



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 04:26 am BST

PDB ID : 5AAM  
Title : Structure of a redesigned cross-reactive antibody to dengue virus with increased in vivo potency  
Authors : Wong, Y.H.; Robinson, L.N.; Lescar, J.; Sasisekharan, R.  
Deposited on : 2015-07-27  
Resolution : 2.49 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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

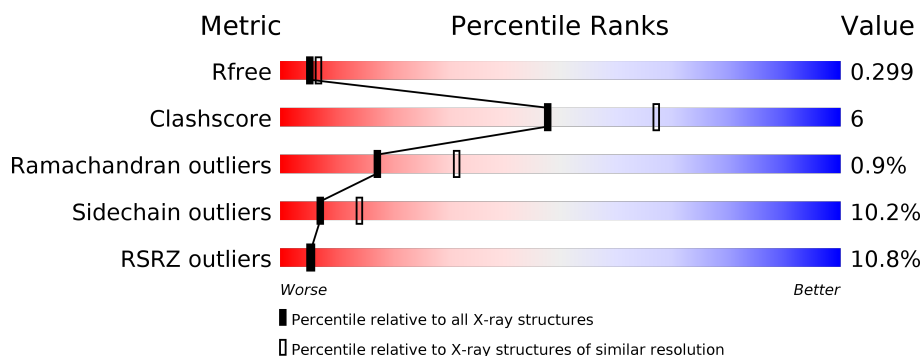
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	A	251	<div> <div>5%</div> <div> <div>73%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	251	<div> <div>%</div> <div> <div>71%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
2	C	115	<div> <div>34%</div> <div> <div>60%</div> <div>22%</div> <div>•</div> <div>17%</div> </div> </div>
2	J	115	<div> <div>14%</div> <div> <div>68%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5137 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 SCFV513.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	0	0
			1775	1113	306	346	10			
1	B	227	Total	C	N	O	S	0	0	0
			1773	1113	306	344	10			

- Molecule 2 is a protein called ENVELOPE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	95	Total	C	N	O	S	0	0	0
			725	458	123	140	4			
2	J	96	Total	C	N	O	S	0	0	0
			737	467	124	142	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	292	MET	-	expression tag	UNP U3N5N6
C	401	HIS	-	expression tag	UNP U3N5N6
C	402	HIS	-	expression tag	UNP U3N5N6
C	403	HIS	-	expression tag	UNP U3N5N6
C	404	HIS	-	expression tag	UNP U3N5N6
C	405	HIS	-	expression tag	UNP U3N5N6
C	406	HIS	-	expression tag	UNP U3N5N6
C	357	LEU	PHE	conflict	UNP U3N5N6
C	384	ASN	ASP	conflict	UNP U3N5N6
J	292	MET	-	expression tag	UNP U3N5N6
J	401	HIS	-	expression tag	UNP U3N5N6
J	402	HIS	-	expression tag	UNP U3N5N6
J	403	HIS	-	expression tag	UNP U3N5N6
J	404	HIS	-	expression tag	UNP U3N5N6
J	405	HIS	-	expression tag	UNP U3N5N6
J	406	HIS	-	expression tag	UNP U3N5N6

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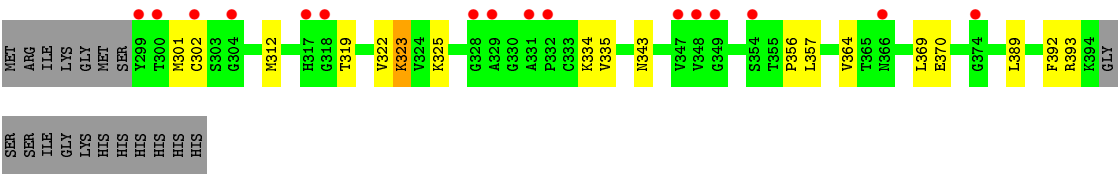
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Chain	Residue	Modelled	Actual	Comment	Reference
J	357	LEU	PHE	conflict	UNP U3N5N6
J	384	ASN	ASP	conflict	UNP U3N5N6

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	0	0
3	B	56	Total O 56 56	0	0
3	C	11	Total O 11 11	0	0
3	J	11	Total O 11 11	0	0





SER  
SER  
ILE  
GLY  
LYS  
HIS  
HIS  
HIS  
HIS  
HIS  
HIS

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.64Å 55.89Å 87.05Å 90.00° 104.58° 90.00°	Depositor
Resolution (Å)	29.55 – 2.49 29.55 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.55-2.49) 98.4 (29.55-2.49)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.51Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0	Depositor
R, $R_{free}$	0.220 , 0.270 0.236 , 0.299	Depositor DCC
$R_{free}$ test set	1188 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.7	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5137	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, 0.333 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	A	0.52	0/1815	0.75	0/2460
1	B	0.51	0/1813	0.77	0/2457
2	C	0.52	0/738	0.76	0/999
2	J	0.50	0/751	0.73	0/1017
All	All	0.51	0/5117	0.76	0/6933

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	A	1775	0	1710	27	0
1	B	1773	0	1713	23	0
2	C	725	0	732	9	0
2	J	737	0	741	7	0
3	A	49	0	0	0	0
3	B	56	0	0	3	0
3	C	11	0	0	0	0
3	J	11	0	0	0	0
All	All	5137	0	4896	60	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 6.



All (60) 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:A:67:ARG:NH2	1:A:90:ASP:OD2	2.19	0.75
1:B:67:ARG:NH2	1:B:90:ASP:OD2	2.20	0.74
1:B:105:TYR:HE1	2:J:325:LYS:HZ2	1.39	0.68
1:A:214:LEU:HD21	1:A:240:LEU:HD21	1.82	0.60
1:B:214:LEU:HD21	1:B:240:LEU:HD21	1.85	0.59
1:A:38:ARG:NH2	1:A:64:LEU:HD21	2.17	0.59
2:C:335:VAL:HB	2:C:356:PRO:HB2	1.88	0.55
2:C:380:ILE:HB	2:C:387:LEU:HB2	1.88	0.55
1:A:178:GLN:NE2	1:B:178:GLN:NE2	2.54	0.55
2:J:335:VAL:HB	2:J:356:PRO:HB2	1.88	0.54
2:J:301:MET:HA	2:J:334:LYS:HB2	1.90	0.53
2:C:301:MET:HA	2:C:334:LYS:HB2	1.91	0.52
2:C:306:PHE:HA	2:C:325:LYS:O	2.11	0.50
1:A:71:THR:OG1	1:A:80:TYR:HB2	2.12	0.50
1:B:6:VAL:HG23	3:B:2002:HOH:O	2.12	0.50
1:A:36:TRP:HD1	1:A:70:MET:CE	2.24	0.49
1:B:97:ALA:HB1	1:B:103:PHE:HB3	1.95	0.48
1:B:147:LEU:HD13	1:B:242:ILE:HD12	1.96	0.48
1:A:33:TYR:OH	2:C:311:GLU:HB2	2.14	0.48
2:C:341:ASP:HB2	2:C:346:LYS:HB2	1.96	0.48
1:B:31:ASP:HB3	2:J:323:LYS:HG2	1.96	0.47
1:A:32:VAL:HG11	1:A:98:ARG:HG3	1.96	0.47
2:J:319:THR:HG22	2:J:370:GLU:HG3	1.95	0.47
1:A:4:GLN:OE1	1:A:5:LEU:N	2.44	0.47
1:B:36:TRP:HD1	1:B:70:MET:CE	2.28	0.47
1:A:97:ALA:HB1	1:A:103:PHE:HB3	1.98	0.46
1:B:170:HIS:O	1:B:224:CYS:HA	2.16	0.45
1:A:146:SER:O	1:A:149:GLN:HB2	2.17	0.45
2:J:312:MET:HE1	2:J:322:VAL:HG13	1.97	0.45
1:A:147:LEU:HD13	1:A:242:ILE:HD12	1.98	0.45
2:C:324:VAL:HG11	2:C:380:ILE:HG12	1.99	0.45
1:B:184:ILE:HA	1:B:189:GLU:O	2.17	0.45
1:A:98:ARG:HB3	1:A:105:TYR:HB2	1.99	0.45
2:C:373:PHE:HA	2:C:393:ARG:HB3	1.98	0.45
1:B:197:ARG:O	1:B:211:ILE:HA	2.17	0.44
3:B:2040:HOH:O	2:J:389:LEU:HA	2.16	0.44
1:A:147:LEU:CD1	1:A:242:ILE:HD12	2.47	0.44
1:A:244:ARG:HH22	1:B:215:GLN:NE2	2.16	0.44
1:B:147:LEU:CD1	1:B:242:ILE:HD12	2.47	0.44
1:B:145:VAL:HG12	1:B:214:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:CG1	1:A:214:LEU:HG	2.49	0.43
1:A:38:ARG:HH22	1:A:64:LEU:HD21	1.84	0.43
1:A:168:PHE:HB2	1:A:228:ASN:HB3	2.01	0.42
1:A:145:VAL:HG12	1:A:214:LEU:HG	2.01	0.42
1:A:15:PRO:HA	1:A:86:LEU:O	2.19	0.42
1:B:98:ARG:HB3	1:B:105:TYR:HB2	2.02	0.42
1:A:184:ILE:HA	1:A:189:GLU:O	2.19	0.42
1:A:163:LYS:HB2	1:A:228:ASN:HB2	2.02	0.42
1:A:67:ARG:HH22	1:A:90:ASP:CG	2.23	0.42
1:B:145:VAL:CG1	1:B:214:LEU:HG	2.50	0.42
1:B:168:PHE:HB2	1:B:228:ASN:HB3	2.01	0.41
1:B:226:ARG:HH22	1:B:229:GLU:HB3	1.85	0.41
1:B:134:ILE:HD12	3:B:2033:HOH:O	2.20	0.41
1:B:15:PRO:HA	1:B:86:LEU:O	2.20	0.41
1:A:160:ASN:H	1:A:160:ASN:HD22	1.68	0.41
1:B:163:LYS:HB2	1:B:228:ASN:HB2	2.03	0.41
1:A:105:TYR:CE1	2:C:325:LYS:HE3	2.56	0.41
1:A:20:LYS:HB2	1:A:82:GLU:OE1	2.21	0.40
1:A:32:VAL:HG11	1:A:98:ARG:CG	2.51	0.40
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.87	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	A	224/251 (89%)	214 (96%)	8 (4%)	2 (1%)	17	31
1	B	223/251 (89%)	215 (96%)	6 (3%)	2 (1%)	17	31
2	C	93/115 (81%)	80 (86%)	11 (12%)	2 (2%)	6	10
2	J	94/115 (82%)	84 (89%)	10 (11%)	0	100	100
All	All	634/732 (87%)	593 (94%)	35 (6%)	6 (1%)	17	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	316	GLN
2	C	318	GLY
1	A	161	VAL
1	B	161	VAL
1	A	204	GLY
1	B	204	GLY

### 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	A	191/202 (95%)	175 (92%)	16 (8%)	11	21
1	B	191/202 (95%)	170 (89%)	21 (11%)	6	12
2	C	82/99 (83%)	71 (87%)	11 (13%)	4	7
2	J	83/99 (84%)	75 (90%)	8 (10%)	8	16
All	All	547/602 (91%)	491 (90%)	56 (10%)	7	14

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	14	LYS
1	A	32	VAL
1	A	50	ARG
1	A	83	LEU
1	A	98	ARG
1	A	133	ASP
1	A	137	THR
1	A	147	LEU
1	A	160	ASN
1	A	178	GLN
1	A	188	SER
1	A	196	ASP
1	A	206	ASP

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Mol	Chain	Res	Type
1	A	214	LEU
1	A	242	ILE
1	B	14	LYS
1	B	38	ARG
1	B	50	ARG
1	B	63	LYS
1	B	73	ASP
1	B	75	SER
1	B	83	LEU
1	B	98	ARG
1	B	133	ASP
1	B	137	THR
1	B	145	VAL
1	B	147	LEU
1	B	150	ARG
1	B	178	GLN
1	B	188	SER
1	B	196	ASP
1	B	206	ASP
1	B	214	LEU
1	B	217	GLU
1	B	239	LYS
1	B	242	ILE
2	C	302	CYS
2	C	317	HIS
2	C	320	THR
2	C	321	VAL
2	C	325	LYS
2	C	357	LEU
2	C	361	THR
2	C	364	VAL
2	C	369	LEU
2	C	375	ASP
2	C	389	LEU
2	J	302	CYS
2	J	323	LYS
2	J	343	ASN
2	J	357	LEU
2	J	364	VAL
2	J	369	LEU
2	J	392	PHE
2	J	393	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	178	GLN
1	B	178	GLN
1	B	215	GLN
2	J	390	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 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 [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, 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	A	228/251 (90%)	0.33	12 (5%) 26 28	45, 73, 106, 128	1 (0%)
1	B	227/251 (90%)	0.01	3 (1%) 77 79	46, 67, 92, 127	1 (0%)
2	C	95/115 (82%)	2.10	39 (41%) 0 0	80, 130, 152, 163	1 (1%)
2	J	96/115 (83%)	1.09	16 (16%) 1 1	74, 114, 137, 145	1 (1%)
All	All	646/732 (88%)	0.59	70 (10%) 5 5	45, 79, 136, 163	4 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	348	VAL	7.4
2	C	349	GLY	7.3
2	C	384	ASN	6.7
2	C	343	ASN	6.2
2	C	317	HIS	6.1
2	J	348	VAL	5.7
2	C	344	LYS	5.7
2	C	331	ALA	5.6
1	B	132	SER	5.3
2	C	359	GLU	5.0
2	C	377	TYR	5.0
2	J	300	THR	4.6
2	C	360	ASN	4.4
2	C	366	ASN	4.4
2	J	328	GLY	4.3
2	J	329	ALA	4.1
1	A	134	ILE	4.1
2	C	381	GLY	4.1
2	J	317	HIS	3.9
2	J	299	TYR	3.8
2	C	330	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	316	GLN	3.6
1	A	133	ASP	3.6
1	A	194	VAL	3.5
2	C	332	PRO	3.4
2	J	366	ASN	3.4
2	C	342	VAL	3.4
2	C	345	GLU	3.2
2	C	392	PHE	3.2
1	A	116	SER	3.2
2	C	391	TRP	3.2
2	C	374	GLY	3.1
1	A	102	GLY	3.1
2	C	346	LYS	3.1
2	C	347	VAL	3.1
1	B	133	ASP	3.0
2	J	318	GLY	3.0
2	C	383	GLY	2.9
2	C	300	THR	2.9
2	J	332	PRO	2.8
2	J	331	ALA	2.8
2	C	302	CYS	2.8
2	J	347	VAL	2.7
2	C	373	PHE	2.6
1	A	104	ALA	2.6
2	C	340	ARG	2.6
2	C	372	PRO	2.5
2	J	354	SER	2.4
1	B	192	TRP	2.4
1	A	132	SER	2.4
2	C	350	ARG	2.4
2	C	301	MET	2.4
2	J	349	GLY	2.4
2	J	374	GLY	2.4
1	A	227	SER	2.4
2	C	337	ILE	2.3
2	C	375	ASP	2.3
2	C	352	ILE	2.3
2	C	357	LEU	2.3
2	J	302	CYS	2.3
1	A	192	TRP	2.2
1	A	214	LEU	2.2
2	C	326	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	169	MET	2.2
2	C	315	THR	2.2
2	J	304	GLY	2.2
2	C	378	ILE	2.1
2	C	387	LEU	2.1
2	C	338	GLU	2.1
1	A	17	ALA	2.1

## 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.