



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:37 AM GMT

PDB ID : 2B1H  
Title : Crystal structure analysis of anti-HIV-1 V3 Fab 2219 in complex with UG29 peptide  
Authors : Stanfield, R.L.; Gorny, M.K.; Zolla-Pazner, S.; Wilson, I.A.  
Deposited on : 2005-09-15  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

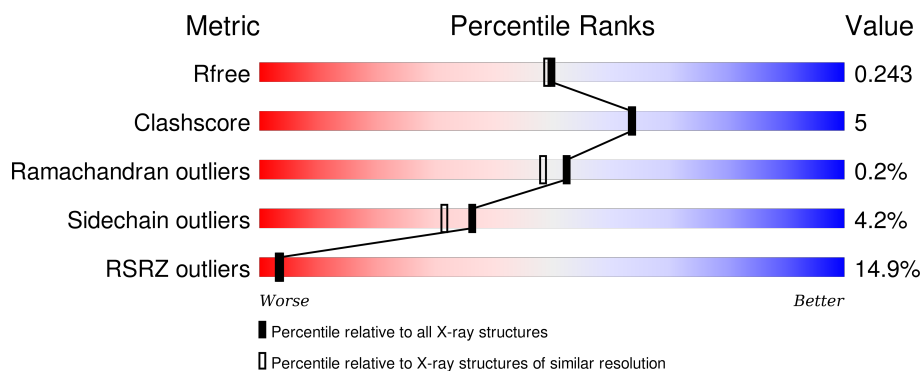
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>12%</div> <div>89%</div> <div>9%</div> </div>
2	H	226	<div> <div>17%</div> <div>86%</div> <div>13%</div> </div>
3	P	23	<div> <div>22%</div> <div>35%</div> <div>26%</div> <div>9%</div> <div>30%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3572 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 UG29 peptide of Exterior membrane glycoprotein GP120.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	16	Total	C	N	O	0	0	0
			134	87	26	21			

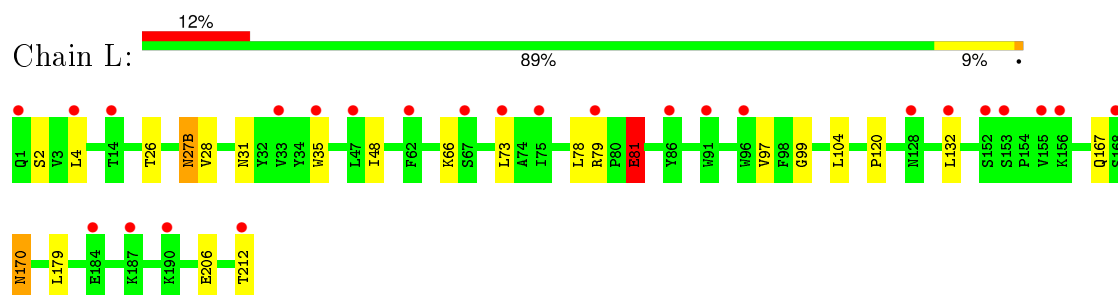
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	81	Total	O	0	0
			81	81		
4	L	42	Total	O	0	0
			42	42		

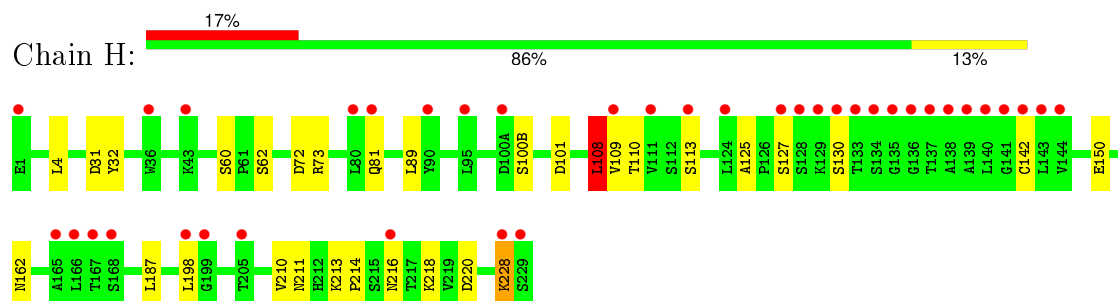
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

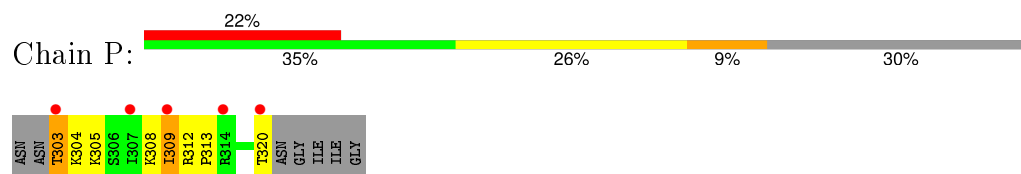
- Molecule 1: Fab 2219, light chain



- Molecule 2: Fab 2219, heavy chain



- Molecule 3: UG29 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, $\alpha$ , $\beta$ , $\gamma$	62.90Å 94.50Å 96.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.42 – 2.00 19.23 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (67.42-2.00) 99.9 (19.23-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.205 , 0.238 0.213 , 0.243	Depositor DCC
$R_{free}$ test set	1982 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 50.4	EDS
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 39559 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	L	0.82	1/1660 (0.1%)	0.78	0/2269
2	H	1.07	9/1744 (0.5%)	0.90	6/2373 (0.3%)
3	P	1.17	1/136 (0.7%)	1.06	0/180
All	All	0.97	11/3540 (0.3%)	0.85	6/4822 (0.1%)

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
3	P	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	309	ILE	C-N	7.91	1.52	1.34
2	H	220	ASP	CG-OD1	7.89	1.43	1.25
2	H	162	ASN	CG-ND2	7.05	1.50	1.32
2	H	210	VAL	C-O	6.80	1.36	1.23
2	H	142	CYS	CB-SG	-6.11	1.71	1.82
2	H	220	ASP	CG-OD2	5.89	1.38	1.25
2	H	150	GLU	CD-OE1	5.69	1.31	1.25
1	L	81	GLU	CB-CG	5.30	1.62	1.52
2	H	218	LYS	CE-NZ	5.25	1.62	1.49
2	H	162	ASN	CG-OD1	5.20	1.35	1.24
2	H	109	VAL	CB-CG2	5.00	1.63	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	72	ASP	CB-CG-OD1	-5.92	112.97	118.30
2	H	73	ARG	NE-CZ-NH1	-5.82	117.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	72	ASP	CB-CG-OD2	5.80	123.53	118.30
2	H	4	LEU	CB-CG-CD2	5.55	120.43	111.00
2	H	108	LEU	CB-CG-CD1	5.52	120.38	111.00
2	H	101	ASP	CB-CG-OD1	5.34	123.11	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	P	309	ILE	Mainchain

## 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	L	1616	0	1554	21	0
2	H	1699	0	1624	10	0
3	P	134	0	148	8	0
4	H	81	0	0	2	0
4	L	42	0	0	0	0
All	All	3572	0	3326	35	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 (35) 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:L:27(B):ASN:HD22	1:L:28:VAL:H	1.15	0.92
1:L:132:LEU:HD12	1:L:179:LEU:HD23	1.61	0.81
1:L:48:ILE:CD1	1:L:73:LEU:HD13	2.14	0.77
1:L:167:GLN:HE21	1:L:170:ASN:HD21	1.31	0.76
1:L:48:ILE:HD11	1:L:73:LEU:CD1	2.17	0.74
2:H:89:LEU:HD13	2:H:108:LEU:HD13	1.72	0.72
1:L:26:THR:H	1:L:27(B):ASN:HD21	1.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:303:THR:OG1	3:P:304:LYS:N	2.25	0.69
1:L:48:ILE:CD1	1:L:73:LEU:CD1	2.72	0.68
1:L:120:PRO:HD3	1:L:132:LEU:CD2	2.29	0.62
2:H:110:THR:HG23	4:H:310:HOH:O	2.01	0.60
1:L:27(B):ASN:ND2	1:L:28:VAL:H	1.95	0.58
3:P:312:ARG:HB2	3:P:313:PRO:HD2	1.86	0.58
1:L:31:ASN:OD1	3:P:312:ARG:NH1	2.36	0.58
1:L:120:PRO:HD3	1:L:132:LEU:HD23	1.88	0.55
2:H:125:ALA:HB3	2:H:228:LYS:HE3	1.89	0.54
1:L:26:THR:H	1:L:27(B):ASN:ND2	2.06	0.53
1:L:48:ILE:HD13	1:L:73:LEU:HD13	1.90	0.50
1:L:167:GLN:HE21	1:L:170:ASN:ND2	2.05	0.50
1:L:2:SER:OG	1:L:97:VAL:HG11	2.12	0.49
1:L:78:LEU:HD11	1:L:104:LEU:HD21	1.96	0.48
2:H:113:SER:OG	2:H:113:SER:O	2.30	0.47
2:H:32:TYR:CZ	3:P:304:LYS:HG3	2.50	0.46
2:H:100(B):SER:O	3:P:308:LYS:NZ	2.41	0.46
2:H:187:LEU:C	2:H:187:LEU:HD12	2.37	0.45
1:L:35:TRP:HB2	1:L:48:ILE:HD12	1.98	0.45
3:P:303:THR:HG23	3:P:305:LYS:CB	2.46	0.45
1:L:167:GLN:NE2	1:L:170:ASN:HD21	2.07	0.44
2:H:31:ASP:O	3:P:304:LYS:HB2	2.18	0.44
2:H:213:LYS:N	2:H:214:PRO:CD	2.82	0.42
1:L:4:LEU:HB2	1:L:99:GLY:HA2	2.01	0.42
2:H:110:THR:CG2	4:H:310:HOH:O	2.67	0.41
1:L:31:ASN:O	1:L:66:LYS:NZ	2.54	0.41
1:L:79:ARG:CZ	1:L:81:GLU:OE2	2.69	0.41
3:P:303:THR:HG23	3:P:305:LYS:H	1.86	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%)	207 (97%)	6 (3%)	0	100	100
2	H	224/226 (99%)	208 (93%)	15 (7%)	1 (0%)	39	33
3	P	14/23 (61%)	14 (100%)	0	0	100	100
All	All	451/464 (97%)	429 (95%)	21 (5%)	1 (0%)	52	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	130	SER

### 5.3.2 Protein sidechains ⓘ

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%)	175 (97%)	5 (3%)	51	50
2	H	191/191 (100%)	182 (95%)	9 (5%)	32	27
3	P	14/19 (74%)	12 (86%)	2 (14%)	4	2
All	All	385/390 (99%)	369 (96%)	16 (4%)	36	31

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	27(B)	ASN
1	L	81	GLU
1	L	170	ASN
1	L	206	GLU
1	L	212	THR
2	H	60	SER
2	H	62	SER
2	H	81	GLN
2	H	108	LEU
2	H	127	SER
2	H	198	LEU
2	H	211	ASN

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Mol	Chain	Res	Type
2	H	216	ASN
2	H	228	LYS
3	P	303	THR
3	P	320	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27(B)	ASN
1	L	170	ASN
1	L	171	ASN
2	H	76	ASN
2	H	79	HIS
2	H	179	GLN
2	H	216	ASN

### 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 carbohydrates 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	L	215/215 (100%)	0.83	25 (11%) 6 7	32, 42, 47, 60	0
2	H	226/226 (100%)	1.22	38 (16%) 2 3	35, 41, 51, 57	0
3	P	16/23 (69%)	1.39	5 (31%) 1 1	35, 42, 57, 59	0
All	All	457/464 (98%)	1.04	68 (14%) 3 3	32, 41, 50, 60	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	130	SER	24.3
2	H	134	SER	13.9
2	H	133	THR	10.4
2	H	199	GLY	9.5
2	H	135	GLY	8.7
1	L	1	GLN	8.1
2	H	127	SER	7.5
1	L	212	THR	7.4
2	H	129	LYS	6.7
3	P	320	THR	6.6
2	H	128	SER	5.2
3	P	303	THR	5.0
1	L	168	SER	4.9
1	L	156	LYS	4.8
2	H	137	THR	4.2
2	H	167	THR	4.1
1	L	152	SER	4.0
2	H	165	ALA	3.7
2	H	205	THR	3.7
2	H	141	GLY	3.7
2	H	198	LEU	3.7
2	H	100(A)	ASP	3.7
2	H	140	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	136	GLY	3.3
1	L	86	TYR	3.2
1	L	73	LEU	3.2
1	L	75	ILE	3.2
2	H	124	LEU	3.2
1	L	67	SER	3.2
2	H	216	ASN	3.0
2	H	166	LEU	3.0
2	H	144	VAL	3.0
2	H	111	VAL	3.0
1	L	47	LEU	3.0
2	H	138	ALA	2.9
1	L	184	GLU	2.9
2	H	168	SER	2.9
1	L	35	TRP	2.8
1	L	4	LEU	2.8
2	H	1	GLU	2.8
1	L	187	LYS	2.8
1	L	79	ARG	2.7
1	L	14	THR	2.7
1	L	33	VAL	2.6
2	H	109	VAL	2.6
2	H	43	LYS	2.5
1	L	132	LEU	2.5
2	H	95	LEU	2.5
2	H	228	LYS	2.4
2	H	90	TYR	2.4
2	H	36	TRP	2.4
1	L	62	PHE	2.4
2	H	142	CYS	2.4
1	L	190	LYS	2.4
2	H	80	LEU	2.3
1	L	91	TRP	2.3
3	P	307	ILE	2.2
3	P	309	ILE	2.2
1	L	153	SER	2.2
1	L	128	ASN	2.2
2	H	143	LEU	2.2
2	H	229	SER	2.2
2	H	139	ALA	2.1
2	H	81	GLN	2.1
3	P	314	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	96	TRP	2.1
1	L	155	VAL	2.0
2	H	113	SER	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 carbohydrates 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.