



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:11 AM GMT

PDB ID : 2ZVY  
Title : Structure of the periplasmic domain of MotB from Salmonella (crystal form II)  
Authors : Kojima, S.; Homma, M.; Namba, K.; Imada, K.  
Deposited on : 2008-11-26  
Resolution : 1.75 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

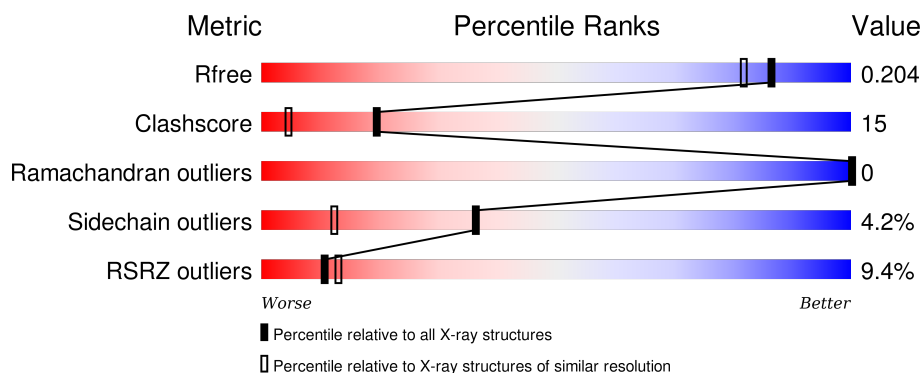
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


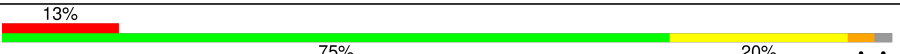
The reported resolution of this entry is 1.75 Å.

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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	A	183	 5% 78% 20% •
1	B	183	 13% 75% 20% ••

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3352 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 Chemotaxis protein motB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	183	Total	C	N	O	S	0	0	0
			1455	898	283	269	5			
1	B	180	Total	C	N	O	S	0	0	0
			1428	882	278	263	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	277	HIS	-	EXPRESSION TAG	UNP P55892
A	278	HIS	-	EXPRESSION TAG	UNP P55892
A	279	HIS	-	EXPRESSION TAG	UNP P55892
A	280	HIS	-	EXPRESSION TAG	UNP P55892
A	281	HIS	-	EXPRESSION TAG	UNP P55892
B	277	HIS	-	EXPRESSION TAG	UNP P55892
B	278	HIS	-	EXPRESSION TAG	UNP P55892
B	279	HIS	-	EXPRESSION TAG	UNP P55892
B	280	HIS	-	EXPRESSION TAG	UNP P55892
B	281	HIS	-	EXPRESSION TAG	UNP P55892

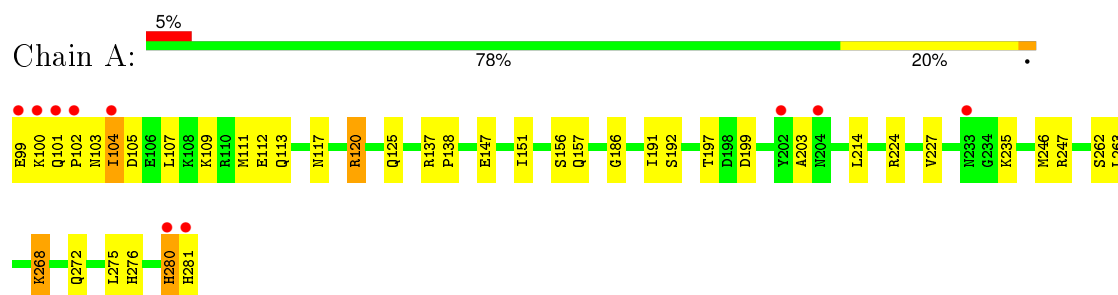
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	280	Total	O	0	0
			280	280		
2	B	189	Total	O	0	0
			189	189		

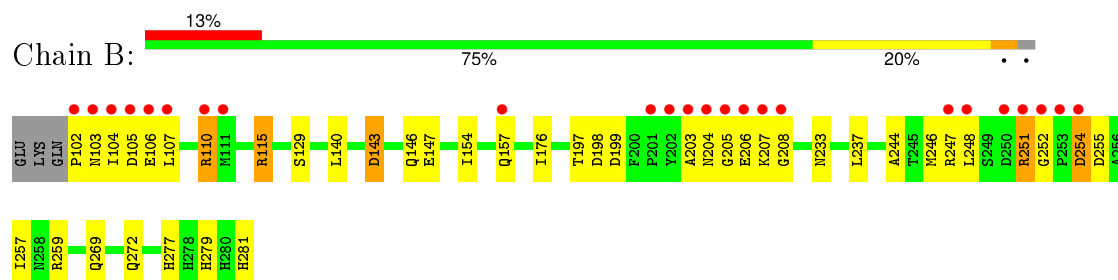
### 3 Residue-property plots [i](#)

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: Chemotaxis protein motB



#### • Molecule 1: Chemotaxis protein motB



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.25Å 86.40Å 129.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.97 – 1.75 35.97 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (35.97-1.75) 99.9 (35.97-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.187 , 0.204 0.186 , 0.204	Depositor DCC
$R_{free}$ test set	1839 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.0	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 36798 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3352	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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	A	0.26	0/1478	0.58	1/1989 (0.1%)
1	B	0.27	0/1451	0.59	0/1953
All	All	0.27	0/2929	0.58	1/3942 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	SER	N-CA-C	-5.39	96.46	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	1455	0	1473	51	0
1	B	1428	0	1447	48	0
2	A	280	0	0	10	1
2	B	189	0	0	9	0
All	All	3352	0	2920	87	1

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 15.

All (87) 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:251:ARG:HD2	1:B:252:GLY:N	1.75	1.00
1:B:251:ARG:HD2	1:B:252:GLY:H	1.30	0.95
1:A:227:VAL:HG11	1:B:206:GLU:HA	1.59	0.84
1:B:115:ARG:HG3	1:B:115:ARG:HH11	1.44	0.81
1:A:109:LYS:HB2	2:A:425:HOH:O	1.83	0.79
1:B:197:THR:HB	2:B:383:HOH:O	1.82	0.78
1:A:111:MET:HG3	2:A:85:HOH:O	1.86	0.74
1:B:199:ASP:OD2	1:B:259:ARG:HD3	1.89	0.73
1:A:268:LYS:NZ	1:A:272:GLN:HG2	2.06	0.71
1:A:101:GLN:N	1:A:102:PRO:HD2	2.06	0.70
1:B:154:ILE:HG21	1:B:257:ILE:HD12	1.75	0.69
1:B:269:GLN:NE2	1:B:269:GLN:H	1.91	0.69
1:A:235:LYS:HD3	2:A:486:HOH:O	1.92	0.68
1:B:254:ASP:HA	2:B:444:HOH:O	1.94	0.68
1:B:129:SER:HB3	2:B:438:HOH:O	1.95	0.66
1:A:203:ALA:HB1	1:B:233:ASN:HD21	1.61	0.63
1:B:103:ASN:O	1:B:107:LEU:HB2	1.98	0.63
1:A:247:ARG:HD2	1:A:247:ARG:C	2.20	0.62
1:B:197:THR:HG22	2:B:9:HOH:O	2.01	0.61
1:B:104:ILE:HG23	1:B:105:ASP:H	1.67	0.59
1:A:268:LYS:HZ3	1:A:272:GLN:HG2	1.64	0.59
1:A:137:ARG:N	1:A:138:PRO:HD2	2.18	0.59
1:B:106:GLU:O	1:B:110:ARG:HG2	2.02	0.58
1:A:101:GLN:O	1:A:104:ILE:HG22	2.03	0.58
1:A:192:SER:OG	1:B:281:HIS:HE1	1.87	0.58
1:B:104:ILE:HG23	1:B:105:ASP:N	2.19	0.58
1:A:157:GLN:HG2	2:A:72:HOH:O	2.03	0.58
1:B:115:ARG:NH1	1:B:115:ARG:HG3	2.18	0.57
1:B:251:ARG:HD3	1:B:255:ASP:OD2	2.04	0.57
1:A:157:GLN:NE2	2:A:383:HOH:O	2.38	0.57
1:B:279:HIS:HB2	2:B:408:HOH:O	2.05	0.56
1:A:191:ILE:HG22	1:A:192:SER:N	2.22	0.55
1:A:104:ILE:O	1:A:104:ILE:HD13	2.07	0.55
1:B:272:GLN:HG3	2:B:78:HOH:O	2.05	0.55
1:B:248:LEU:HD12	1:B:257:ILE:HG13	1.88	0.54
1:A:109:LYS:O	1:A:113:GLN:HG3	2.07	0.54
1:A:109:LYS:HD2	2:A:425:HOH:O	2.07	0.53
1:A:247:ARG:HD2	1:A:247:ARG:O	2.08	0.53
1:A:227:VAL:CG1	1:B:206:GLU:HA	2.34	0.53
1:A:280:HIS:ND1	1:A:280:HIS:O	2.42	0.52
1:A:117:ASN:HB2	2:A:58:HOH:O	2.10	0.52
1:B:102:PRO:HG2	1:B:103:ASN:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:GLY:C	1:B:207:LYS:H	2.14	0.51
1:A:268:LYS:HA	1:A:268:LYS:HE2	1.93	0.50
1:B:154:ILE:HD13	1:B:257:ILE:CD1	2.42	0.50
1:B:146:GLN:HG3	1:B:147:GLU:OE2	2.12	0.50
1:A:281:HIS:CE1	1:B:143:ASP:HB2	2.47	0.49
1:A:224:ARG:HD2	1:B:208:GLY:HA2	1.94	0.49
1:B:110:ARG:N	1:B:110:ARG:HD3	2.27	0.49
1:A:104:ILE:HA	1:A:107:LEU:HD12	1.94	0.49
1:A:262:SER:OG	1:B:281:HIS:HD2	1.95	0.49
1:A:197:THR:HG21	1:A:214:LEU:HD23	1.95	0.49
1:A:191:ILE:HD13	1:A:263:LEU:HD21	1.95	0.49
1:A:275:LEU:HD23	1:B:246:MET:CE	2.43	0.48
1:B:157:GLN:HG2	2:B:444:HOH:O	2.12	0.48
1:B:204:ASN:O	1:B:207:LYS:HB2	2.13	0.48
1:B:140:LEU:HD21	1:B:176:ILE:HD13	1.96	0.48
1:A:157:GLN:HA	2:A:371:HOH:O	2.13	0.47
1:A:99:GLU:OE2	1:A:99:GLU:N	2.47	0.47
1:A:147:GLU:HG2	1:B:277:HIS:CE1	2.49	0.47
1:A:101:GLN:N	1:A:102:PRO:CD	2.77	0.46
1:A:247:ARG:HG3	2:A:373:HOH:O	2.16	0.46
1:B:146:GLN:HG3	1:B:147:GLU:CD	2.36	0.46
1:A:120:ARG:HD3	1:A:120:ARG:C	2.37	0.45
1:A:281:HIS:HE1	1:B:143:ASP:HB2	1.81	0.45
1:A:280:HIS:O	1:A:281:HIS:HB3	2.17	0.44
1:A:191:ILE:CG2	1:A:192:SER:N	2.81	0.43
1:A:280:HIS:C	1:A:281:HIS:O	2.52	0.43
1:A:276:HIS:CE1	1:A:280:HIS:HB3	2.52	0.43
1:A:151:ILE:HD12	1:A:263:LEU:HD22	2.00	0.43
1:A:147:GLU:HG2	1:B:277:HIS:ND1	2.33	0.43
1:B:248:LEU:HD12	1:B:257:ILE:CG1	2.49	0.43
1:B:203:ALA:C	1:B:205:GLY:H	2.23	0.42
1:A:186:GLY:HA3	2:A:22:HOH:O	2.19	0.42
1:B:279:HIS:HD2	2:B:33:HOH:O	2.02	0.41
1:A:268:LYS:HZ2	1:A:272:GLN:HG2	1.82	0.41
1:A:280:HIS:NE2	1:B:147:GLU:OE1	2.53	0.41
1:B:205:GLY:C	1:B:207:LYS:N	2.72	0.41
1:A:157:GLN:HA	1:A:157:GLN:OE1	2.20	0.41
1:A:100:LYS:HG3	1:A:101:GLN:N	2.35	0.41
1:B:198:ASP:N	2:B:383:HOH:O	2.52	0.41
1:A:112:GLU:CD	1:A:268:LYS:H	2.24	0.41
1:B:244:ALA:O	1:B:247:ARG:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:O	1:A:107:LEU:HG	2.20	0.41
1:A:281:HIS:CD2	1:A:281:HIS:OXT	2.74	0.41
1:B:237:LEU:HD23	1:B:237:LEU:O	2.20	0.40
1:B:115:ARG:CG	1:B:115:ARG:NH1	2.80	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:283:HOH:O	2:A:283:HOH:O[3_555]	1.51	0.69

## 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	181/183 (99%)	177 (98%)	4 (2%)	0	100	100
1	B	178/183 (97%)	170 (96%)	8 (4%)	0	100	100
All	All	359/366 (98%)	347 (97%)	12 (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	156/156 (100%)	148 (95%)	8 (5%)	29	8
1	B	153/156 (98%)	148 (97%)	5 (3%)	45	19
All	All	309/312 (99%)	296 (96%)	13 (4%)	36	12

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	ILE
1	A	105	ASP
1	A	120	ARG
1	A	125	GLN
1	A	199	ASP
1	A	246	MET
1	A	268	LYS
1	A	280	HIS
1	B	110	ARG
1	B	115	ARG
1	B	143	ASP
1	B	251	ARG
1	B	254	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	204	ASN
1	A	281	HIS
1	B	125	GLN
1	B	233	ASN
1	B	269	GLN
1	B	279	HIS
1	B	281	HIS

### 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 [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	183/183 (100%)	0.30	10 (5%) 29 34	6, 13, 38, 73	0
1	B	180/183 (98%)	0.67	24 (13%) 4 6	7, 17, 53, 68	0
All	All	363/366 (99%)	0.49	34 (9%) 11 13	6, 15, 49, 73	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	PRO	11.6
1	B	202	TYR	10.5
1	A	99	GLU	7.6
1	A	100	LYS	6.7
1	B	103	ASN	6.3
1	B	207	LYS	6.0
1	A	281	HIS	6.0
1	B	107	LEU	5.9
1	B	250	ASP	5.1
1	B	206	GLU	5.0
1	B	253	PRO	4.6
1	B	252	GLY	4.2
1	A	101	GLN	4.2
1	B	104	ILE	4.0
1	A	202	TYR	3.7
1	B	208	GLY	3.7
1	A	102	PRO	3.5
1	B	248	LEU	3.2
1	B	251	ARG	3.2
1	B	205	GLY	3.1
1	B	203	ALA	3.0
1	B	110	ARG	2.9
1	A	204	ASN	2.7
1	B	254	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	111	MET	2.6
1	A	280	HIS	2.6
1	A	233	ASN	2.5
1	B	157	GLN	2.5
1	B	105	ASP	2.4
1	B	204	ASN	2.4
1	B	247	ARG	2.3
1	B	106	GLU	2.2
1	B	201	PRO	2.2
1	A	104	ILE	2.2

## 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.