Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1LY7
Title	:	The solution structure of the the c-terminal domain of frataxin, the protein responsible for friedreich ataxia
Authors	:	Musco, G.; Stier, G.; Kolmerer, B.; Adinolfi, S.; Martin, S.; Frenkiel, T.; Gibson, T.; Pastore, A.
Deposited on	:	2002-06-07

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

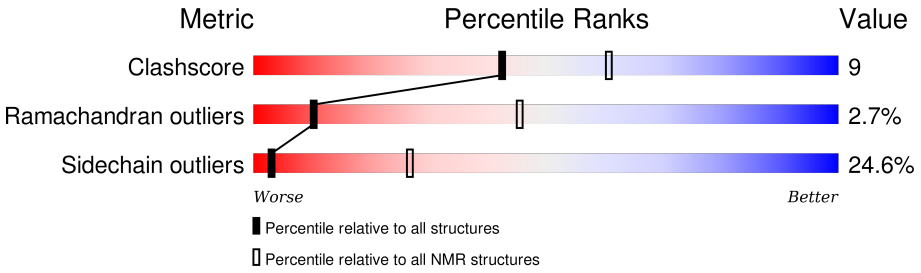
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 90%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	121	50% 34% • 14%

2 Ensemble composition and analysis

This entry contains 15 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:94-A:147, A:152-A:175, A:181-A:206 (104)	0.29	15

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 and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 5, 9, 13, 15
2	3, 4, 10, 11, 12, 14
3	6, 7
Single-model clusters	8

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1863 atoms, of which 909 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called frataxin.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1863	608	909	149	196	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	-	INITIATING MET	UNP Q16595

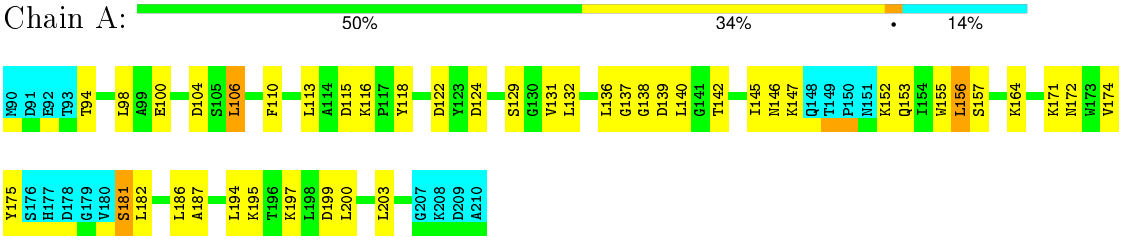
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: frataxin

Chain A:



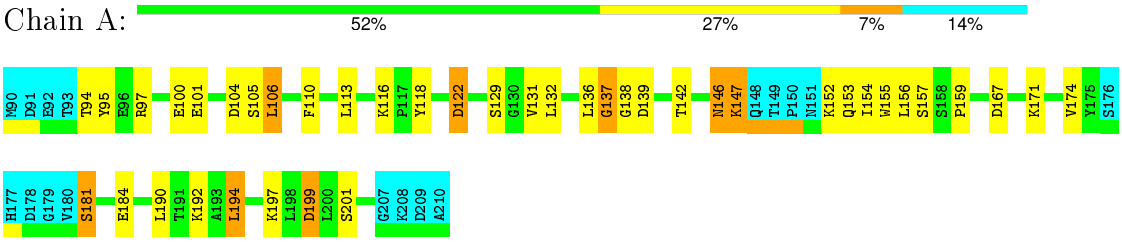
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: frataxin

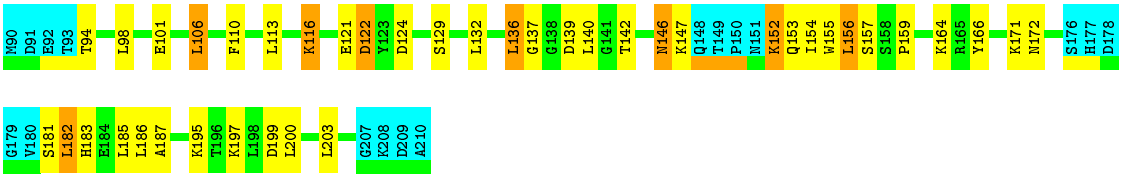
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: frataxin

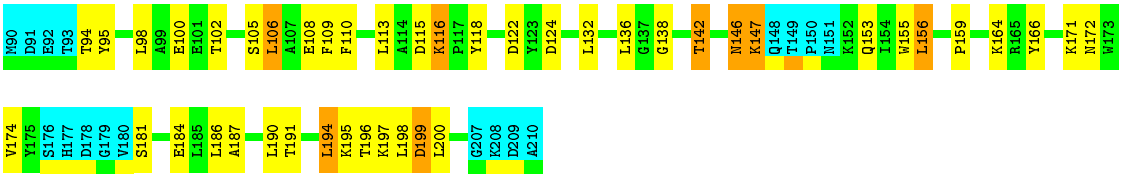
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: frataxin

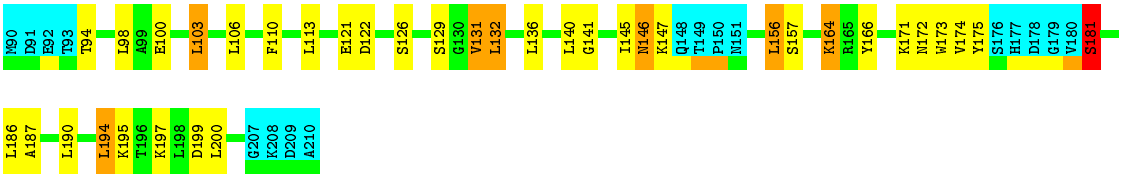
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: frataxin

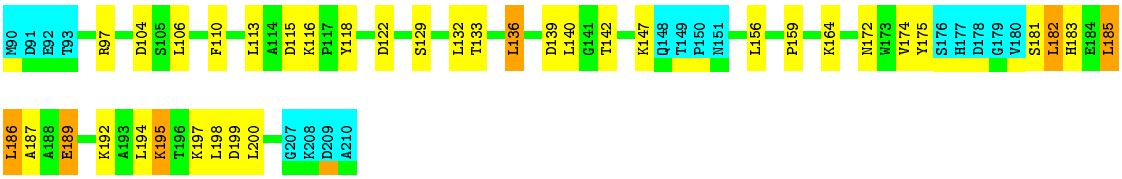
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: frataxin

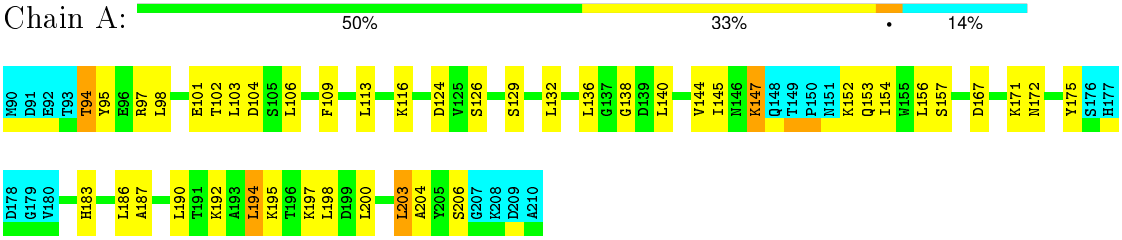
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: frataxin

Chain A:



4.2.7 Score per residue for model 7

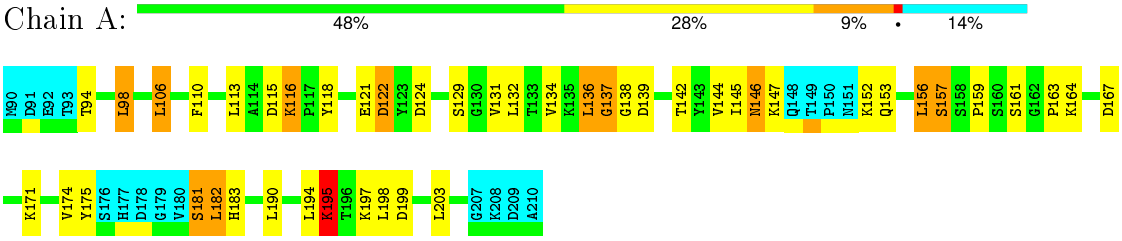
- Molecule 1: frataxin

Chain A:

4.2.8 Score per residue for model 8

- Molecule 1: frataxin

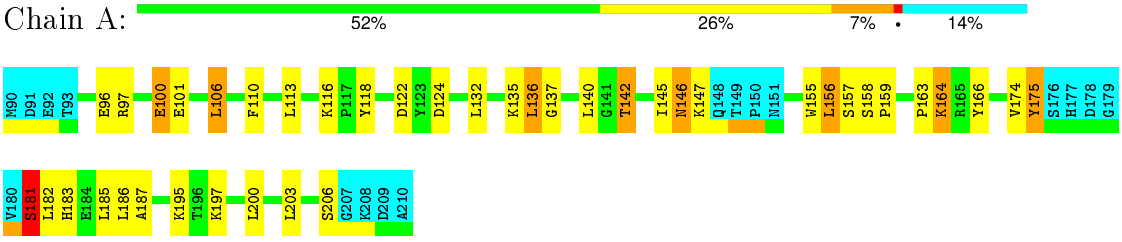
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: frataxin

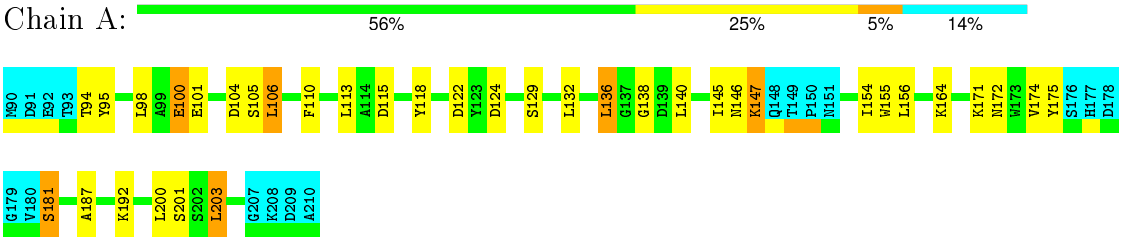
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: frataxin

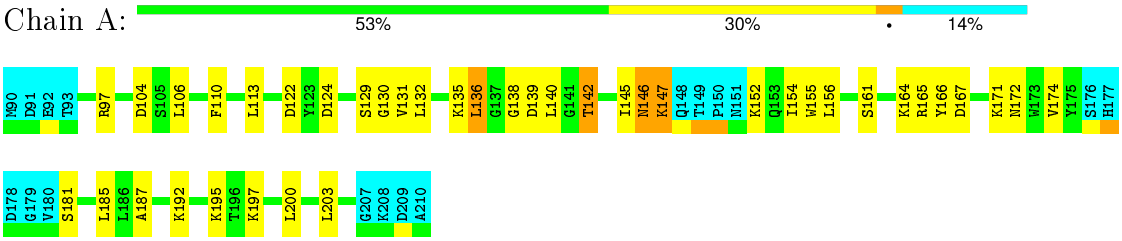
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: frataxin

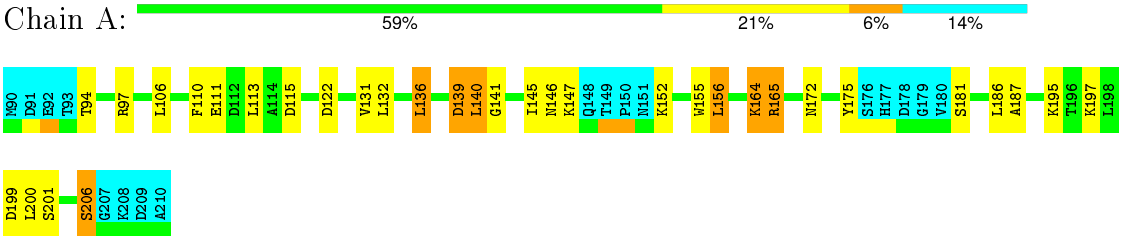
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: frataxin

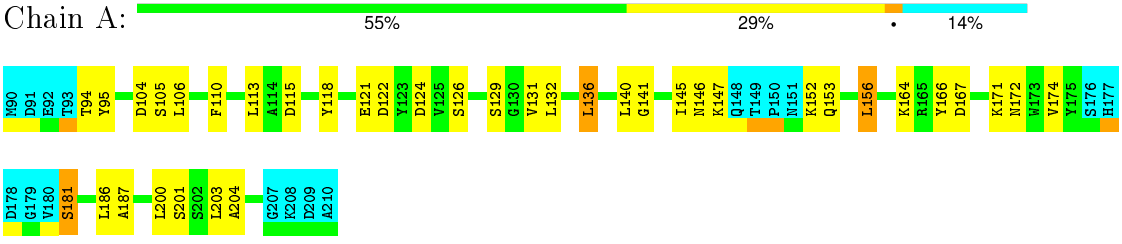
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: frataxin

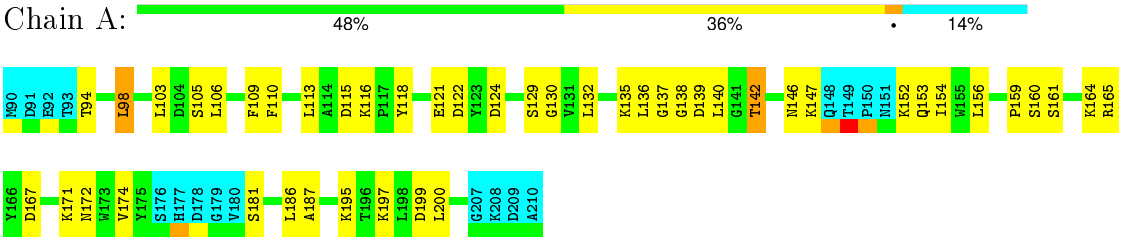
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: frataxin

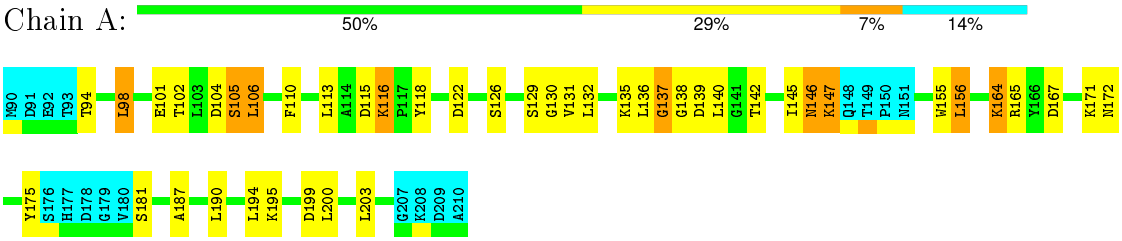
Chain A:



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: frataxin

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *structures with favorable non-bond energy*.

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

Software name	Classification	Version
aria	structure solution	1.0
aria	refinement	1.0

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)	BMRB entry 4342
Number of chemical shift lists	1
Total number of shifts	1463
Number of shifts mapped to atoms	1452
Number of unparsed shifts	0
Number of shifts with mapping errors	11
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 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	829	811	810	14±3
All	All	12435	12156	12150	214

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:HD13	1:A:140:LEU:HD23	0.80	1.53	9	9
1:A:131:VAL:HG23	1:A:146:ASN:HB3	0.74	1.57	11	6
1:A:166:TYR:HA	1:A:175:TYR:HB2	0.67	1.67	7	2
1:A:174:VAL:HG22	1:A:181:SER:HB2	0.67	1.65	7	5
1:A:156:LEU:HB3	1:A:164:LYS:HB2	0.65	1.68	12	7
1:A:94:THR:HG22	1:A:98:LEU:HD13	0.64	1.70	8	6
1:A:157:SER:HA	1:A:163:PRO:HA	0.62	1.70	8	2
1:A:110:PHE:HA	1:A:113:LEU:HD12	0.62	1.69	15	13
1:A:187:ALA:HB2	1:A:200:LEU:HB2	0.60	1.72	4	6
1:A:110:PHE:CZ	1:A:186:LEU:HD21	0.60	2.32	5	1
1:A:106:LEU:HG	1:A:203:LEU:HD21	0.59	1.72	10	4
1:A:130:GLY:HA2	1:A:147:LYS:HD3	0.59	1.73	11	2
1:A:113:LEU:HA	1:A:116:LYS:HD2	0.59	1.75	3	1
1:A:122:ASP:HB3	1:A:137:GLY:HA3	0.58	1.74	2	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LYS:HD2	1:A:154:ILE:HG12	0.57	1.76	10	1
1:A:146:ASN:ND2	1:A:155:TRP:HB2	0.57	2.14	9	6
1:A:113:LEU:HD23	1:A:116:LYS:HE2	0.56	1.76	2	1
1:A:187:ALA:HA	1:A:200:LEU:HD13	0.56	1.77	11	9
1:A:147:LYS:HA	1:A:154:ILE:HG12	0.56	1.77	11	4
1:A:174:VAL:HG13	1:A:181:SER:N	0.55	2.17	3	2
1:A:146:ASN:HD21	1:A:155:TRP:HB2	0.54	1.63	11	2
1:A:105:SER:HB2	1:A:203:LEU:HG	0.54	1.78	15	1
1:A:136:LEU:CD2	1:A:136:LEU:N	0.54	2.70	8	1
1:A:134:VAL:HG12	1:A:136:LEU:CD2	0.54	2.32	8	1
1:A:174:VAL:HA	1:A:181:SER:HA	0.54	1.79	14	3
1:A:95:TYR:HB2	1:A:152:LYS:HD3	0.53	1.80	6	3
1:A:200:LEU:HD23	1:A:203:LEU:HD22	0.53	1.79	6	1
1:A:200:LEU:HD23	1:A:203:LEU:HD11	0.53	1.81	11	2
1:A:190:LEU:HD12	1:A:198:LEU:HD11	0.52	1.81	3	1
1:A:174:VAL:HG22	1:A:181:SER:HB3	0.52	1.80	13	5
1:A:135:LYS:HA	1:A:142:THR:HG23	0.51	1.82	15	3
1:A:145:ILE:HG13	1:A:156:LEU:HD23	0.51	1.83	4	2
1:A:113:LEU:HA	1:A:116:LYS:HD3	0.50	1.83	2	1
1:A:190:LEU:O	1:A:194:LEU:HB2	0.49	2.07	1	6
1:A:142:THR:H	1:A:159:PRO:HG3	0.49	1.67	9	7
1:A:103:LEU:HD11	1:A:147:LYS:HB3	0.49	1.85	14	2
1:A:174:VAL:HG22	1:A:181:SER:CB	0.49	2.38	7	1
1:A:103:LEU:HA	1:A:106:LEU:HB2	0.49	1.85	6	1
1:A:102:THR:O	1:A:106:LEU:HD12	0.48	2.08	15	2
1:A:131:VAL:HG12	1:A:146:ASN:HB2	0.48	1.85	4	1
1:A:130:GLY:HA3	1:A:147:LYS:HE2	0.48	1.83	15	1
1:A:153:GLN:HB3	1:A:165:ARG:HG2	0.48	1.84	7	1
1:A:190:LEU:HB2	1:A:198:LEU:HD12	0.48	1.85	6	2
1:A:145:ILE:CG1	1:A:156:LEU:HD23	0.47	2.39	11	10
1:A:106:LEU:HD11	1:A:183:HIS:CD2	0.47	2.44	9	1
1:A:103:LEU:N	1:A:103:LEU:HD13	0.47	2.24	4	1
1:A:106:LEU:HD22	1:A:203:LEU:HG	0.47	1.87	6	1
1:A:155:TRP:HA	1:A:164:LYS:O	0.47	2.10	12	5
1:A:155:TRP:NE1	1:A:165:ARG:HG3	0.46	2.25	7	1
1:A:156:LEU:HD13	1:A:156:LEU:O	0.46	2.11	2	1
1:A:182:LEU:HD23	1:A:186:LEU:HD23	0.46	1.87	2	2
1:A:166:TYR:HB3	1:A:173:TRP:HB3	0.46	1.86	4	1
1:A:106:LEU:CD1	1:A:203:LEU:HD21	0.45	2.41	6	1
1:A:118:TYR:CE2	1:A:196:THR:HG21	0.45	2.46	3	1
1:A:109:PHE:HZ	1:A:198:LEU:HD22	0.45	1.71	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:VAL:HG12	1:A:136:LEU:HD21	0.45	1.88	8	1
1:A:144:VAL:HB	1:A:157:SER:HB3	0.45	1.88	6	1
1:A:191:THR:HA	1:A:196:THR:O	0.44	2.12	3	1
1:A:134:VAL:O	1:A:136:LEU:HD23	0.44	2.11	8	1
1:A:201:SER:HA	1:A:206:SER:OG	0.44	2.12	12	1
1:A:146:ASN:OD1	1:A:155:TRP:HB2	0.44	2.13	7	1
1:A:153:GLN:HA	1:A:166:TYR:O	0.44	2.13	13	2
1:A:194:LEU:O	1:A:195:LYS:C	0.44	2.56	8	1
1:A:156:LEU:HD12	1:A:164:LYS:HG3	0.43	1.89	5	1
1:A:113:LEU:HD22	1:A:118:TYR:OH	0.43	2.12	5	2
1:A:102:THR:O	1:A:106:LEU:HD23	0.43	2.13	6	1
1:A:126:SER:O	1:A:132:LEU:HD23	0.43	2.14	4	1
1:A:183:HIS:HB3	1:A:203:LEU:HD12	0.43	1.91	9	1
1:A:174:VAL:HG13	1:A:181:SER:HA	0.43	1.90	7	1
1:A:109:PHE:O	1:A:113:LEU:HG	0.43	2.14	6	2
1:A:136:LEU:HD12	1:A:141:GLY:C	0.43	2.35	4	3
1:A:106:LEU:HD11	1:A:203:LEU:HD21	0.42	1.89	6	1
1:A:116:LYS:HB3	1:A:118:TYR:HD1	0.42	1.74	3	2
1:A:102:THR:HA	1:A:204:ALA:HB3	0.42	1.91	6	1
1:A:198:LEU:HD13	1:A:200:LEU:HD11	0.42	1.91	5	1
1:A:144:VAL:O	1:A:156:LEU:HA	0.42	2.14	7	1
1:A:166:TYR:OH	1:A:185:LEU:HD22	0.42	2.15	11	2
1:A:96:GLU:O	1:A:100:GLU:HB2	0.42	2.15	9	1
1:A:146:ASN:O	1:A:154:ILE:HA	0.41	2.15	14	1
1:A:165:ARG:HG3	1:A:175:TYR:HE1	0.41	1.75	12	1
1:A:154:ILE:O	1:A:166:TYR:HB2	0.41	2.15	2	1
1:A:156:LEU:O	1:A:156:LEU:HD13	0.41	2.16	4	1
1:A:113:LEU:HA	1:A:116:LYS:HE2	0.41	1.91	15	1
1:A:194:LEU:C	1:A:195:LYS:HD2	0.41	2.36	5	1
1:A:185:LEU:O	1:A:189:GLU:HB2	0.41	2.16	5	1
1:A:187:ALA:CA	1:A:200:LEU:HD13	0.41	2.46	6	3
1:A:182:LEU:O	1:A:185:LEU:HB3	0.41	2.15	5	1
1:A:106:LEU:HD23	1:A:110:PHE:HE2	0.41	1.75	1	1
1:A:95:TYR:OH	1:A:147:LYS:HB2	0.40	2.15	3	1
1:A:100:GLU:O	1:A:104:ASP:HB2	0.40	2.16	10	1
1:A:185:LEU:HD23	1:A:186:LEU:HD22	0.40	1.93	2	1

6.3 Torsion angles

6.3.1 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 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	104/121 (86%)	82±2 (79±2%)	19±3 (19±3%)	3±2 (3±2%)	10 45
All	All	1560/1815 (86%)	1228 (79%)	290 (19%)	42 (3%)	10 45

All 13 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	138	GLY	8
1	A	199	ASP	7
1	A	152	LYS	5
1	A	129	SER	4
1	A	182	LEU	4
1	A	139	ASP	3
1	A	137	GLY	3
1	A	140	LEU	2
1	A	181	SER	2
1	A	187	ALA	1
1	A	153	GLN	1
1	A	204	ALA	1
1	A	195	LYS	1

6.3.2 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 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	90/104 (87%)	68±2 (75±3%)	22±2 (25±3%)	3 27
All	All	1350/1560 (87%)	1018 (75%)	332 (25%)	3 27

All 58 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	132	LEU	15
1	A	106	LEU	14
1	A	147	LYS	14
1	A	172	ASN	12
1	A	197	LYS	12
1	A	136	LEU	12
1	A	171	LYS	12
1	A	195	LYS	11
1	A	122	ASP	11
1	A	156	LEU	10
1	A	116	LYS	10
1	A	124	ASP	10
1	A	181	SER	10
1	A	146	ASN	9
1	A	186	LEU	8
1	A	129	SER	8
1	A	115	ASP	8
1	A	175	TYR	7
1	A	97	ARG	7
1	A	167	ASP	7
1	A	104	ASP	7
1	A	101	GLU	6
1	A	139	ASP	6
1	A	100	GLU	6
1	A	98	LEU	6
1	A	164	LYS	6
1	A	105	SER	6
1	A	192	LYS	6
1	A	94	THR	6
1	A	157	SER	5
1	A	118	TYR	5
1	A	121	GLU	5
1	A	199	ASP	4
1	A	142	THR	4
1	A	165	ARG	4
1	A	194	LEU	4
1	A	183	HIS	4
1	A	161	SER	3
1	A	184	GLU	3
1	A	206	SER	3
1	A	126	SER	3
1	A	201	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	203	LEU	3
1	A	153	GLN	2
1	A	131	VAL	2
1	A	144	VAL	1
1	A	185	LEU	1
1	A	158	SER	1
1	A	135	LYS	1
1	A	140	LEU	1
1	A	182	LEU	1
1	A	189	GLU	1
1	A	152	LYS	1
1	A	111	GLU	1
1	A	160	SER	1
1	A	103	LEU	1
1	A	108	GLU	1
1	A	133	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4342

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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	1463
Number of shifts mapped to atoms	1452
Number of unparsed shifts	0
Number of shifts with mapping errors	11
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 11 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1	PRO	CB	32.2	-1.0	1
A	1	PRO	HB3	2.3	-1.0	1
A	1	PRO	CA	62.7	-1.0	1
A	1	PRO	HA	4.45	-1.0	1
A	1	PRO	HD2	3.62	-1.0	2
A	1	PRO	HG2	1.95	-1.0	1
A	1	PRO	HB2	2.3	-1.0	1
A	1	PRO	HG3	1.95	-1.0	1
A	1	PRO	CD	50.6	-1.0	1
A	1	PRO	HD3	3.27	-1.0	2
A	1	PRO	CG	27.0	-1.0	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	122	-0.68 ± 0.13	Should be applied
$^{13}C_{\beta}$	113	0.06 ± 0.22	None needed (< 0.5 ppm)
$^{13}C'$	75	0.02 ± 0.34	None needed (< 0.5 ppm)
^{15}N	117	-2.44 ± 0.37	Should be applied

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 90%, i.e. 1126 atoms were assigned a chemical shift out of a possible 1258. 21 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	475/514 (92%)	205/205 (100%)	169/208 (81%)	101/101 (100%)
Sidechain	544/608 (89%)	335/354 (95%)	206/236 (87%)	3/18 (17%)
Aromatic	107/136 (79%)	68/70 (97%)	36/61 (59%)	3/5 (60%)
Overall	1126/1258 (90%)	608/629 (97%)	411/505 (81%)	107/124 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1281 atoms were assigned a chemical shift out of a possible 1437. 22 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	551/597 (92%)	238/238 (100%)	196/242 (81%)	117/117 (100%)
Sidechain	619/696 (89%)	383/405 (95%)	231/270 (86%)	5/21 (24%)
Aromatic	111/144 (77%)	70/74 (95%)	38/63 (60%)	3/7 (43%)
Overall	1281/1437 (89%)	691/717 (96%)	465/575 (81%)	125/145 (86%)

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.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	170	GLY	H	4.38	11.63 – 5.03	-6.0
1	A	165	ARG	HG3	-0.09	3.00 – 0.10	-5.7
1	A	168	TRP	HE3	5.08	9.33 – 5.33	-5.6

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	148	GLN	HB3	0.61	3.37 – 0.67	-5.2
1	A	155	TRP	CD2	120.20	134.55 – 120.45	-5.2

7.1.5 Random Coil Index (RCI) plots

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.

Random coil index (RCI) for chain A: