



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 04:13 PM JST

PDB ID : 23VJ / pdb\_000023vj  
Title : Crystal structure of the MafR protein from *Enterococcus faecalis*  
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Deposited on : 2026-02-20  
Resolution : 2.30 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

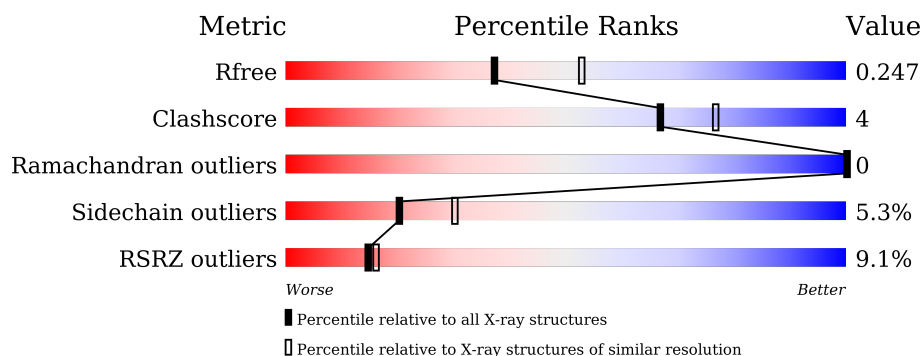
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	488	 6% 85% 11% ..
1	B	488	 10% 71% 9% • 18%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6916 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 M protein trans-acting positive regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3720	2423	589	702	6			
1	B	398	Total	C	N	O	S	0	2	0
			3136	2050	498	584	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP A0A3N3PGJ5
A	-4	SER	-	expression tag	UNP A0A3N3PGJ5
A	-3	ALA	-	expression tag	UNP A0A3N3PGJ5
A	-2	LYS	-	expression tag	UNP A0A3N3PGJ5
A	-1	ASP	-	expression tag	UNP A0A3N3PGJ5
A	0	PRO	-	expression tag	UNP A0A3N3PGJ5
B	-5	GLY	-	expression tag	UNP A0A3N3PGJ5
B	-4	SER	-	expression tag	UNP A0A3N3PGJ5
B	-3	ALA	-	expression tag	UNP A0A3N3PGJ5
B	-2	LYS	-	expression tag	UNP A0A3N3PGJ5
B	-1	ASP	-	expression tag	UNP A0A3N3PGJ5
B	0	PRO	-	expression tag	UNP A0A3N3PGJ5

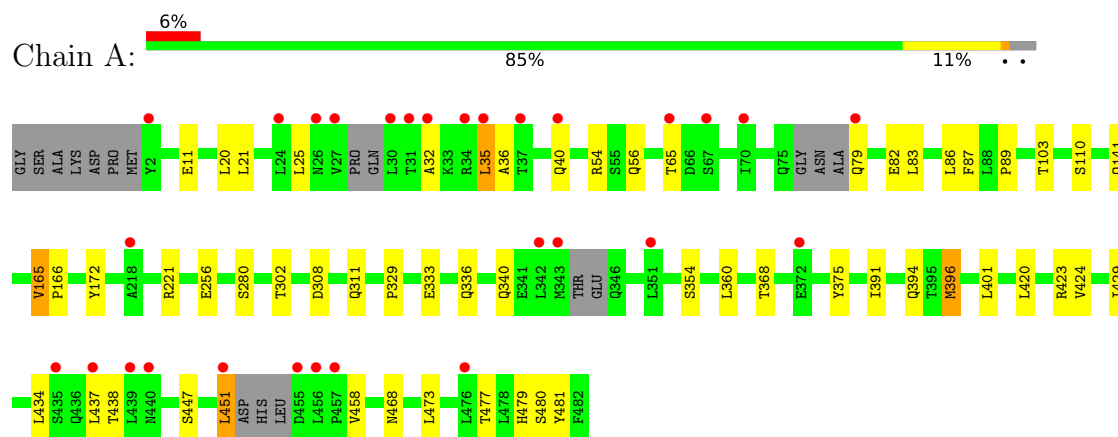
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	32	Total	O	0	0
			32	32		
2	B	28	Total	O	0	0
			28	28		

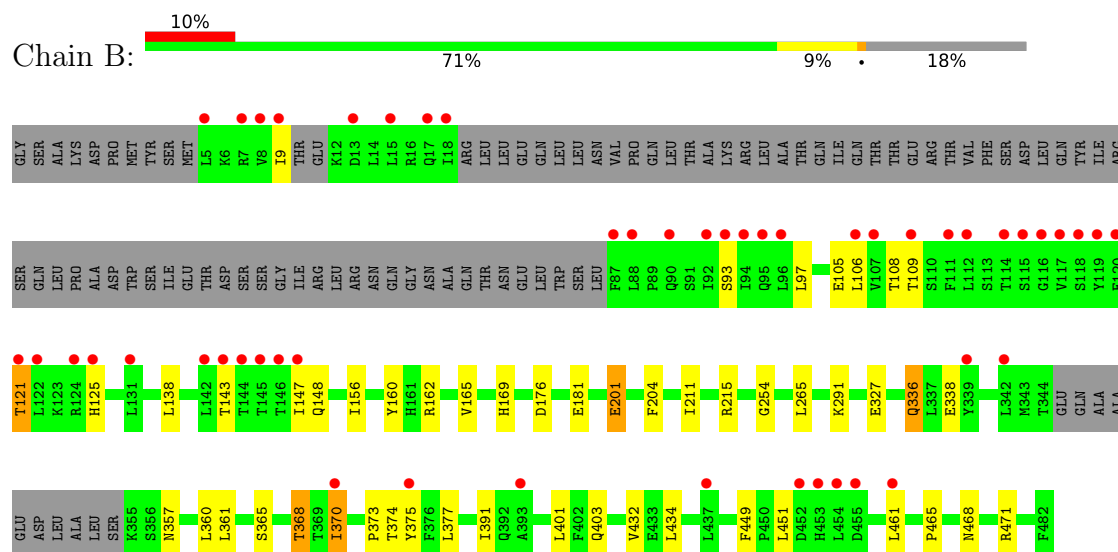
### 3 Residue-property plots [i](#)

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: M protein trans-acting positive regulator



- Molecule 1: M protein trans-acting positive regulator



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.18Å 102.47Å 90.75Å 90.00° 96.76° 90.00°	Depositor
Resolution (Å)	29.47 – 2.30 29.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.47-2.30) 99.7 (29.47-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.211 , 0.248 0.211 , 0.247	Depositor DCC
$R_{free}$ test set	2547 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6916	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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	0.29	0/3801	0.47	0/5177
1	B	0.30	0/3218	0.46	1/4384 (0.0%)
All	All	0.30	0/7019	0.47	1/9561 (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	B	254	GLY	CA-C-O	-5.49	115.40	121.05

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	3720	0	3540	25	0
1	B	3136	0	2918	24	0
2	A	32	0	0	0	0
2	B	28	0	0	0	0
All	All	6916	0	6458	49	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 (49) 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:108:THR:HG22	1:B:147:ILE:HG13	1.55	0.88
1:A:54:ARG:HH12	1:A:65:THR:HG22	1.52	0.74
1:A:165:VAL:HG12	1:A:166:PRO:HD3	1.81	0.62
1:B:9:ILE:HA	1:B:93:SER:CB	2.30	0.61
1:A:420:LEU:HD13	1:A:424:VAL:HG11	1.84	0.60
1:B:138:LEU:HD11	1:B:156:ILE:HA	1.85	0.58
1:A:396:MET:HE2	1:A:479:HIS:CE1	2.39	0.58
1:B:357:ASN:OD1	1:B:377:LEU:HD22	2.03	0.57
1:B:105:GLU:HG3	1:B:148:GLN:HG2	1.87	0.57
1:A:451:LEU:HD21	1:A:458:VAL:HG21	1.87	0.56
1:B:201:GLU:HB2	1:B:204:PHE:HB3	1.89	0.55
1:B:108:THR:HG21	1:B:143:THR:O	2.07	0.54
1:B:336:GLN:HB2	1:B:375:TYR:CD1	2.42	0.54
1:A:329:PRO:HG3	1:A:368:THR:OG1	2.12	0.50
1:A:221:ARG:HA	1:A:256:GLU:OE1	2.11	0.50
1:A:36:ALA:O	1:A:40:GLN:N	2.45	0.49
1:B:361:LEU:HD11	1:B:373:PRO:HB3	1.94	0.49
1:B:434:LEU:HD21	1:B:451:LEU:HD13	1.94	0.49
1:B:121:THR:HG22	1:B:125:HIS:CE1	2.48	0.48
1:A:420:LEU:HD22	1:A:477:THR:HG21	1.95	0.48
1:A:308:ASP:HB2	1:A:391:ILE:HD12	1.96	0.48
1:A:423:ARG:HD3	1:A:481:TYR:CD2	2.48	0.48
1:A:401:LEU:O	1:A:447:SER:HA	2.14	0.47
1:B:162:ARG:HB2	1:B:338:GLU:HG3	1.96	0.47
1:A:32:ALA:O	1:A:35:LEU:HD23	2.13	0.47
1:B:461:LEU:HD11	1:B:465:PRO:HB3	1.97	0.47
1:B:357:ASN:CG	1:B:377:LEU:HD22	2.39	0.47
1:A:86:LEU:HD23	1:A:87:PHE:CE2	2.51	0.46
1:A:396:MET:HE3	1:A:480:SER:HB2	1.98	0.46
1:A:473:LEU:O	1:A:477:THR:HG23	2.17	0.45
1:A:21:LEU:HD12	1:A:21:LEU:HA	1.62	0.45
1:B:169:HIS:NE2	1:B:181:GLU:OE2	2.40	0.45
1:B:401:LEU:HD23	1:B:401:LEU:HA	1.89	0.44
1:A:336:GLN:HG2	1:A:375:TYR:CD2	2.54	0.43
1:B:370:ILE:HD11	1:B:373:PRO:HA	2.01	0.43
1:B:336:GLN:HB2	1:B:375:TYR:CG	2.53	0.43
1:A:360:LEU:HD23	1:A:360:LEU:HA	1.86	0.43
1:A:429:ILE:HD11	1:A:434:LEU:HD13	2.00	0.42
1:B:360:LEU:HD12	1:B:360:LEU:HA	1.87	0.42
1:B:403:GLN:HG3	1:B:449:PHE:CE2	2.54	0.42
1:A:89:PRO:HB3	1:A:172:TYR:CZ	2.55	0.42
1:A:451:LEU:HD21	1:A:458:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:SER:HA	1:B:368:THR:O	2.20	0.42
1:B:211:ILE:O	1:B:215:ARG:HG2	2.19	0.42
1:B:265:LEU:CD2	1:B:327:GLU:HG3	2.49	0.41
1:A:396:MET:HE1	1:A:477:THR:HA	2.02	0.41
1:B:97:LEU:O	1:B:160:TYR:OH	2.29	0.41
1:A:221:ARG:HA	1:A:221:ARG:HD3	1.90	0.41
1:A:79:GLN:O	1:A:82:GLU:HG2	2.22	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	461/488 (94%)	453 (98%)	8 (2%)	0	100	100
1	B	392/488 (80%)	378 (96%)	14 (4%)	0	100	100
All	All	853/976 (87%)	831 (97%)	22 (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	388/448 (87%)	366 (94%)	22 (6%)	18	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	317/448 (71%)	302 (95%)	15 (5%)	23	35
All	All	705/896 (79%)	668 (95%)	37 (5%)	20	31

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	20	LEU
1	A	25	LEU
1	A	35	LEU
1	A	56	GLN
1	A	83	LEU
1	A	103	THR
1	A	110	SER
1	A	141	GLN
1	A	165	VAL
1	A	280	SER
1	A	302	THR
1	A	311	GLN
1	A	333	GLU
1	A	340	GLN
1	A	354	SER
1	A	394	GLN
1	A	396	MET
1	A	437	LEU
1	A	438	THR
1	A	451	LEU
1	A	468	ASN
1	B	106	LEU
1	B	109	THR
1	B	121	THR
1	B	165	VAL
1	B	176	ASP
1	B	201	GLU
1	B	291	LYS
1	B	336	GLN
1	B	368	THR
1	B	370	ILE
1	B	374	THR
1	B	391	ILE
1	B	432	VAL
1	B	468	ASN

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Mol	Chain	Res	Type
1	B	471	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	190	GLN
1	A	216	ASN
1	A	224	GLN
1	A	235	GLN
1	A	269	ASN
1	A	285	HIS
1	A	336	GLN
1	A	357	ASN
1	A	413	GLN
1	B	125	HIS
1	B	171	ASN
1	B	453	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 ⓘ

There are no oligosaccharides 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	471/488 (96%)	0.31	29 (6%) 26 28	27, 55, 103, 134	0
1	B	398/488 (81%)	0.65	50 (12%) 8 9	28, 61, 112, 126	2 (0%)
All	All	869/976 (89%)	0.46	79 (9%) 15 16	27, 57, 110, 134	2 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	GLU	6.1
1	A	2	TYR	5.3
1	B	144	THR	4.4
1	B	8	VAL	4.4
1	B	92	ILE	4.3
1	B	112	LEU	4.3
1	B	342	LEU	4.1
1	B	122	LEU	4.0
1	B	147	ILE	3.9
1	B	393	ALA	3.7
1	A	35	LEU	3.6
1	B	107	VAL	3.5
1	B	116	GLY	3.5
1	B	115	SER	3.5
1	B	119	TYR	3.5
1	B	145	THR	3.4
1	A	27	VAL	3.4
1	B	142	LEU	3.4
1	B	117	VAL	3.3
1	B	18	ILE	3.3
1	B	9	ILE	3.3
1	A	30	LEU	3.3
1	A	476	LEU	3.3
1	B	111	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	90	GLN	3.2
1	B	121	THR	3.2
1	B	370	ILE	3.1
1	B	453	HIS	3.1
1	B	454	LEU	3.1
1	A	37	THR	3.0
1	A	65	THR	3.0
1	B	94	ILE	2.9
1	A	343	MET	2.9
1	B	96	LEU	2.9
1	B	106	LEU	2.8
1	A	67	SER	2.8
1	B	15	LEU	2.7
1	B	114	THR	2.7
1	B	339	TYR	2.7
1	A	455	ASP	2.6
1	B	375	TYR	2.6
1	A	70	ILE	2.6
1	B	95	GLN	2.5
1	A	342	LEU	2.5
1	B	109	THR	2.5
1	B	7	ARG	2.5
1	A	79	GLN	2.5
1	B	17	GLN	2.5
1	A	451	LEU	2.5
1	A	439	LEU	2.4
1	B	131	LEU	2.4
1	A	32	ALA	2.4
1	A	34	ARG	2.4
1	B	118	SER	2.4
1	B	93	SER	2.4
1	B	88	LEU	2.4
1	B	124	ARG	2.4
1	B	143	THR	2.3
1	A	26	ASN	2.3
1	A	456	LEU	2.3
1	B	455	ASP	2.2
1	A	437	LEU	2.2
1	B	452	ASP	2.2
1	A	457	PRO	2.2
1	A	435	SER	2.1
1	B	461	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	125	HIS	2.1
1	B	87	PHE	2.1
1	A	31	THR	2.1
1	A	218	ALA	2.1
1	B	146	THR	2.1
1	A	351	LEU	2.1
1	A	24	LEU	2.0
1	A	440	ASN	2.0
1	B	5	LEU	2.0
1	B	13	ASP	2.0
1	A	372	GLU	2.0
1	A	40	GLN	2.0
1	B	437	LEU	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 oligosaccharides 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.