



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:31 AM GMT

PDB ID : 2NXN
Title : T. thermophilus ribosomal protein L11 methyltransferase (PrmA) in complex with ribosomal protein L11
Authors : Demirci, H.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2006-11-17
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

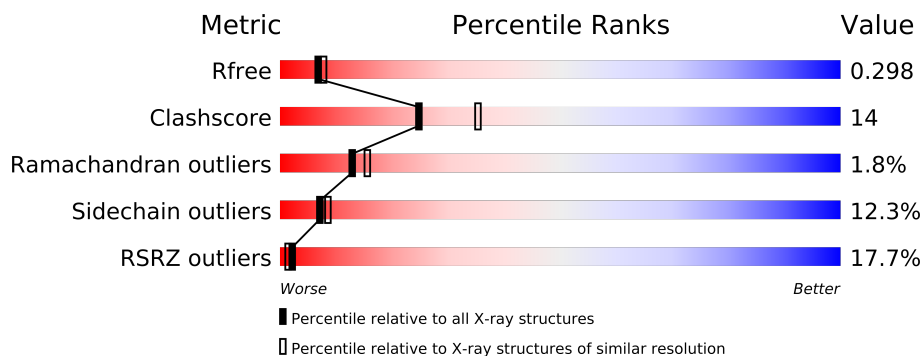
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	254	
2	B	147	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3054 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Ribosomal protein L11 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1926	1250	335	337	4			

- Molecule 2 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1033	659	182	186	6			

- Molecule 3 is water.

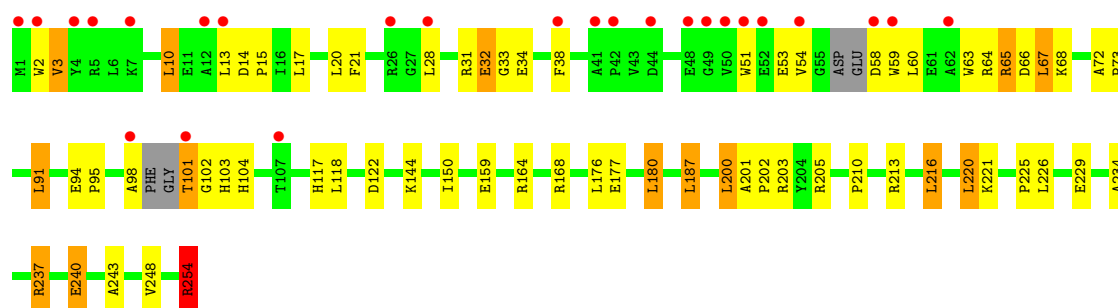
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	27	Total	O	0	0
			27	27		

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 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 ($\text{RSRZ} > 2$). 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.

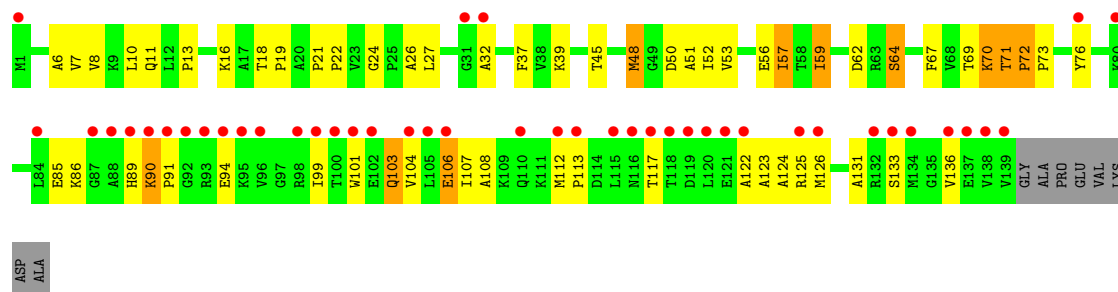
- Molecule 1: Ribosomal protein L11 methyltransferase

Chain A: 



- Molecule 2: 50S ribosomal protein L11

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	132.84Å 132.84Å 46.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40 28.76 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.40) 98.9 (28.76-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.273 0.230 , 0.298	Depositor DCC
R_{free} test set	941 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.2	EDS
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 18330 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3054	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.83	1/1980 (0.1%)	0.89	8/2697 (0.3%)
2	B	0.53	0/1052	0.73	2/1425 (0.1%)
All	All	0.74	1/3032 (0.0%)	0.84	10/4122 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	LEU	C-N	6.11	1.48	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	122	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	220	LEU	CA-CB-CG	5.99	129.06	115.30
1	A	254	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	B	71	THR	N-CA-C	5.18	124.98	111.00
1	A	187	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	216	LEU	CB-CG-CD1	5.10	119.67	111.00
2	B	71	THR	C-N-CD	-5.08	109.44	120.60
1	A	91	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	200	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	70	LYS	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1926	0	1931	48	0
2	B	1033	0	1086	42	0
3	A	68	0	0	10	0
3	B	27	0	0	1	0
All	All	3054	0	3017	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:72:PRO:HB2	2:B:73:PRO:CD	1.82	1.08
1:A:31:ARG:HG2	1:A:32:GLU:H	1.31	0.93
2:B:72:PRO:HB2	2:B:73:PRO:HD2	1.57	0.86
2:B:72:PRO:HB2	2:B:73:PRO:HD3	1.64	0.79
1:A:101:THR:HG23	3:A:257:HOH:O	1.82	0.78
1:A:68:LYS:O	1:A:103:HIS:NE2	2.17	0.76
2:B:104:VAL:HG11	2:B:124:ALA:HA	1.68	0.74
2:B:62:ASP:OD1	2:B:64:SER:HB2	1.86	0.74
1:A:31:ARG:HG2	1:A:32:GLU:N	2.03	0.73
2:B:16:LYS:O	2:B:16:LYS:HG3	1.89	0.71
1:A:59:TRP:CZ2	2:B:21:PRO:HG3	2.26	0.70
1:A:98:ALA:HA	3:A:296:HOH:O	1.91	0.70
2:B:18:THR:HB	2:B:19:PRO:HD2	1.72	0.70
1:A:13:LEU:O	1:A:17:LEU:HG	1.92	0.69
2:B:27:LEU:HB3	2:B:32:ALA:HB3	1.75	0.68
1:A:53:GLU:HG3	1:A:54:VAL:H	1.58	0.68
1:A:17:LEU:HA	1:A:20:LEU:HD12	1.76	0.67
2:B:6:ALA:HB3	2:B:59:ILE:HG13	1.78	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:LEU:HD22	1:A:103:HIS:CE1	2.32	0.64
1:A:68:LYS:O	1:A:103:HIS:CE1	2.51	0.63
2:B:72:PRO:CB	2:B:73:PRO:CD	2.67	0.62
2:B:90:LYS:HG3	2:B:91:PRO:HD3	1.81	0.62
2:B:85:GLU:HG3	2:B:86:LYS:H	1.64	0.62
1:A:176:LEU:O	1:A:180:LEU:HD23	1.99	0.62
1:A:237:ARG:NH1	3:A:305:HOH:O	2.31	0.62
1:A:59:TRP:HZ2	2:B:21:PRO:HG3	1.63	0.62
1:A:159:GLU:HA	1:A:159:GLU:OE1	2.00	0.61
1:A:225:PRO:O	1:A:229:GLU:HG3	2.00	0.61
1:A:51:TRP:HB3	3:A:275:HOH:O	2.03	0.58
2:B:52:ILE:O	2:B:72:PRO:HB3	2.04	0.57
1:A:221:LYS:HE2	1:A:243:ALA:HB1	1.87	0.57
2:B:10:LEU:HD11	2:B:22:PRO:HB2	1.85	0.57
1:A:118:LEU:HD13	1:A:187:LEU:HD23	1.87	0.57
1:A:31:ARG:HB3	1:A:34:GLU:HB2	1.87	0.57
2:B:108:ALA:HB1	2:B:123:ALA:HB1	1.89	0.55
2:B:90:LYS:HG3	2:B:91:PRO:CD	2.38	0.54
2:B:8:VAL:HG13	2:B:57:ILE:HG12	1.89	0.54
1:A:221:LYS:HD3	1:A:248:VAL:CG1	2.38	0.53
1:A:32:GLU:HB2	3:A:316:HOH:O	2.08	0.53
2:B:103:GLN:HA	3:B:153:HOH:O	2.10	0.52
1:A:2:TRP:HB3	3:A:275:HOH:O	2.10	0.52
1:A:177:GLU:OE2	1:A:203:ARG:NE	2.44	0.51
2:B:37:PHE:CE1	2:B:57:ILE:HD12	2.46	0.51
1:A:2:TRP:HE3	3:A:275:HOH:O	1.94	0.51
1:A:210:PRO:HA	1:A:254:ARG:HD2	1.93	0.51
1:A:59:TRP:CD1	2:B:24:GLY:HA3	2.46	0.51
1:A:14:ASP:HA	1:A:17:LEU:HD12	1.93	0.50
1:A:205:ARG:HD2	1:A:234:ALA:O	2.12	0.50
2:B:72:PRO:CB	2:B:73:PRO:HD3	2.36	0.50
2:B:52:ILE:O	2:B:72:PRO:CB	2.60	0.50
2:B:8:VAL:CG1	2:B:57:ILE:HB	2.44	0.48
2:B:45:THR:HG22	2:B:48:MET:HE3	1.95	0.48
2:B:8:VAL:HG21	2:B:26:ALA:HB1	1.96	0.47
1:A:21:PHE:HE2	2:B:13:PRO:HG3	1.80	0.47
1:A:14:ASP:N	1:A:15:PRO:CD	2.78	0.47
2:B:56:GLU:O	2:B:67:PHE:HA	2.16	0.45
1:A:10:LEU:HA	3:A:298:HOH:O	2.16	0.45
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.43	0.45
2:B:131:ALA:HB1	2:B:136:VAL:HB	1.98	0.45
2:B:112:MET:HB3	2:B:113:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:104:HIS:CE1	2:B:39:LYS:HG2	2.52	0.45
2:B:48:MET:H	2:B:48:MET:HG2	1.42	0.45
1:A:144:LYS:NZ	3:A:307:HOH:O	2.48	0.44
1:A:28:LEU:HD12	2:B:11:GLN:HB2	2.00	0.44
2:B:51:ALA:HA	2:B:76:TYR:CZ	2.51	0.44
1:A:3:VAL:HB	1:A:38:PHE:CE2	2.52	0.44
1:A:14:ASP:HA	1:A:17:LEU:CD1	2.47	0.43
1:A:17:LEU:HD21	3:A:298:HOH:O	2.17	0.43
1:A:28:LEU:HB2	2:B:11:GLN:HB2	2.00	0.43
1:A:31:ARG:NH1	1:A:32:GLU:HB3	2.34	0.43
2:B:117:THR:HG21	2:B:122:ALA:HB3	2.01	0.42
1:A:63:TRP:HE3	1:A:64:ARG:HG2	1.84	0.42
2:B:104:VAL:C	2:B:106:GLU:H	2.23	0.42
1:A:221:LYS:HD3	1:A:248:VAL:HG13	2.02	0.42
1:A:117:HIS:NE2	1:A:240:GLU:OE2	2.42	0.41
1:A:201:ALA:HB3	1:A:202:PRO:HD3	2.01	0.41
2:B:27:LEU:HD21	2:B:57:ILE:HG13	2.03	0.41
2:B:7:VAL:O	2:B:7:VAL:HG13	2.20	0.41
2:B:8:VAL:HG13	2:B:57:ILE:CG1	2.50	0.41
1:A:177:GLU:HG2	1:A:203:ARG:NH2	2.37	0.40
1:A:94:GLU:HA	1:A:95:PRO:HD3	1.91	0.40
1:A:72:ALA:O	1:A:73:PRO:C	2.59	0.40
2:B:90:LYS:CG	2:B:91:PRO:HD3	2.49	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	244/254 (96%)	227 (93%)	14 (6%)	3 (1%)	19	26
2	B	137/147 (93%)	107 (78%)	26 (19%)	4 (3%)	7	6
All	All	381/401 (95%)	334 (88%)	40 (10%)	7 (2%)	13	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	33	GLY
2	B	72	PRO
2	B	101	TRP
2	B	106	GLU
2	B	99	ILE
1	A	102	GLY

5.3.2 Protein sidechains ⓘ

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	186/189 (98%)	167 (90%)	19 (10%)	11	15
2	B	106/111 (96%)	89 (84%)	17 (16%)	3	4
All	All	292/300 (97%)	256 (88%)	36 (12%)	7	8

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	58	ASP
1	A	60	LEU
1	A	65	ARG
1	A	66	ASP
1	A	67	LEU
1	A	91	LEU
1	A	101	THR
1	A	150	ILE
1	A	164	ARG
1	A	180	LEU
1	A	200	LEU
1	A	213	ARG
1	A	216	LEU
1	A	220	LEU
1	A	226	LEU
1	A	237	ARG
1	A	240	GLU
1	A	254	ARG

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Mol	Chain	Res	Type
2	B	48	MET
2	B	50	ASP
2	B	53	VAL
2	B	57	ILE
2	B	59	ILE
2	B	64	SER
2	B	69	THR
2	B	70	LYS
2	B	71	THR
2	B	89	HIS
2	B	90	LYS
2	B	94	GLU
2	B	103	GLN
2	B	107	ILE
2	B	125	ARG
2	B	126	MET
2	B	133	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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, 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	250/254 (98%)	0.39	25 (10%) 8 7	28, 39, 100, 100	0
2	B	139/147 (94%)	1.67	44 (31%) 1 1	51, 71, 100, 100	0
All	All	389/401 (97%)	0.85	69 (17%) 2 1	28, 56, 100, 100	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	95	LYS	13.0
2	B	105	LEU	12.3
1	A	49	GLY	11.5
2	B	92	GLY	10.6
1	A	7	LYS	9.3
2	B	139	VAL	9.1
2	B	93	ARG	8.6
2	B	89	HIS	8.1
2	B	101	TRP	7.4
2	B	96	VAL	7.3
2	B	87	GLY	6.6
1	A	51	TRP	6.3
1	A	54	VAL	6.1
2	B	112	MET	6.1
2	B	88	ALA	6.0
1	A	48	GLU	6.0
1	A	59	TRP	5.9
1	A	2	TRP	5.6
2	B	134	MET	5.4
1	A	44	ASP	5.3
2	B	100	THR	5.3
1	A	50	VAL	5.1
2	B	118	THR	5.0
2	B	117	THR	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	98	ARG	4.7
1	A	41	ALA	4.5
2	B	113	PRO	4.2
2	B	106	GLU	4.2
2	B	84	LEU	4.0
2	B	115	LEU	3.8
2	B	99	ILE	3.7
2	B	137	GLU	3.5
2	B	138	VAL	3.5
2	B	116	ASN	3.4
2	B	120	LEU	3.4
1	A	101	THR	3.2
2	B	125	ARG	3.2
1	A	12	ALA	3.2
2	B	121	GLU	3.1
2	B	133	SER	3.1
1	A	5	ARG	3.0
2	B	94	GLU	3.0
2	B	31	GLY	3.0
1	A	28	LEU	3.0
2	B	122	ALA	2.9
2	B	104	VAL	2.9
1	A	52	GLU	2.9
2	B	136	VAL	2.9
2	B	110	GLN	2.9
2	B	132	ARG	2.9
1	A	62	ALA	2.7
2	B	102	GLU	2.7
2	B	119	ASP	2.6
2	B	76	TYR	2.6
1	A	26	ARG	2.6
1	A	4	TYR	2.6
2	B	32	ALA	2.5
2	B	80	LYS	2.5
1	A	107	THR	2.5
2	B	90	LYS	2.4
2	B	1	MET	2.3
1	A	38	PHE	2.2
1	A	98	ALA	2.2
2	B	91	PRO	2.1
1	A	13	LEU	2.1
2	B	126	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	58	ASP	2.1
1	A	1	MET	2.0
1	A	42	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.