



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:38 pm GMT

PDB ID : 4Z29
Title : Crystal structure of the magnetobacterial protein MtxA C-terminal domain
Authors : Zarivach, R.; Davidov, G.
Deposited on : 2015-03-29
Resolution : 2.03 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

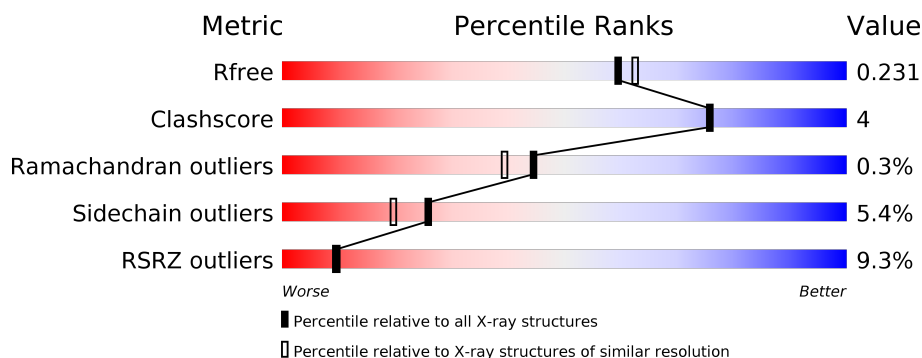
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	100719	8396 (2.04-2.00)
Clashscore	112137	9678 (2.04-2.00)
Ramachandran outliers	110173	9566 (2.04-2.00)
Sidechain outliers	110143	9565 (2.04-2.00)
RSRZ outliers	101464	8490 (2.04-2.00)

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 ≥ 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	325	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 9%; height: 10px; background-color: red;"></div> <div style="width: 47%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 46%; height: 10px; background-color: grey;"></div> </div> </div> </div>
1	B	325	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%;"></div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 10px;"> <div style="width: 9%; height: 10px; background-color: red;"></div> <div style="width: 48%; height: 10px; background-color: green;"></div> <div style="width: 48%; height: 10px; background-color: grey;"></div> </div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2800 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 Magnetotaxis protein MtxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	4	0
			1363	861	233	265	4			
1	B	169	Total	C	N	O	S	0	1	0
			1297	815	223	255	4			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A4TUL6
A	2	ALA	-	expression tag	UNP A4TUL6
A	3	SER	-	expression tag	UNP A4TUL6
A	4	TRP	-	expression tag	UNP A4TUL6
A	5	SER	-	expression tag	UNP A4TUL6
A	6	HIS	-	expression tag	UNP A4TUL6
A	7	PRO	-	expression tag	UNP A4TUL6
A	8	GLN	-	expression tag	UNP A4TUL6
A	9	PHE	-	expression tag	UNP A4TUL6
A	10	GLU	-	expression tag	UNP A4TUL6
A	11	LYS	-	expression tag	UNP A4TUL6
A	12	GLY	-	expression tag	UNP A4TUL6
A	13	ALA	-	expression tag	UNP A4TUL6
A	14	ASP	-	expression tag	UNP A4TUL6
A	15	ASP	-	expression tag	UNP A4TUL6
A	16	ASP	-	expression tag	UNP A4TUL6
A	17	ASP	-	expression tag	UNP A4TUL6
A	18	LYS	-	expression tag	UNP A4TUL6
A	308	PRO	-	expression tag	UNP A4TUL6
A	309	GLY	-	expression tag	UNP A4TUL6
A	310	PHE	-	expression tag	UNP A4TUL6
A	311	SER	-	expression tag	UNP A4TUL6
A	312	SER	-	expression tag	UNP A4TUL6
A	313	ILE	-	expression tag	UNP A4TUL6
A	314	SER	-	expression tag	UNP A4TUL6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	315	ALA	-	expression tag	UNP A4TUL6
A	316	HIS	-	expression tag	UNP A4TUL6
A	317	HIS	-	expression tag	UNP A4TUL6
A	318	HIS	-	expression tag	UNP A4TUL6
A	319	HIS	-	expression tag	UNP A4TUL6
A	320	HIS	-	expression tag	UNP A4TUL6
A	321	HIS	-	expression tag	UNP A4TUL6
A	322	HIS	-	expression tag	UNP A4TUL6
A	323	HIS	-	expression tag	UNP A4TUL6
A	324	HIS	-	expression tag	UNP A4TUL6
A	325	HIS	-	expression tag	UNP A4TUL6
B	1	MET	-	initiating methionine	UNP A4TUL6
B	2	ALA	-	expression tag	UNP A4TUL6
B	3	SER	-	expression tag	UNP A4TUL6
B	4	TRP	-	expression tag	UNP A4TUL6
B	5	SER	-	expression tag	UNP A4TUL6
B	6	HIS	-	expression tag	UNP A4TUL6
B	7	PRO	-	expression tag	UNP A4TUL6
B	8	GLN	-	expression tag	UNP A4TUL6
B	9	PHE	-	expression tag	UNP A4TUL6
B	10	GLU	-	expression tag	UNP A4TUL6
B	11	LYS	-	expression tag	UNP A4TUL6
B	12	GLY	-	expression tag	UNP A4TUL6
B	13	ALA	-	expression tag	UNP A4TUL6
B	14	ASP	-	expression tag	UNP A4TUL6
B	15	ASP	-	expression tag	UNP A4TUL6
B	16	ASP	-	expression tag	UNP A4TUL6
B	17	ASP	-	expression tag	UNP A4TUL6
B	18	LYS	-	expression tag	UNP A4TUL6
B	308	PRO	-	expression tag	UNP A4TUL6
B	309	GLY	-	expression tag	UNP A4TUL6
B	310	PHE	-	expression tag	UNP A4TUL6
B	311	SER	-	expression tag	UNP A4TUL6
B	312	SER	-	expression tag	UNP A4TUL6
B	313	ILE	-	expression tag	UNP A4TUL6
B	314	SER	-	expression tag	UNP A4TUL6
B	315	ALA	-	expression tag	UNP A4TUL6
B	316	HIS	-	expression tag	UNP A4TUL6
B	317	HIS	-	expression tag	UNP A4TUL6
B	318	HIS	-	expression tag	UNP A4TUL6
B	319	HIS	-	expression tag	UNP A4TUL6
B	320	HIS	-	expression tag	UNP A4TUL6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	321	HIS	-	expression tag	UNP A4TUL6
B	322	HIS	-	expression tag	UNP A4TUL6
B	323	HIS	-	expression tag	UNP A4TUL6
B	324	HIS	-	expression tag	UNP A4TUL6
B	325	HIS	-	expression tag	UNP A4TUL6

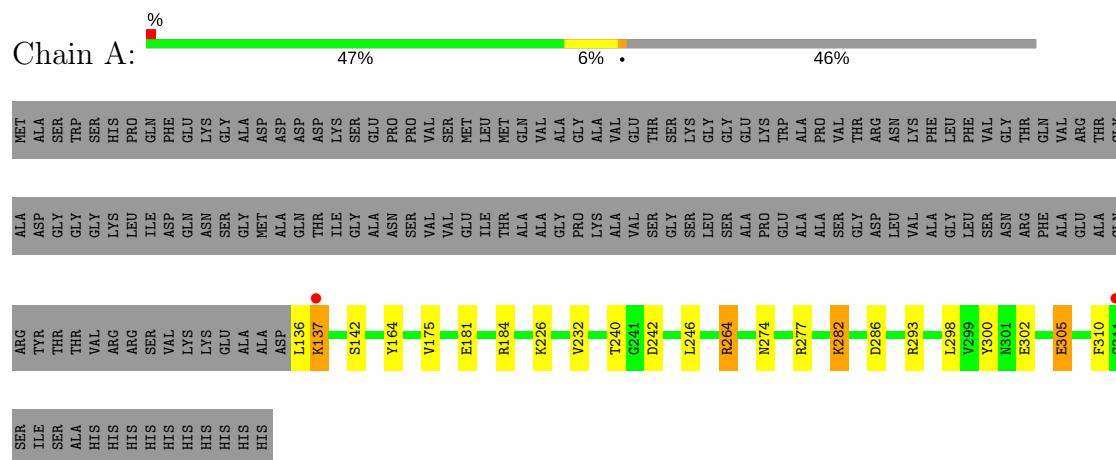
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		
2	B	35	Total	O	0	0
			35	35		

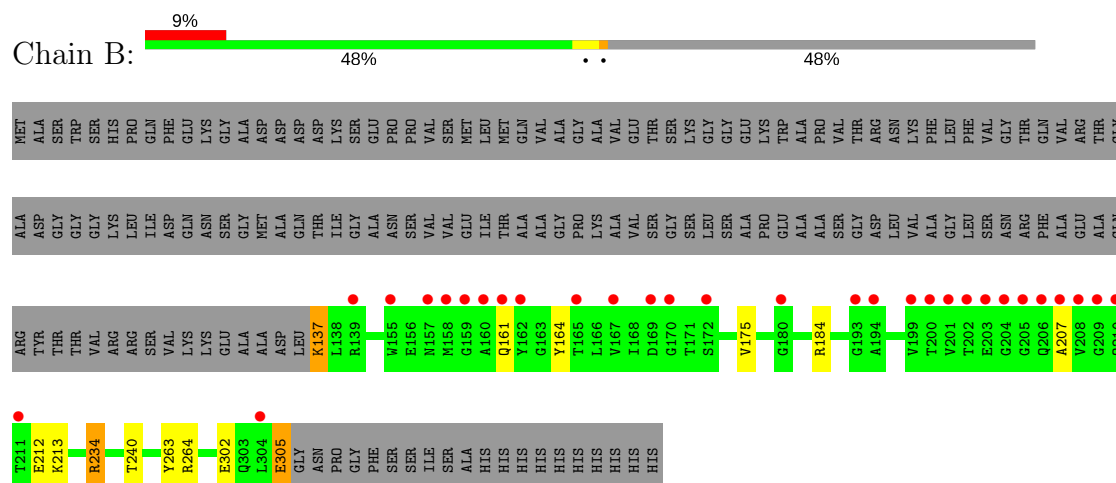
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Magnetotaxis protein MtxA



• Molecule 1: Magnetotaxis protein MtxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.34Å 88.95Å 95.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.70 – 2.03 42.04 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.70-2.03) 98.4 (42.04-2.03)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.03Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.227 0.193 , 0.231	Depositor DCC
R_{free} test set	1163 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2800	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.01	0/1401	0.98	3/1899 (0.2%)
1	B	0.78	1/1324 (0.1%)	0.90	3/1797 (0.2%)
All	All	0.90	1/2725 (0.0%)	0.94	6/3696 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	TYR	CE1-CZ	5.60	1.45	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	B	184	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	184	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	264	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	242	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	264	ARG	NE-CZ-NH1	5.05	122.83	120.30

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	1363	0	1361	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1297	0	1283	7	0
2	A	105	0	0	1	1
2	B	35	0	0	1	0
All	All	2800	0	2644	19	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 4.

All (19) 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:274:ASN:HD22	1:A:277:ARG:HH21	1.36	0.72
1:A:274:ASN:HD21	1:A:300:TYR:HA	1.62	0.65
1:A:137:LYS:HA	1:A:137:LYS:HE3	1.84	0.60
1:A:181[A]:GLU:OE1	1:A:264:ARG:NH2	2.32	0.54
1:B:240[A]:THR:HB	2:B:412:HOH:O	2.11	0.50
1:A:305:GLU:HA	1:A:310:PHE:CD2	2.47	0.50
1:A:142:SER:O	1:B:213:LYS:NZ	2.46	0.48
1:A:286:ASP:OD1	1:A:286:ASP:O	2.32	0.47
1:A:282[B]:LYS:HG3	2:A:450:HOH:O	2.17	0.45
1:B:164:TYR:HB2	1:B:175:VAL:HB	2.00	0.44
1:B:137:LYS:NZ	1:B:137:LYS:HB3	2.33	0.43
1:B:305:GLU:OE1	1:B:305:GLU:N	2.52	0.43
1:A:164:TYR:HB2	1:A:175:VAL:HB	2.03	0.41
1:A:232:VAL:HG13	1:A:246:LEU:CD1	2.51	0.41
1:A:274:ASN:ND2	1:A:277:ARG:HH21	2.13	0.40
1:A:286:ASP:OD1	1:A:286:ASP:C	2.60	0.40
1:A:282[B]:LYS:NZ	1:A:286:ASP:OD2	2.54	0.40
1:A:310:PHE:CZ	1:B:234:ARG:HG2	2.56	0.40
1:B:137:LYS:CB	1:B:137:LYS:NZ	2.85	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:485:HOH:O	2:A:487:HOH:O[4_565]	2.05	0.15

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	178/325 (55%)	174 (98%)	4 (2%)	0	100	100
1	B	168/325 (52%)	161 (96%)	6 (4%)	1 (1%)	28	21
All	All	346/650 (53%)	335 (97%)	10 (3%)	1 (0%)	44	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	ALA

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	146/256 (57%)	135 (92%)	11 (8%)	16	9
1	B	138/256 (54%)	132 (96%)	6 (4%)	33	28
All	All	284/512 (56%)	267 (94%)	17 (6%)	26	16

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	137	LYS
1	A	226[A]	LYS
1	A	226[B]	LYS
1	A	240	THR

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Mol	Chain	Res	Type
1	A	282[A]	LYS
1	A	282[B]	LYS
1	A	293	ARG
1	A	298	LEU
1	A	302	GLU
1	A	305	GLU
1	B	137	LYS
1	B	161	GLN
1	B	212	GLU
1	B	234	ARG
1	B	302	GLU
1	B	305	GLU

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

Mol	Chain	Res	Type
1	A	274	ASN

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 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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	176/325 (54%)	-0.16	2 (1%) 80 80	16, 26, 57, 65	0
1	B	169/325 (52%)	0.69	30 (17%) 2 1	25, 51, 101, 123	0
All	All	345/650 (53%)	0.26	32 (9%) 9 10	16, 36, 92, 123	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	ALA	5.9
1	B	170	GLY	5.2
1	B	159	GLY	5.0
1	B	161	GLN	4.3
1	B	211	THR	4.0
1	B	172	SER	3.9
1	B	202	THR	3.8
1	B	180	GLY	3.7
1	B	162	TYR	3.6
1	B	206	GLN	3.4
1	B	210	GLN	3.4
1	B	199	VAL	3.1
1	B	208	VAL	3.1
1	B	158	MET	3.1
1	B	157	ASN	3.0
1	B	209	GLY	2.9
1	B	201	VAL	2.8
1	B	169	ASP	2.8
1	B	204	GLY	2.8
1	B	200	THR	2.7
1	B	203	GLU	2.6
1	B	205	GLY	2.5
1	B	139	ARG	2.5
1	B	207	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	193	GLY	2.5
1	B	167	VAL	2.4
1	B	194	ALA	2.4
1	A	311	SER	2.1
1	B	165	THR	2.1
1	A	137	LYS	2.1
1	B	155	TRP	2.0
1	B	304	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 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.