Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:42 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 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:

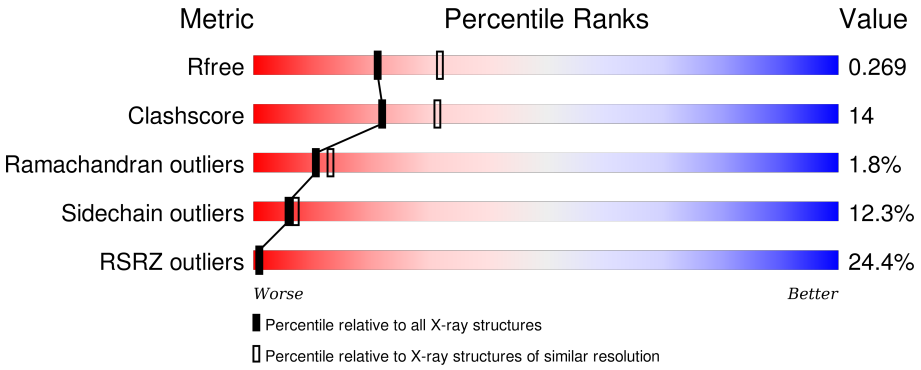
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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. 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 <=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	254	18% 72% 21% 6%
2	B	147	34% 54% 33% 7% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3054 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 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.

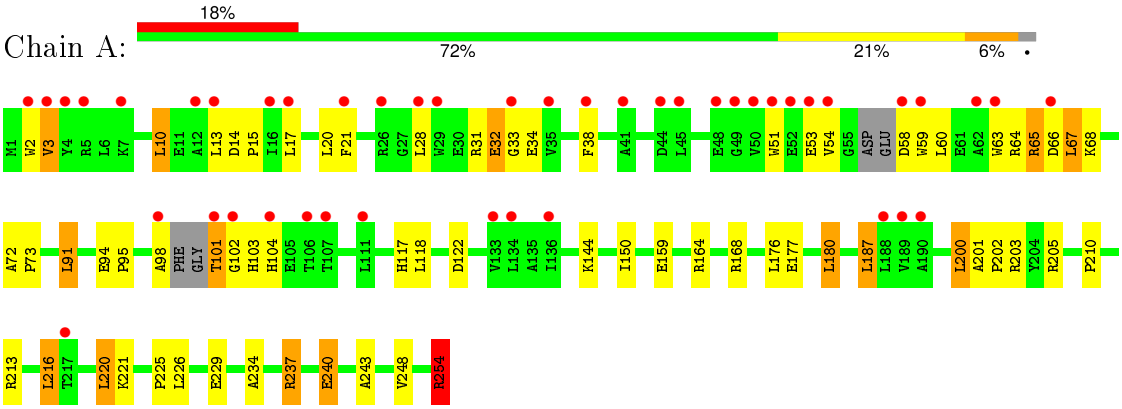
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	27	Total	O	0	0
			27	27		

3 Residue-property plots (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.

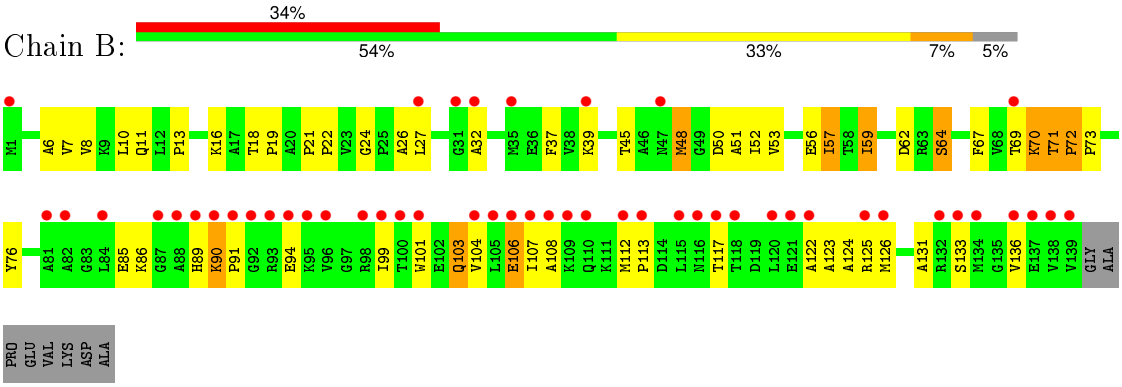
- Molecule 1: Ribosomal protein L11 methyltransferase

Chain A:



- Molecule 2: 50S ribosomal protein L11

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.11 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.273 0.215 , 0.269	Depositor DCC
R_{free} test set	940 reflections (5.43%)	DCC
Wilson B-factor (Å^2)	46.5	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 60.4	EDS
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 18330 reflections	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.83	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(^{o})	Ideal(^{o})
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 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	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

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 14.

All (83) 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)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:ALA:HB3	2:B:59:ILE:HG13	1.78	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	244/254 (96%)	227 (93%)	14 (6%)	3 (1%)	16 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	137/147 (93%)	107 (78%)	26 (19%)	4 (3%)	6 5
All	All	381/401 (95%)	334 (88%)	40 (10%)	7 (2%)	11 13

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 (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	186/189 (98%)	167 (90%)	19 (10%)	9 13
2	B	106/111 (96%)	89 (84%)	17 (16%)	3 3
All	All	292/300 (97%)	256 (88%)	36 (12%)	6 7

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

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Mol	Chain	Res	Type
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
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 (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

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, 95^{th} 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%)	0.79	45 (18%)	2	2	28, 39, 100, 100	0
2	B	139/147 (94%)	2.20	50 (35%)	0	0	51, 71, 100, 100	0
All	All	389/401 (97%)	1.29	95 (24%)	1	1	28, 56, 100, 100	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	105	LEU	19.6
2	B	92	GLY	13.8
2	B	88	ALA	12.4
2	B	96	VAL	12.0
2	B	89	HIS	11.2
2	B	95	LYS	10.7
1	A	59	TRP	10.5
1	A	7	LYS	10.4
2	B	93	ARG	10.3
1	A	44	ASP	9.1
2	B	104	VAL	9.1
2	B	139	VAL	8.7
1	A	12	ALA	8.6
2	B	112	MET	8.5
2	B	134	MET	7.7
2	B	100	THR	7.1
2	B	106	GLU	6.3
2	B	84	LEU	6.2
1	A	49	GLY	6.1
2	B	113	PRO	5.9
2	B	87	GLY	5.8
1	A	4	TYR	5.8
1	A	5	ARG	5.5
2	B	115	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	51	TRP	5.1
2	B	133	SER	5.1
2	B	91	PRO	5.0
1	A	101	THR	4.8
1	A	2	TRP	4.7
2	B	101	TRP	4.5
2	B	125	ARG	4.5
2	B	126	MET	4.4
1	A	52	GLU	4.1
2	B	108	ALA	3.9
1	A	62	ALA	3.9
2	B	117	THR	3.8
1	A	50	VAL	3.4
2	B	137	GLU	3.4
1	A	33	GLY	3.4
2	B	99	ILE	3.4
2	B	132	ARG	3.3
2	B	118	THR	3.2
2	B	121	GLU	3.2
1	A	58	ASP	3.2
1	A	35	VAL	3.2
2	B	122	ALA	3.2
1	A	3	VAL	3.1
2	B	138	VAL	3.1
2	B	90	LYS	3.1
1	A	21	PHE	3.1
2	B	98	ARG	3.1
2	B	31	GLY	3.0
1	A	38	PHE	3.0
2	B	81	ALA	3.0
1	A	53	GLU	3.0
2	B	94	GLU	3.0
2	B	109	LYS	2.9
1	A	98	ALA	2.8
1	A	41	ALA	2.8
1	A	48	GLU	2.7
2	B	107	ILE	2.7
2	B	110	GLN	2.7
1	A	217	THR	2.7
2	B	39	LYS	2.7
1	A	107	THR	2.7
1	A	190	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	120	LEU	2.6
2	B	116	ASN	2.5
2	B	82	ALA	2.5
2	B	32	ALA	2.4
1	A	106	THR	2.4
2	B	1	MET	2.4
1	A	134	LEU	2.4
1	A	28	LEU	2.4
1	A	54	VAL	2.4
2	B	27	LEU	2.3
1	A	104	HIS	2.3
1	A	111	LEU	2.3
1	A	63	TRP	2.3
1	A	102	GLY	2.3
1	A	133	VAL	2.2
2	B	136	VAL	2.2
1	A	29	TRP	2.2
2	B	35	MET	2.2
1	A	189	VAL	2.2
1	A	45	LEU	2.1
2	B	69	THR	2.1
1	A	66	ASP	2.1
1	A	16	ILE	2.1
1	A	136	ILE	2.1
1	A	188	LEU	2.0
2	B	47	ASN	2.0
1	A	13	LEU	2.0
1	A	17	LEU	2.0
1	A	26	ARG	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.