Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:57 pm BST

PDB ID	:	2MSL
Title	:	Solution Structure and Chemical Shift Assignments for the Apo form of the Receiver Domain of Nitrogen Regulatory Protein C (NTRC) at 35C
Authors	:	Clarkson, M.W.; Pontiggia, F.; Villali, J.; Kern, D.
Deposited on	:	2014-08-04

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 ⓘ symbol.

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

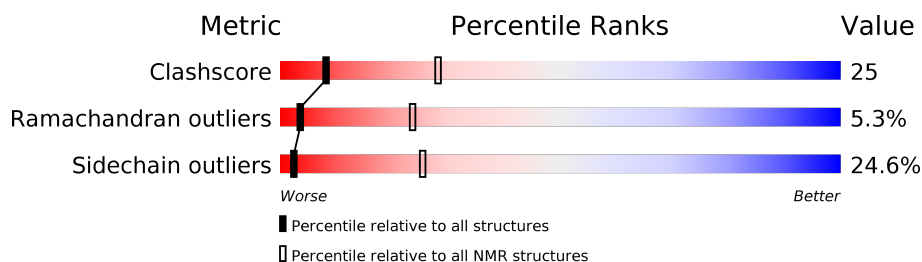|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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

The overall completeness of chemical shifts assignment is 92%.

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	Percentile Ranks	Value
Clashscore		25
Ramachandran outliers		5.3%
Sidechain outliers		24.6%

Worse   *Better*

■ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	124	40% 44% 8% 8%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 5 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:3-A:55, A:62-A:122 (114)	0.30	5

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 4 clusters and 6 single-model clusters were found.

Cluster number	Models
1	1, 2, 7, 13, 15, 22
2	3, 6, 10, 14, 23
3	5, 18, 20, 24
4	8, 17, 21, 25
Single-model clusters	4; 9; 11; 12; 16; 19

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1910 atoms, of which 955 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nitrogen regulation protein NR(I).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	124	1910	606	955	162	181	6	0

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.
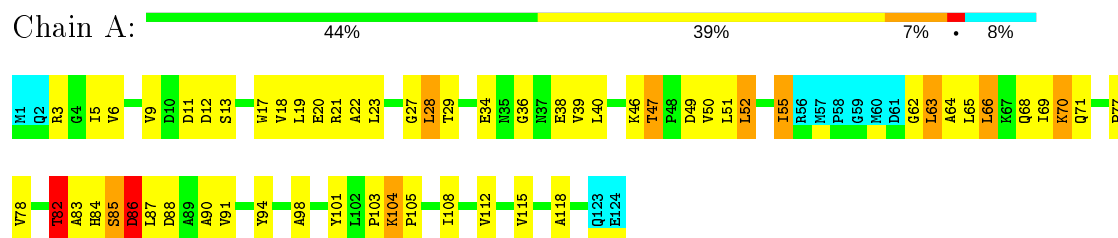
• Molecule 1: Nitrogen regulation protein NR(I)
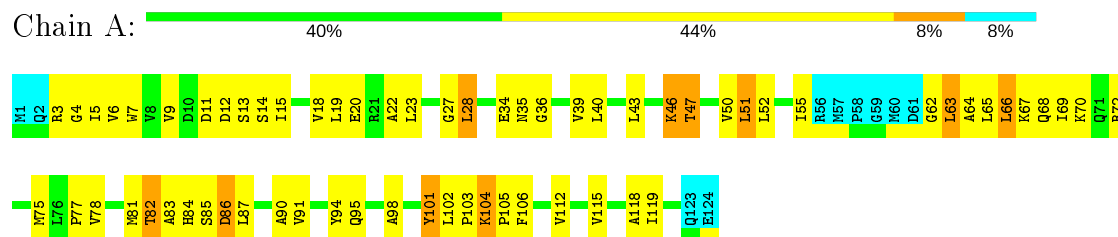
4.2   Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.
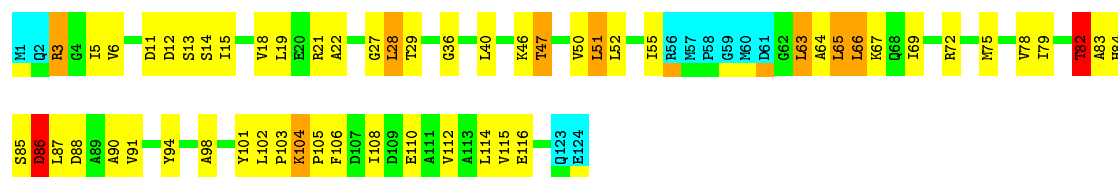
4.2.1   Score per residue for model 1

• Molecule 1: Nitrogen regulation protein NR(I)
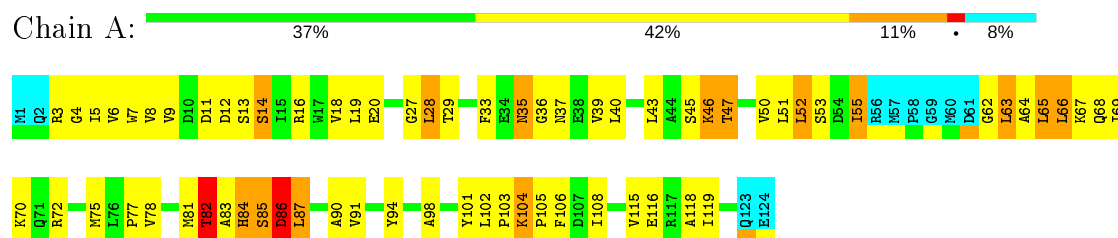

4.2.2   Score per residue for model 2

• Molecule 1: Nitrogen regulation protein NR(I)

4.2.3 Score per residue for model 3

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A:

4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A: 40% 43% 9% · 8%

4.2.7 Score per residue for model 7

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A: 49% 35% 6% · 8%

4.2.8 Score per residue for model 8

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A: 42% 37% 12% · 8%

4.2.9 Score per residue for model 9

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A: 40% 43% 10% 8%

4.2.10 Score per residue for model 10

• Molecule 1: Nitrogen regulation protein NR(I)

4.2.11 Score per residue for model 11

• Molecule 1: Nitrogen regulation protein NR(I)

4.2.12 Score per residue for model 12

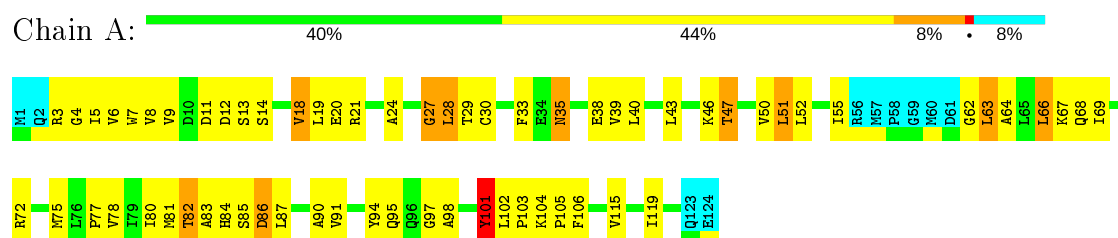• Molecule 1: Nitrogen regulation protein NR(I)

4.2.13 Score per residue for model 13

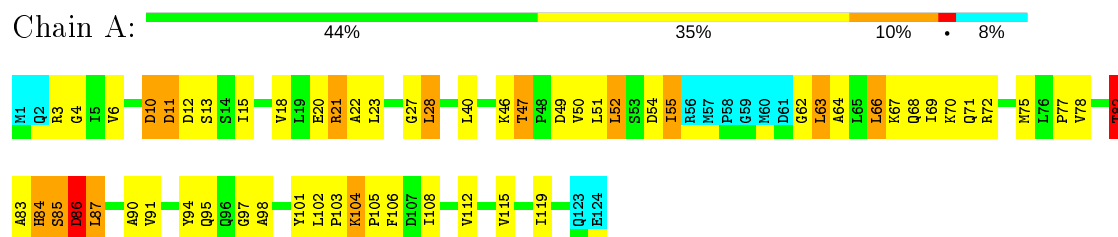• Molecule 1: Nitrogen regulation protein NR(I)

4.2.14 Score per residue for model 14
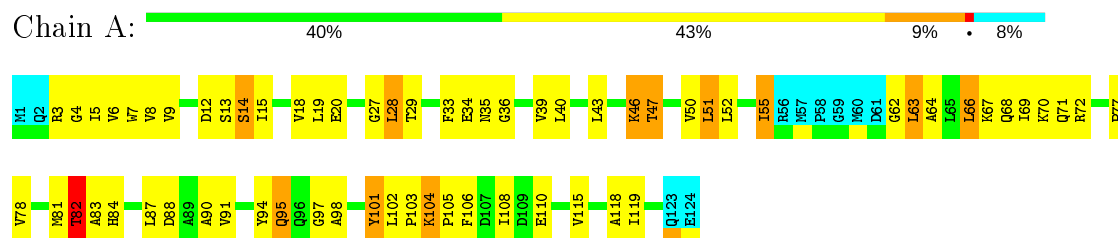
• Molecule 1: Nitrogen regulation protein NR(I)

4.2.15 Score per residue for model 15

• Molecule 1: Nitrogen regulation protein NR(I)
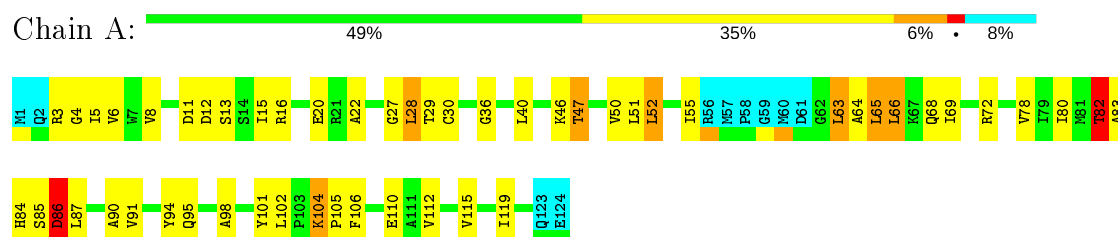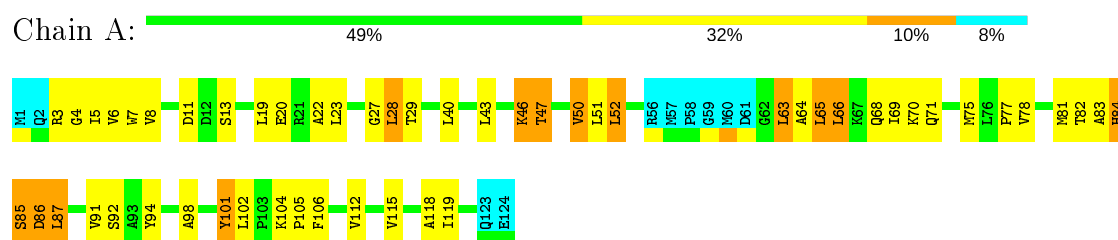

4.2.16 Score per residue for model 16

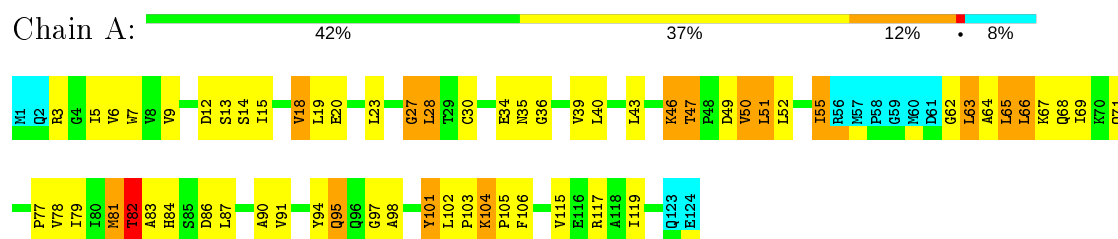• Molecule 1: Nitrogen regulation protein NR(I)
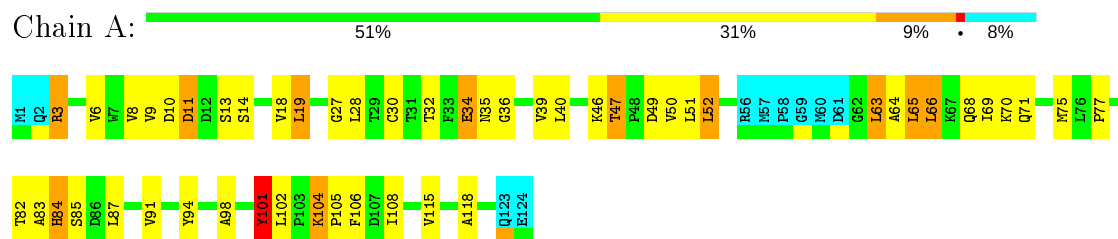
4.2.17 Score per residue for model 17

• Molecule 1: Nitrogen regulation protein NR(I)
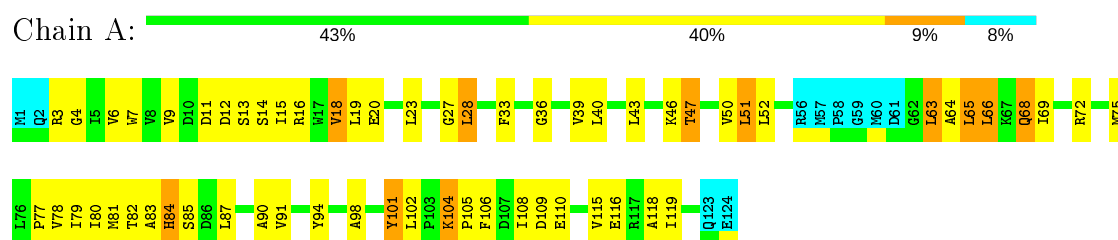
4.2.18 Score per residue for model 18

• Molecule 1: Nitrogen regulation protein NR(I)
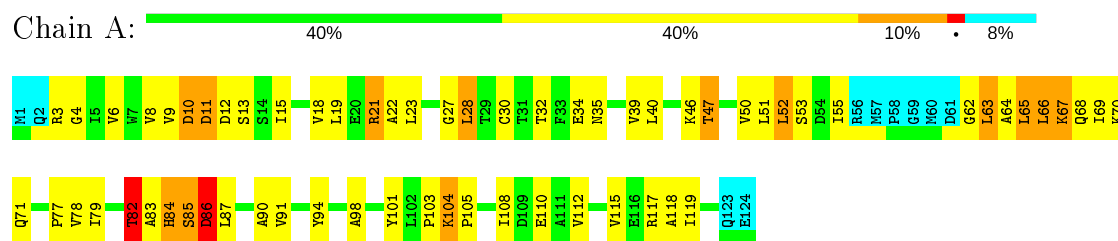
4.2.19 Score per residue for model 19

• Molecule 1: Nitrogen regulation protein NR(I)
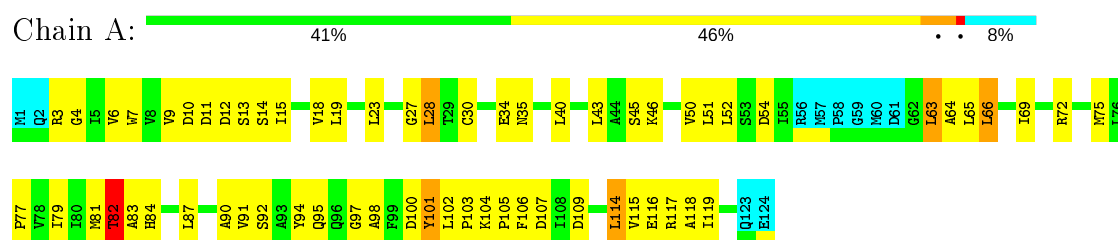
4.2.20 Score per residue for model 20

• Molecule 1: Nitrogen regulation protein NR(I)
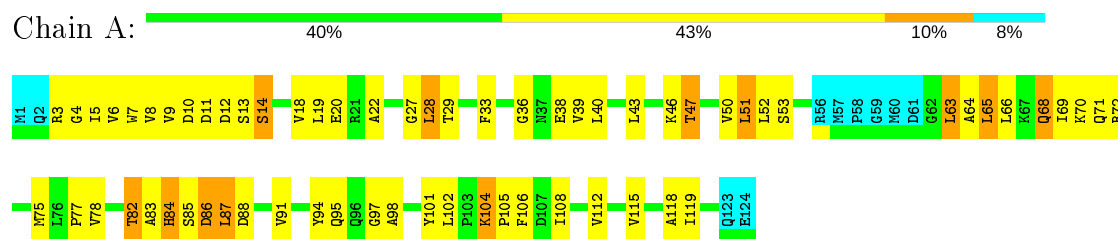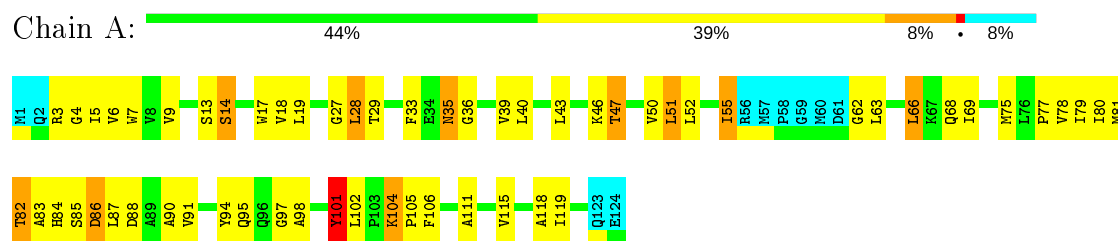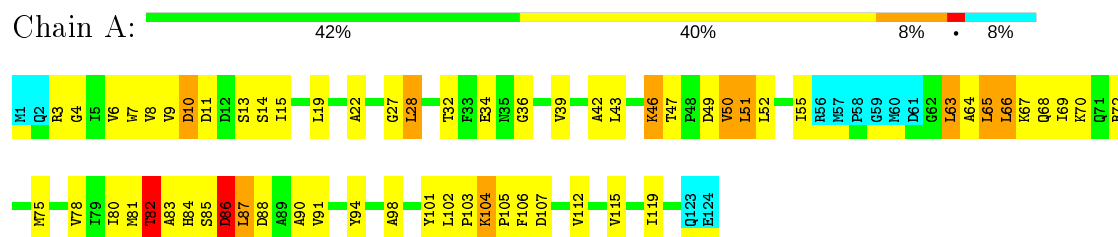

4.2.21 Score per residue for model 21

• Molecule 1: Nitrogen regulation protein NR(I)
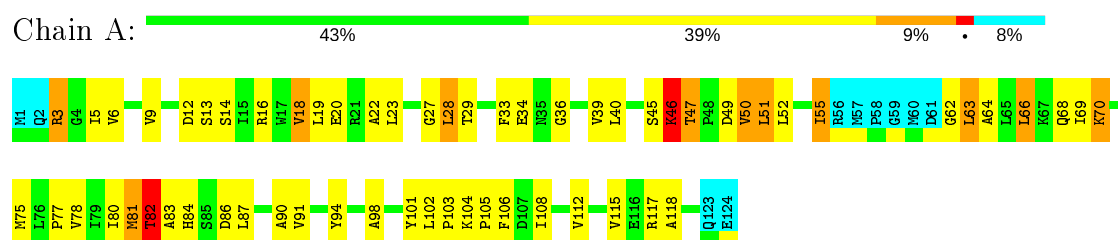
4.2.22 Score per residue for model 22

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A:
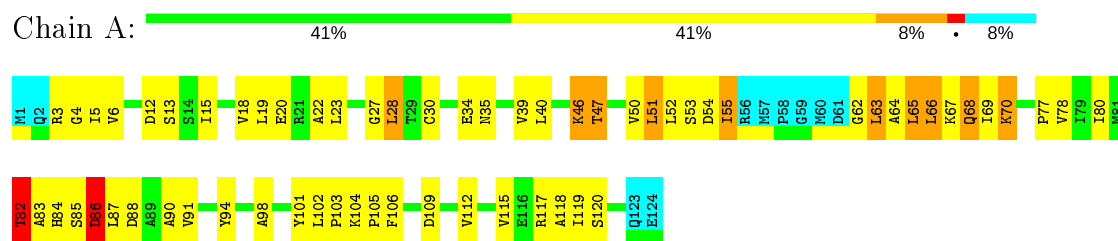
4.2.23 Score per residue for model 23

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A:
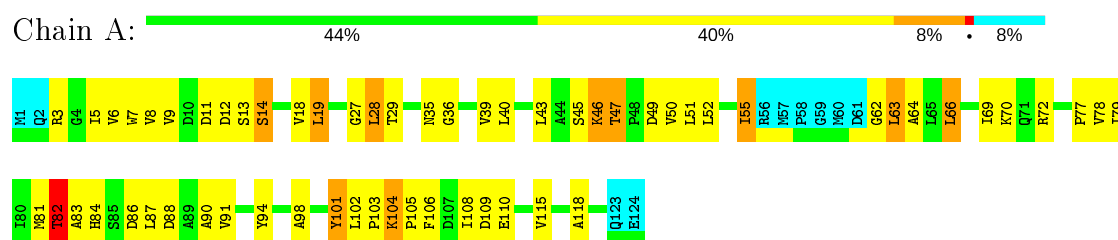
4.2.24 Score per residue for model 24

• Molecule 1: Nitrogen regulation protein NR(I)

Chain A:
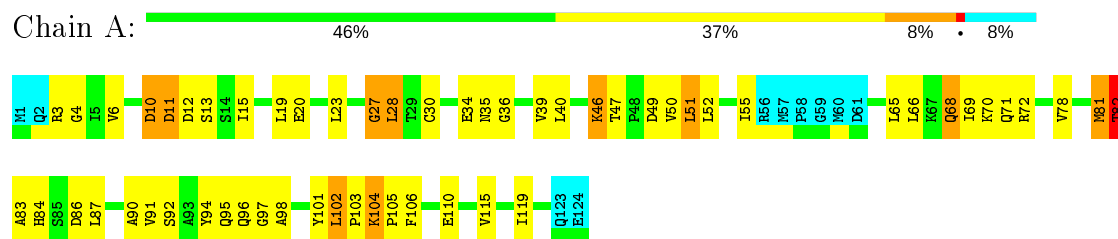
4.2.25 Score per residue for model 25
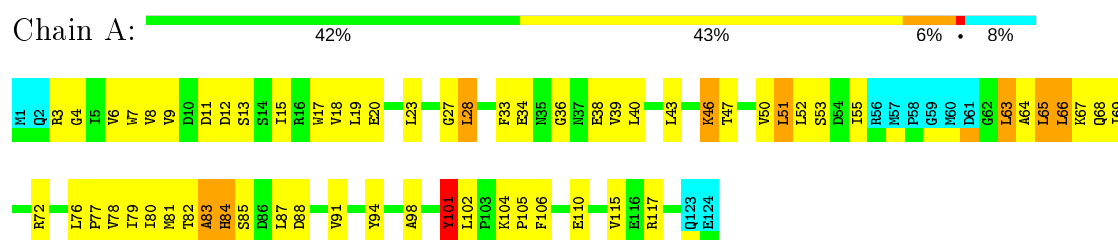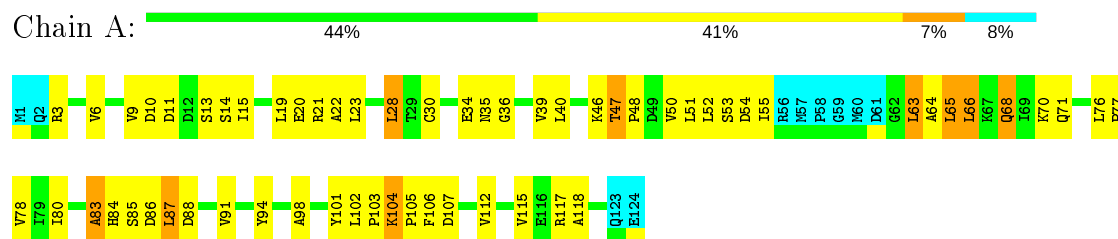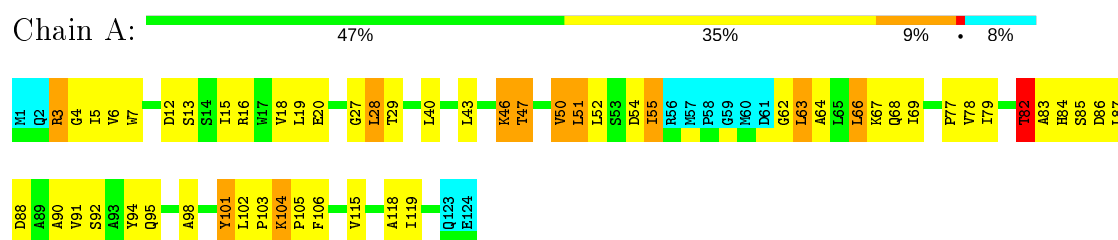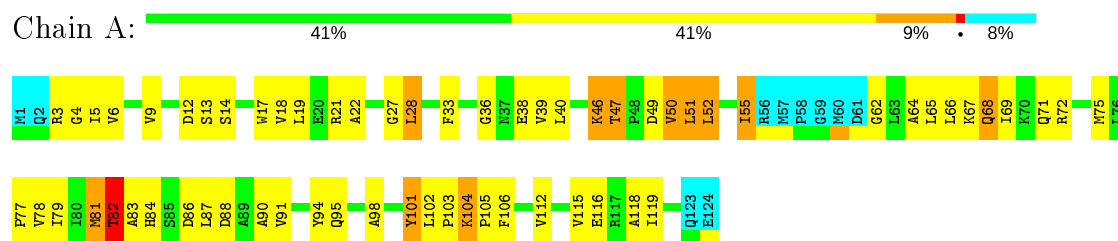
• Molecule 1: Nitrogen regulation protein NR(I)

Chain A:
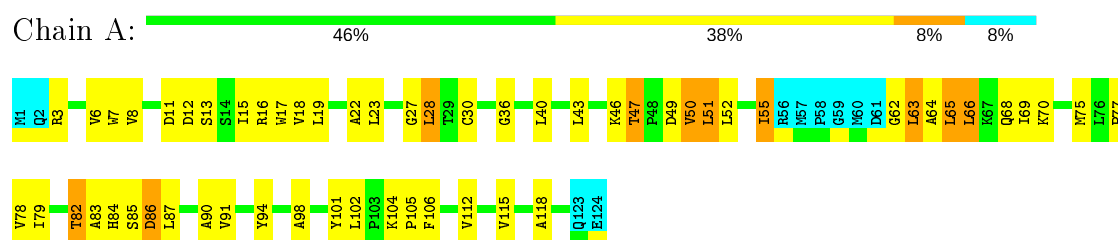
5 Refinement protocol and experimental data overview (i)

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

Of the 300 calculated structures, 25 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
CYANA	structure solution	
CYANA	refinement	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1557
Number of shifts mapped to atoms	1557
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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

6 Model quality (i)

6.1 Standard geometry (i)

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 (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	874	879	879	43±6
All	All	21850	21975	21975	1079

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:23:LEU:HD22	1:A:28:LEU:HD12	1.05	1.29	24	10
1:A:8:VAL:HG11	1:A:19:LEU:HD13	0.97	1.31	4	3
1:A:19:LEU:HD21	1:A:52:LEU:HD22	0.91	1.42	23	2
1:A:19:LEU:HD22	1:A:52:LEU:HD13	0.90	1.41	14	5
1:A:50:VAL:HG11	1:A:115:VAL:HG23	0.83	1.50	20	22
1:A:18:VAL:HG23	1:A:108:ILE:HD11	0.83	1.51	23	7
1:A:66:LEU:HD22	1:A:69:ILE:HD12	0.78	1.56	8	13
1:A:6:VAL:HG13	1:A:50:VAL:HG13	0.76	1.55	19	11
1:A:69:ILE:HG21	1:A:78:VAL:HG21	0.74	1.57	4	19
1:A:63:LEU:HD13	1:A:63:LEU:C	0.74	2.03	18	1
1:A:55:ILE:HD11	1:A:80:ILE:HD12	0.73	1.61	21	4
1:A:4:GLY:HA3	1:A:119:ILE:HD13	0.72	1.61	18	16
1:A:8:VAL:HG22	1:A:52:LEU:HD13	0.70	1.62	7	1
1:A:14:SER:O	1:A:18:VAL:HG12	0.70	1.87	23	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG11	1:A:115:VAL:CG2	0.69	2.16	11	17
1:A:9:VAL:HG11	1:A:39:VAL:HG21	0.69	1.62	18	3
1:A:63:LEU:HD22	1:A:63:LEU:O	0.69	1.88	18	1
1:A:6:VAL:HG13	1:A:52:LEU:HD13	0.68	1.65	11	1
1:A:102:LEU:HD12	1:A:103:PRO:HD2	0.68	1.65	4	8
1:A:6:VAL:HG21	1:A:115:VAL:HG21	0.67	1.65	8	16
1:A:94:TYR:O	1:A:98:ALA:HB3	0.67	1.89	2	25
1:A:87:LEU:O	1:A:91:VAL:HG23	0.67	1.90	19	25
1:A:102:LEU:HD21	1:A:106:PHE:CG	0.66	2.25	23	20
1:A:22:ALA:HB1	1:A:112:VAL:HG22	0.66	1.68	18	9
1:A:50:VAL:HG11	1:A:115:VAL:HG21	0.65	1.67	10	2
1:A:19:LEU:HD11	1:A:81:MET:HE1	0.64	1.70	10	3
1:A:33:PHE:CG	1:A:39:VAL:HG22	0.64	2.26	4	9
1:A:4:GLY:HA3	1:A:119:ILE:HG21	0.64	1.70	18	2
1:A:9:VAL:HG21	1:A:36:GLY:HA2	0.63	1.70	23	6
1:A:19:LEU:HD11	1:A:81:MET:CE	0.63	2.23	10	11
1:A:22:ALA:HB1	1:A:112:VAL:CG2	0.63	2.24	15	13
1:A:15:ILE:HD12	1:A:104:LYS:HE2	0.63	1.70	11	1
1:A:9:VAL:HB	1:A:39:VAL:HG21	0.63	1.71	17	11
1:A:39:VAL:HG11	1:A:51:LEU:HD21	0.63	1.70	24	2
1:A:6:VAL:CG1	1:A:52:LEU:HD13	0.62	2.24	11	11
1:A:27:GLY:O	1:A:28:LEU:HD23	0.62	1.94	4	12
1:A:102:LEU:HD11	1:A:106:PHE:CB	0.62	2.23	10	16
1:A:6:VAL:CG2	1:A:115:VAL:HG21	0.62	2.25	25	15
1:A:51:LEU:O	1:A:52:LEU:HD12	0.62	1.95	25	8
1:A:6:VAL:HG22	1:A:50:VAL:CG1	0.62	2.24	9	7
1:A:36:GLY:CA	1:A:65:LEU:HD13	0.61	2.25	14	13
1:A:40:LEU:HD22	1:A:68:GLN:NE2	0.61	2.11	4	16
1:A:65:LEU:HD23	1:A:66:LEU:N	0.61	2.11	12	12
1:A:79:ILE:CD1	1:A:114:LEU:HD11	0.61	2.25	19	1
1:A:39:VAL:HG11	1:A:51:LEU:HD11	0.60	1.72	14	2
1:A:23:LEU:CD2	1:A:28:LEU:HD12	0.60	2.26	1	3
1:A:36:GLY:HA3	1:A:65:LEU:HD13	0.59	1.73	12	11
1:A:82:THR:O	1:A:83:ALA:HB3	0.59	1.98	13	10
1:A:18:VAL:CG2	1:A:108:ILE:HD11	0.59	2.27	16	1
1:A:15:ILE:HG21	1:A:54:ASP:CG	0.59	2.17	19	3
1:A:66:LEU:HG	1:A:69:ILE:HD12	0.59	1.74	10	2
1:A:6:VAL:HB	1:A:23:LEU:HD11	0.59	1.72	17	5
1:A:39:VAL:CG1	1:A:51:LEU:HD11	0.59	2.28	22	4
1:A:51:LEU:C	1:A:52:LEU:HD12	0.58	2.18	13	13
1:A:6:VAL:CG1	1:A:52:LEU:HD11	0.57	2.29	1	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LEU:HD21	1:A:106:PHE:CD2	0.57	2.33	15	13
1:A:7:TRP:CZ3	1:A:43:LEU:HD23	0.57	2.34	11	14
1:A:15:ILE:HG23	1:A:104:LYS:CE	0.57	2.29	2	1
1:A:8:VAL:HB	1:A:32:THR:HG22	0.57	1.76	16	3
1:A:27:GLY:C	1:A:28:LEU:HD23	0.57	2.20	5	23
1:A:40:LEU:HD22	1:A:68:GLN:OE1	0.57	2.00	11	2
1:A:62:GLY:O	1:A:65:LEU:HD23	0.57	2.00	18	1
1:A:82:THR:HG23	1:A:87:LEU:HD13	0.56	1.76	3	5
1:A:77:PRO:HG3	1:A:118:ALA:HB1	0.56	1.76	6	4
1:A:84:HIS:CD2	1:A:84:HIS:N	0.56	2.72	16	2
1:A:79:ILE:HD13	1:A:114:LEU:HD11	0.56	1.75	19	1
1:A:40:LEU:O	1:A:40:LEU:HD12	0.56	2.00	18	10
1:A:65:LEU:HD23	1:A:65:LEU:H	0.56	1.60	24	2
1:A:66:LEU:HD22	1:A:69:ILE:CD1	0.55	2.29	8	8
1:A:35:ASN:O	1:A:39:VAL:HG23	0.55	2.01	3	1
1:A:82:THR:HG21	1:A:86:ASP:CB	0.55	2.31	13	4
1:A:76:LEU:HD12	1:A:77:PRO:HD2	0.55	1.77	11	1
1:A:9:VAL:HG13	1:A:9:VAL:O	0.55	2.02	21	8
1:A:23:LEU:HD22	1:A:28:LEU:CD1	0.55	2.31	15	2
1:A:66:LEU:HA	1:A:69:ILE:HD12	0.55	1.77	24	5
1:A:40:LEU:HD12	1:A:40:LEU:O	0.55	2.02	16	12
1:A:102:LEU:HD11	1:A:106:PHE:HB2	0.55	1.79	4	5
1:A:4:GLY:O	1:A:23:LEU:HD13	0.55	2.02	11	1
1:A:50:VAL:HG23	1:A:77:PRO:O	0.54	2.01	13	13
1:A:5:ILE:HG23	1:A:29:THR:HB	0.54	1.78	2	12
1:A:83:ALA:CA	1:A:87:LEU:HD13	0.54	2.32	21	7
1:A:83:ALA:N	1:A:87:LEU:HD13	0.54	2.16	23	7
1:A:83:ALA:HB2	1:A:103:PRO:CB	0.54	2.32	22	7
1:A:5:ILE:HD12	1:A:46:LYS:NZ	0.54	2.17	13	1
1:A:66:LEU:HD13	1:A:80:ILE:CD1	0.54	2.32	11	3
1:A:82:THR:HG21	1:A:86:ASP:HB3	0.54	1.80	1	8
1:A:5:ILE:HD13	1:A:46:LYS:HE2	0.54	1.80	14	5
1:A:77:PRO:CB	1:A:118:ALA:HB1	0.53	2.33	16	13
1:A:91:VAL:HG22	1:A:101:TYR:OH	0.53	2.04	15	15
1:A:114:LEU:HD12	1:A:114:LEU:O	0.53	2.02	19	1
1:A:21:ARG:NE	1:A:108:ILE:HD13	0.53	2.19	5	3
1:A:8:VAL:HG21	1:A:19:LEU:HB3	0.53	1.80	25	5
1:A:50:VAL:CG1	1:A:115:VAL:HG23	0.53	2.33	14	5
1:A:82:THR:HG23	1:A:87:LEU:CD1	0.53	2.34	13	5
1:A:8:VAL:HG13	1:A:52:LEU:O	0.53	2.03	4	1
1:A:63:LEU:HD12	1:A:64:ALA:N	0.53	2.18	1	21

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LEU:HD21	1:A:106:PHE:CB	0.53	2.33	4	4
1:A:82:THR:HG23	1:A:83:ALA:H	0.52	1.64	21	12
1:A:55:ILE:HD11	1:A:80:ILE:CD1	0.52	2.33	21	1
1:A:69:ILE:CG2	1:A:78:VAL:HG21	0.52	2.34	4	1
1:A:10:ASP:OD2	1:A:15:ILE:HG21	0.52	2.04	18	4
1:A:83:ALA:HB2	1:A:103:PRO:HB3	0.52	1.80	12	2
1:A:115:VAL:HG22	1:A:119:ILE:CD1	0.52	2.35	8	2
1:A:6:VAL:HG13	1:A:50:VAL:O	0.52	2.04	8	1
1:A:77:PRO:CG	1:A:118:ALA:HB1	0.52	2.34	6	16
1:A:83:ALA:HB2	1:A:103:PRO:HB2	0.51	1.83	5	7
1:A:66:LEU:HD13	1:A:69:ILE:HD12	0.51	1.81	18	6
1:A:62:GLY:O	1:A:66:LEU:HD23	0.51	2.05	14	1
1:A:63:LEU:HD21	1:A:67:LYS:HE3	0.51	1.82	18	1
1:A:83:ALA:H	1:A:87:LEU:HD13	0.51	1.66	23	8
1:A:83:ALA:HB2	1:A:104:LYS:N	0.51	2.21	17	3
1:A:8:VAL:CG1	1:A:19:LEU:HD13	0.51	2.35	23	2
1:A:15:ILE:HG23	1:A:104:LYS:HE2	0.50	1.83	2	2
1:A:83:ALA:HA	1:A:87:LEU:HD13	0.50	1.82	6	6
1:A:102:LEU:HD11	1:A:106:PHE:HB3	0.50	1.83	11	6
1:A:40:LEU:CD1	1:A:65:LEU:HD12	0.50	2.36	19	1
1:A:9:VAL:O	1:A:9:VAL:HG13	0.50	2.06	8	5
1:A:63:LEU:HD21	1:A:67:LYS:CE	0.50	2.36	18	1
1:A:50:VAL:HG21	1:A:115:VAL:HG23	0.50	1.83	9	1
1:A:55:ILE:HG23	1:A:62:GLY:HA3	0.50	1.83	21	12
1:A:84:HIS:N	1:A:84:HIS:CD2	0.50	2.79	11	1
1:A:15:ILE:O	1:A:18:VAL:HG22	0.49	2.07	22	5
1:A:4:GLY:CA	1:A:119:ILE:HG21	0.49	2.37	18	1
1:A:15:ILE:HG23	1:A:104:LYS:HE3	0.49	1.84	25	1
1:A:15:ILE:HD12	1:A:104:LYS:CE	0.49	2.38	7	2
1:A:94:TYR:CZ	1:A:98:ALA:HB1	0.49	2.43	19	16
1:A:33:PHE:CD2	1:A:39:VAL:HG22	0.49	2.42	10	4
1:A:19:LEU:CD2	1:A:52:LEU:HD22	0.49	2.37	10	2
1:A:15:ILE:O	1:A:19:LEU:HD12	0.48	2.07	17	3
1:A:9:VAL:HG21	1:A:36:GLY:CA	0.48	2.37	10	4
1:A:6:VAL:HG22	1:A:50:VAL:HG13	0.48	1.84	11	1
1:A:18:VAL:HG23	1:A:108:ILE:CD1	0.48	2.38	6	2
1:A:66:LEU:HD13	1:A:80:ILE:HD13	0.48	1.85	11	2
1:A:8:VAL:CG2	1:A:19:LEU:HD13	0.48	2.39	23	1
1:A:66:LEU:HD21	1:A:78:VAL:HG11	0.48	1.86	2	4
1:A:104:LYS:HA	1:A:105:PRO:C	0.47	2.30	22	25
1:A:6:VAL:HG12	1:A:52:LEU:HD11	0.47	1.85	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:TRP:HZ3	1:A:43:LEU:HD23	0.47	1.69	11	4
1:A:23:LEU:HD12	1:A:30:CYS:HB3	0.47	1.85	19	3
1:A:5:ILE:HD13	1:A:46:LYS:HE3	0.47	1.86	22	1
1:A:19:LEU:HD11	1:A:81:MET:SD	0.47	2.49	15	3
1:A:21:ARG:HA	1:A:24:ALA:HB3	0.47	1.87	4	1
1:A:70:LYS:HE3	1:A:98:ALA:HB2	0.47	1.87	15	3
1:A:63:LEU:HD13	1:A:64:ALA:N	0.47	2.24	18	1
1:A:77:PRO:HB2	1:A:118:ALA:HB1	0.47	1.86	12	4
1:A:15:ILE:HD12	1:A:104:LYS:HE3	0.47	1.86	2	3
1:A:114:LEU:C	1:A:114:LEU:HD12	0.47	2.30	19	1
1:A:82:THR:O	1:A:83:ALA:CB	0.46	2.63	13	4
1:A:63:LEU:C	1:A:63:LEU:CD1	0.46	2.76	18	1
1:A:53:SER:HB3	1:A:66:LEU:HD11	0.46	1.88	11	1
1:A:8:VAL:HG13	1:A:19:LEU:HD13	0.46	1.88	16	1
1:A:17:TRP:CE3	1:A:18:VAL:HG13	0.46	2.45	25	5
1:A:66:LEU:CD2	1:A:69:ILE:HD12	0.46	2.40	13	3
1:A:40:LEU:HD22	1:A:68:GLN:CD	0.46	2.31	13	7
1:A:66:LEU:HG	1:A:80:ILE:HD11	0.46	1.87	17	1
1:A:39:VAL:O	1:A:42:ALA:HB3	0.46	2.11	20	1
1:A:8:VAL:HG21	1:A:19:LEU:HD13	0.46	1.88	23	1
1:A:4:GLY:CA	1:A:119:ILE:HD13	0.46	2.36	18	1
1:A:18:VAL:HG12	1:A:108:ILE:HD11	0.46	1.87	1	1
1:A:79:ILE:HD13	1:A:114:LEU:CD2	0.46	2.41	2	1
1:A:66:LEU:HD22	1:A:80:ILE:HD11	0.46	1.88	12	2
1:A:4:GLY:HA3	1:A:28:LEU:HD13	0.45	1.87	11	1
1:A:55:ILE:CD1	1:A:80:ILE:HD12	0.45	2.39	21	1
1:A:70:LYS:CE	1:A:98:ALA:HB2	0.45	2.41	22	2
1:A:90:ALA:O	1:A:94:TYR:CB	0.45	2.64	25	20
1:A:9:VAL:HG21	1:A:39:VAL:CG2	0.45	2.42	18	3
1:A:9:VAL:CG1	1:A:39:VAL:HG21	0.45	2.38	18	1
1:A:8:VAL:HG22	1:A:52:LEU:CD1	0.45	2.42	15	1
1:A:83:ALA:HA	1:A:87:LEU:HD22	0.45	1.87	3	2
1:A:65:LEU:HD23	1:A:66:LEU:H	0.45	1.70	20	1
1:A:102:LEU:HD12	1:A:103:PRO:CD	0.45	2.42	24	1
1:A:78:VAL:C	1:A:94:TYR:HH	0.45	2.15	6	4
1:A:14:SER:O	1:A:18:VAL:HG22	0.45	2.11	10	2
1:A:70:LYS:HE2	1:A:98:ALA:HB2	0.44	1.89	1	1
1:A:65:LEU:CD2	1:A:66:LEU:HD12	0.44	2.43	12	1
1:A:52:LEU:HD11	1:A:79:ILE:HD12	0.44	1.88	8	3
1:A:19:LEU:HD22	1:A:52:LEU:HD22	0.44	1.89	10	5
1:A:79:ILE:HG23	1:A:101:TYR:HA	0.44	1.90	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:15:ILE:HG21	1:A:54:ASP:OD2	0.44	2.13	19	1
1:A:53:SER:OG	1:A:80:ILE:HD13	0.44	2.13	22	1
1:A:22:ALA:HB1	1:A:112:VAL:HG23	0.43	1.90	22	1
1:A:80:ILE:HG22	1:A:80:ILE:O	0.43	2.13	17	1
1:A:18:VAL:HG23	1:A:108:ILE:CG1	0.43	2.42	3	1
1:A:78:VAL:HG12	1:A:79:ILE:N	0.43	2.29	10	7
1:A:95:GLN:C	1:A:97:GLY:H	0.43	2.17	5	8
1:A:53:SER:OG	1:A:66:LEU:HD21	0.43	2.14	9	1
1:A:76:LEU:HD12	1:A:77:PRO:CD	0.42	2.44	11	1
1:A:19:LEU:HD22	1:A:52:LEU:CD1	0.42	2.35	12	1
1:A:94:TYR:O	1:A:98:ALA:CB	0.42	2.67	13	6
1:A:85:SER:O	1:A:86:ASP:CB	0.42	2.68	7	2
1:A:39:VAL:HG11	1:A:51:LEU:CD2	0.42	2.42	24	1
1:A:33:PHE:CE2	1:A:39:VAL:HG13	0.42	2.50	10	1
1:A:106:PHE:CD1	1:A:111:ALA:HB2	0.41	2.50	10	1
1:A:84:HIS:O	1:A:86:ASP:N	0.41	2.53	18	3
1:A:63:LEU:HD12	1:A:63:LEU:C	0.41	2.36	10	1
1:A:83:ALA:HB2	1:A:104:LYS:H	0.41	1.75	4	1
1:A:80:ILE:O	1:A:80:ILE:HG22	0.41	2.16	10	1
1:A:84:HIS:O	1:A:84:HIS:CG	0.41	2.73	13	1
1:A:48:PRO:O	1:A:76:LEU:HD13	0.41	2.15	12	1
1:A:6:VAL:HG11	1:A:52:LEU:HD11	0.41	1.91	3	1
1:A:82:THR:HG23	1:A:83:ALA:N	0.41	2.31	10	3
1:A:83:ALA:O	1:A:84:HIS:CD2	0.41	2.73	15	2
1:A:66:LEU:HD21	1:A:78:VAL:CG1	0.40	2.47	12	1
1:A:19:LEU:HD13	1:A:52:LEU:HD13	0.40	1.93	18	1
1:A:23:LEU:HD13	1:A:28:LEU:HB2	0.40	1.92	25	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	114/124 (92%)	93±3 (82±2%)	15±3 (13±2%)	6±2 (5±2%)	3	23
All	All	2850/3100 (92%)	2332 (82%)	367 (13%)	151 (5%)	3	23

All 16 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	82	THR	24
1	A	47	THR	21
1	A	84	HIS	18
1	A	86	ASP	14
1	A	55	ILE	14
1	A	85	SER	11
1	A	50	VAL	7
1	A	34	GLU	7
1	A	101	TYR	6
1	A	46	LYS	6
1	A	11	ASP	5
1	A	10	ASP	5
1	A	35	ASN	5
1	A	3	ARG	3
1	A	27	GLY	3
1	A	83	ALA	2

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	93/102 (91%)	70±3 (75±3%)	23±3 (25±3%)	2	25
All	All	2325/2550 (91%)	1754 (75%)	571 (25%)	2	25

All 55 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	13	SER	25
1	A	46	LYS	25
1	A	51	LEU	25
1	A	3	ARG	25
1	A	47	THR	24
1	A	28	LEU	24
1	A	63	LEU	22
1	A	66	LEU	22

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Mol	Chain	Res	Type	Models (Total)
1	A	12	ASP	20
1	A	101	TYR	20
1	A	86	ASP	18
1	A	104	LYS	18
1	A	11	ASP	17
1	A	82	THR	16
1	A	20	GLU	16
1	A	65	LEU	14
1	A	72	ARG	14
1	A	70	LYS	14
1	A	75	MET	14
1	A	67	LYS	12
1	A	88	ASP	12
1	A	71	GLN	11
1	A	49	ASP	10
1	A	68	GLN	10
1	A	85	SER	10
1	A	14	SER	9
1	A	35	ASN	9
1	A	52	LEU	8
1	A	110	GLU	8
1	A	30	CYS	7
1	A	117	ARG	7
1	A	81	MET	6
1	A	16	ARG	6
1	A	87	LEU	6
1	A	34	GLU	6
1	A	84	HIS	6
1	A	116	GLU	5
1	A	38	GLU	5
1	A	21	ARG	5
1	A	95	GLN	5
1	A	18	VAL	4
1	A	109	ASP	4
1	A	45	SER	4
1	A	92	SER	4
1	A	107	ASP	3
1	A	53	SER	3
1	A	10	ASP	3
1	A	54	ASP	2
1	A	19	LEU	2
1	A	100	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	120	SER	1
1	A	37	ASN	1
1	A	114	LEU	1
1	A	102	LEU	1
1	A	96	GLN	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 (i)

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: input_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	1557
Number of shifts mapped to atoms	1557
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	124	-0.03 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_\beta$	117	0.11 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	109	0.08 ± 0.12	None needed (< 0.5 ppm)
^{15}N	114	0.06 ± 0.38	None needed (< 0.5 ppm)

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 92%, i.e. 1249 atoms were assigned a chemical shift out of a possible 1353. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	545/560 (97%)	221/223 (99%)	217/228 (95%)	107/109 (98%)
Sidechain	617/697 (89%)	372/402 (93%)	239/270 (89%)	6/25 (24%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	87/96 (91%)	45/51 (88%)	40/40 (100%)	2/5 (40%)
Overall	1249/1353 (92%)	638/676 (94%)	496/538 (92%)	115/139 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1358 atoms were assigned a chemical shift out of a possible 1483. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	585/608 (96%)	238/242 (98%)	233/248 (94%)	114/118 (97%)
Sidechain	686/779 (88%)	417/452 (92%)	261/297 (88%)	8/30 (27%)
Aromatic	87/96 (91%)	45/51 (88%)	40/40 (100%)	2/5 (40%)
Overall	1358/1483 (92%)	700/745 (94%)	534/585 (91%)	124/153 (81%)

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	48	PRO	HB2	-0.34	$3.82 - 0.32$	-6.9
1	A	48	PRO	HD3	1.23	$5.52 - 1.72$	-6.3

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.

Random coil index (RCI) for chain A: