
1	A	363	VAL
1	A	392	ARG
1	A	412	THR
1	A	462	VAL
1	A	526	THR
1	A	530	GLU
1	A	595	VAL
1	A	625	SER
1	A	636	THR
1	A	638	VAL
1	A	660	THR
1	A	685	VAL

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Mol	Chain	Res	Type
1	A	686	GLU
1	A	687	VAL
1	A	689	GLU
1	A	690	THR
1	A	691	ILE
1	A	696	THR
1	A	703	GLU
1	A	715	ARG
1	A	731	ARG
1	A	733	ASN
1	A	734	GLN
1	A	735	LEU
1	A	736	HIS
1	A	738	LEU
1	A	739	LYS

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

Mol	Chain	Res	Type
1	A	535	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 monosaccharides 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.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	572/702 (81%)	0.20	24 (4%) 36 18	38, 92, 165, 341	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	635	GLY	18.5
1	A	636	THR	16.4
1	A	252	ALA	15.8
1	A	253	LEU	12.7
1	A	251	ASN	11.1
1	A	637	GLY	10.1
1	A	606	GLY	6.0
1	A	634	ASN	6.0
1	A	147	TYR	4.3
1	A	605	ARG	3.7
1	A	638	VAL	3.7
1	A	254	GLY	3.5
1	A	521	HIS	3.1
1	A	250	LEU	2.6
1	A	145	PRO	2.4
1	A	146	GLU	2.4
1	A	268	ILE	2.2
1	A	620	ARG	2.2
1	A	316	GLU	2.2
1	A	615	ARG	2.2
1	A	678	ASP	2.1
1	A	189	THR	2.1
1	A	523	ARG	2.0
1	A	604	VAL	2.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.