Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 07:07 PM EDT

PDB ID	:	2B1A
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:

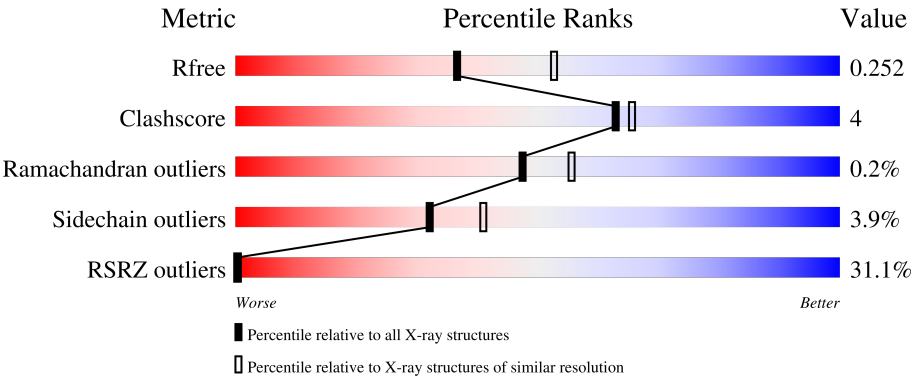
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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	26% 87% 13%
2	H	226	36% 89% 11%
3	P	23	22% 48% 22% 30%

2 Entry composition (i)

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			

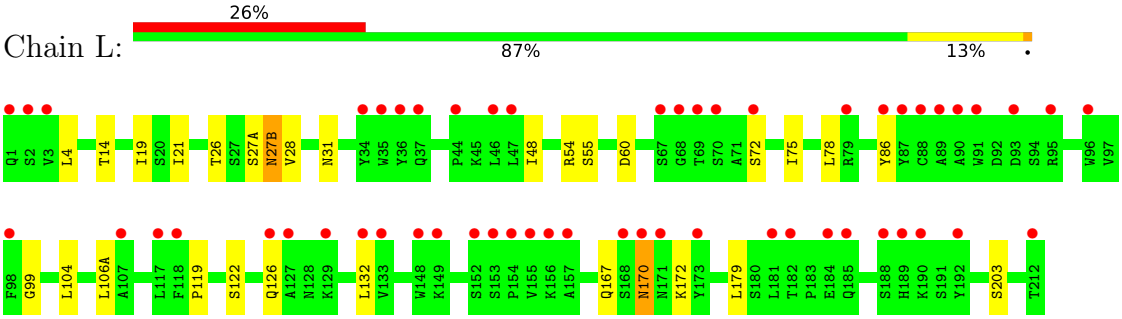
- Molecule 4 is water.

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

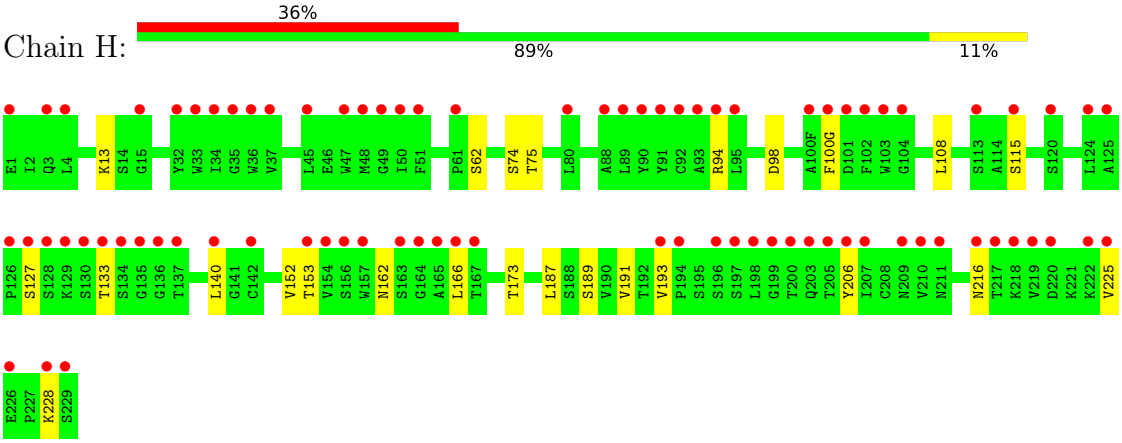
3 Residue-property plots (i)

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.

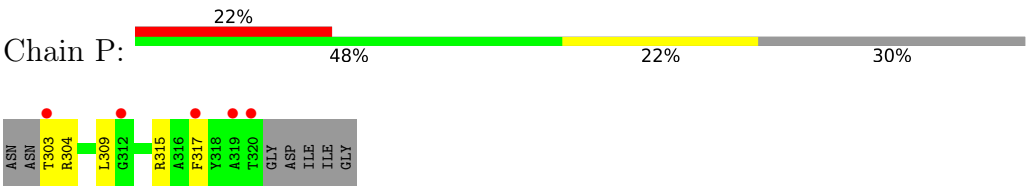
• Molecule 1: Fab 2219, light chain



• Molecule 2: Fab 2219, heavy chain



• Molecule 3: UG1033 peptide of Exterior membrane glycoprotein GP120



4 Data and refinement statistics (i)

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 31.36 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (31.31-2.35) 98.5 (31.36-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [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)	0.28 , 61.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	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.*

[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	L	0.47	0/1660	0.60	0/2269
2	H	0.67	3/1744 (0.2%)	0.69	1/2373 (0.0%)
3	P	1.82	1/128 (0.8%)	1.07	0/171
All	All	0.67	4/3532 (0.1%)	0.67	1/4813 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	309	LEU	C-N	18.86	1.67	1.33
2	H	162	ASN	CG-ND2	9.35	1.56	1.32
2	H	162	ASN	CG-OD1	8.48	1.42	1.24
2	H	13	LYS	CD-CE	5.12	1.64	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	98	ASP	CB-CG-OD1	5.18	122.97	118.30

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	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	29	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 (29) 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:167:GLN:HE21	1:L:170:ASN:HD21	1.52	0.57
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:170:ASN:HD22	1:L:170:ASN:C	2.11	0.52
2:H:187:LEU:C	2:H:187:LEU:HD12	2.30	0.52
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:173:THR:HA	2:H:189:SER:HA	2.03	0.41
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%)	34 38
3	P	14/23 (61%)	13 (93%)	1 (7%)	0	100 100
All	All	451/464 (97%)	429 (95%)	21 (5%)	1 (0%)	47 55

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%)	38 46
2	H	191/191 (100%)	183 (96%)	8 (4%)	30 37
3	P	12/17 (71%)	11 (92%)	1 (8%)	11 11
All	All	383/388 (99%)	368 (96%)	15 (4%)	32 41

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	27(A)	SER
1	L	27(B)	ASN
1	L	55	SER
1	L	72	SER
1	L	170	ASN
1	L	203	SER
2	H	62	SER
2	H	108	LEU
2	H	115	SER
2	H	133	THR
2	H	152	VAL
2	H	153	THR
2	H	216	ASN
2	H	228	LYS
3	P	317	PHE

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

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

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)

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, 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	L	215/215 (100%)	1.54	55 (25%)	0 1	65, 71, 74, 80	0
2	H	226/226 (100%)	2.05	82 (36%)	0 0	64, 70, 77, 81	0
3	P	16/23 (69%)	2.52	5 (31%)	0 0	66, 71, 83, 87	0
All	All	457/464 (98%)	1.83	142 (31%)	0 0	64, 71, 77, 87	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	133	THR	14.3
2	H	165	ALA	14.0
3	P	320	THR	13.3
2	H	136	GLY	12.5
2	H	130	SER	11.6
2	H	166	LEU	10.8
2	H	134	SER	9.6
2	H	198	LEU	7.8
3	P	303	THR	7.5
2	H	135	GLY	7.4
2	H	229	SER	7.4
2	H	205	THR	7.1
2	H	100(G)	PHE	6.4
2	H	222	LYS	6.3
1	L	156	LYS	6.0
2	H	207	ILE	5.9
2	H	128	SER	5.9
2	H	219	VAL	5.7
2	H	217	THR	5.7
1	L	36	TYR	5.7
2	H	129	LYS	5.6
2	H	210	VAL	5.5
2	H	37	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	197	SER	5.4
2	H	216	ASN	5.2
1	L	96	TRP	5.1
2	H	157	TRP	5.0
2	H	206	TYR	4.9
2	H	93	ALA	4.8
2	H	45	LEU	4.7
2	H	103	TRP	4.7
2	H	164	GLY	4.6
1	L	190	LYS	4.6
1	L	47	LEU	4.4
1	L	67	SER	4.3
1	L	1	GLN	4.2
2	H	91	TYR	4.2
1	L	168	SER	4.1
1	L	126	GLN	4.1
2	H	95	LEU	4.1
1	L	154	PRO	4.0
1	L	98	PHE	4.0
1	L	192	TYR	4.0
2	H	193	VAL	4.0
1	L	107	ALA	3.9
2	H	218	LYS	3.9
3	P	319	ALA	3.9
1	L	184	GLU	3.8
2	H	126	PRO	3.8
1	L	212	THR	3.8
2	H	211	ASN	3.8
1	L	155	VAL	3.8
1	L	3	VAL	3.7
1	L	157	ALA	3.7
1	L	70	SER	3.6
2	H	142	CYS	3.5
1	L	185	GLN	3.5
2	H	92	CYS	3.5
2	H	124	LEU	3.5
1	L	87	TYR	3.5
1	L	72	SER	3.5
1	L	89	ALA	3.4
1	L	118	PHE	3.4
2	H	196	SER	3.4
2	H	226	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	L	68	GLY	3.4
1	L	91	TRP	3.3
2	H	36	TRP	3.3
1	L	182	THR	3.2
2	H	100(F)	ALA	3.2
1	L	188	SER	3.1
2	H	35	GLY	3.1
2	H	125	ALA	3.1
1	L	129	LYS	3.1
2	H	47	TRP	3.0
1	L	2	SER	3.0
2	H	228	LYS	3.0
1	L	46	LEU	3.0
2	H	127	SER	2.9
2	H	50	ILE	2.8
2	H	34	ILE	2.8
1	L	133	VAL	2.8
1	L	189	HIS	2.8
1	L	171	ASN	2.8
1	L	153	SER	2.7
1	L	149	LYS	2.7
1	L	34	TYR	2.7
2	H	104	GLY	2.7
1	L	35	TRP	2.7
2	H	194	PRO	2.6
2	H	80	LEU	2.6
1	L	127	ALA	2.6
1	L	132	LEU	2.6
2	H	4	LEU	2.6
2	H	209	ASN	2.6
2	H	94	ARG	2.6
1	L	173	TYR	2.6
1	L	93	ASP	2.5
2	H	48	MET	2.5
2	H	203	GLN	2.5
1	L	86	TYR	2.5
1	L	170	ASN	2.5
3	P	317	PHE	2.5
1	L	152	SER	2.5
1	L	88	CYS	2.5
2	H	199	GLY	2.5
2	H	167	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	H	137	THR	2.4
2	H	49	GLY	2.4
1	L	95	ARG	2.4
1	L	117	LEU	2.4
2	H	90	TYR	2.4
2	H	154	VAL	2.4
2	H	225	VAL	2.4
2	H	113	SER	2.3
2	H	140	LEU	2.3
2	H	120	SER	2.3
2	H	1	GLU	2.3
2	H	102	PHE	2.3
2	H	220	ASP	2.2
2	H	163	SER	2.2
1	L	69	THR	2.2
2	H	32	TYR	2.2
2	H	61	PRO	2.2
1	L	148	TRP	2.2
2	H	33	TRP	2.2
3	P	312	GLY	2.2
1	L	44	PRO	2.1
1	L	37	GLN	2.1
1	L	90	ALA	2.1
2	H	51	PHE	2.1
2	H	115	SER	2.1
1	L	181	LEU	2.0
2	H	88	ALA	2.0
2	H	156	SER	2.0
1	L	79	ARG	2.0
2	H	3	GLN	2.0
2	H	200	THR	2.0
2	H	89	LEU	2.0
2	H	15	GLY	2.0
2	H	101	ASP	2.0
2	H	153	THR	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.