



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 12:04 AM JST

PDB ID : 7VMC  
Title : Crystal structure of EF-Tu/CdiA/CdiI  
Authors : Wang, J.; Yashiro, Y.; Tomita, K.  
Deposited on : 2021-10-08  
Resolution : 3.41 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	:	2.27
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)	:	2.27



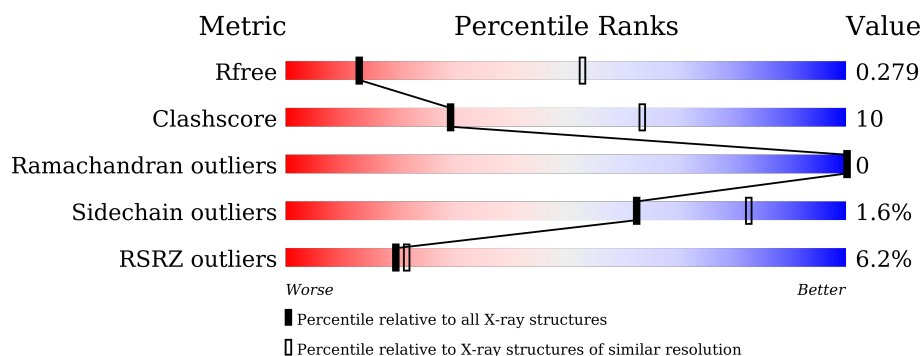
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)

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  $\geq 3$ , 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	402	<div> <div> <div></div> <div>78%</div> <div>18%</div> <div>.</div> </div> </div>
2	B	306	<div> <div> <div>3%</div> <div>30%</div> <div>6%</div> <div>64%</div> </div> </div>
3	C	179	<div> <div> <div>16%</div> <div>64%</div> <div>34%</div> <div>..</div> </div> </div>



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5190 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 Elongation factor Tu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	2955	1868	508	566	13	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	394	LEU	-	expression tag	UNP E2QJ06
A	395	GLU	-	expression tag	UNP E2QJ06
A	396	HIS	-	expression tag	UNP E2QJ06
A	397	HIS	-	expression tag	UNP E2QJ06
A	398	HIS	-	expression tag	UNP E2QJ06
A	399	HIS	-	expression tag	UNP E2QJ06
A	400	HIS	-	expression tag	UNP E2QJ06
A	401	HIS	-	expression tag	UNP E2QJ06

- Molecule 2 is a protein called tRNA nuclease CdiA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	111	861	545	150	163	3	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	initiating methionine	UNP B3BM48
B	-19	GLY	-	expression tag	UNP B3BM48
B	-18	SER	-	expression tag	UNP B3BM48
B	-17	SER	-	expression tag	UNP B3BM48
B	-16	HIS	-	expression tag	UNP B3BM48
B	-15	HIS	-	expression tag	UNP B3BM48
B	-14	HIS	-	expression tag	UNP B3BM48
B	-13	HIS	-	expression tag	UNP B3BM48

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP B3BM48
B	-11	HIS	-	expression tag	UNP B3BM48
B	-10	SER	-	expression tag	UNP B3BM48
B	-9	SER	-	expression tag	UNP B3BM48
B	-8	GLY	-	expression tag	UNP B3BM48
B	-7	LEU	-	expression tag	UNP B3BM48
B	-6	VAL	-	expression tag	UNP B3BM48
B	-5	PRO	-	expression tag	UNP B3BM48
B	-4	ARG	-	expression tag	UNP B3BM48
B	-3	GLY	-	expression tag	UNP B3BM48
B	-2	SER	-	expression tag	UNP B3BM48
B	-1	HIS	-	expression tag	UNP B3BM48
B	0	MET	-	expression tag	UNP B3BM48

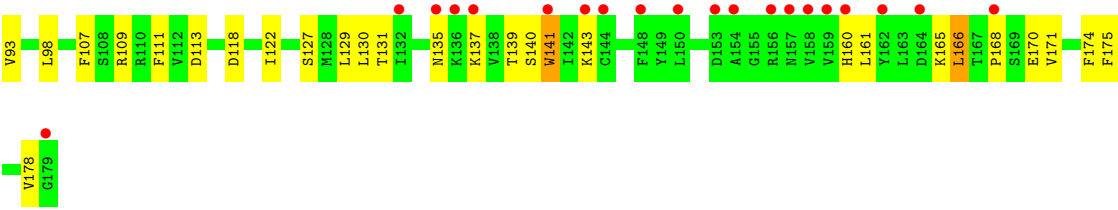
- Molecule 3 is a protein called Contact-dependent inhibitor I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	177	Total	C	N	O	S	0	0	0
			1374	879	219	272	4			











## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.93Å 102.76Å 88.14Å 90.00° 111.86° 90.00°	Depositor
Resolution (Å)	35.60 – 3.41 49.76 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.6 (35.60-3.41) 98.4 (49.76-3.40)	Depositor EDS
$R_{merge}$	0.31	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.237 , 0.274 0.238 , 0.279	Depositor DCC
$R_{free}$ test set	577 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.2	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 84.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5190	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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

### 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	A	0.27	0/3010	0.48	0/4077
2	B	0.27	0/882	0.45	0/1195
3	C	0.27	0/1401	0.52	0/1904
All	All	0.27	0/5293	0.49	0/7176

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

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	2955	0	2965	49	0
2	B	861	0	850	15	0
3	C	1374	0	1378	41	0
All	All	5190	0	5193	99	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 10.

All (99) 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:16:THR:CG2	1:A:80:ASP:HB3	1.70	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:THR:HG22	1:A:80:ASP:HB3	1.20	1.13
1:A:318:ARG:NH2	1:A:326:TYR:CE1	2.42	0.88
3:C:127:SER:HA	3:C:166:LEU:HD21	1.56	0.86
3:C:59:GLY:HA3	3:C:93:VAL:HG13	1.61	0.82
1:A:16:THR:CG2	1:A:80:ASP:CB	2.58	0.81
1:A:318:ARG:NH2	1:A:326:TYR:HE1	1.80	0.79
1:A:16:THR:HG21	1:A:80:ASP:HB3	1.65	0.79
1:A:16:THR:HG22	1:A:80:ASP:CB	2.12	0.71
1:A:288:ARG:NH2	1:A:334:THR:O	2.25	0.70
3:C:69:ILE:HG13	3:C:178:VAL:HG23	1.73	0.69
3:C:27:ILE:HD11	3:C:64:ILE:HG12	1.76	0.67
1:A:341:ILE:HG22	1:A:360:VAL:HG22	1.77	0.67
2:B:194:ILE:HG23	2:B:234:SER:HB3	1.77	0.67
1:A:67:VAL:HG23	1:A:78:HIS:HB3	1.77	0.67
3:C:41:ARG:HG2	3:C:51:GLU:HG2	1.80	0.63
1:A:63:ASN:ND2	1:A:86:ASP:OD2	2.32	0.63
1:A:246:GLY:HA3	1:A:290:GLN:HG2	1.82	0.62
1:A:213:PRO:HG3	1:A:333:ARG:HD3	1.81	0.61
3:C:135:ASN:HB3	3:C:137:LYS:HD3	1.81	0.60
1:A:283:ARG:NH2	2:B:284:TYR:OH	2.34	0.60
3:C:34:LYS:H	3:C:34:LYS:HD2	1.67	0.60
1:A:16:THR:HB	1:A:78:HIS:NE2	2.20	0.57
3:C:35:LEU:HD23	3:C:36:PRO:HD2	1.88	0.56
1:A:132:VAL:HB	1:A:169:ILE:HG12	1.88	0.56
3:C:19:ILE:HD12	3:C:170:GLU:HG3	1.87	0.55
1:A:321:PRO:HB3	1:A:351:MET:HA	1.88	0.55
3:C:139:THR:HG22	3:C:140:SER:H	1.70	0.54
1:A:140:VAL:HG21	1:A:146:LEU:HD11	1.88	0.54
3:C:3:LEU:HA	3:C:98:LEU:HD11	1.90	0.54
1:A:30:ALA:HB2	1:A:178:LEU:HD23	1.90	0.54
3:C:17:ILE:HG12	3:C:27:ILE:HG22	1.89	0.54
3:C:9:ILE:O	3:C:90:GLY:HA3	2.08	0.54
2:B:223:ARG:NH1	3:C:36:PRO:O	2.40	0.54
3:C:41:ARG:HB2	3:C:113:ASP:HB3	1.88	0.54
1:A:15:GLY:HA3	1:A:98:MET:SD	2.48	0.53
3:C:35:LEU:HD22	3:C:56:PRO:HG3	1.90	0.53
1:A:131:ILE:HG22	1:A:168:PRO:HD2	1.91	0.52
1:A:80:ASP:N	1:A:80:ASP:OD1	2.42	0.52
3:C:50:LEU:HA	3:C:66:LEU:HA	1.91	0.52
1:A:34:VAL:HB	1:A:188:ILE:HD11	1.90	0.51
1:A:213:PRO:HA	1:A:291:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLU:HG2	1:A:254:THR:HG22	1.91	0.51
3:C:38:LEU:HD12	3:C:54:VAL:HG13	1.93	0.51
1:A:87:TYR:O	1:A:91:MET:HG2	2.12	0.50
1:A:231:VAL:HG13	1:A:270:ALA:HA	1.93	0.50
3:C:113:ASP:N	3:C:113:ASP:OD1	2.45	0.50
3:C:175:PHE:HA	3:C:178:VAL:HG12	1.94	0.50
3:C:122:ILE:HB	3:C:129:LEU:HG	1.93	0.49
3:C:41:ARG:NH1	3:C:51:GLU:OE2	2.45	0.49
1:A:26:THR:HG21	1:A:175:LEU:HG	1.95	0.49
1:A:245:VAL:HG13	1:A:250:THR:HG22	1.93	0.49
2:B:278:VAL:HG11	3:C:22:TYR:HD1	1.77	0.49
2:B:259:MET:HB2	2:B:266:LEU:H	1.77	0.49
2:B:220:TYR:HA	3:C:107:PHE:CE1	2.48	0.48
3:C:26:ASP:HA	3:C:65:THR:HG22	1.96	0.48
3:C:29:ILE:HG13	3:C:30:ILE:HG13	1.96	0.48
1:A:16:THR:HG21	1:A:80:ASP:CB	2.39	0.47
2:B:267:VAL:HG22	2:B:281:HIS:HB2	1.96	0.47
3:C:166:LEU:HD23	3:C:166:LEU:H	1.78	0.47
3:C:39:TYR:HB2	3:C:111:PHE:CE1	2.49	0.47
3:C:130:LEU:HB2	3:C:161:LEU:HB3	1.97	0.47
2:B:194:ILE:HG22	2:B:238:LEU:HD11	1.98	0.46
2:B:198:PHE:HE1	2:B:200:LEU:HD12	1.79	0.46
2:B:265:GLU:HG3	2:B:283:LEU:HB2	1.98	0.45
2:B:243:SER:HA	2:B:246:LYS:HG2	1.99	0.45
1:A:149:VAL:HA	1:A:152:GLU:HG2	1.98	0.45
1:A:282:LYS:HE2	1:A:282:LYS:HB2	1.79	0.45
1:A:34:VAL:CB	1:A:188:ILE:HD11	2.47	0.44
3:C:80:LEU:CD2	3:C:127:SER:HB2	2.47	0.44
2:B:281:HIS:CE1	2:B:283:LEU:HD23	2.52	0.44
2:B:278:VAL:HG11	3:C:22:TYR:CD1	2.53	0.44
1:A:372:LEU:O	1:A:388:VAL:HG12	2.18	0.43
1:A:123:ARG:HD3	1:A:160:TYR:O	2.17	0.43
1:A:150:GLU:HG3	1:A:169:ILE:HG21	2.00	0.43
1:A:65:SER:OG	1:A:80:ASP:O	2.24	0.43
1:A:214:ILE:HD12	1:A:290:GLN:HB2	2.00	0.43
2:B:242:GLN:HA	2:B:245:VAL:HG12	2.00	0.43
3:C:7:SER:OG	3:C:8:VAL:N	2.52	0.42
3:C:131:THR:HG23	3:C:160:HIS:CD2	2.54	0.42
1:A:323:PHE:CE1	1:A:349:MET:HB3	2.54	0.42
1:A:319:HIS:CD2	1:A:320:THR:HG23	2.55	0.42
1:A:62:ILE:HD12	1:A:89:LYS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:VAL:HA	3:C:174:PHE:HB3	2.02	0.42
1:A:142:ASP:O	1:A:146:LEU:HD13	2.19	0.42
1:A:294:LYS:HD3	1:A:295:PRO:HD2	2.00	0.41
1:A:141:ASP:OD1	1:A:141:ASP:N	2.49	0.41
3:C:168:PRO:O	3:C:171:VAL:HG22	2.20	0.41
3:C:87:SER:HB3	3:C:141:TRP:O	2.21	0.41
1:A:56:LYS:O	1:A:382:THR:HG21	2.20	0.41
1:A:244:ILE:HG13	1:A:244:ILE:O	2.21	0.41
1:A:78:HIS:CE1	1:A:102:ILE:HD12	2.56	0.41
3:C:52:LEU:HG	3:C:64:ILE:HB	2.03	0.41
1:A:123:ARG:HD2	1:A:161:ASP:HB2	2.03	0.40
3:C:86:SER:HA	3:C:143:LYS:HE3	2.02	0.40
2:B:223:ARG:NH1	3:C:37:PRO:O	2.54	0.40
3:C:41:ARG:HB3	3:C:49:LEU:HD11	2.03	0.40
1:A:329:GLN:HB3	1:A:336:ASP:HB3	2.04	0.40
3:C:165:LYS:HB3	3:C:165:LYS:HE2	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	A	382/402 (95%)	369 (97%)	13 (3%)	0	100	100
2	B	109/306 (36%)	108 (99%)	1 (1%)	0	100	100
3	C	175/179 (98%)	161 (92%)	14 (8%)	0	100	100
All	All	666/887 (75%)	638 (96%)	28 (4%)	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	A	317/335 (95%)	314 (99%)	3 (1%)	78	90
2	B	95/238 (40%)	94 (99%)	1 (1%)	73	87
3	C	162/164 (99%)	157 (97%)	5 (3%)	40	70
All	All	574/737 (78%)	565 (98%)	9 (2%)	62	82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	216	ASP
1	A	259	GLU
2	B	284	TYR
3	C	89	CYS
3	C	109	ARG
3	C	118	ASP
3	C	141	TRP
3	C	166	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

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	A	384/402 (95%)	0.19	5 (1%) 77 75	59, 95, 129, 154	0
2	B	111/306 (36%)	0.51	9 (8%) 12 15	84, 108, 146, 160	0
3	C	177/179 (98%)	0.91	28 (15%) 2 3	89, 141, 177, 196	0
All	All	672/887 (75%)	0.43	42 (6%) 20 21	59, 105, 164, 196	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	85	PRO	5.0
3	C	154	ALA	4.9
3	C	90	GLY	4.3
3	C	162	TYR	4.1
1	A	47	ASP	4.0
3	C	83	SER	3.9
2	B	277	PRO	3.7
2	B	206	THR	3.6
3	C	141	TRP	3.5
3	C	60	PHE	3.5
3	C	159	VAL	3.4
3	C	144	CYS	3.3
3	C	148	PHE	3.3
2	B	276	TYR	3.3
3	C	153	ASP	3.3
3	C	150	LEU	3.3
3	C	158	VAL	3.3
3	C	156	ARG	3.2
3	C	157	ASN	2.9
3	C	164	ASP	2.9
3	C	132	ILE	2.9
1	A	223	ARG	2.6
3	C	61	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	216	ASP	2.6
3	C	135	ASN	2.6
2	B	208	TRP	2.6
3	C	179	GLY	2.5
3	C	168	PRO	2.4
2	B	190	PRO	2.4
3	C	160	HIS	2.4
3	C	136	LYS	2.4
2	B	195	PRO	2.4
3	C	84	LEU	2.3
1	A	246	GLY	2.3
1	A	287	GLU	2.3
3	C	89	CYS	2.3
3	C	20	ASP	2.2
2	B	280	LYS	2.2
3	C	137	LYS	2.2
2	B	237	MET	2.1
2	B	268	PHE	2.0
3	C	143	LYS	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.