



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 01:20 PM JST

PDB ID : 7FIV  
Title : Crystal structure of the complex formed by Wolbachia cytoplasmic incompatibility factors CidA and CidBND1-ND2 from wPip(Tunis)  
Authors : Xiao, Y.J.; Wang, W.; Chen, X.; Ji, X.Y.; Yang, H.T.  
Deposited on : 2021-08-01  
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

<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>.

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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 : 2.36  
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) : 2.36

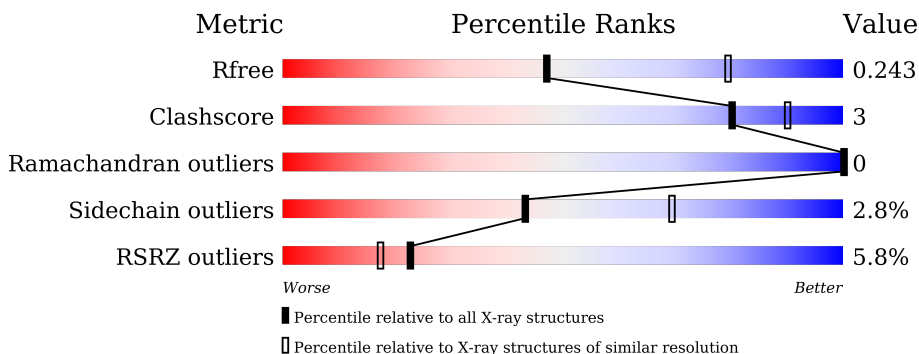
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 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	499	
2	B	769	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9425 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 CidA\_I gamma/2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3299	2115	551	616	17	0	2	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LEU	-	expression tag	UNP A0A2K9VS01
A	493	GLU	-	expression tag	UNP A0A2K9VS01
A	494	HIS	-	expression tag	UNP A0A2K9VS01
A	495	HIS	-	expression tag	UNP A0A2K9VS01
A	496	HIS	-	expression tag	UNP A0A2K9VS01
A	497	HIS	-	expression tag	UNP A0A2K9VS01
A	498	HIS	-	expression tag	UNP A0A2K9VS01
A	499	HIS	-	expression tag	UNP A0A2K9VS01

- Molecule 2 is a protein called CidB\_I b/2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	741	5943	3728	1096	1104	15	0	13	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	762	LEU	-	expression tag	UNP A0A2K9VS18
B	763	GLU	-	expression tag	UNP A0A2K9VS18
B	764	HIS	-	expression tag	UNP A0A2K9VS18
B	765	HIS	-	expression tag	UNP A0A2K9VS18
B	766	HIS	-	expression tag	UNP A0A2K9VS18
B	767	HIS	-	expression tag	UNP A0A2K9VS18
B	768	HIS	-	expression tag	UNP A0A2K9VS18
B	769	HIS	-	expression tag	UNP A0A2K9VS18

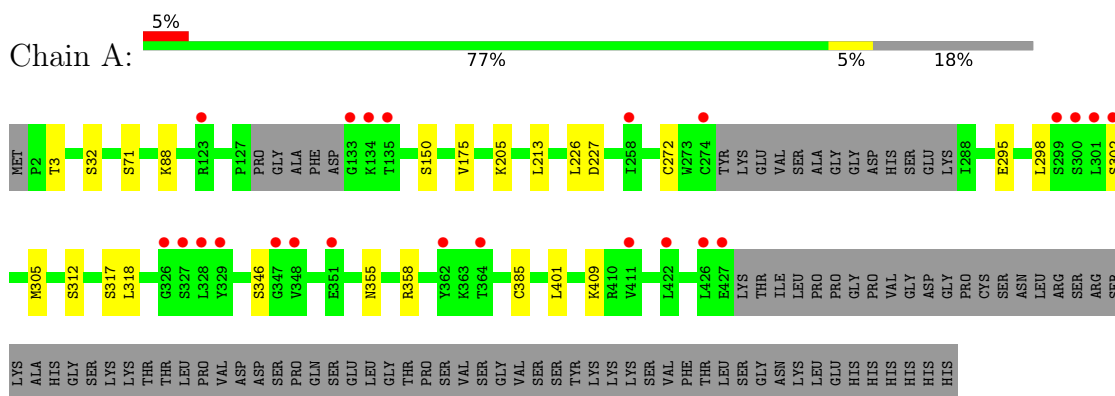
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	160	Total O 160 160	0	0

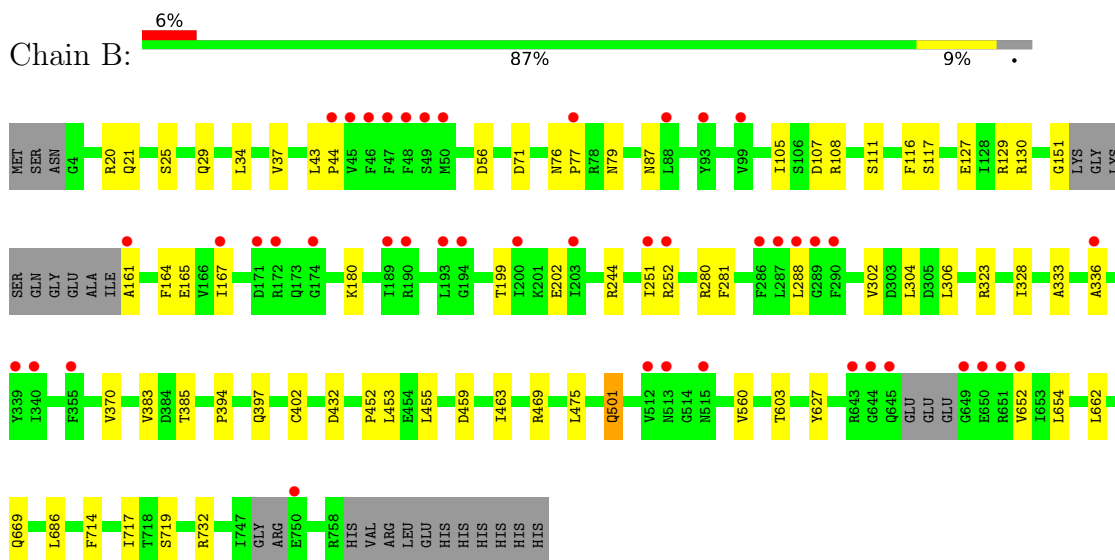
### 3 Residue-property plots

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: CidA\_I gamma/2 protein



- Molecule 2: CidB\_I b/2 protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.58Å 181.58Å 54.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.61 – 2.59 35.61 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.61-2.59) 99.7 (35.61-2.59)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.196 , 0.244 0.199 , 0.243	Depositor DCC
$R_{free}$ test set	1998 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.3	Xtrriage
Anisotropy	0.167	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.054 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9425	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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	0.35	0/3373	0.46	0/4539
2	B	0.34	0/6102	0.51	0/8278
All	All	0.35	0/9475	0.49	0/12817

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	3299	0	3213	9	0
2	B	5943	0	5662	40	0
3	A	23	0	0	0	0
3	B	160	0	0	0	0
All	All	9425	0	8875	48	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 3.

All (48) 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:B:469[A]:ARG:HB2	2:B:603:THR:HG22	1.11	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469[B]:ARG:HB2	2:B:603:THR:HG22	1.08	1.05
2:B:469[A]:ARG:HB2	2:B:603:THR:CG2	2.04	0.86
2:B:469[A]:ARG:CB	2:B:603:THR:HG22	2.01	0.83
2:B:469[B]:ARG:HB2	2:B:603:THR:CG2	2.03	0.80
2:B:475:LEU:HD21	2:B:501:GLN:NE2	2.04	0.72
2:B:469[B]:ARG:CB	2:B:603:THR:HG22	2.01	0.68
2:B:453:LEU:HB2	2:B:463:ILE:HD11	1.77	0.66
2:B:288:LEU:HD21	2:B:302:VAL:HG11	1.79	0.65
2:B:76[B]:ASN:OD1	2:B:77:PRO:HD2	2.02	0.59
2:B:34:LEU:HB3	2:B:161:ALA:HA	1.85	0.57
2:B:469[A]:ARG:HG3	2:B:603:THR:HA	1.87	0.57
2:B:76[A]:ASN:ND2	2:B:77:PRO:HD2	2.21	0.56
2:B:333:ALA:HB1	2:B:336:ALA:HB3	1.89	0.54
1:A:295:GLU:HA	1:A:298:LEU:HD12	1.91	0.53
2:B:165:GLU:HB3	2:B:654:LEU:HD12	1.90	0.53
1:A:302:SER:HA	1:A:305:MET:HE3	1.92	0.49
2:B:252:ARG:HD3	2:B:383:VAL:HB	1.94	0.49
2:B:167:ILE:HG23	2:B:652:VAL:HG22	1.97	0.47
1:A:401:LEU:O	1:A:409:LYS:NZ	2.39	0.46
2:B:34:LEU:HA	2:B:37:VAL:HG13	1.98	0.46
1:A:205:LYS:HD3	1:A:205:LYS:HA	1.84	0.45
2:B:151:GLY:HA3	2:B:161:ALA:HB3	1.98	0.45
1:A:355:ASN:HA	1:A:358:ARG:HG3	1.98	0.45
2:B:25:SER:O	2:B:29:GLN:HG3	2.16	0.45
2:B:180:LYS:HB3	2:B:180:LYS:HE2	1.75	0.45
2:B:627:TYR:CG	2:B:669[A]:GLN:HB3	2.53	0.44
2:B:71:ASP:HB3	2:B:87:ASN:HB2	2.00	0.44
2:B:455:LEU:HD12	2:B:459:ASP:HB3	1.99	0.44
2:B:288:LEU:HD11	2:B:304:LEU:HD22	1.99	0.44
1:A:312:SER:HB2	1:A:355:ASN:HD21	1.83	0.44
2:B:370:VAL:HG22	2:B:383:VAL:HG22	2.00	0.43
2:B:244:ARG:HD2	2:B:385:THR:HG21	2.00	0.43
2:B:43:LEU:HB3	2:B:44:PRO:HD3	2.01	0.43
2:B:469[B]:ARG:NH2	2:B:603:THR:HG23	2.32	0.43
2:B:108:ARG:CB	2:B:111:SER:HB2	2.49	0.43
2:B:714:PHE:O	2:B:717:ILE:HG12	2.19	0.43
2:B:251:ILE:HD11	2:B:328:ILE:HG12	2.02	0.42
2:B:394:PRO:HB2	2:B:397:GLN:HB3	2.01	0.42
2:B:662:LEU:HD23	2:B:662:LEU:HA	1.88	0.42
1:A:150:SER:HB2	2:B:452:PRO:HD2	2.01	0.41
2:B:306:LEU:HD23	2:B:306:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:GLU:HA	2:B:130:ARG:HG3	2.02	0.41
2:B:199:THR:HG22	2:B:202:GLU:HG3	2.02	0.41
2:B:280:ARG:HH21	2:B:281:PHE:HE1	1.69	0.41
1:A:175:VAL:HG13	1:A:205:LYS:HE3	2.03	0.40
1:A:213:LEU:HB2	1:A:226:LEU:HD21	2.03	0.40
2:B:560:VAL:HG21	2:B:603:THR:HG21	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	A	404/499 (81%)	395 (98%)	9 (2%)	0	100	100
2	B	746/769 (97%)	722 (97%)	24 (3%)	0	100	100
All	All	1150/1268 (91%)	1117 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	354/448 (79%)	344 (97%)	10 (3%)	43	69
2	B	628/678 (93%)	611 (97%)	17 (3%)	44	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	982/1126 (87%)	955 (97%)	27 (3%)	43 71

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	32	SER
1	A	71	SER
1	A	88	LYS
1	A	227	ASP
1	A	272	CYS
1	A	317	SER
1	A	318	LEU
1	A	346	SER
1	A	385	CYS
2	B	20	ARG
2	B	21	GLN
2	B	56	ASP
2	B	79	ASN
2	B	105	ILE
2	B	107	ASP
2	B	116	PHE
2	B	117	SER
2	B	129	ARG
2	B	164	PHE
2	B	323	ARG
2	B	402	CYS
2	B	432	ASP
2	B	501	GLN
2	B	686	LEU
2	B	719	SER
2	B	732	ARG

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

Mol	Chain	Res	Type
1	A	355	ASN
2	B	501	GLN

### 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](#)

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	408/499 (81%)	0.23	23 (5%) 24 19	45, 79, 119, 141	0
2	B	741/769 (96%)	0.17	44 (5%) 22 17	32, 64, 108, 138	0
All	All	1149/1268 (90%)	0.19	67 (5%) 23 17	32, 69, 114, 141	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	651	ARG	4.5
2	B	193	LEU	4.0
2	B	652	VAL	3.9
1	A	327	SER	3.8
2	B	644	GLY	3.8
2	B	161	ALA	3.7
1	A	347	GLY	3.5
1	A	426	LEU	3.5
1	A	329	TYR	3.5
2	B	649	GLY	3.3
1	A	328	LEU	3.3
2	B	49	SER	3.2
1	A	364	THR	3.2
2	B	289	GLY	3.2
2	B	167	ILE	3.0
1	A	301	LEU	3.0
2	B	513	ASN	3.0
2	B	47	PHE	3.0
2	B	50	MET	2.9
2	B	99	VAL	2.9
1	A	348	VAL	2.9
1	A	302	SER	2.9
2	B	643	ARG	2.9
1	A	133	GLY	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	512	VAL	2.7
2	B	340	ILE	2.7
2	B	88	LEU	2.6
2	B	252	ARG	2.6
2	B	200	ILE	2.6
1	A	351	GLU	2.6
1	A	422	LEU	2.5
2	B	46	PHE	2.5
2	B	339	TYR	2.5
2	B	189	ILE	2.5
2	B	172	ARG	2.5
2	B	203	ILE	2.5
2	B	645	GLN	2.5
1	A	135	THR	2.5
2	B	171	ASP	2.4
2	B	287	LEU	2.4
2	B	93	TYR	2.4
1	A	362	TYR	2.4
1	A	299	SER	2.4
2	B	77	PRO	2.4
1	A	411	VAL	2.4
2	B	290	PHE	2.3
2	B	515	ASN	2.3
2	B	174	GLY	2.2
1	A	300	SER	2.2
2	B	251	ILE	2.2
2	B	750	GLU	2.2
1	A	326	GLY	2.2
2	B	355	PHE	2.2
2	B	48	PHE	2.2
1	A	134	LYS	2.2
2	B	194	GLY	2.1
2	B	190	ARG	2.1
2	B	650	GLU	2.1
2	B	45	VAL	2.1
2	B	336	ALA	2.1
2	B	288	LEU	2.1
1	A	427	GLU	2.1
1	A	123	ARG	2.1
2	B	44	PRO	2.1
2	B	286	PHE	2.1
1	A	274	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	258	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 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.