



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2024 – 12:18 PM EDT

PDB ID : 8V5L
Title : Structure of the Varicella Zoster Virus (VZV) gI binding domain of glycoprotein E (gE) in complex with human Fab 1A2 and 1E12
Authors : Seraj, N.; Holzapfel, G.; Harshbarger, W.
Deposited on : 2023-11-30
Resolution : 3.09 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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) : 1.20.1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

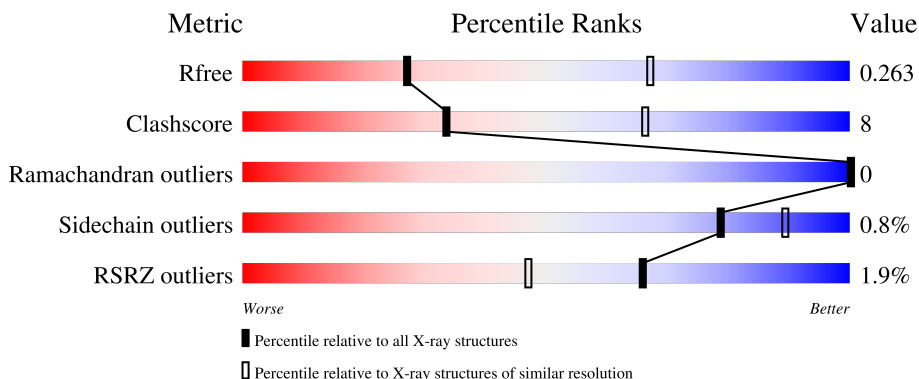
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (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 $\leq 5\%$. 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	H	243	 3% 72% 19% 8%
2	L	214	 88% 11%
3	A	203	 3% 46% 16% 38%
4	B	248	 3% 74% 19% 7%
5	C	219	 3% 85% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7752 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 Fab 1A2 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	224	1721	1089	291	334	7	0	0	0

- Molecule 2 is a protein called Fab 1A2 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1634	1019	279	331	5	0	0	0

- Molecule 3 is a protein called Envelope glycoprotein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	126	1030	661	168	199	2	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	308	GLU	-	expression tag	UNP Q77JX0
A	309	ASN	-	expression tag	UNP Q77JX0
A	310	LEU	-	expression tag	UNP Q77JX0
A	311	TYR	-	expression tag	UNP Q77JX0
A	312	PHE	-	expression tag	UNP Q77JX0
A	313	GLN	-	expression tag	UNP Q77JX0
A	314	GLY	-	expression tag	UNP Q77JX0
A	315	HIS	-	expression tag	UNP Q77JX0
A	316	HIS	-	expression tag	UNP Q77JX0
A	317	HIS	-	expression tag	UNP Q77JX0
A	318	HIS	-	expression tag	UNP Q77JX0
A	319	HIS	-	expression tag	UNP Q77JX0
A	320	HIS	-	expression tag	UNP Q77JX0

- Molecule 4 is a protein called Fab 1E12 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	231	1735	1100	286	343	6	0	0	0

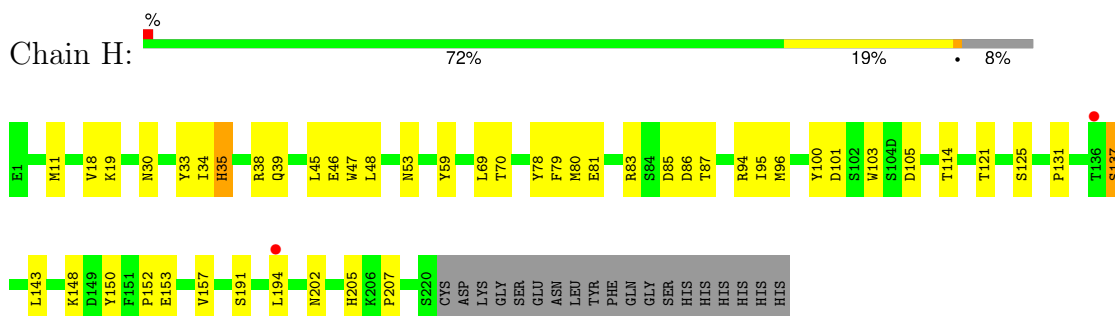
- Molecule 5 is a protein called Fab 1E12 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	217	1632	1015	279	334	4	0	0	0

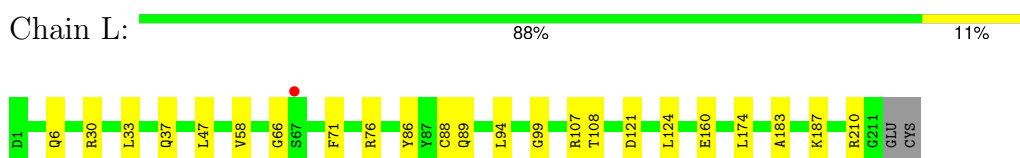
3 Residue-property plots [i](#)

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.

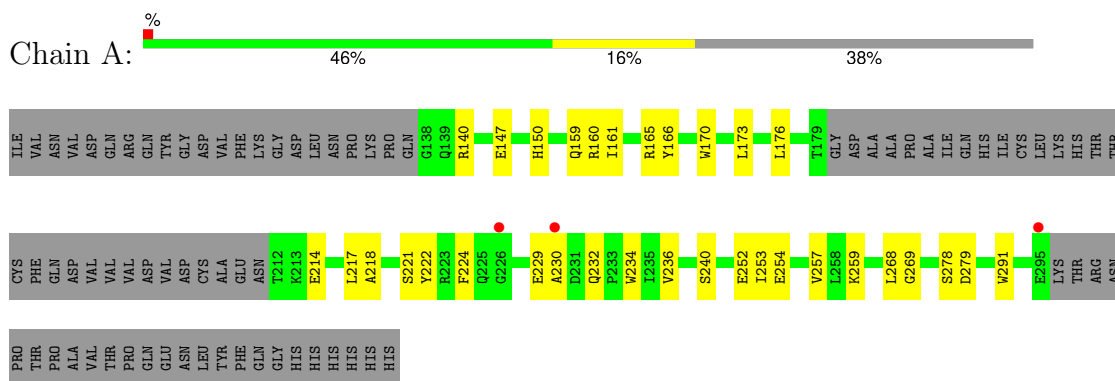
- Molecule 1: Fab 1A2 Heavy Chain



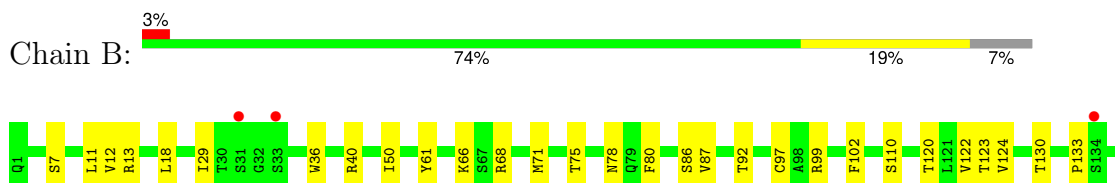
- Molecule 2: Fab 1A2 Light Chain



- Molecule 3: Envelope glycoprotein E

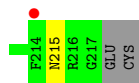
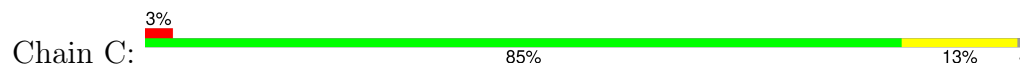


- Molecule 4: Fab 1E12 Heavy Chain





● Molecule 5: Fab 1E12 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.78Å 63.49Å 96.48Å 90.00° 99.96° 90.00°	Depositor
Resolution (Å)	47.57 – 3.09 47.57 – 3.09	Depositor EDS
% Data completeness (in resolution range)	76.0 (47.57-3.09) 90.8 (47.57-3.09)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.07Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.269 0.231 , 0.263	Depositor DCC
R_{free} test set	23042 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7752	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	H	0.27	0/1766	0.52	0/2406
2	L	0.27	0/1669	0.51	0/2267
3	A	0.26	0/1055	0.52	0/1435
4	B	0.27	0/1780	0.53	0/2427
5	C	0.27	0/1669	0.53	0/2277
All	All	0.27	0/7939	0.52	0/10812

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 [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	H	1721	0	1676	31	1
2	L	1634	0	1590	16	0
3	A	1030	0	1004	20	1
4	B	1735	0	1700	32	0
5	C	1632	0	1578	22	0
All	All	7752	0	7548	116	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 8.

The worst 5 of 116 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:H:38:ARG:HH22	1:H:86:ASP:HA	1.39	0.87
4:B:140:PRO:HD2	4:B:227:PRO:HA	1.68	0.75
4:B:40:ARG:HB3	4:B:50:ILE:HD11	1.70	0.72
1:H:11:MET:HB2	1:H:152:PRO:HG2	1.74	0.68
2:L:33:LEU:HD11	2:L:88:CYS:HB2	1.76	0.67

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:H:100:TYR:OH	3:A:236:VAL:O[2_554]	2.06	0.14

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	H	222/243 (91%)	216 (97%)	6 (3%)	0	100	100
2	L	210/214 (98%)	206 (98%)	4 (2%)	0	100	100
3	A	122/203 (60%)	117 (96%)	5 (4%)	0	100	100
4	B	229/248 (92%)	224 (98%)	5 (2%)	0	100	100
5	C	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
All	All	998/1127 (89%)	971 (97%)	27 (3%)	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	H	192/209 (92%)	189 (98%)	3 (2%)	58	79
2	L	188/190 (99%)	187 (100%)	1 (0%)	86	92
3	A	114/182 (63%)	112 (98%)	2 (2%)	54	76
4	B	199/214 (93%)	199 (100%)	0	100	100
5	C	186/188 (99%)	185 (100%)	1 (0%)	86	92
All	All	879/983 (89%)	872 (99%)	7 (1%)	79	89

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	76	ARG
3	A	140	ARG
5	C	181	SER
3	A	240	SER
1	H	137	SER

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

Mol	Chain	Res	Type
4	B	16	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 [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	H	224/243 (92%)	0.09	2 (0%) 81 66	33, 52, 92, 136	0
2	L	212/214 (99%)	0.09	1 (0%) 87 75	36, 53, 70, 78	0
3	A	126/203 (62%)	0.27	3 (2%) 59 41	36, 58, 105, 121	0
4	B	231/248 (93%)	0.42	7 (3%) 52 33	35, 60, 98, 139	0
5	C	217/219 (99%)	0.37	6 (2%) 55 35	37, 64, 110, 131	0
All	All	1010/1127 (89%)	0.25	19 (1%) 66 47	33, 56, 104, 139	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	143	LYS	3.7
4	B	33	SER	3.1
3	A	230	ALA	3.1
4	B	144	SER	3.0
5	C	196	VAL	3.0

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.