



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:54 AM GMT

PDB ID : 3GI8  
Title : Crystal Structure of ApcT K158A Transporter Bound to 7F11 Monoclonal Fab Fragment  
Authors : Shaffer, P.L.; Goehring, A.S.; Shankaranarayanan, A.; Gouaux, E.; New York Consortium on Membrane Protein Structure (NYCOMPS)  
Deposited on : 2009-03-05  
Resolution : 2.59 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

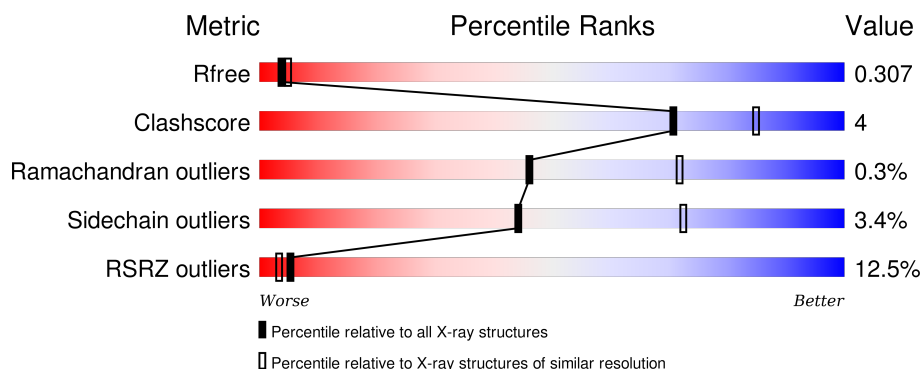
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.59 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	C	444	
2	L	220	
3	H	223	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6924 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 Uncharacterized protein MJ0609.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	435	Total	C	N	O	S	0	0	0
			3351	2261	512	567	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	158	ALA	LYS	ENGINEERED	UNP Q58026
C	436	LEU	-	EXPRESSION TAG	UNP Q58026
C	437	GLU	-	EXPRESSION TAG	UNP Q58026
C	438	SER	-	EXPRESSION TAG	UNP Q58026
C	439	SER	-	EXPRESSION TAG	UNP Q58026
C	440	GLY	-	EXPRESSION TAG	UNP Q58026
C	441	LEU	-	EXPRESSION TAG	UNP Q58026
C	442	VAL	-	EXPRESSION TAG	UNP Q58026
C	443	PRO	-	EXPRESSION TAG	UNP Q58026
C	444	ARG	-	EXPRESSION TAG	UNP Q58026

- Molecule 2 is a protein called 7F11 Anti-ApcT Monoclonal Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	220	Total	C	N	O	S	0	0	0
			1705	1061	285	351	8			

- Molecule 3 is a protein called 7F11 Anti-ApcT Monoclonal Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	220	Total	C	N	O	S	0	0	0
			1664	1057	264	334	9			

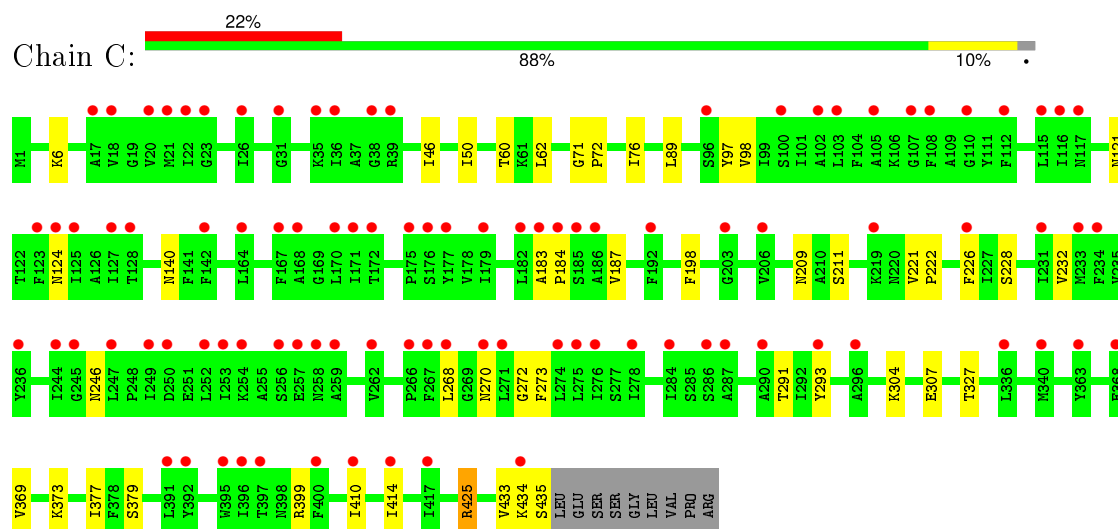
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	57	Total 57	O 57	0	0
4	H	71	Total 71	O 71	0	0
4	L	76	Total 76	O 76	0	0

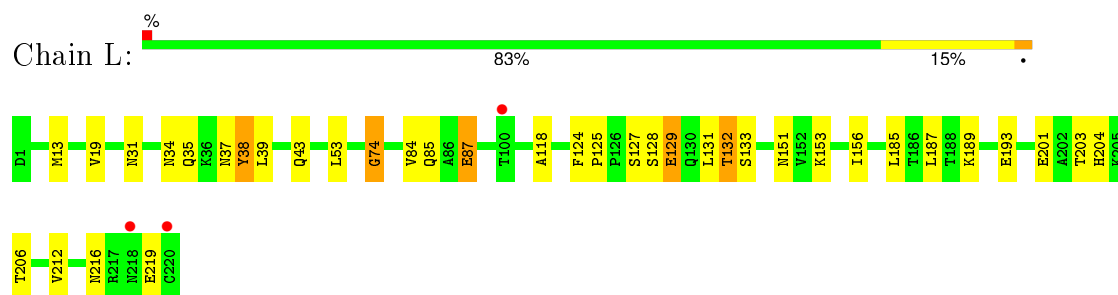
### 3 Residue-property plots

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.

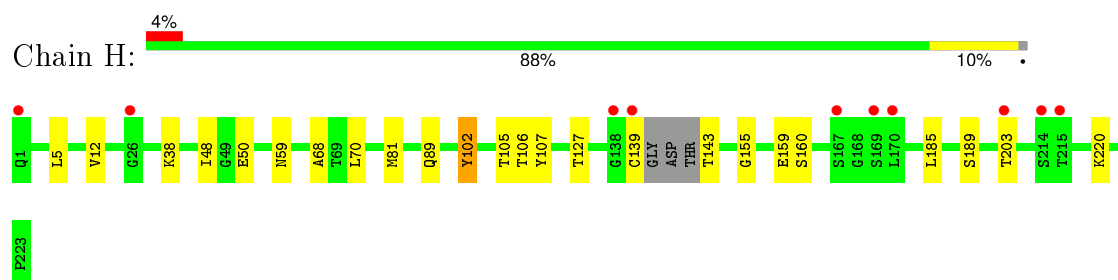
#### • Molecule 1: Uncharacterized protein MJ0609



#### • Molecule 2: 7F11 Anti-ApcT Monoclonal Fab Light Chain



#### • Molecule 3: 7F11 Anti-ApcT Monoclonal Fab Heavy Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.04Å 111.19Å 115.67Å 90.00° 90.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.59 40.11 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.59) 99.6 (40.11-2.59)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.254 , 0.307 0.252 , 0.307	Depositor DCC
$R_{free}$ test set	1805 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtriage
Anisotropy	0.549	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.9	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.013 for -h,-l,-k 0.029 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 36116 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6924	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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	C	0.36	0/3432	0.44	0/4660
2	L	0.35	0/1742	0.53	0/2361
3	H	0.34	0/1713	0.50	0/2345
All	All	0.35	0/6887	0.48	0/9366

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	C	3351	0	3510	29	0
2	L	1705	0	1635	20	0
3	H	1664	0	1592	10	0
4	C	57	0	0	2	0
4	H	71	0	0	0	0
4	L	76	0	0	1	0
All	All	6924	0	6737	59	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 (59) 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:C:425:ARG:HG2	1:C:425:ARG:HH11	1.38	0.87
2:L:216:ASN:HB2	2:L:219:GLU:HG3	1.59	0.81
3:H:70:LEU:HD21	3:H:81:MET:HE3	1.68	0.75
2:L:216:ASN:HB2	2:L:219:GLU:CG	2.21	0.70
2:L:13:MET:HG3	2:L:19:VAL:HG22	1.72	0.70
1:C:121:ASN:HB2	1:C:124:ASN:H	1.57	0.68
3:H:102:TYR:O	3:H:105:THR:HG22	1.96	0.66
1:C:434:LYS:HB3	1:C:435:SER:HA	1.77	0.66
2:L:43:GLN:HB2	2:L:53:LEU:HD11	1.82	0.61
2:L:31:ASN:O	2:L:35:GLN:HA	2.00	0.60
2:L:131:LEU:O	2:L:189:LYS:HE3	2.02	0.60
1:C:433:VAL:HG12	1:C:434:LYS:O	2.02	0.59
1:C:425:ARG:HH11	1:C:425:ARG:CG	2.14	0.58
1:C:268:LEU:HB3	1:C:272:GLY:HA3	1.84	0.58
2:L:131:LEU:C	2:L:133:SER:H	2.11	0.53
1:C:433:VAL:O	1:C:434:LYS:HB2	2.08	0.53
3:H:105:THR:HG23	3:H:107:TYR:H	1.74	0.52
1:C:270:ASN:HA	1:C:273:PHE:HB3	1.91	0.51
1:C:97:TYR:HD1	1:C:291:THR:HG23	1.77	0.50
2:L:151:ASN:HB3	2:L:203:THR:HB	1.95	0.49
1:C:97:TYR:OH	1:C:209:ASN:ND2	2.40	0.49
3:H:203:THR:HG23	3:H:220:LYS:HE3	1.96	0.48
1:C:98:VAL:HG22	1:C:327:THR:HG23	1.96	0.47
1:C:304:LYS:O	1:C:425:ARG:HD3	2.16	0.46
1:C:140:ASN:HB2	1:C:293:TYR:OH	2.15	0.46
1:C:183:ALA:HA	1:C:184:PRO:HD3	1.87	0.45
2:L:37:ASN:HD21	2:L:74:GLY:H	1.63	0.45
3:H:159:GLU:HA	3:H:160:SER:HA	1.75	0.45
2:L:127:SER:C	2:L:129:GLU:H	2.20	0.44
3:H:68:ALA:HB1	3:H:81:MET:HE2	2.00	0.44
2:L:118:ALA:HA	2:L:206:THR:HG21	1.99	0.44
1:C:414:ILE:HA	4:C:488:HOH:O	2.17	0.44
1:C:71:GLY:HA3	1:C:72:PRO:HD2	1.85	0.43
1:C:76:ILE:HD13	1:C:89:LEU:HD13	1.99	0.43
2:L:153:LYS:HB2	2:L:201:GLU:HB2	2.01	0.43
3:H:155:GLY:HA2	3:H:185:LEU:HB3	1.99	0.43
2:L:156:ILE:HD11	2:L:185:LEU:HD21	2.01	0.43
3:H:38:LYS:HB2	3:H:48:ILE:HD11	2.00	0.42
2:L:124:PHE:HA	2:L:125:PRO:HD3	1.92	0.42
2:L:87:GLU:HG3	2:L:87:GLU:H	1.71	0.42
1:C:379:SER:HB2	4:C:490:HOH:O	2.19	0.42
3:H:50:GLU:HG2	3:H:59:ASN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:VAL:HB	1:C:222:PRO:HD3	2.02	0.42
1:C:46:ILE:O	1:C:50:ILE:HG12	2.19	0.42
2:L:201:GLU:HG2	2:L:212:VAL:HG22	2.00	0.42
1:C:60:THR:HG22	1:C:222:PRO:HA	2.01	0.41
2:L:34:ASN:HB2	4:L:288:HOH:O	2.20	0.41
1:C:373:LYS:O	1:C:377:ILE:HG13	2.20	0.41
2:L:38:TYR:N	2:L:38:TYR:CD2	2.88	0.41
1:C:434:LYS:CB	1:C:435:SER:HA	2.46	0.41
1:C:211:SER:HB2	1:C:221:VAL:HG21	2.02	0.41
2:L:37:ASN:ND2	2:L:74:GLY:H	2.19	0.41
1:C:62:LEU:HD23	1:C:369:VAL:HG11	2.03	0.41
1:C:410:ILE:O	1:C:414:ILE:HG12	2.20	0.41
1:C:425:ARG:HG2	1:C:425:ARG:NH1	2.18	0.41
3:H:48:ILE:HG21	3:H:81:MET:CE	2.51	0.41
2:L:204:HIS:HB3	2:L:206:THR:HG22	2.02	0.41
1:C:228:SER:O	1:C:232:VAL:HG22	2.21	0.40
1:C:184:PRO:HA	1:C:187:VAL:HB	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	C	433/444 (98%)	414 (96%)	19 (4%)	0	100	100
2	L	218/220 (99%)	204 (94%)	11 (5%)	3 (1%)	14	28
3	H	216/223 (97%)	210 (97%)	6 (3%)	0	100	100
All	All	867/887 (98%)	828 (96%)	36 (4%)	3 (0%)	46	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	132	THR
2	L	128	SER
2	L	74	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	C	352/360 (98%)	345 (98%)	7 (2%)	63	85
2	L	198/198 (100%)	189 (96%)	9 (4%)	34	62
3	H	191/194 (98%)	182 (95%)	9 (5%)	32	59
All	All	741/752 (98%)	716 (97%)	25 (3%)	44	72

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	6	LYS
1	C	198	PHE
1	C	226	PHE
1	C	246	ASN
1	C	307	GLU
1	C	399	ARG
1	C	425	ARG
2	L	38	TYR
2	L	39	LEU
2	L	84	VAL
2	L	85	GLN
2	L	87	GLU
2	L	129	GLU
2	L	132	THR
2	L	187	LEU
2	L	193	GLU
3	H	5	LEU
3	H	12	VAL
3	H	89	GLN
3	H	102	TYR

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Mol	Chain	Res	Type
3	H	106	THR
3	H	127	THR
3	H	139	CYS
3	H	143	THR
3	H	189	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	5	ASN
1	C	209	ASN
1	C	246	ASN
1	C	394	GLN
1	C	430	ASN
2	L	27	GLN
2	L	37	ASN
2	L	143	ASN
2	L	144	ASN
2	L	162	GLN
2	L	163	ASN
2	L	167	ASN
3	H	62	GLN
3	H	175	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

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	C	435/444 (97%)	1.19	96 (22%) 1 0	36, 71, 101, 104	0
2	L	220/220 (100%)	0.01	3 (1%) 78 74	28, 41, 54, 68	0
3	H	220/223 (98%)	0.19	10 (4%) 37 29	29, 43, 64, 67	0
All	All	875/887 (98%)	0.64	109 (12%) 5 3	28, 53, 96, 104	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	220	CYS	9.1
1	C	168	ALA	8.8
1	C	127	ILE	8.4
1	C	278	ILE	6.8
1	C	271	LEU	6.3
1	C	392	TYR	5.6
2	L	100	THR	5.1
1	C	267	PHE	4.9
1	C	124	ASN	4.7
1	C	396	ILE	4.7
1	C	39	ARG	4.6
1	C	167	PHE	4.4
1	C	182	LEU	4.4
1	C	177	TYR	4.3
3	H	139	CYS	4.2
1	C	142	PHE	4.2
1	C	250	ASP	4.1
1	C	125	ILE	4.1
1	C	259	ALA	4.0
1	C	244	ILE	4.0
1	C	172	THR	3.9
1	C	414	ILE	3.9
1	C	117	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	184	PRO	3.7
1	C	185	SER	3.7
3	H	1	GLN	3.6
1	C	254	LYS	3.6
1	C	107	GLY	3.6
1	C	270	ASN	3.6
1	C	31	GLY	3.6
1	C	176	SER	3.6
1	C	123	PHE	3.5
1	C	256	SER	3.5
1	C	38	GLY	3.5
1	C	262	VAL	3.4
1	C	368	GLU	3.4
1	C	410	ILE	3.3
1	C	22	ILE	3.3
1	C	274	LEU	3.2
1	C	192	PHE	3.2
1	C	35	LYS	3.1
1	C	284	ILE	3.1
1	C	21	MET	3.1
3	H	167	SER	3.1
1	C	234	PHE	3.0
1	C	112	PHE	3.0
1	C	17	ALA	3.0
1	C	186	ALA	3.0
1	C	340	MET	3.0
1	C	276	ILE	3.0
1	C	258	ASN	3.0
1	C	116	ILE	3.0
1	C	100	SER	3.0
3	H	138	GLY	3.0
1	C	266	PRO	2.9
1	C	115	LEU	2.9
1	C	226	PHE	2.9
3	H	169	SER	2.8
1	C	128	THR	2.8
1	C	26	ILE	2.8
1	C	434	LYS	2.8
1	C	170	LEU	2.8
1	C	183	ALA	2.7
1	C	290	ALA	2.6
1	C	23	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	397	THR	2.6
1	C	257	GLU	2.6
3	H	170	LEU	2.6
1	C	253	ILE	2.6
1	C	175	PRO	2.6
1	C	336	LEU	2.6
1	C	20	VAL	2.5
2	L	218	ASN	2.5
1	C	108	PHE	2.5
1	C	400	PHE	2.5
3	H	26	GLY	2.5
1	C	247	LEU	2.5
1	C	179	ILE	2.5
1	C	249	ILE	2.4
1	C	233	MET	2.4
1	C	206	VAL	2.4
1	C	275	LEU	2.4
1	C	203	GLY	2.4
1	C	287	ALA	2.4
1	C	245	GLY	2.4
1	C	395	TRP	2.3
3	H	214	SER	2.3
1	C	36	ILE	2.3
1	C	391	LEU	2.3
1	C	164	LEU	2.3
1	C	18	VAL	2.3
1	C	110	GLY	2.2
1	C	293	TYR	2.2
1	C	219	LYS	2.2
1	C	171	ILE	2.2
1	C	231	ILE	2.1
1	C	103	LEU	2.1
1	C	252	LEU	2.1
1	C	96	SER	2.1
1	C	105	ALA	2.1
1	C	268	LEU	2.1
3	H	215	THR	2.1
1	C	417	ILE	2.1
1	C	236	TYR	2.0
3	H	203	THR	2.0
1	C	286	SER	2.0
1	C	102	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	296	ALA	2.0
1	C	363	TYR	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.