



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:21 PM UTC

PDB ID : 6MTT / pdb_00006mtt
Title : Crystal structure of VRC46.01 Fab in complex with gp41 peptide
Authors : Kwon, Y.D.; Druz, A.; Law, W.H.; Peng, D.; Veradi, R.; Doria-Rose, N.A.;
Kwong, P.D.
Deposited on : 2018-10-21
Resolution : 1.70 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

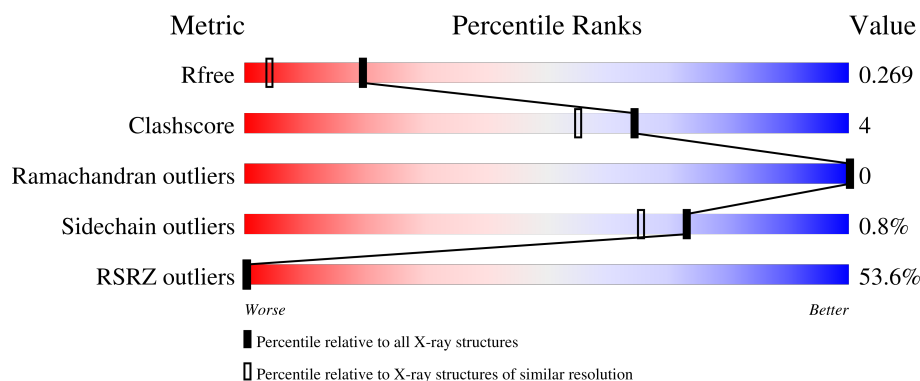
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	214	48% 91% 7%
2	H	224	56% 89% 9%
3	P	28	46% 46% 21% 32%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3676 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 Antibody VRC46.01 Fb light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1601	1000	265	329	7			

- Molecule 2 is a protein called Antibody VRC46.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1620	1033	267	314	6			

- Molecule 3 is a protein called RV217 founder virus gp41 peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	19	Total	C	N	O	0	0	0
			182	130	27	25			

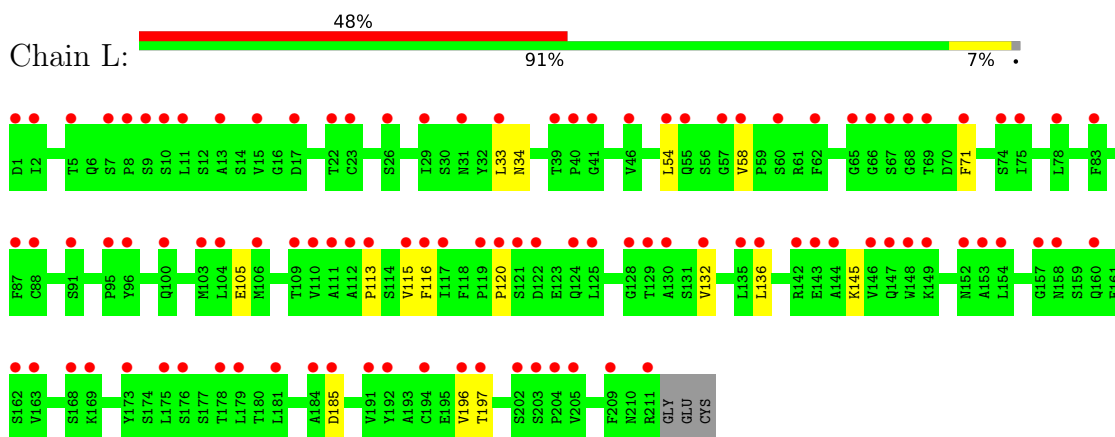
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	145	Total	O	0	0
			145	145		
4	H	112	Total	O	0	0
			112	112		
4	P	16	Total	O	0	0
			16	16		

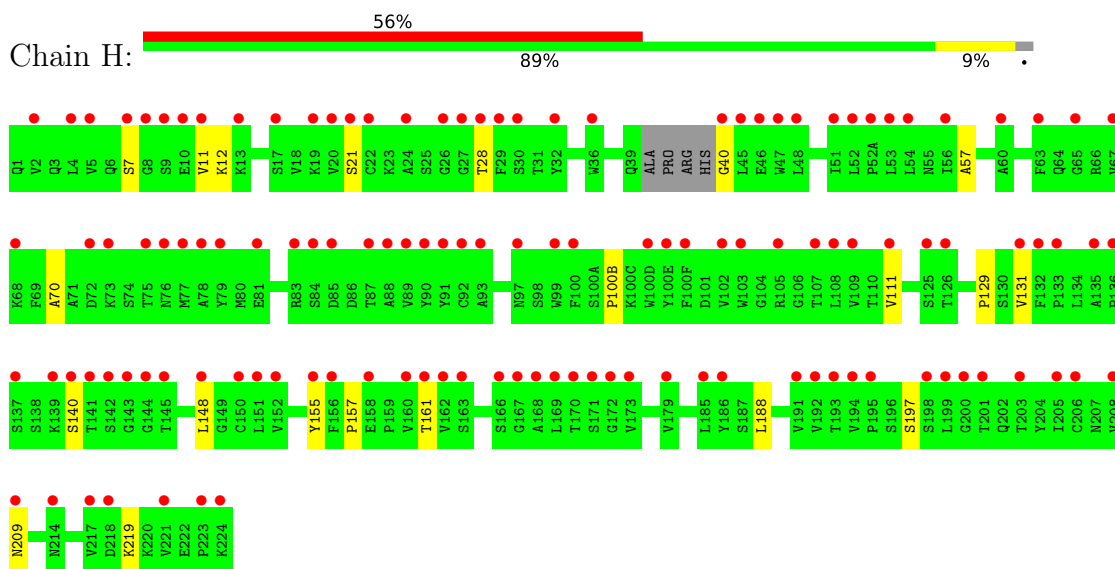
3 Residue-property plots

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: Antibody VRC46.01 Fb light chain



- Molecule 2: Antibody VRC46.01 Fab heavy chain



- Molecule 3: RV217 founder virus gp41 peptide



ASN	ASN
GLU	K665
LYS	W666
GLU	A667
LEU	S668
LEU	L669
GLU	W670
LEU	N671
LEU	W672
LEU	F673
LEU	D674
ASP	I675
	W676
	L679
	W680
	Y681
	I682
	K683

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.60Å 49.16Å 99.97Å 90.00° 97.10° 90.00°	Depositor
Resolution (Å)	41.26 – 1.70 41.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	94.4 (41.26-1.70) 94.4 (41.26-1.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.235 , 0.265 0.242 , 0.269	Depositor DCC
R_{free} test set	2000 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3676	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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	L	0.19	0/1636	0.44	0/2223
2	H	0.17	0/1663	0.40	0/2271
3	P	0.17	0/193	0.36	0/266
All	All	0.18	0/3492	0.42	0/4760

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	L	1601	0	1533	10	0
2	H	1620	0	1549	15	0
3	P	182	0	166	5	0
4	H	112	0	0	5	1
4	L	145	0	0	1	1
4	P	16	0	0	1	0
All	All	3676	0	3248	26	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 4.

All (26) 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)
2:H:28:THR:O	4:H:301:HOH:O	1.98	0.81
2:H:40:GLY:N	4:H:303:HOH:O	2.15	0.78
1:L:136:LEU:HD21	1:L:196:VAL:HG21	1.67	0.77
2:H:70:ALA:HB2	3:P:665:LYS:HA	1.71	0.73
2:H:197:SER:OG	4:H:302:HOH:O	2.08	0.71
1:L:185:ASP:OD1	4:L:301:HOH:O	2.12	0.65
2:H:7:SER:OG	4:H:304:HOH:O	2.15	0.64
2:H:11:VAL:HG21	2:H:157:PRO:HG3	1.85	0.57
1:L:120:PRO:HD3	1:L:132:VAL:HG22	1.88	0.55
2:H:131:VAL:O	2:H:219:LYS:NZ	2.39	0.54
2:H:219:LYS:NZ	4:H:305:HOH:O	2.18	0.54
3:P:678:TRP:CE2	3:P:679:LEU:HG	2.45	0.52
3:P:683:LYS:O	4:P:701:HOH:O	2.19	0.51
1:L:116:PHE:HD1	2:H:140:SER:HA	1.76	0.49
1:L:33:LEU:HG	1:L:34:ASN:N	2.27	0.49
2:H:7:SER:HB3	2:H:21:SER:HB3	1.97	0.46
2:H:100(B):PRO:HD3	3:P:680:TRP:CD2	2.53	0.44
2:H:57:ALA:HB3	3:P:669:LEU:HD23	2.00	0.44
1:L:33:LEU:HD22	1:L:71:PHE:CG	2.53	0.43
2:H:129:PRO:HB3	2:H:155:TYR:HB3	2.00	0.43
1:L:145:LYS:HB2	1:L:197:THR:HB	2.00	0.43
1:L:54:LEU:HG	1:L:58:VAL:HB	2.01	0.43
2:H:12:LYS:O	2:H:111:VAL:HA	2.19	0.43
1:L:113:PRO:HB2	1:L:136:LEU:HD22	2.00	0.42
2:H:161:THR:OG1	2:H:209:ASN:HB2	2.20	0.42
1:L:115:VAL:HG22	1:L:136:LEU:CD2	2.50	0.42

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)
4:L:315:HOH:O	4:H:403:HOH:O[1_565]	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	L	209/214 (98%)	204 (98%)	5 (2%)	0	100	100
2	H	216/224 (96%)	211 (98%)	5 (2%)	0	100	100
3	P	17/28 (61%)	16 (94%)	1 (6%)	0	100	100
All	All	442/466 (95%)	431 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	183/188 (97%)	182 (100%)	1 (0%)	81	76
2	H	176/190 (93%)	174 (99%)	2 (1%)	65	54
3	P	17/27 (63%)	17 (100%)	0	100	100
All	All	376/405 (93%)	373 (99%)	3 (1%)	73	65

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	105	GLU
2	H	148	LEU
2	H	188	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	79	GLN
2	H	76	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 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	L	211/214 (98%)	2.11	102 (48%) 0 0	28, 39, 58, 69	0
2	H	220/224 (98%)	2.24	126 (57%) 0 0	29, 40, 68, 89	0
3	P	19/28 (67%)	2.63	13 (68%) 0 0	38, 43, 75, 76	0
All	All	450/466 (96%)	2.20	241 (53%) 0 0	28, 40, 65, 89	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	666	TRP	6.3
1	L	67	SER	6.2
1	L	154	LEU	5.6
2	H	29	PHE	5.1
1	L	146	VAL	5.0
2	H	198	SER	4.8
3	P	667	ALA	4.7
1	L	1	ASP	4.6
2	H	199	LEU	4.5
1	L	181	LEU	4.5
2	H	144	GLY	4.4
2	H	92	CYS	4.4
2	H	140	SER	4.4
1	L	104	LEU	4.4
2	H	125	SER	4.3
3	P	682	ILE	4.3
2	H	99	TRP	4.2
2	H	20	VAL	4.2
2	H	22	CYS	4.2
2	H	161	THR	4.2
2	H	150	CYS	4.2
2	H	67	VAL	4.1
1	L	184	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	10	SER	4.0
1	L	69	THR	4.0
2	H	136	PRO	4.0
2	H	40	GLY	4.0
2	H	36	TRP	3.9
1	L	202	SER	3.9
1	L	203	SER	3.9
1	L	23	CYS	3.9
2	H	27	GLY	3.9
3	P	665	LYS	3.9
2	H	90	TYR	3.8
1	L	153	ALA	3.8
2	H	201	THR	3.8
1	L	58	VAL	3.8
2	H	89	VAL	3.8
1	L	11	LEU	3.8
3	P	683	LYS	3.7
1	L	116	PHE	3.7
1	L	115	VAL	3.7
2	H	224	LYS	3.7
2	H	5	VAL	3.7
2	H	21	SER	3.7
2	H	160	VAL	3.6
1	L	185	ASP	3.6
2	H	54	LEU	3.6
2	H	8	GLY	3.6
1	L	204	PRO	3.6
2	H	193	THR	3.6
1	L	15	VAL	3.6
1	L	205	VAL	3.6
1	L	112	ALA	3.5
2	H	45	LEU	3.5
2	H	73	LYS	3.5
2	H	47	TRP	3.5
2	H	100(D)	TRP	3.5
1	L	39	THR	3.5
2	H	194	VAL	3.4
1	L	129	THR	3.4
1	L	111	ALA	3.4
1	L	125	LEU	3.4
1	L	135	LEU	3.4
2	H	148	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	P	678	TRP	3.4
1	L	109	THR	3.3
3	P	679	LEU	3.3
2	H	142	SER	3.3
2	H	107	THR	3.3
2	H	126	THR	3.3
1	L	22	THR	3.3
2	H	217	VAL	3.3
2	H	76	ASN	3.3
2	H	11	VAL	3.2
1	L	60	SER	3.2
2	H	79	TYR	3.2
1	L	29	ILE	3.2
2	H	9	SER	3.2
1	L	122	ASP	3.2
1	L	144	ALA	3.1
2	H	100(F)	PHE	3.1
2	H	91	TYR	3.1
1	L	120	PRO	3.1
2	H	171	SER	3.0
1	L	197	THR	3.0
2	H	88	ALA	3.0
2	H	168	ALA	3.0
1	L	26	SER	3.0
1	L	209	PHE	3.0
2	H	63	PHE	3.0
2	H	24	ALA	3.0
1	L	8	PRO	3.0
2	H	218	ASP	2.9
1	L	96	TYR	2.9
1	L	13	ALA	2.9
1	L	136	LEU	2.9
2	H	52	LEU	2.9
1	L	83	PHE	2.9
2	H	132	PHE	2.9
1	L	68	GLY	2.9
2	H	209	ASN	2.9
2	H	78	ALA	2.8
1	L	106	MET	2.8
3	P	675	ILE	2.8
2	H	170	THR	2.8
2	H	100	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	167	GLY	2.8
1	L	54	LEU	2.8
1	L	87	PHE	2.8
2	H	93	ALA	2.8
1	L	211	ARG	2.8
2	H	77	MET	2.8
2	H	156	PHE	2.7
1	L	191	VAL	2.7
2	H	53	LEU	2.7
2	H	7	SER	2.7
2	H	84	SER	2.7
2	H	200	GLY	2.7
1	L	130	ALA	2.7
1	L	71	PHE	2.7
2	H	103	TRP	2.7
2	H	155	TYR	2.7
2	H	13	LYS	2.7
1	L	196	VAL	2.7
2	H	28	THR	2.7
2	H	102	VAL	2.7
2	H	111	VAL	2.7
2	H	105	ARG	2.6
1	L	176	SER	2.6
1	L	57	GLY	2.6
1	L	175	LEU	2.6
2	H	109	VAL	2.6
2	H	83	ARG	2.6
1	L	149	LYS	2.6
1	L	143	GLU	2.6
1	L	95	PRO	2.6
2	H	195	PRO	2.6
1	L	142	ARG	2.6
1	L	147	GLN	2.6
1	L	160	GLN	2.6
2	H	108	LEU	2.6
2	H	173	VAL	2.6
2	H	133	PRO	2.6
2	H	158	GLU	2.6
1	L	110	VAL	2.5
2	H	131	VAL	2.5
1	L	117	ILE	2.5
1	L	74	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	17	SER	2.5
2	H	10	GLU	2.5
1	L	179	LEU	2.5
1	L	192	TYR	2.5
1	L	113	PRO	2.5
2	H	2	VAL	2.5
2	H	52(A)	PRO	2.5
2	H	214	ASN	2.5
1	L	33	LEU	2.5
2	H	32	TYR	2.5
2	H	172	GLY	2.5
2	H	191	VAL	2.5
2	H	208	VAL	2.5
1	L	132	VAL	2.4
1	L	162	SER	2.4
2	H	30	SER	2.4
2	H	141	THR	2.4
2	H	166	SER	2.4
1	L	152	ASN	2.4
1	L	9	SER	2.4
1	L	31	ASN	2.4
2	H	85	ASP	2.4
1	L	103	MET	2.4
2	H	97	ASN	2.4
3	P	673	PHE	2.4
1	L	17	ASP	2.4
2	H	81	GLU	2.4
2	H	179	VAL	2.4
2	H	143	GLY	2.3
2	H	163	SER	2.3
2	H	60	ALA	2.3
1	L	148	TRP	2.3
1	L	168	SER	2.3
2	H	145	THR	2.3
2	H	100(E)	TYR	2.3
1	L	88	CYS	2.3
1	L	194	CYS	2.3
2	H	206	CYS	2.3
2	H	68	LYS	2.3
1	L	65	GLY	2.3
1	L	157	GLY	2.3
2	H	26	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	221	VAL	2.3
3	P	670	TRP	2.2
3	P	672	TRP	2.2
1	L	178	THR	2.2
1	L	78	LEU	2.2
2	H	48	LEU	2.2
1	L	169	LYS	2.2
1	L	128	GLY	2.2
2	H	87	THR	2.2
2	H	203	THR	2.2
2	H	135	ALA	2.2
1	L	7	SER	2.2
2	H	151	LEU	2.2
1	L	173	TYR	2.2
2	H	186	TYR	2.2
2	H	51	ILE	2.2
1	L	40	PRO	2.2
2	H	19	LYS	2.2
2	H	139	LYS	2.2
1	L	91	SER	2.2
2	H	4	LEU	2.2
2	H	205	ILE	2.2
2	H	223	PRO	2.2
1	L	121	SER	2.2
2	H	72	ASP	2.1
2	H	152	VAL	2.1
3	P	671	ASN	2.1
1	L	100	GLN	2.1
1	L	2	ILE	2.1
1	L	46	VAL	2.1
2	H	192	VAL	2.1
1	L	41	GLY	2.1
1	L	124	GLN	2.1
1	L	5	THR	2.1
1	L	119	PRO	2.1
1	L	163	VAL	2.1
1	L	158	ASN	2.1
2	H	137	SER	2.1
2	H	185	LEU	2.1
1	L	62	PHE	2.1
2	H	56	ILE	2.1
3	P	681	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	66	GLY	2.0
2	H	65	GLY	2.0
2	H	46	GLU	2.0
1	L	55	GLN	2.0
2	H	162	VAL	2.0
2	H	169	LEU	2.0
2	H	75	THR	2.0
1	L	75	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.