



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:07 AM UTC

PDB ID : 8Q0E / pdb_00008q0e
Title : Crystal Structure of the N-terminal Domain of Variant Surface Glycoprotein 545 (VSG545) of Trypanosome brucei brucei Lister 427
Authors : van Straaten, M.; Stebbins, C.E.
Deposited on : 2023-07-28
Resolution : 3.15 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

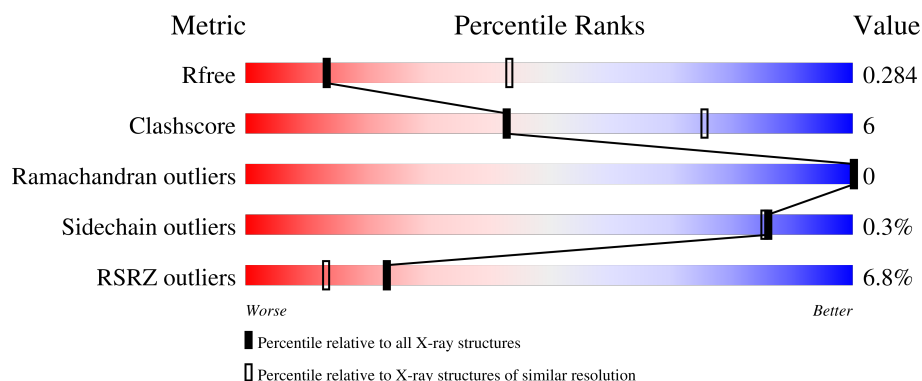
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 $\leq 5\%$. 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	489	4% 42% 7% 51%
1	B	489	3% 41% 8% 51%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3452 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.

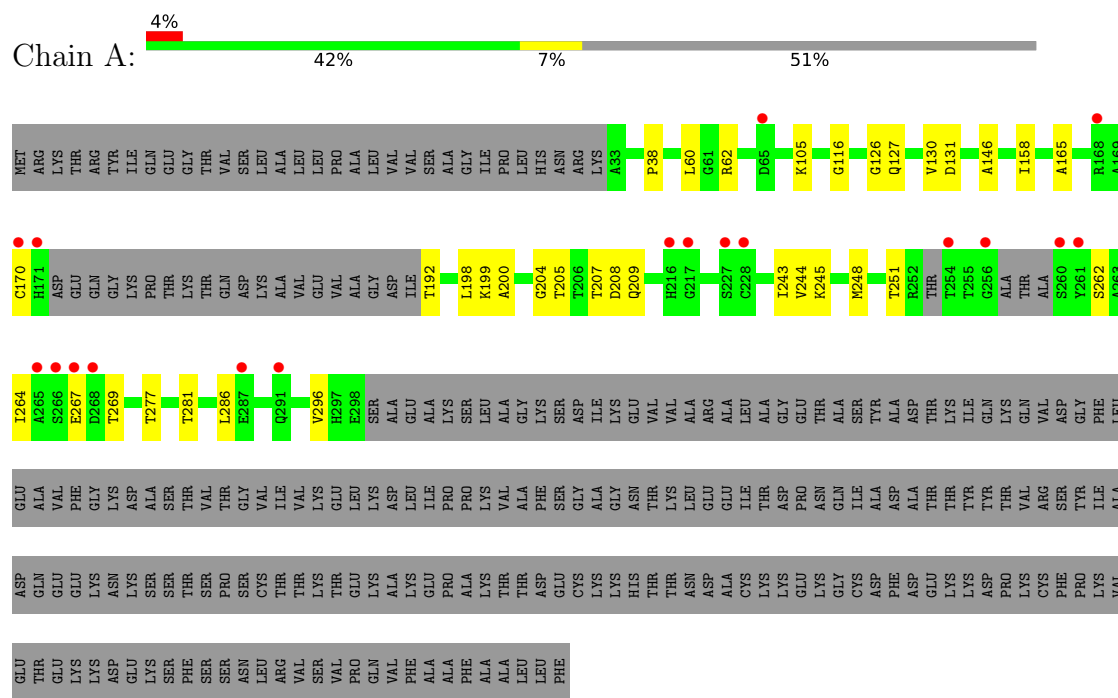
- Molecule 1 is a protein called Variant surface glycoprotein 545.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1726	1065	306	349	6			
1	B	241	Total	C	N	O	S	0	0	0
			1726	1065	305	350	6			

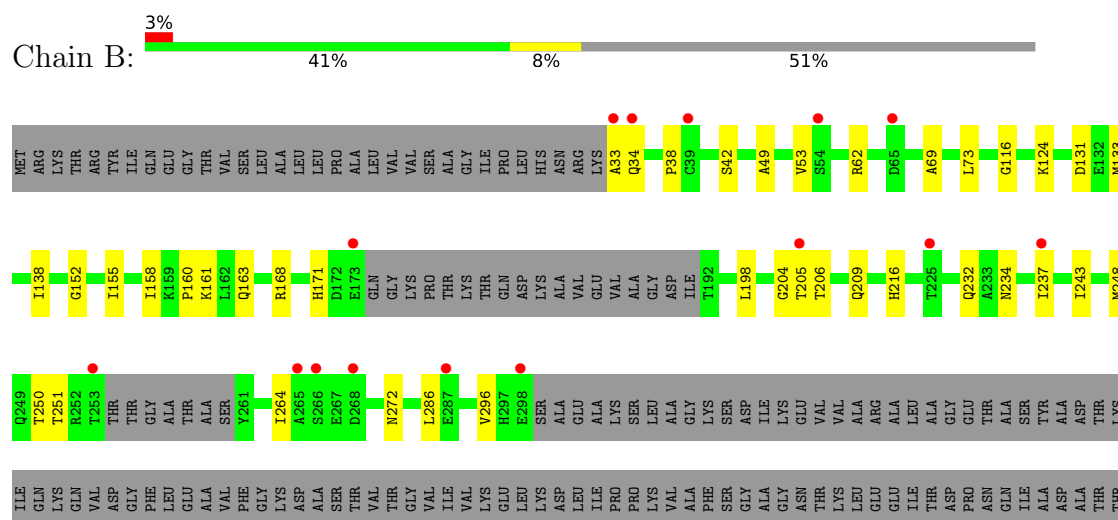
3 Residue-property plots [i](#)

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: Variant surface glycoprotein 545



• Molecule 1: Variant surface glycoprotein 545



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.41Å 52.28Å 305.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 3.15 46.52 – 3.15	Depositor EDS
% Data completeness (in resolution range)	75.5 (46.52-3.15) 75.5 (46.52-3.15)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.236 , 0.287 0.239 , 0.284	Depositor DCC
R_{free} test set	538 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3452	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.14	0/1743	0.32	0/2364
1	B	0.15	0/1744	0.33	0/2367
All	All	0.14	0/3487	0.32	0/4731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1726	0	1741	24	0
1	B	1726	0	1737	23	0
All	All	3452	0	3478	43	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 6.

All (43) 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:158:ILE:HD11	1:B:237:ILE:HD12	1.66	0.76
1:A:116:GLY:HA3	1:A:286:LEU:HB2	1.71	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:PRO:HB2	1:A:131:ASP:HB2	1.77	0.66
1:B:205:THR:HG23	1:B:206:THR:HG23	1.80	0.63
1:B:116:GLY:HA3	1:B:286:LEU:HB2	1.80	0.62
1:A:248:MET:HB3	1:A:264:ILE:HD13	1.81	0.61
1:A:192:THR:HA	1:A:251:THR:HA	1.81	0.61
1:B:216:HIS:O	1:B:234:ASN:HB2	2.01	0.61
1:A:207:THR:OG1	1:A:208:ASP:N	2.35	0.60
1:B:250:THR:HG22	1:B:251:THR:H	1.66	0.59
1:B:62:ARG:NH1	1:B:296:VAL:O	2.34	0.58
1:B:198:LEU:HD13	1:B:243:ILE:HD12	1.88	0.54
1:A:192:THR:HG22	1:A:251:THR:HG23	1.89	0.54
1:A:199:LYS:HB3	1:A:244:VAL:HG23	1.89	0.54
1:A:192:THR:O	1:A:192:THR:OG1	2.25	0.52
1:A:127:GLN:HA	1:A:130:VAL:HG22	1.89	0.52
1:A:205:THR:N	1:A:209:GLN:OE1	2.29	0.52
1:B:42:SER:HB2	1:B:124:LYS:HG3	1.91	0.52
1:A:165:ALA:O	1:B:272:ASN:ND2	2.43	0.51
1:B:33:ALA:O	1:B:34:GLN:HG2	2.12	0.50
1:A:38:PRO:HD3	1:A:245:LYS:HD2	1.93	0.49
1:A:277:THR:O	1:A:281:THR:HG23	2.12	0.49
1:B:138:ILE:HD12	1:B:158:ILE:HG22	1.95	0.49
1:A:200:ALA:HB1	1:B:160:PRO:HB2	1.95	0.48
1:A:267:GLU:OE2	1:A:269:THR:OG1	2.30	0.48
1:A:126:GLY:O	1:A:130:VAL:HG13	2.15	0.47
1:A:251:THR:O	1:A:262:SER:HB2	2.15	0.47
1:A:198:LEU:HD22	1:A:243:ILE:HG21	1.95	0.47
1:B:248:MET:HB3	1:B:264:ILE:CD1	2.45	0.46
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.84	0.45
1:B:168:ARG:HB2	1:B:171:HIS:HB2	1.99	0.44
1:A:105:LYS:HD3	1:A:296:VAL:HG12	1.99	0.44
1:A:62:ARG:NH1	1:A:296:VAL:O	2.50	0.44
1:B:38:PRO:HB2	1:B:131:ASP:HB2	2.00	0.44
1:B:133:MET:HE3	1:B:133:MET:HB3	1.90	0.44
1:B:49:ALA:O	1:B:53:VAL:HG23	2.19	0.43
1:B:152:GLY:O	1:B:155:ILE:HG12	2.19	0.42
1:A:146:ALA:O	1:B:232:GLN:HG2	2.18	0.42
1:B:204:GLY:HA3	1:B:209:GLN:HB3	2.02	0.41
1:B:116:GLY:CA	1:B:286:LEU:HB2	2.49	0.41
1:B:161:LYS:HG3	1:B:163:GLN:HE21	1.86	0.41
1:B:69:ALA:O	1:B:73:LEU:HB2	2.21	0.40
1:A:204:GLY:HA3	1:A:209:GLN:HB3	2.04	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	234/489 (48%)	223 (95%)	11 (5%)	0	100	100
1	B	235/489 (48%)	229 (97%)	6 (3%)	0	100	100
All	All	469/978 (48%)	452 (96%)	17 (4%)	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 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	176/382 (46%)	175 (99%)	1 (1%)	78	81
1	B	176/382 (46%)	176 (100%)	0	100	100
All	All	352/764 (46%)	351 (100%)	1 (0%)	86	85

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	127	GLN
1	A	297	HIS
1	B	58	GLN
1	B	209	GLN
1	B	229	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 oligosaccharides 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, 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	242/489 (49%)	0.70	18 (7%) 20 12	12, 42, 73, 97	0
1	B	241/489 (49%)	0.57	15 (6%) 26 15	12, 42, 74, 99	0
All	All	483/978 (49%)	0.64	33 (6%) 23 13	12, 42, 74, 99	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	SER	5.0
1	B	266	SER	4.1
1	A	256	GLY	3.7
1	B	287	GLU	3.4
1	A	254	THR	3.2
1	B	265	ALA	3.2
1	A	265	ALA	3.1
1	A	267	GLU	3.1
1	A	268	ASP	2.9
1	B	253	THR	2.9
1	A	287	GLU	2.9
1	B	225	THR	2.8
1	A	168	ARG	2.8
1	B	54	SER	2.7
1	A	65	ASP	2.7
1	A	260	SER	2.5
1	B	34	GLN	2.5
1	A	170	CYS	2.4
1	A	217	GLY	2.4
1	A	261	TYR	2.4
1	B	173	GLU	2.4
1	A	227	SER	2.4
1	A	171	HIS	2.3
1	B	33	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	65	ASP	2.2
1	B	298	GLU	2.2
1	A	228	CYS	2.2
1	B	39	CYS	2.2
1	A	291	GLN	2.2
1	B	237	ILE	2.1
1	B	205	THR	2.1
1	A	216	HIS	2.0
1	B	268	ASP	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 oligosaccharides 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.