Full wwPDB NMR Structure Validation Report (i)

Jun 11, 2024 – 07:10 PM EDT

PDB ID	:	2JVR
BMRB ID	:	15487
Title	:	Segmental Isotope Labeling of Npl3p
Authors	:	Skrisovska, L.; Allain, F.H.-T.
Deposited on	:	2007-09-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

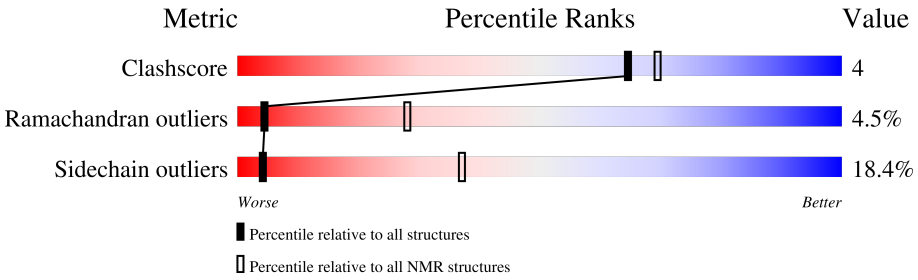
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 78%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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%

Mol	Chain	Length	Quality of chain
1	A	111	41% 15% • 14% 28%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:27-A:35, A:40-A:61, A:69-A:102 (65)	0.44	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 7, 8, 9, 10, 11, 12, 13, 15, 16, 17, 19
2	6, 14
3	18, 20

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1262 atoms, of which 620 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nucleolar protein 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	80	1262	396	620	112	132	2	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q01560
A	2	GLY	-	expression tag	UNP Q01560
A	3	SER	-	expression tag	UNP Q01560
A	4	SER	-	expression tag	UNP Q01560
A	5	HIS	-	expression tag	UNP Q01560
A	6	HIS	-	expression tag	UNP Q01560
A	7	HIS	-	expression tag	UNP Q01560
A	8	HIS	-	expression tag	UNP Q01560
A	9	HIS	-	expression tag	UNP Q01560
A	10	HIS	-	expression tag	UNP Q01560
A	11	SER	-	expression tag	UNP Q01560
A	12	SER	-	expression tag	UNP Q01560
A	13	GLY	-	expression tag	UNP Q01560
A	14	LEU	-	expression tag	UNP Q01560
A	15	VAL	-	expression tag	UNP Q01560
A	16	PRO	-	expression tag	UNP Q01560
A	17	ARG	-	expression tag	UNP Q01560
A	18	GLY	-	expression tag	UNP Q01560
A	19	SER	-	expression tag	UNP Q01560
A	20	HIS	-	expression tag	UNP Q01560
A	21	MET	-	expression tag	UNP Q01560

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Nucleolar protein 3

Chain A: 41% 15% • 14% 28%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS LEU P25 A26 K27 R28 Y29 R30 K34 N35 L36 P37 E38 G39 D47 L48 A49 R50 S53 L54 E55 T56 T57 F58 S59 N62 T63 R64 D65 F66 D67 G68 L72

R86 L87 F92 R93 V96 E100 R101 D102 D103 N104 PRO PRO PRO ILE ARG ARG SER

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Nucleolar protein 3

Chain A: 37% 20% • 14% 28%

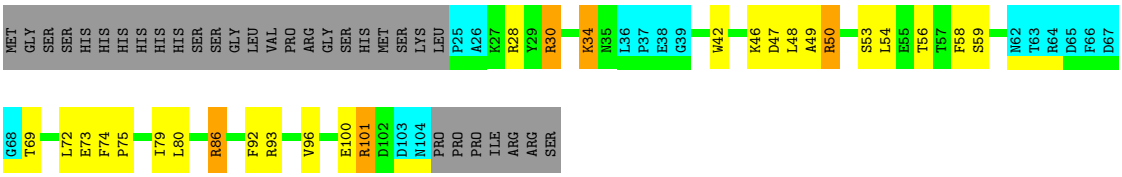
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS LEU P25 A26 K27 R28 Y29 R30 I31 K34 N35 L36 P37 E38 G39 C40 S41 L48 A49 R50 S53 L54 E55 T56 T57 F58 S59 S60 V61 N62 T63 R64 D65 F66 D67

G68 A71 L72 E73 L80 L84 E85 R86 E91 F92 R93 E100 D103 N104 PRO PRO PRO ILE ARG ARG SER

4.2.2 Score per residue for model 2

• Molecule 1: Nucleolar protein 3

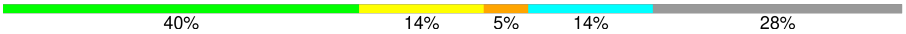
Chain A: 34% 20% 5% 14% 28%

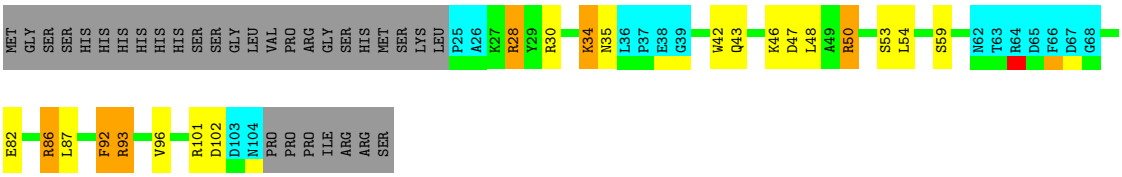


4.2.3 Score per residue for model 3

- Molecule 1: Nucleolar protein 3

Chain A:

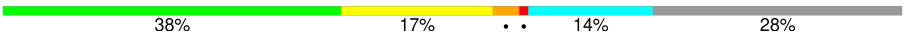


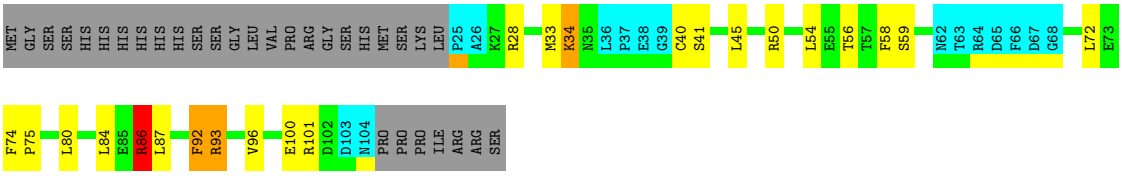


4.2.4 Score per residue for model 4

- Molecule 1: Nucleolar protein 3

Chain A:

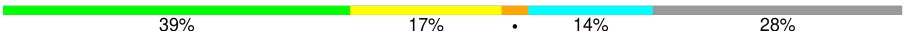


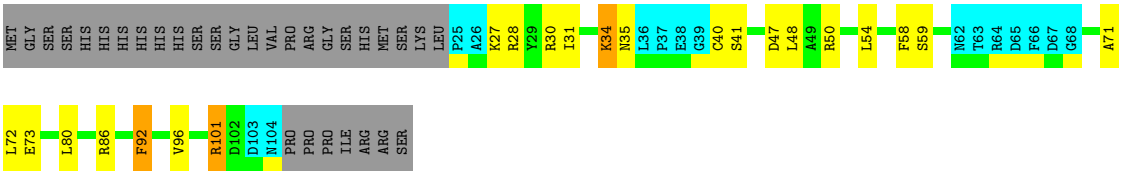


4.2.5 Score per residue for model 5

- Molecule 1: Nucleolar protein 3

Chain A:





4.2.6 Score per residue for model 6

- Molecule 1: Nucleolar protein 3

Chain A: 40% 16% • 14% 28%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS LEU P25 A26 K27 R28 Y29 R30 K34 N35 L36 P37 E38 G39 D47 L48 A49 R50 S53 L54 F58 S59 S60 V61 N62 T63 R64 D65 F66 D67 G68 L72

L84 E85 R86 L87 I90 E91 F92 R93 V96 E100 D103 N104 PRO PRO PRO ILE ARG ARG SER

4.2.7 Score per residue for model 7

- Molecule 1: Nucleolar protein 3

Chain A: 36% 19% • 14% 28%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS LEU P25 A26 K27 R28 Y29 R30 K34 N35 L36 P37 E38 G39 C40 D44 L45 K46 D47 L48 A49 R50 S53 L54 F58 S59 S60 V61 N62 T63 R64 D65 F66 D67

G68 L72 E73 F74 P75 L84 E85 R86 F92 R93 V96 D103 N104 PRO PRO PRO ILE ARG ARG SER

4.2.8 Score per residue for model 8

- Molecule 1: Nucleolar protein 3

Chain A: 33% 21% 5% 14% 28%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS LEU P25 A26 K27 R28 I31 K34 N35 L36 P37 E38 G39 C40 S41 W42 Q43 D44 D47 L48 A49 R50 E51 N52 S53 L54 E55 T56 T57 F58 S59 N62 T63 R64

D65 F66 D67 G68 A71 L72 L84 E85 R86 L87 F92 R93 V96 E100 R101 D102 D103 N104 PRO PRO PRO ILE ARG ARG SER

4.2.9 Score per residue for model 9

- Molecule 1: Nucleolar protein 3

Chain A: 34% 21% • 14% 28%

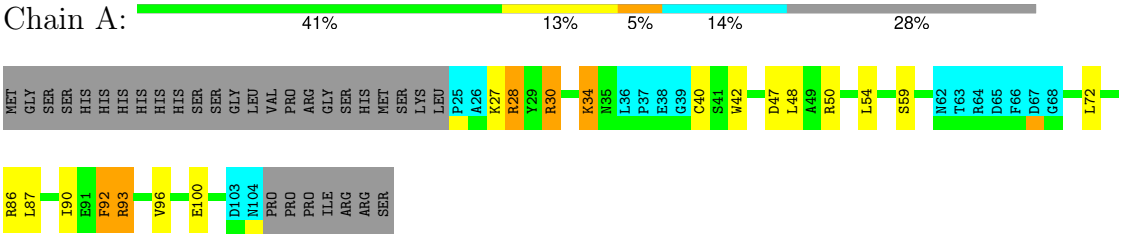
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET SER LYS LEU P25 A26 K27 R28 Y29 R30 K34 N35 L36 P37 E38 G39 W42 Q43 K46 D47 L48 A49 R50 S53 L54 E55 T56 T57 F58 S59 S60 V61 N62 T63 R64 D65

F66 D67 G68 L72 E73 F74 L84 E85 R86 I90 E91 F92 R93 E100 D103 N104 PRO PRO PRO ILE ARG ARG SER

4.2.10 Score per residue for model 10

- Molecule 1: Nucleolar protein 3

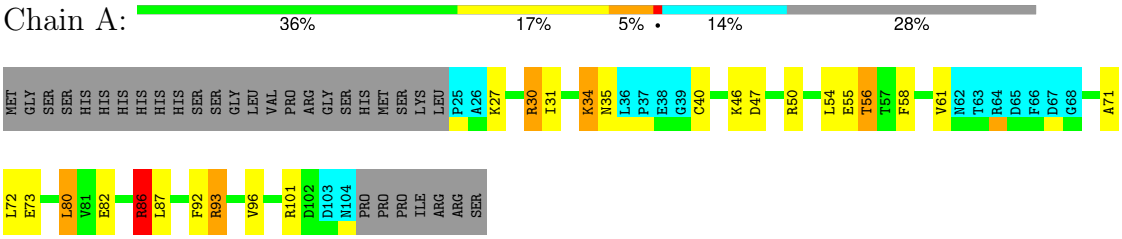
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: Nucleolar protein 3

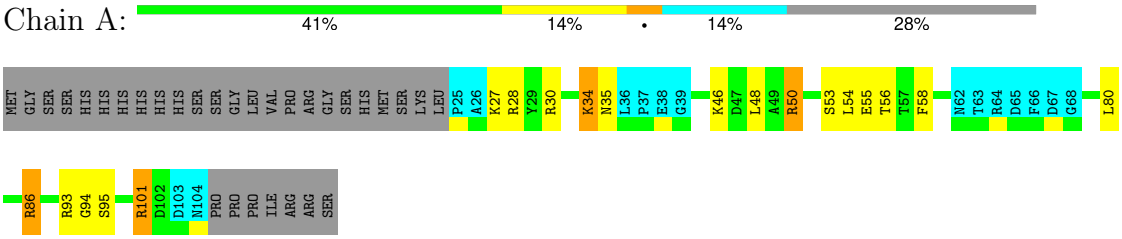
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Nucleolar protein 3

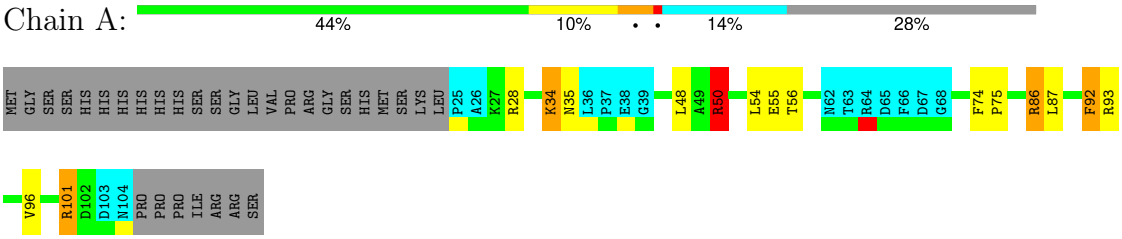
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: Nucleolar protein 3

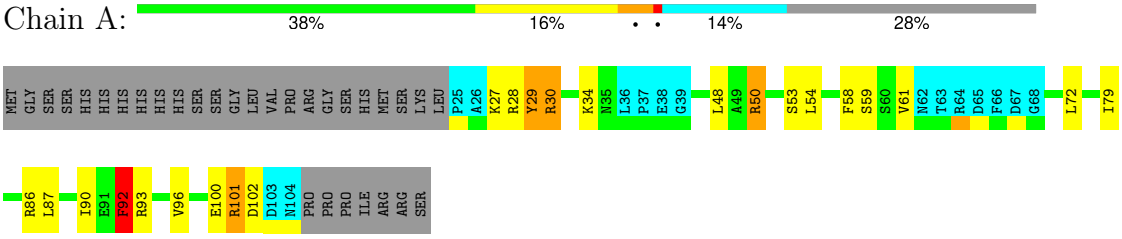
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: Nucleolar protein 3

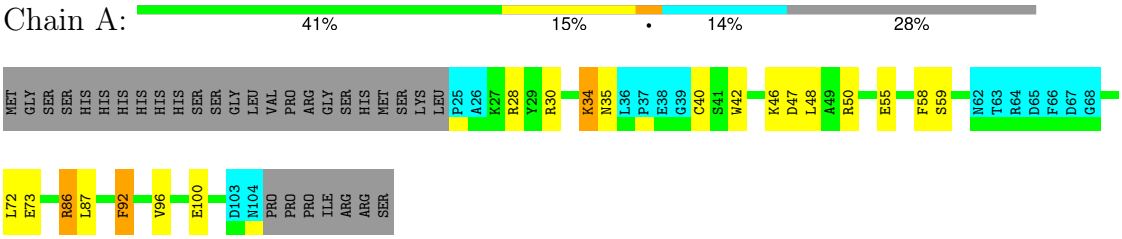
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: Nucleolar protein 3

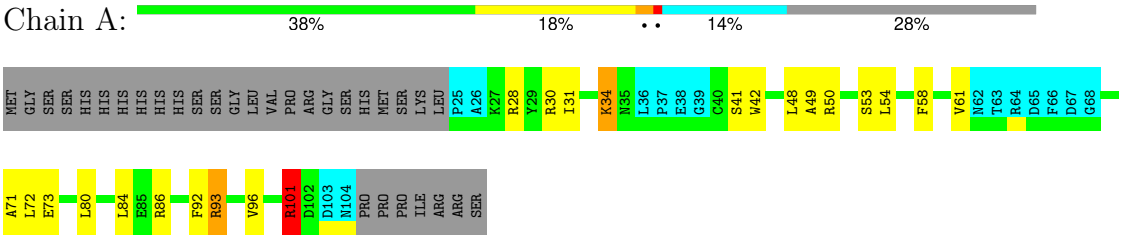
Chain A:



4.2.16 Score per residue for model 16

- Molecule 1: Nucleolar protein 3

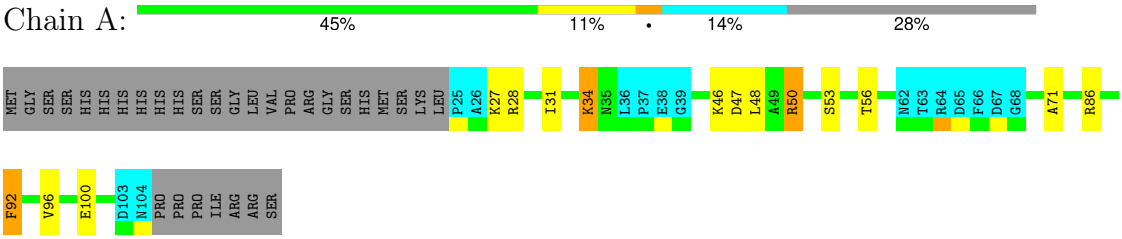
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: Nucleolar protein 3

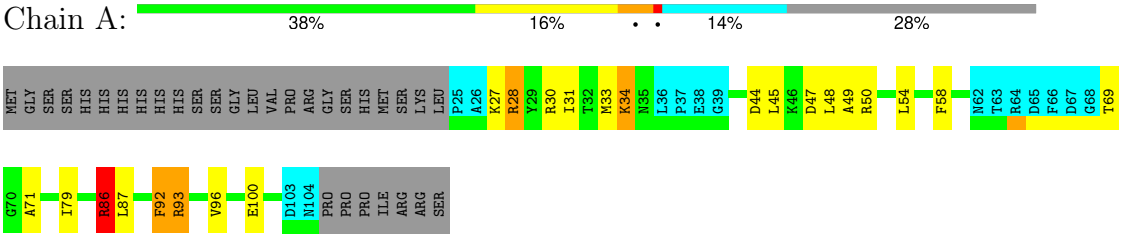
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Nucleolar protein 3

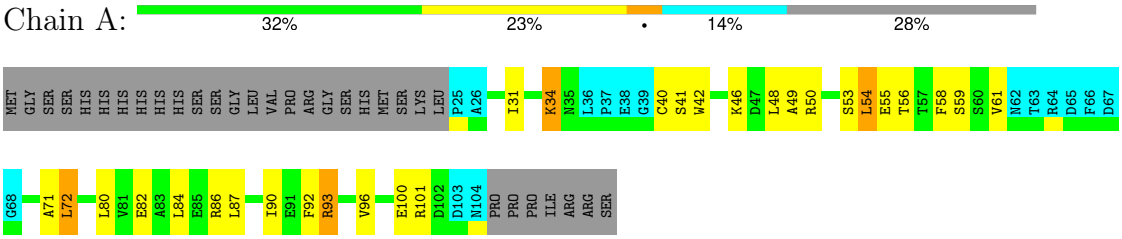
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Nucleolar protein 3

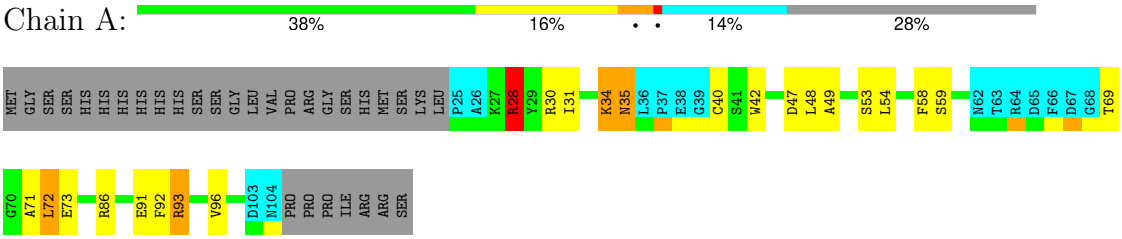
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Nucleolar protein 3

Chain A:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	**Classification**	**Version**
ATNOS/CANDID	structure calculation	
Amber	refinement	7.0

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	813
Number of shifts mapped to atoms	813
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	78%

6 Model quality (i)

6.1 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 (average) 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	0.73±0.01	0±0/536 (0.0± 0.0%)	1.43±0.04	6±2/723 (0.8± 0.2%)
All	All	0.73	0/10720 (0.0%)	1.43	114/14460 (0.8%)

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	Planarity
1	A	0.0±0.0	1.2±0.7
All	All	0	25

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	93	ARG	NE-CZ-NH1	12.85	126.73	120.30	7	15
1	A	30	ARG	NE-CZ-NH1	12.33	126.46	120.30	2	14
1	A	28	ARG	NE-CZ-NH1	9.95	125.27	120.30	20	17
1	A	50	ARG	NE-CZ-NH1	9.42	125.01	120.30	16	14
1	A	101	ARG	NE-CZ-NH1	7.93	124.26	120.30	4	9
1	A	30	ARG	CD-NE-CZ	7.77	134.48	123.60	2	2
1	A	34	LYS	N-CA-CB	-7.21	97.61	110.60	9	9
1	A	82	GLU	CA-CB-CG	6.81	128.38	113.40	11	1
1	A	48	LEU	CB-CG-CD1	6.62	122.25	111.00	12	3
1	A	93	ARG	CD-NE-CZ	6.54	132.75	123.60	7	2
1	A	34	LYS	CB-CA-C	-6.27	97.87	110.40	4	9
1	A	82	GLU	N-CA-CB	-6.18	99.48	110.60	11	1
1	A	86	ARG	NE-CZ-NH1	6.16	123.38	120.30	18	4
1	A	29	TYR	CB-CG-CD1	-6.09	117.34	121.00	14	1
1	A	101	ARG	CD-NE-CZ	5.93	131.91	123.60	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	35	ASN	CB-CA-C	5.70	121.80	110.40	3	3
1	A	50	ARG	CD-NE-CZ	5.57	131.40	123.60	14	1
1	A	93	ARG	NE-CZ-NH2	-5.43	117.58	120.30	7	1
1	A	28	ARG	NE-CZ-NH2	-5.43	117.59	120.30	16	2
1	A	30	ARG	NE-CZ-NH2	-5.38	117.61	120.30	14	1
1	A	28	ARG	NH1-CZ-NH2	-5.27	113.61	119.40	3	1
1	A	92	PHE	CB-CG-CD2	-5.10	117.23	120.80	4	3

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	86	ARG	Sidechain	18
1	A	101	ARG	Sidechain	3
1	A	58	PHE	Sidechain	1
1	A	50	ARG	Sidechain	1
1	A	29	TYR	Sidechain	1
1	A	28	ARG	Sidechain	1

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	529	525	525	4±2
All	All	10580	10500	10500	89

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 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:SER:HB2	1:A:72:LEU:HD13	0.70	1.62	9	13
1:A:49:ALA:HB1	1:A:54:LEU:HB2	0.64	1.68	16	5
1:A:48:LEU:HD23	1:A:48:LEU:C	0.58	2.19	1	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD12	1:A:92:PHE:CD1	0.55	2.36	7	9
1:A:49:ALA:HB1	1:A:54:LEU:HB3	0.51	1.83	19	2
1:A:48:LEU:HD12	1:A:92:PHE:CG	0.50	2.42	6	2
1:A:42:TRP:CZ3	1:A:72:LEU:HD11	0.47	2.44	16	1
1:A:74:PHE:CD1	1:A:75:PRO:HD2	0.47	2.45	2	4
1:A:42:TRP:CE3	1:A:59:SER:HB3	0.47	2.45	10	6
1:A:56:THR:HG21	1:A:72:LEU:HD12	0.47	1.86	11	2
1:A:31:ILE:O	1:A:71:ALA:HA	0.45	2.11	17	9
1:A:31:ILE:CG2	1:A:80:LEU:HD13	0.44	2.41	11	1
1:A:42:TRP:CZ2	1:A:46:LYS:HE3	0.44	2.48	9	1
1:A:86:ARG:C	1:A:87:LEU:HD12	0.44	2.33	8	5
1:A:87:LEU:HA	1:A:90:ILE:HG12	0.43	1.91	14	4
1:A:49:ALA:HB1	1:A:54:LEU:CB	0.43	2.43	19	2
1:A:86:ARG:HB3	1:A:87:LEU:HD12	0.42	1.91	18	2
1:A:48:LEU:HD11	1:A:90:ILE:HD11	0.41	1.91	9	1
1:A:33:MET:CE	1:A:45:LEU:HD22	0.41	2.45	4	2
1:A:29:TYR:CE2	1:A:74:PHE:HB3	0.41	2.50	9	1
1:A:74:PHE:CD2	1:A:79:ILE:HG13	0.41	2.51	2	1
1:A:42:TRP:CZ2	1:A:46:LYS:HE2	0.41	2.51	19	1
1:A:52:ASN:HB3	1:A:87:LEU:HD11	0.40	1.92	8	1

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	65/111 (59%)	55±1 (85±2%)	7±1 (11±2%)	3±1 (4±2%)	4 28
All	All	1300/2220 (59%)	1099 (85%)	143 (11%)	58 (4%)	4 28

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	53	SER	13
1	A	56	THR	8

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Mol	Chain	Res	Type	Models (Total)
1	A	93	ARG	8
1	A	40	CYS	8
1	A	35	ASN	6
1	A	55	GLU	5
1	A	69	THR	3
1	A	82	GLU	2
1	A	92	PHE	2
1	A	94	GLY	1
1	A	30	ARG	1
1	A	28	ARG	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	60/100 (60%)	49±2 (82±4%)	11±2 (18±4%)	4 37
All	All	1200/2000 (60%)	979 (82%)	221 (18%)	4 37

All 31 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	34	LYS	20
1	A	92	PHE	19
1	A	96	VAL	17
1	A	58	PHE	15
1	A	50	ARG	13
1	A	54	LEU	13
1	A	100	GLU	12
1	A	47	ASP	12
1	A	73	GLU	9
1	A	27	LYS	9
1	A	61	VAL	8
1	A	80	LEU	8
1	A	84	LEU	8
1	A	46	LYS	8
1	A	101	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	41	SER	5
1	A	28	ARG	5
1	A	86	ARG	4
1	A	30	ARG	4
1	A	35	ASN	3
1	A	91	GLU	3
1	A	102	ASP	3
1	A	44	ASP	3
1	A	93	ARG	3
1	A	72	LEU	3
1	A	43	GLN	2
1	A	79	ILE	2
1	A	56	THR	1
1	A	40	CYS	1
1	A	95	SER	1
1	A	55	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 78% for the well-defined parts and 74% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	813
Number of shifts mapped to atoms	813
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	67	2.68 ± 0.18	Should be applied
$^{13}C_{\beta}$	71	2.31 ± 0.13	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	75	0.91 ± 0.49	None needed (imprecise)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 78%, i.e. 718 atoms were assigned a chemical shift out of a possible 916. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	247/325 (76%)	126/131 (96%)	57/130 (44%)	64/64 (100%)
Sidechain	441/540 (82%)	300/347 (86%)	137/167 (82%)	4/26 (15%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	30/51 (59%)	18/25 (72%)	11/25 (44%)	1/1 (100%)
Overall	718/916 (78%)	444/503 (88%)	205/322 (64%)	69/91 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 813 atoms were assigned a chemical shift out of a possible 1094. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	292/398 (73%)	150/161 (93%)	67/160 (42%)	75/77 (97%)
Sidechain	483/635 (76%)	328/406 (81%)	149/198 (75%)	6/31 (19%)
Aromatic	38/61 (62%)	23/30 (77%)	14/30 (47%)	1/1 (100%)
Overall	813/1094 (74%)	501/597 (84%)	230/388 (59%)	82/109 (75%)

7.1.4 Statistically unusual chemical shifts (i)

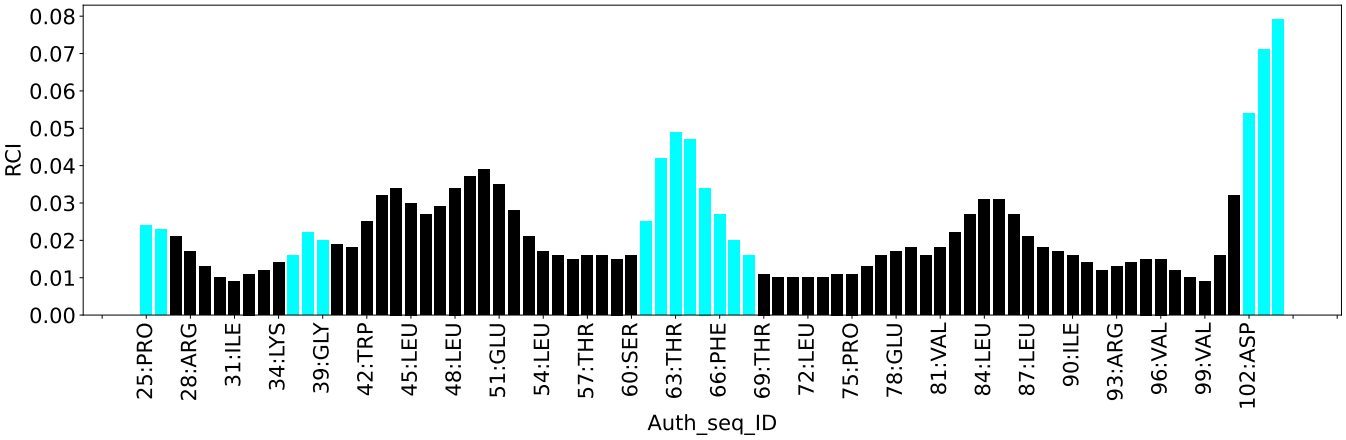
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	54	LEU	CD2	11.71	15.73 – 32.47	-7.4
1	A	46	LYS	HD3	2.95	0.54 – 2.65	6.4
1	A	46	LYS	HD2	2.84	0.58 – 2.64	6.0
1	A	38	GLU	CG	29.25	30.20 – 42.01	-5.8
1	A	54	LEU	CD1	15.85	16.71 – 32.55	-5.5
1	A	87	LEU	CD2	15.20	15.73 – 32.47	-5.3
1	A	65	ASP	HB2	1.34	1.41 – 4.01	-5.3

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
25:PRO
28:ARG
31:ILE
34:LYS
39:GLY
42:TRP
45:LEU
48:LEU
51:GLU
54:LEU
57:THR
60:SER
63:THR
66:PHE
69:THR
72:LEU
75:PRO
78:GLU
81:VAL
84:LEU
87:LEU
90:ILE
93:ARG
96:VAL
99:VAL
102:ASP
Auth_seq_ID