



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:32 AM EDT

PDB ID : 7MX5  
Title : Crystal structure of TolB from *Acinetobacter baumannii*  
Authors : Stogios, P.J.; Evdokimova, E.; Endres, M.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CS-GID)  
Deposited on : 2021-05-18  
Resolution : 2.42 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 : 2.35.1  
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) : 2.35.1

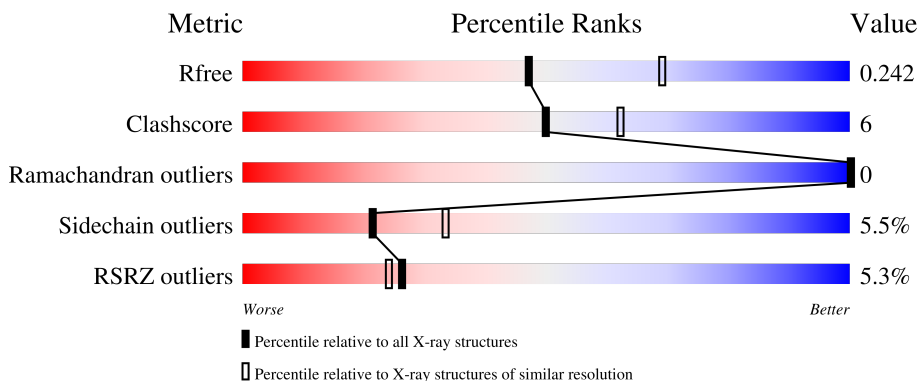
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	400	 6% 83% 16%
1	B	400	 5% 81% 17%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6504 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 Tol-Pal system protein TolB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	400	Total 3095	C 1942	N 544	O 601	S 8	0	1	0
1	B	399	Total 3104	C 1949	N 547	O 600	S 8	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP A0A6F8TCJ6
B	27	GLY	-	expression tag	UNP A0A6F8TCJ6

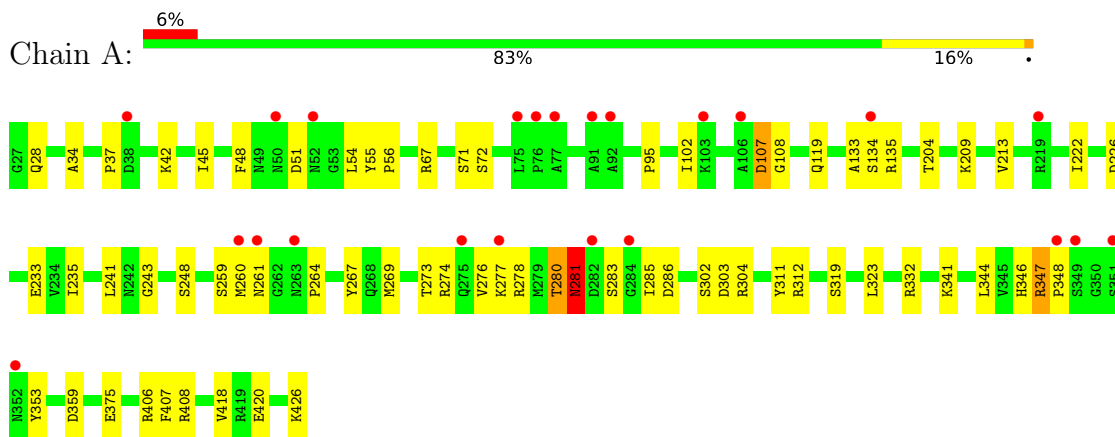
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	143	Total 145	O 145	0	2
2	B	159	Total 160	O 160	0	1

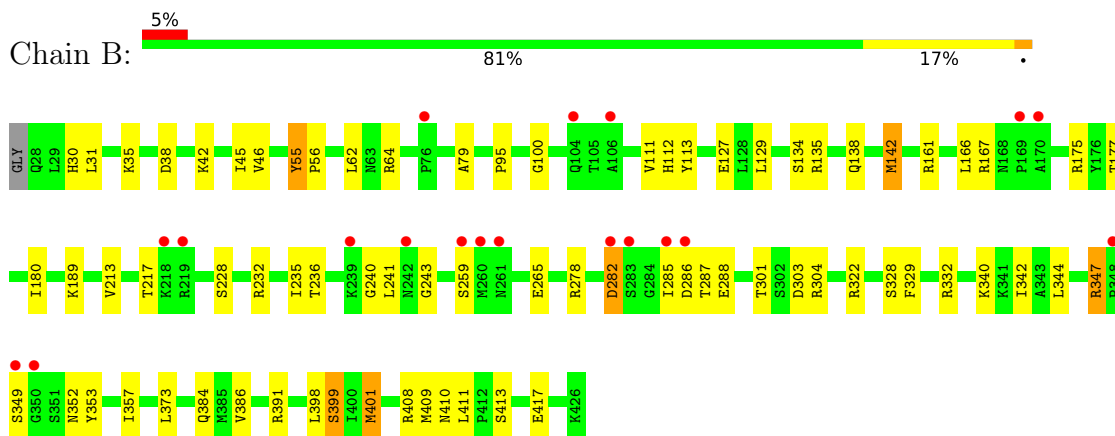
### 3 Residue-property plots [i](#)

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: Tol-Pal system protein TolB



- Molecule 1: Tol-Pal system protein TolB



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.50Å 98.44Å 83.83Å 90.00° 92.07° 90.00°	Depositor
Resolution (Å)	29.63 – 2.42 29.63 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.7 (29.63-2.42) 98.7 (29.63-2.42)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.194 , 0.244 0.193 , 0.242	Depositor DCC
$R_{free}$ test set	1344 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtrriage
Anisotropy	0.176	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6504	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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, 0.333 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	0.26	0/3165	0.55	2/4296 (0.0%)
1	B	0.25	0/3180	0.54	0/4315
All	All	0.26	0/6345	0.55	2/8611 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASN	N-CA-C	8.31	133.44	111.00
1	A	280	THR	N-CA-C	5.73	126.47	111.00

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	3095	0	3055	33	0
1	B	3104	0	3076	39	0
2	A	145	0	0	2	0
2	B	160	0	0	5	0
All	All	6504	0	6131	72	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 (72) 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:B:111:VAL:HG12	1:B:129:LEU:HB3	1.67	0.76
1:A:108:GLY:HA3	1:A:133:ALA:H	1.59	0.68
1:A:107:ASP:N	1:A:107:ASP:OD1	2.29	0.65
1:B:282:ASP:OD2	1:B:287:THR:HG21	2.00	0.60
1:A:45:ILE:HD11	1:A:55:TYR:HB2	1.83	0.60
1:B:35:LYS:NZ	2:B:503:HOH:O	2.27	0.58
1:B:329:PHE:HB3	1:B:347:ARG:HG3	1.86	0.57
1:A:408:ARG:NH2	2:A:502:HOH:O	2.28	0.57
1:B:287:THR:HG22	1:B:301:THR:O	2.06	0.56
1:B:322:ARG:NH2	2:B:508:HOH:O	2.39	0.56
1:B:240:GLY:O	1:B:259:SER:N	2.32	0.55
1:A:267:TYR:CE2	1:A:278:ARG:HB3	2.41	0.55
1:A:285:ILE:HG12	1:A:303:ASP:HB2	1.89	0.55
1:B:213:VAL:HG21	1:B:243:GLY:HA3	1.88	0.55
1:B:285:ILE:HG13	1:B:303:ASP:OD2	2.09	0.53
1:B:347:ARG:HB3	1:B:353:TYR:HA	1.90	0.53
1:A:281:ASN:OD1	1:A:283:SER:HB3	2.09	0.52
1:A:222:ILE:HG13	1:A:241:LEU:HD21	1.90	0.52
1:A:34:ALA:HB3	1:A:408:ARG:HB3	1.91	0.52
1:B:111:VAL:CG1	1:B:129:LEU:HB3	2.38	0.50
1:B:167:ARG:HB2	1:B:417:GLU:HG3	1.93	0.50
1:A:233:GLU:OE1	1:A:274:ARG:NH2	2.44	0.50
1:A:347:ARG:HG3	1:A:353:TYR:CD1	2.47	0.50
1:B:42:LYS:O	1:B:95:PRO:HD2	2.13	0.49
1:B:342:ILE:HG22	1:B:344:LEU:HD23	1.95	0.49
1:A:55:TYR:CD2	1:A:56:PRO:HD3	2.48	0.49
1:B:64:ARG:HB2	1:B:409:MET:HE2	1.94	0.49
1:B:265:GLU:OE2	1:B:278:ARG:NH2	2.45	0.48
1:B:138:GLN:HE21	1:B:142:MET:HE1	1.79	0.48
1:B:398:LEU:HB2	1:B:411:LEU:HB2	1.95	0.48
1:A:302:SER:OG	1:A:304:ARG:HG2	2.14	0.48
1:B:401:MET:HG3	1:B:408:ARG:HG3	1.95	0.48
1:A:302:SER:HB3	1:A:311:TYR:CD1	2.50	0.47
1:A:259:SER:HB3	1:A:264:PRO:HA	1.95	0.47
1:B:55:TYR:CD2	1:B:56:PRO:HD3	2.49	0.47
1:B:180:ILE:O	1:B:189:LYS:N	2.47	0.46
1:B:161:ARG:HH22	1:B:189:LYS:HB2	1.80	0.46
1:B:288:GLU:OE2	1:B:332:ARG:NH1	2.47	0.46
1:B:46:VAL:HG21	1:B:79:ALA:HB3	1.98	0.46
1:A:375:GLU:OE2	1:A:420:GLU:N	2.42	0.46
1:B:285:ILE:HG22	1:B:286:ASP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LYS:HG2	1:A:226:ASP:HA	1.98	0.45
1:A:341:LYS:NZ	1:A:359:ASP:OD2	2.42	0.45
1:B:373:LEU:HD21	1:B:391[B]:ARG:NH2	2.31	0.45
1:B:357:ILE:HD11	1:B:386:VAL:HG21	1.98	0.45
1:B:235:ILE:HG22	1:B:236:THR:HG22	1.98	0.45
1:B:399:SER:OG	1:B:410:ASN:OD1	2.35	0.44
1:A:45:ILE:HG23	1:A:72:SER:HB3	2.00	0.44
1:A:48:PHE:HE2	1:A:54:LEU:HD12	1.84	0.43
1:A:37:PRO:HD3	1:A:407:PHE:HD1	1.83	0.43
1:A:319:SER:H	1:A:319:SER:HG	1.61	0.43
1:B:340:LYS:O	2:B:501:HOH:O	2.21	0.43
1:A:213:VAL:HG21	1:A:243:GLY:HA3	2.01	0.43
1:B:135:ARG:NH1	2:B:521:HOH:O	2.52	0.43
1:A:42:LYS:O	1:A:95:PRO:HD2	2.19	0.42
1:A:235:ILE:O	1:A:269:MET:HE1	2.19	0.42
1:A:312:ARG:HB2	1:A:323:LEU:HD11	2.01	0.42
1:B:30:HIS:O	1:B:411:LEU:HA	2.18	0.42
1:B:31:LEU:HD11	1:B:64:ARG:HD3	2.01	0.42
1:B:45:ILE:HD11	1:B:62:LEU:HD12	2.01	0.42
1:B:166:LEU:HB2	1:B:177:THR:HB	2.01	0.42
1:A:264:PRO:O	1:A:281:ASN:O	2.38	0.42
1:B:285:ILE:HG22	1:B:286:ASP:H	1.84	0.41
1:A:135:ARG:HA	1:A:135:ARG:HD2	1.89	0.41
1:A:51:ASP:HA	1:A:102:ILE:HD12	2.02	0.41
1:B:384:GLN:NE2	2:B:522:HOH:O	2.52	0.41
1:A:67:ARG:HE	1:A:67:ARG:HB3	1.61	0.41
1:A:269:MET:HG3	1:A:276:VAL:CG1	2.51	0.41
1:A:346:HIS:CD2	1:A:348:PRO:HD3	2.56	0.41
1:B:113:TYR:CZ	1:B:127:GLU:HB2	2.55	0.41
1:B:100:GLY:HA2	1:B:112:HIS:O	2.21	0.40
1:A:119:GLN:NE2	2:A:519:HOH:O	2.55	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	A	399/400 (100%)	377 (94%)	22 (6%)	0	100	100
1	B	400/400 (100%)	380 (95%)	20 (5%)	0	100	100
All	All	799/800 (100%)	757 (95%)	42 (5%)	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	335/334 (100%)	316 (94%)	19 (6%)	20	32
1	B	337/334 (101%)	318 (94%)	19 (6%)	21	32
All	All	672/668 (101%)	634 (94%)	38 (6%)	21	32

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	71	SER
1	A	107	ASP
1	A	134	SER
1	A	204	THR
1	A	248	SER
1	A	260	MET
1	A	261	ASN
1	A	273	THR
1	A	277	LYS
1	A	280	THR
1	A	281	ASN
1	A	286	ASP
1	A	332	ARG
1	A	344	LEU

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Mol	Chain	Res	Type
1	A	347	ARG
1	A	406	ARG
1	A	418	VAL
1	A	426	LYS
1	B	38	ASP
1	B	55	TYR
1	B	134	SER
1	B	142	MET
1	B	175	ARG
1	B	217	THR
1	B	228	SER
1	B	232	ARG
1	B	241	LEU
1	B	282	ASP
1	B	304	ARG
1	B	328	SER
1	B	347	ARG
1	B	349	SER
1	B	352[A]	ASN
1	B	352[B]	ASN
1	B	399	SER
1	B	401	MET
1	B	413	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	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	400/400 (100%)	-0.00	23 (5%) 23 21	31, 47, 89, 146	0
1	B	399/400 (99%)	0.04	19 (4%) 30 28	25, 44, 100, 171	0
All	All	799/800 (99%)	0.02	42 (5%) 26 24	25, 46, 94, 171	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	285	ILE	8.4
1	B	286	ASP	5.5
1	A	349	SER	5.1
1	B	349	SER	5.0
1	B	169	PRO	5.0
1	A	50	ASN	4.7
1	B	350	GLY	4.6
1	B	261	ASN	4.4
1	A	260	MET	4.3
1	A	261	ASN	4.0
1	A	76	PRO	3.5
1	A	351	SER	3.4
1	A	77	ALA	3.3
1	B	259	SER	3.3
1	A	282	ASP	3.2
1	B	260	MET	3.2
1	B	282	ASP	3.1
1	B	219	ARG	2.9
1	B	348	PRO	2.8
1	A	75	LEU	2.8
1	A	106	ALA	2.7
1	A	38	ASP	2.7
1	B	76	PRO	2.6
1	B	239	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	263	ASN	2.6
1	A	275	GLN	2.5
1	A	352	ASN	2.5
1	A	277	LYS	2.4
1	A	134	SER	2.4
1	B	170	ALA	2.4
1	A	348	PRO	2.3
1	A	92	ALA	2.3
1	B	218	LYS	2.3
1	B	104	GLN	2.3
1	B	106	ALA	2.3
1	A	219	ARG	2.2
1	B	283	SER	2.2
1	A	52	ASN	2.2
1	A	103	LYS	2.2
1	A	91	ALA	2.2
1	B	242	ASN	2.1
1	A	284	GLY	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 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.