



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:37 PM UTC

PDB ID : 2B1A / pdb_00002b1a
Title : Crystal structure analysis of anti-HIV-1 V3 Fab 2219 in complex with UG1033 peptide
Authors : Stanfield, R.L.; Gorny, M.K.; Zolla-Pazner, S.; Wilson, I.A.
Deposited on : 2005-09-15
Resolution : 2.35 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

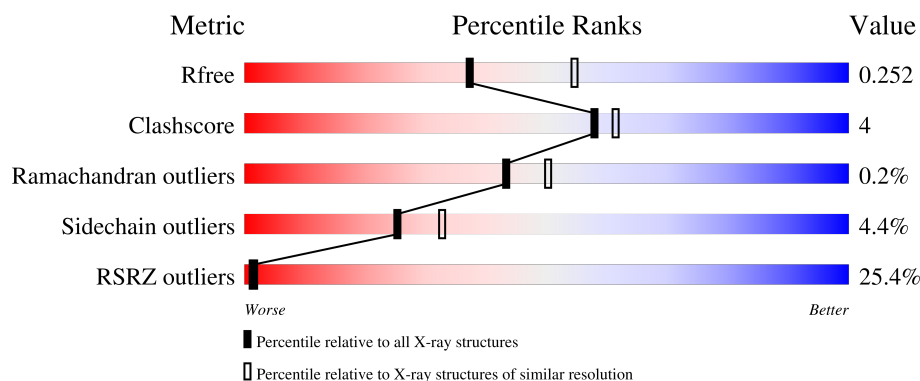
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	L	215	22% 86% 13%
2	H	226	28% 88% 12%
3	P	23	17% 52% 13% • 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3500 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 2219, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1616	1011	274	327	4			

- Molecule 2 is a protein called Fab 2219, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1699	1070	277	345	7			

- Molecule 3 is a protein called UG1033 peptide of Exterior membrane glycoprotein GP120.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	16	Total	C	N	O	0	0	0
			125	80	25	20			

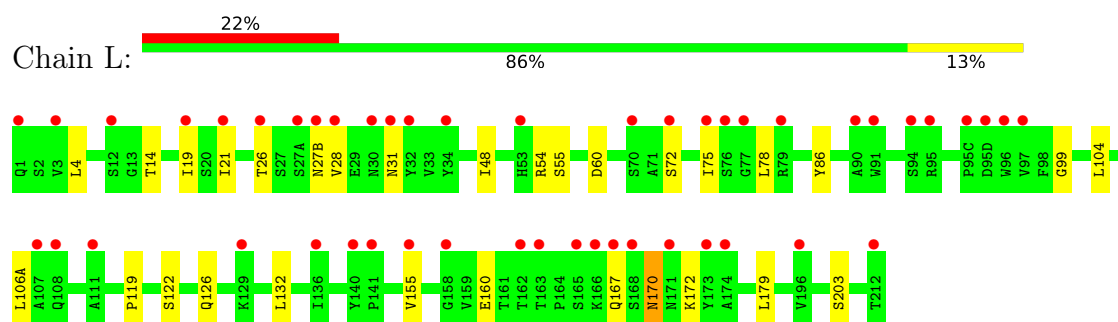
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	11	Total	O	0	0
			11	11		
4	H	49	Total	O	0	0
			49	49		

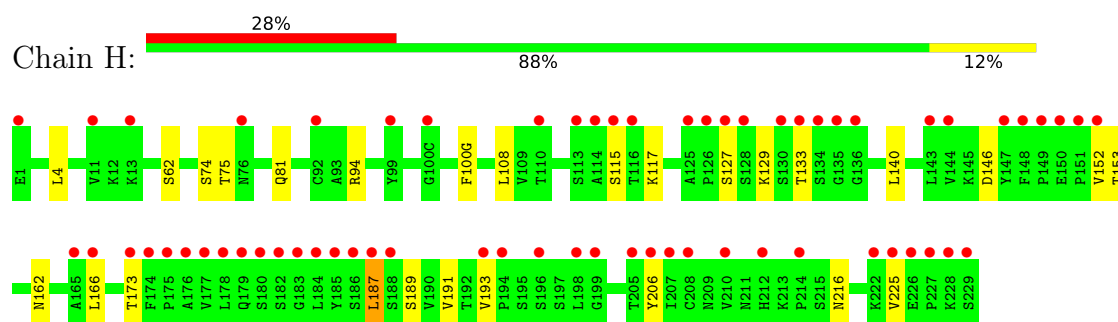
3 Residue-property plots [i](#)

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 2219, light chain



- Molecule 2: Fab 2219, heavy chain



- Molecule 3: UG1033 peptide of Exterior membrane glycoprotein GP120



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.72Å 96.89Å 97.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.31 – 2.35 31.31 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.31-2.35) 98.3 (31.31-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2, CNS 1.1	Depositor
R, R_{free}	0.211 , 0.244 0.218 , 0.252	Depositor DCC
R_{free} test set	1208 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3500	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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	L	0.55	0/1660	0.75	0/2269
2	H	0.80	2/1744 (0.1%)	0.83	2/2373 (0.1%)
3	P	2.12	1/128 (0.8%)	1.26	3/171 (1.8%)
All	All	0.79	3/3532 (0.1%)	0.81	5/4813 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	309	LEU	C-N	22.49	1.67	1.33
2	H	162	ASN	CG-ND2	10.94	1.56	1.33
2	H	162	ASN	CG-OD1	10.03	1.42	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	162	ASN	OD1-CG-ND2	9.12	131.72	122.60
3	P	309	LEU	O-C-N	8.20	131.50	122.15
3	P	309	LEU	CA-C-N	-5.82	112.73	121.87
3	P	309	LEU	C-N-CA	-5.82	112.73	121.87
2	H	81	GLN	N-CA-C	5.43	117.65	109.23

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	L	1616	0	1554	19	0
2	H	1699	0	1624	9	0
3	P	125	0	127	3	0
4	H	49	0	0	0	0
4	L	11	0	0	0	0
All	All	3500	0	3305	30	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 4.

All (30) 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)
3:P:303:THR:OG1	3:P:304:ARG:N	2.15	0.79
1:L:31:ASN:OD1	3:P:315:ARG:NH2	2.30	0.64
3:P:303:THR:HG1	3:P:304:ARG:H	1.49	0.61
2:H:166:LEU:HD21	2:H:191:VAL:HG21	1.85	0.58
1:L:170:ASN:HD22	1:L:170:ASN:C	2.11	0.57
1:L:167:GLN:HE21	1:L:170:ASN:HD21	1.52	0.57
2:H:187:LEU:C	2:H:187:LEU:HD12	2.30	0.56
1:L:14:THR:HG22	1:L:106(A):LEU:HD12	1.88	0.55
1:L:27(B):ASN:HD22	1:L:28:VAL:H	1.54	0.53
1:L:119:PRO:HA	1:L:132:LEU:HD23	1.90	0.53
1:L:26:THR:H	1:L:27(B):ASN:ND2	2.09	0.50
1:L:21:ILE:HD13	1:L:86:TYR:HB2	1.93	0.50
1:L:122:SER:O	1:L:126:GLN:HG3	2.12	0.50
1:L:78:LEU:HD11	1:L:104:LEU:HD21	1.95	0.49
2:H:94:ARG:O	2:H:100(G):PHE:HA	2.11	0.49
1:L:4:LEU:HB2	1:L:99:GLY:HA2	1.94	0.49
1:L:54:ARG:NE	1:L:60:ASP:HA	2.27	0.49
2:H:140:LEU:HD13	2:H:225:VAL:HG11	1.96	0.47
2:H:193:VAL:HG11	2:H:206:TYR:CE1	2.51	0.46
1:L:167:GLN:HE21	1:L:170:ASN:ND2	2.13	0.46
1:L:26:THR:H	1:L:27(B):ASN:HD21	1.64	0.45
1:L:170:ASN:ND2	1:L:172:LYS:H	2.14	0.45
1:L:170:ASN:HD22	1:L:172:LYS:H	1.65	0.44
2:H:74:SER:OG	2:H:75:THR:HG23	2.18	0.44
2:H:140:LEU:HD13	2:H:225:VAL:CG1	2.48	0.44
1:L:132:LEU:HD12	1:L:179:LEU:HD23	2.01	0.43
1:L:48:ILE:HD13	1:L:54:ARG:HA	2.00	0.42
2:H:117:LYS:NZ	2:H:146:ASP:O	2.50	0.41
2:H:173:THR:HA	2:H:189:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:19:ILE:HD11	1:L:75:ILE:HD12	2.03	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	L	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
2	H	224/226 (99%)	210 (94%)	13 (6%)	1 (0%)	30	32
3	P	14/23 (61%)	13 (93%)	1 (7%)	0	100	100
All	All	451/464 (97%)	429 (95%)	21 (5%)	1 (0%)	43	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	127	SER

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	L	180/180 (100%)	174 (97%)	6 (3%)	33	43
2	H	191/191 (100%)	181 (95%)	10 (5%)	21	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P	12/17 (71%)	11 (92%)	1 (8%)	10	11
All	All	383/388 (99%)	366 (96%)	17 (4%)	25	33

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	55	SER
1	L	72	SER
1	L	155	VAL
1	L	160	GLU
1	L	170	ASN
1	L	203	SER
2	H	4	LEU
2	H	62	SER
2	H	108	LEU
2	H	115	SER
2	H	129	LYS
2	H	133	THR
2	H	152	VAL
2	H	153	THR
2	H	187	LEU
2	H	216	ASN
3	P	309	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27(B)	ASN
1	L	170	ASN
1	L	171	ASN
2	H	79	HIS
2	H	172	HIS
2	H	203	GLN
2	H	211	ASN
2	H	216	ASN
3	P	308	HIS

5.3.3 RNA ⓘ

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	309:LEU	C	312:GLY	N	1.67

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	L	215/215 (100%)	1.45	48 (22%)  	65, 71, 74, 80	0
2	H	226/226 (100%)	1.70	64 (28%)  	64, 70, 77, 81	0
3	P	16/23 (69%)	1.53	4 (25%)  	66, 71, 83, 87	0
All	All	457/464 (98%)	1.58	116 (25%)  	64, 71, 77, 87	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	114	ALA	8.3
2	H	178	LEU	6.3
2	H	185	TYR	6.0
2	H	134	SER	5.6
1	L	107	ALA	5.5
2	H	148	PHE	5.3
3	P	320	THR	5.1
2	H	184	LEU	5.0
2	H	176	ALA	5.0
2	H	113	SER	4.8
2	H	133	THR	4.6
2	H	228	LYS	4.6
2	H	180	SER	4.5
2	H	135	GLY	4.4
2	H	183	GLY	4.4
3	P	303	THR	4.1
2	H	115	SER	4.1
1	L	212	THR	4.1
2	H	186	SER	4.0
2	H	225	VAL	4.0
2	H	175	PRO	4.0
2	H	229	SER	4.0
2	H	151	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
2	H	150	GLU	3.9
1	L	140	TYR	3.8
2	H	147	TYR	3.8
2	H	199	GLY	3.8
2	H	177	VAL	3.8
2	H	152	VAL	3.7
1	L	96	TRP	3.6
2	H	128	SER	3.6
2	H	130	SER	3.5
2	H	149	PRO	3.4
2	H	182	SER	3.3
1	L	90	ALA	3.3
2	H	144	VAL	3.2
3	P	317	PHE	3.2
2	H	179	GLN	3.2
1	L	97	VAL	3.1
2	H	174	PHE	3.1
1	L	21	ILE	3.1
2	H	193	VAL	3.1
2	H	126	PRO	3.0
1	L	3	VAL	3.0
1	L	19	ILE	3.0
2	H	13	LYS	2.9
1	L	108	GLN	2.9
2	H	110	THR	2.9
2	H	187	LEU	2.9
2	H	208	CYS	2.9
1	L	76	SER	2.8
2	H	198	LEU	2.8
2	H	206	TYR	2.8
2	H	125	ALA	2.8
1	L	91	TRP	2.8
2	H	214	PRO	2.8
1	L	174	ALA	2.7
2	H	210	VAL	2.7
1	L	94	SER	2.7
1	L	163	THR	2.7
1	L	171	ASN	2.7
1	L	111	ALA	2.6
2	H	226	GLU	2.6
2	H	100(C)	GLY	2.6
2	H	173	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	L	26	THR	2.6
1	L	166	LYS	2.6
1	L	168	SER	2.5
2	H	1	GLU	2.5
1	L	53	HIS	2.5
2	H	227	PRO	2.5
1	L	27(B)	ASN	2.5
1	L	141	PRO	2.5
2	H	127	SER	2.4
1	L	28	VAL	2.4
2	H	166	LEU	2.4
1	L	167	GLN	2.4
1	L	31	ASN	2.4
1	L	12	SER	2.4
2	H	143	LEU	2.4
2	H	212	HIS	2.4
1	L	72	SER	2.3
2	H	92	CYS	2.3
1	L	77	GLY	2.3
2	H	116	THR	2.3
2	H	207	ILE	2.3
1	L	173	TYR	2.3
2	H	136	GLY	2.3
1	L	70	SER	2.3
2	H	194	PRO	2.3
1	L	32	TYR	2.3
1	L	129	LYS	2.3
2	H	165	ALA	2.2
1	L	162	THR	2.2
1	L	27(A)	SER	2.2
2	H	222	LYS	2.2
1	L	75	ILE	2.2
1	L	158	GLY	2.2
1	L	34	TYR	2.2
2	H	99	TYR	2.2
1	L	95(D)	ASP	2.2
1	L	95(C)	PRO	2.2
1	L	155	VAL	2.2
2	H	76	ASN	2.2
2	H	188	SER	2.2
2	H	205	THR	2.2
3	P	319	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	165	SER	2.1
1	L	1	GLN	2.1
1	L	30	ASN	2.1
1	L	196	VAL	2.1
1	L	79	ARG	2.0
1	L	95	ARG	2.0
2	H	11	VAL	2.0
2	H	196	SER	2.0
1	L	136	ILE	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.