Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 10:22 pm BST

PDB ID	:	2K06
Title	:	Solution structure of the aminoterminal domain of E. coli NusG
Authors	:	Schweimer, K.; Scheckenhofer, U.; Roesch, P.
Deposited on	:	2008-01-25

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

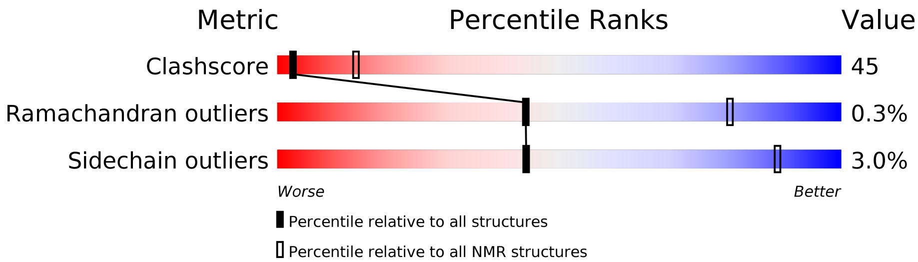
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	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 88%.

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	123	30% 36% • 32%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 6 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:7-A:44, A:67-A:112 (84)	0.34	6

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 2 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1981 atoms, of which 993 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription antitermination protein nusG.

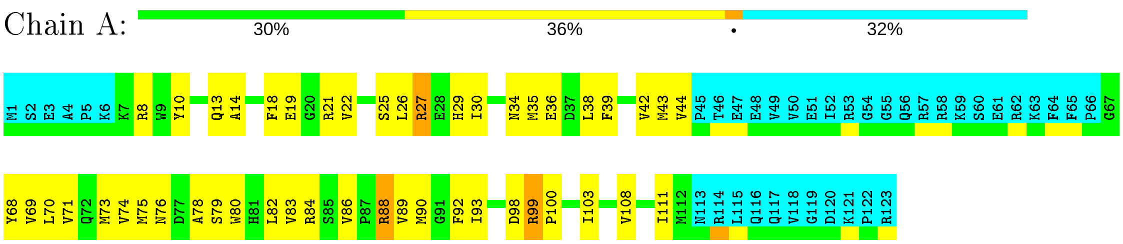
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	123	1981	622	993	182	177	7	0

4 Residue-property plots

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: Transcription antitermination protein nusG

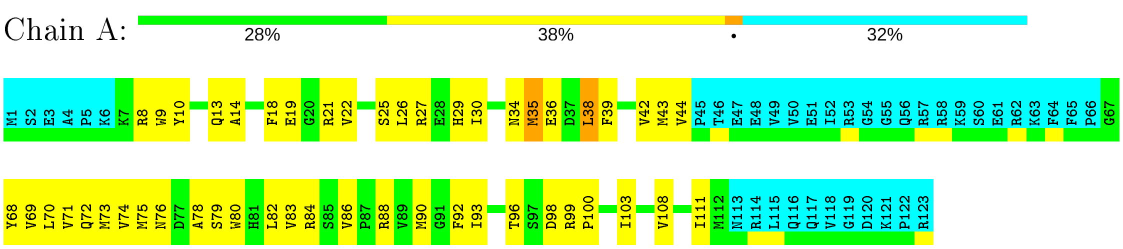


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

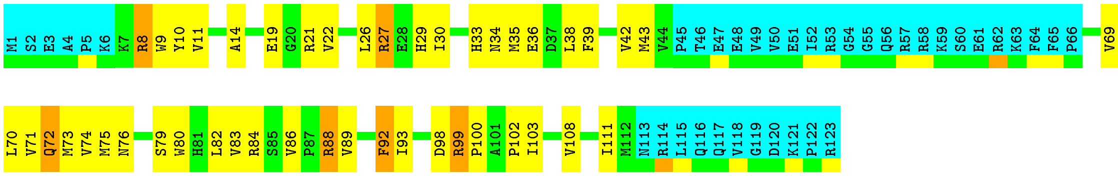
4.2.1 Score per residue for model 1

- Molecule 1: Transcription antitermination protein nusG



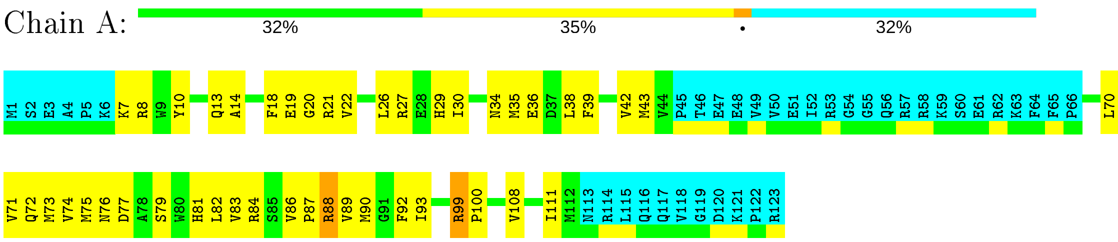
4.2.2 Score per residue for model 2

- Molecule 1: Transcription antitermination protein nusG



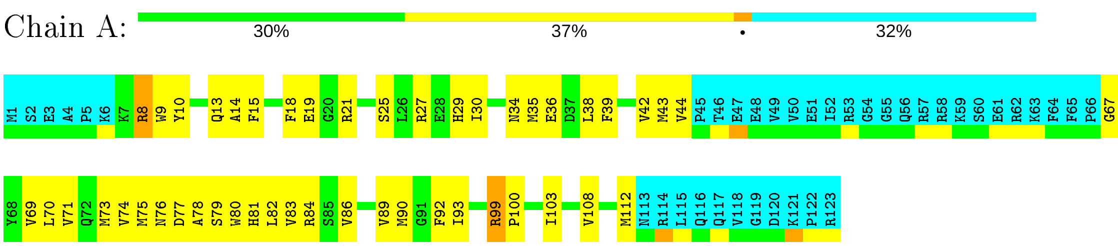
4.2.3 Score per residue for model 3

- Molecule 1: Transcription antitermination protein nusG



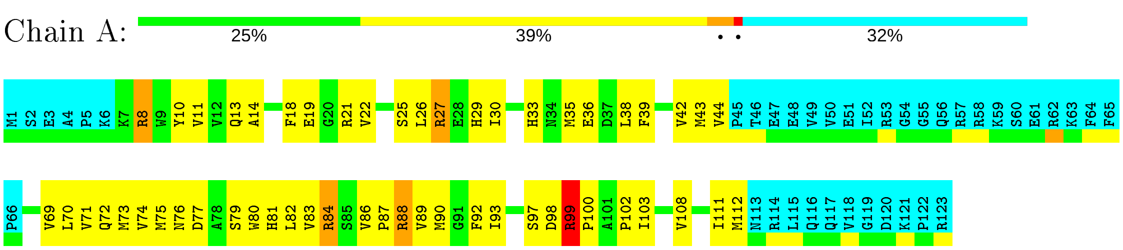
4.2.4 Score per residue for model 4

- Molecule 1: Transcription antitermination protein nusG



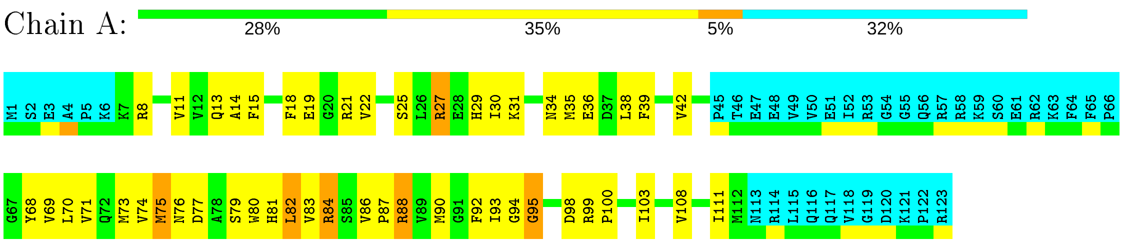
4.2.5 Score per residue for model 5

- Molecule 1: Transcription antitermination protein nusG



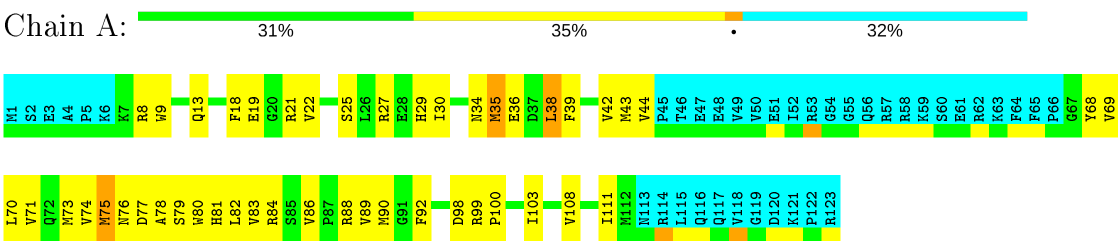
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Transcription antitermination protein nusG



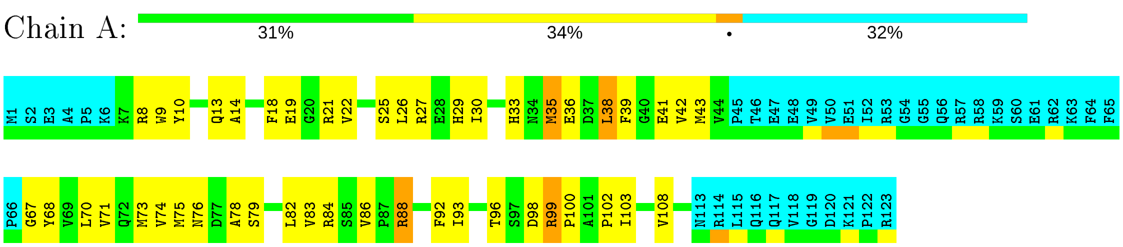
4.2.7 Score per residue for model 7

- Molecule 1: Transcription antitermination protein nusG



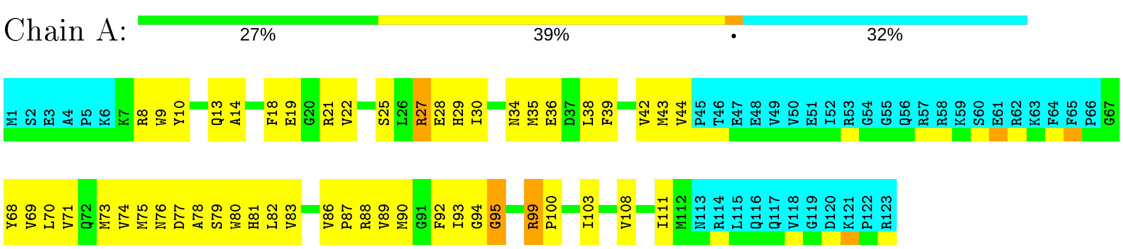
4.2.8 Score per residue for model 8

- Molecule 1: Transcription antitermination protein nusG



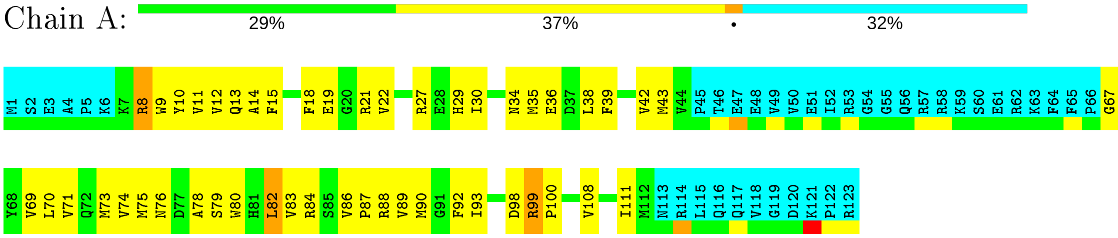
4.2.9 Score per residue for model 9

- Molecule 1: Transcription antitermination protein nusG



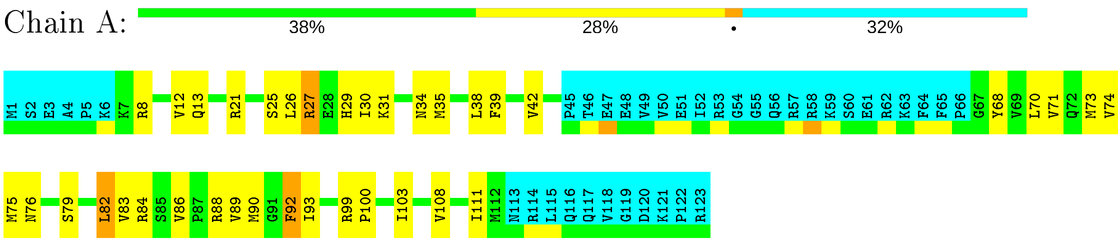
4.2.10 Score per residue for model 10

- Molecule 1: Transcription antitermination protein nusG



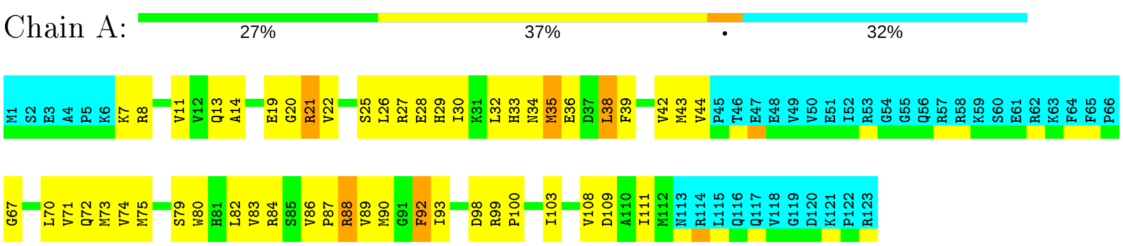
4.2.11 Score per residue for model 11

- Molecule 1: Transcription antitermination protein nusG



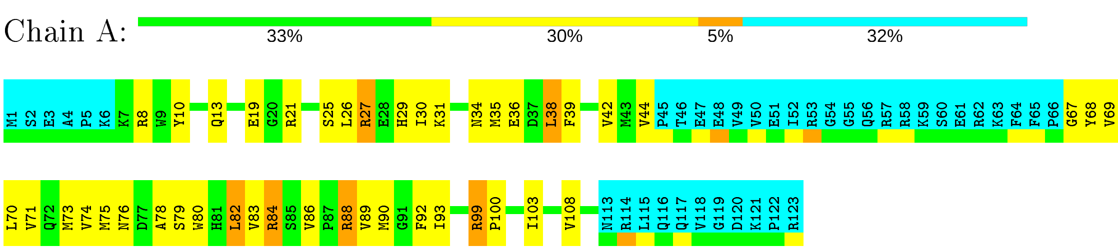
4.2.12 Score per residue for model 12

- Molecule 1: Transcription antitermination protein nusG



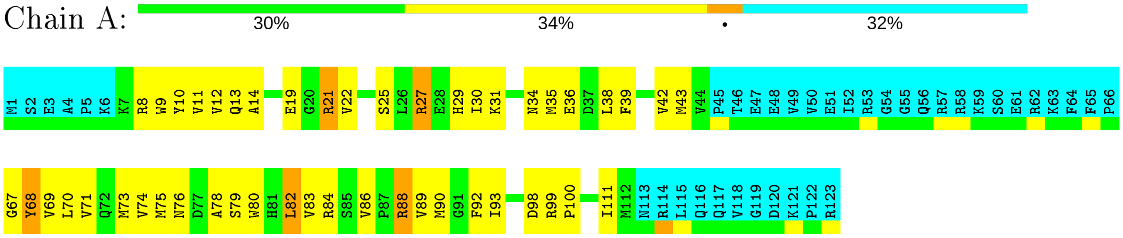
4.2.13 Score per residue for model 13

- Molecule 1: Transcription antitermination protein nusG



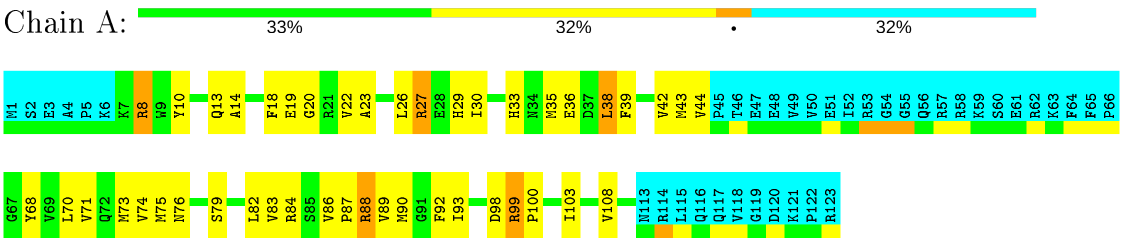
4.2.14 Score per residue for model 14

- Molecule 1: Transcription antitermination protein nusG



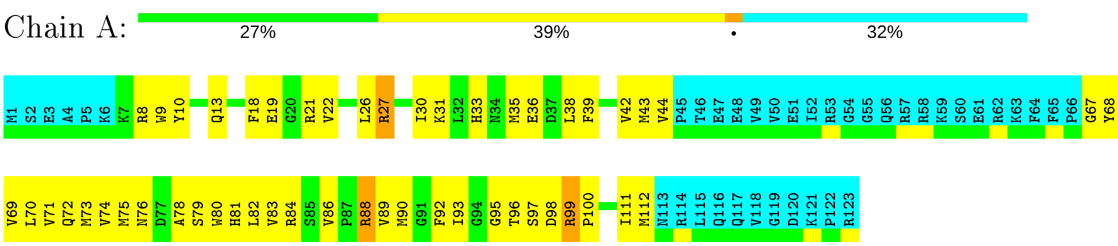
4.2.15 Score per residue for model 15

- Molecule 1: Transcription antitermination protein nusG



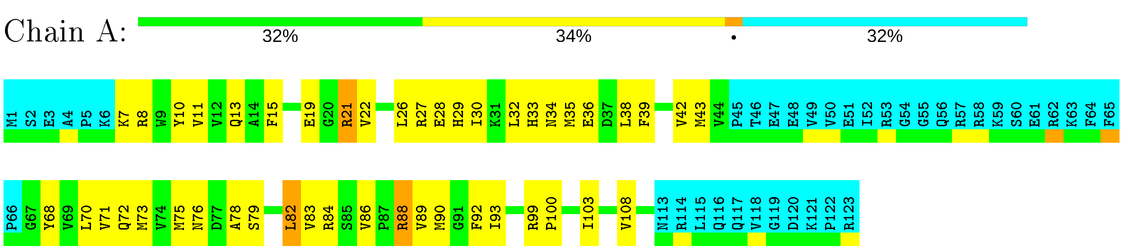
4.2.16 Score per residue for model 16

- Molecule 1: Transcription antitermination protein nusG



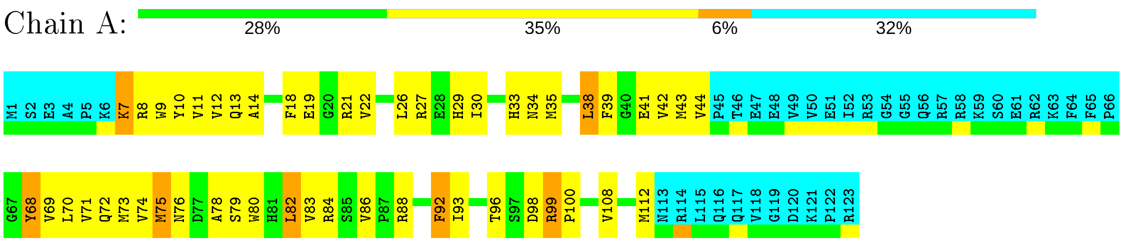
4.2.17 Score per residue for model 17

- Molecule 1: Transcription antitermination protein nusG



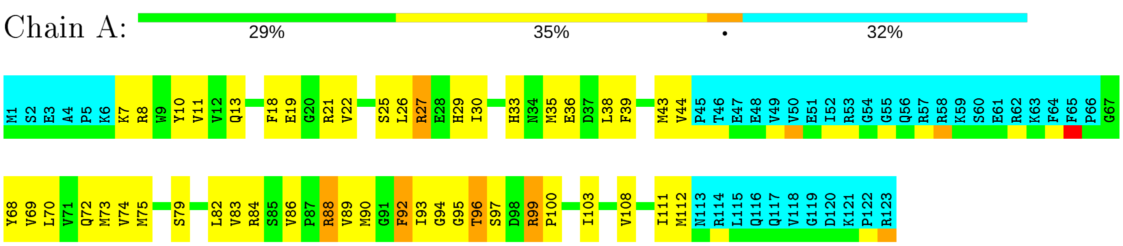
4.2.18 Score per residue for model 18

• Molecule 1: Transcription antitermination protein nusG



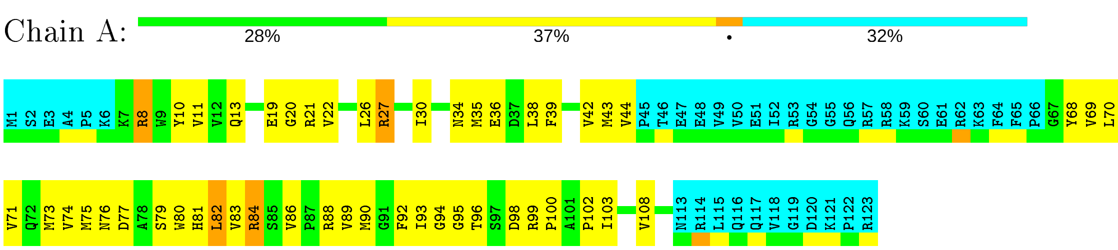
4.2.19 Score per residue for model 19

• Molecule 1: Transcription antitermination protein nusG



4.2.20 Score per residue for model 20

• Molecule 1: Transcription antitermination protein nusG



5 Refinement protocol and experimental data overview (i)

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

Of the 80 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
X-PLOR NIH	structure solution	
X-PLOR NIH	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	1410
Number of shifts mapped to atoms	1410
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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.

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	5.8±0.4
All	All	0	116

There are no bond-length outliers.

There are no bond-angle outliers.

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	8	ARG	Sidechain	20
1	A	99	ARG	Sidechain	20
1	A	88	ARG	Sidechain	19
1	A	21	ARG	Sidechain	19
1	A	27	ARG	Sidechain	19
1	A	84	ARG	Sidechain	19

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	666	662	662	60±7
All	All	13320	13240	13240	1206

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 45.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:LEU:HD21	1:A:111:ILE:HD12	1.08	1.18	11	9
1:A:42:VAL:HG23	1:A:71:VAL:HG22	1.06	1.20	7	3
1:A:42:VAL:HG13	1:A:71:VAL:HG22	1.01	1.33	8	16
1:A:83:VAL:HG21	1:A:92:PHE:CZ	0.96	1.94	3	16
1:A:30:ILE:HD12	1:A:39:PHE:CD1	0.96	1.95	16	6
1:A:38:LEU:HD13	1:A:79:SER:OG	0.92	1.63	12	6
1:A:30:ILE:HD12	1:A:39:PHE:CD2	0.92	1.98	8	1
1:A:83:VAL:HG11	1:A:92:PHE:CE2	0.90	2.01	2	10
1:A:13:GLN:CG	1:A:93:ILE:HD11	0.90	1.96	18	3
1:A:38:LEU:HD12	1:A:73:MET:SD	0.86	2.11	18	1
1:A:29:HIS:HB3	1:A:82:LEU:HD11	0.86	1.48	3	7
1:A:35:MET:HG3	1:A:82:LEU:HD13	0.86	1.47	11	8
1:A:83:VAL:CG1	1:A:89:VAL:HG11	0.84	2.02	10	2
1:A:42:VAL:HG22	1:A:71:VAL:HG13	0.84	1.47	8	7
1:A:11:VAL:HG11	1:A:93:ILE:HD12	0.83	1.47	5	3
1:A:33:HIS:CD2	1:A:82:LEU:HD11	0.83	2.08	5	4
1:A:70:LEU:CD2	1:A:111:ILE:HD12	0.82	2.02	11	2
1:A:11:VAL:CG1	1:A:93:ILE:HD12	0.82	2.05	19	4
1:A:23:ALA:HB1	1:A:42:VAL:HG11	0.82	1.46	15	1
1:A:33:HIS:CG	1:A:82:LEU:HD11	0.82	2.09	5	1
1:A:26:LEU:HD23	1:A:86:VAL:HG21	0.82	1.50	11	6
1:A:26:LEU:CD2	1:A:86:VAL:HG21	0.81	2.06	11	6
1:A:26:LEU:HD12	1:A:86:VAL:HG21	0.81	1.53	17	2
1:A:70:LEU:CD2	1:A:108:VAL:HG13	0.81	2.06	17	9
1:A:26:LEU:CD1	1:A:86:VAL:HG21	0.80	2.05	17	1
1:A:13:GLN:HB2	1:A:93:ILE:HD11	0.80	1.53	4	11
1:A:83:VAL:HG21	1:A:92:PHE:CE2	0.80	2.10	3	11
1:A:30:ILE:HD13	1:A:39:PHE:CD2	0.79	2.12	3	3
1:A:22:VAL:HG13	1:A:86:VAL:HG11	0.79	1.53	20	3
1:A:70:LEU:HD22	1:A:70:LEU:N	0.79	1.93	4	1
1:A:18:PHE:O	1:A:22:VAL:HG23	0.79	1.77	8	10
1:A:43:MET:O	1:A:69:VAL:HG13	0.78	1.78	18	11
1:A:70:LEU:HD12	1:A:70:LEU:N	0.78	1.93	11	8
1:A:70:LEU:N	1:A:70:LEU:HD12	0.78	1.93	15	9
1:A:70:LEU:HD21	1:A:111:ILE:CD1	0.78	2.07	11	3
1:A:11:VAL:HB	1:A:93:ILE:HD12	0.77	1.54	19	2
1:A:30:ILE:HG23	1:A:35:MET:HB2	0.77	1.55	17	9
1:A:11:VAL:CB	1:A:93:ILE:HD12	0.77	2.10	19	2
1:A:13:GLN:CD	1:A:93:ILE:HD11	0.76	1.99	11	3
1:A:70:LEU:N	1:A:70:LEU:HD22	0.76	1.94	12	2
1:A:38:LEU:HB2	1:A:74:VAL:HG12	0.76	1.57	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LEU:HD12	1:A:73:MET:CG	0.75	2.12	7	3
1:A:26:LEU:HD12	1:A:86:VAL:CG2	0.74	2.12	17	1
1:A:42:VAL:CG1	1:A:71:VAL:HG22	0.74	2.11	8	2
1:A:35:MET:HG3	1:A:82:LEU:HD22	0.74	1.58	9	6
1:A:83:VAL:HG21	1:A:92:PHE:HZ	0.73	1.43	13	9
1:A:103:ILE:HD11	1:A:108:VAL:CG2	0.73	2.14	6	14
1:A:82:LEU:O	1:A:86:VAL:HG23	0.73	1.84	6	5
1:A:103:ILE:HD11	1:A:108:VAL:HG22	0.72	1.60	6	12
1:A:42:VAL:HG23	1:A:71:VAL:CG2	0.72	2.12	1	3
1:A:30:ILE:HD13	1:A:39:PHE:CD1	0.72	2.20	12	6
1:A:30:ILE:HD12	1:A:39:PHE:CE1	0.72	2.20	5	6
1:A:26:LEU:CD2	1:A:30:ILE:HD11	0.71	2.15	16	2
1:A:30:ILE:HD13	1:A:39:PHE:CG	0.71	2.21	3	6
1:A:44:VAL:HG13	1:A:44:VAL:O	0.71	1.85	4	1
1:A:38:LEU:HD11	1:A:39:PHE:CE2	0.70	2.21	8	1
1:A:35:MET:SD	1:A:82:LEU:HD22	0.70	2.27	1	3
1:A:28:GLU:O	1:A:32:LEU:HD12	0.69	1.86	12	2
1:A:38:LEU:HD12	1:A:73:MET:HG3	0.69	1.64	7	2
1:A:30:ILE:HD12	1:A:39:PHE:CE2	0.69	2.23	8	1
1:A:15:PHE:CD2	1:A:18:PHE:CD2	0.69	2.81	10	2
1:A:29:HIS:HB3	1:A:82:LEU:HD21	0.68	1.64	8	1
1:A:70:LEU:HD23	1:A:108:VAL:HG13	0.68	1.65	1	7
1:A:14:ALA:HB1	1:A:22:VAL:HG21	0.68	1.64	15	9
1:A:35:MET:HB3	1:A:38:LEU:HD12	0.68	1.65	20	8
1:A:35:MET:CG	1:A:38:LEU:HD21	0.68	2.19	8	2
1:A:38:LEU:HD13	1:A:79:SER:HB3	0.67	1.66	16	2
1:A:75:MET:HE1	1:A:100:PRO:HG2	0.67	1.65	6	3
1:A:42:VAL:HG13	1:A:71:VAL:CG2	0.67	2.17	8	6
1:A:39:PHE:CZ	1:A:82:LEU:HD22	0.66	2.26	18	8
1:A:30:ILE:CD1	1:A:39:PHE:CE1	0.64	2.81	5	7
1:A:43:MET:HE1	1:A:108:VAL:HG11	0.64	1.68	8	4
1:A:83:VAL:HG13	1:A:89:VAL:HG11	0.64	1.67	10	2
1:A:29:HIS:NE2	1:A:86:VAL:HG23	0.64	2.07	10	1
1:A:26:LEU:HD21	1:A:30:ILE:HD11	0.64	1.69	16	1
1:A:83:VAL:HG11	1:A:92:PHE:CZ	0.64	2.27	19	3
1:A:9:TRP:CB	1:A:108:VAL:HG21	0.63	2.23	1	2
1:A:30:ILE:CD1	1:A:39:PHE:CD2	0.63	2.81	3	4
1:A:86:VAL:O	1:A:89:VAL:HG12	0.63	1.94	14	9
1:A:33:HIS:CD2	1:A:82:LEU:CD1	0.63	2.82	16	4
1:A:9:TRP:CG	1:A:108:VAL:HG21	0.63	2.29	1	4
1:A:68:TYR:OH	1:A:93:ILE:HG21	0.63	1.94	15	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:HIS:CD2	1:A:82:LEU:N	0.62	2.67	16	1
1:A:30:ILE:CD1	1:A:39:PHE:CD1	0.62	2.82	12	10
1:A:75:MET:HE2	1:A:100:PRO:CG	0.62	2.24	2	2
1:A:10:TYR:CE2	1:A:75:MET:CG	0.62	2.83	5	2
1:A:10:TYR:CZ	1:A:75:MET:CG	0.61	2.82	2	3
1:A:29:HIS:CB	1:A:82:LEU:HD11	0.61	2.25	12	4
1:A:73:MET:HE2	1:A:79:SER:HB3	0.61	1.70	9	1
1:A:30:ILE:HG22	1:A:36:GLU:HG3	0.61	1.73	7	4
1:A:30:ILE:HG23	1:A:35:MET:CB	0.61	2.26	1	8
1:A:80:TRP:NE1	1:A:92:PHE:CE2	0.61	2.68	16	1
1:A:25:SER:HB2	1:A:86:VAL:HG13	0.61	1.73	11	1
1:A:33:HIS:CD2	1:A:82:LEU:HD12	0.61	2.30	18	2
1:A:26:LEU:HD13	1:A:86:VAL:HG21	0.60	1.70	2	2
1:A:35:MET:HG3	1:A:38:LEU:HD21	0.60	1.73	7	2
1:A:30:ILE:CD1	1:A:39:PHE:CE2	0.58	2.86	8	2
1:A:92:PHE:O	1:A:96:THR:HG22	0.58	1.98	16	1
1:A:70:LEU:N	1:A:70:LEU:CD1	0.58	2.67	15	8
1:A:29:HIS:CD2	1:A:86:VAL:HG22	0.58	2.34	18	5
1:A:19:GLU:OE2	1:A:69:VAL:HG23	0.58	1.99	2	1
1:A:86:VAL:HB	1:A:89:VAL:HG21	0.58	1.76	7	3
1:A:77:ASP:O	1:A:81:HIS:CD2	0.58	2.57	9	7
1:A:70:LEU:CD2	1:A:70:LEU:N	0.58	2.67	12	3
1:A:19:GLU:CG	1:A:69:VAL:CG2	0.58	2.81	16	3
1:A:75:MET:CE	1:A:100:PRO:CG	0.57	2.82	16	7
1:A:39:PHE:CZ	1:A:73:MET:SD	0.57	2.97	15	15
1:A:29:HIS:NE2	1:A:86:VAL:CG2	0.57	2.67	15	2
1:A:75:MET:HE3	1:A:100:PRO:HG2	0.57	1.76	13	3
1:A:30:ILE:CG2	1:A:36:GLU:N	0.57	2.67	12	14
1:A:30:ILE:HG22	1:A:36:GLU:CG	0.57	2.28	2	4
1:A:25:SER:O	1:A:29:HIS:CD2	0.57	2.57	19	11
1:A:9:TRP:CE2	1:A:72:GLN:OE1	0.57	2.57	1	1
1:A:70:LEU:CD1	1:A:70:LEU:N	0.57	2.67	18	9
1:A:30:ILE:HG23	1:A:35:MET:C	0.57	2.20	9	7
1:A:39:PHE:CE1	1:A:73:MET:SD	0.57	2.98	1	5
1:A:39:PHE:CE2	1:A:82:LEU:HD22	0.57	2.35	14	2
1:A:22:VAL:HG21	1:A:88:ARG:O	0.57	1.99	19	2
1:A:39:PHE:CE2	1:A:73:MET:SD	0.56	2.98	2	10
1:A:10:TYR:CG	1:A:75:MET:SD	0.56	2.98	10	3
1:A:75:MET:HE3	1:A:100:PRO:HG3	0.56	1.77	9	2
1:A:11:VAL:CG1	1:A:68:TYR:CE1	0.56	2.88	17	1
1:A:10:TYR:CE2	1:A:73:MET:O	0.56	2.58	3	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLN:HG3	1:A:93:ILE:HD11	0.56	1.74	11	2
1:A:70:LEU:HD21	1:A:111:ILE:HG13	0.56	1.78	16	1
1:A:81:HIS:C	1:A:81:HIS:CD2	0.56	2.78	16	1
1:A:35:MET:CE	1:A:38:LEU:CD1	0.56	2.83	20	7
1:A:38:LEU:HD22	1:A:76:ASN:ND2	0.56	2.16	6	4
1:A:83:VAL:CG1	1:A:92:PHE:CE2	0.56	2.87	19	4
1:A:39:PHE:CE1	1:A:82:LEU:HD22	0.56	2.36	11	5
1:A:70:LEU:HD12	1:A:70:LEU:H	0.56	1.58	2	1
1:A:10:TYR:CE2	1:A:75:MET:SD	0.56	2.99	2	2
1:A:18:PHE:CB	1:A:22:VAL:HG23	0.56	2.31	10	1
1:A:33:HIS:CD2	1:A:82:LEU:HD13	0.55	2.36	2	2
1:A:44:VAL:O	1:A:44:VAL:HG12	0.55	2.01	18	2
1:A:39:PHE:CZ	1:A:82:LEU:CD2	0.55	2.90	11	6
1:A:26:LEU:HD23	1:A:86:VAL:CG2	0.55	2.30	11	2
1:A:44:VAL:HG23	1:A:69:VAL:HG22	0.55	1.79	4	1
1:A:10:TYR:CE1	1:A:73:MET:O	0.55	2.60	5	2
1:A:10:TYR:CE1	1:A:100:PRO:O	0.55	2.59	15	2
1:A:10:TYR:CD2	1:A:75:MET:SD	0.55	2.99	2	3
1:A:70:LEU:HD22	1:A:108:VAL:HG13	0.55	1.77	5	5
1:A:13:GLN:NE2	1:A:93:ILE:HD11	0.55	2.17	12	3
1:A:11:VAL:HG13	1:A:68:TYR:CE1	0.55	2.37	17	1
1:A:75:MET:HE3	1:A:100:PRO:CG	0.55	2.31	9	4
1:A:35:MET:HB3	1:A:38:LEU:HD21	0.55	1.79	18	1
1:A:9:TRP:CH2	1:A:43:MET:SD	0.54	3.00	4	1
1:A:25:SER:CB	1:A:86:VAL:HG13	0.54	2.32	11	1
1:A:35:MET:CG	1:A:38:LEU:CD1	0.54	2.86	1	2
1:A:26:LEU:C	1:A:26:LEU:HD23	0.54	2.23	16	1
1:A:26:LEU:HD21	1:A:39:PHE:CE1	0.54	2.38	3	1
1:A:103:ILE:CD1	1:A:108:VAL:CG2	0.54	2.86	12	2
1:A:10:TYR:CZ	1:A:75:MET:HG2	0.53	2.38	5	5
1:A:10:TYR:CD2	1:A:75:MET:HE2	0.53	2.38	4	1
1:A:76:ASN:OD1	1:A:79:SER:CB	0.53	2.57	17	9
1:A:75:MET:HE2	1:A:100:PRO:HG2	0.53	1.78	2	3
1:A:30:ILE:CD1	1:A:39:PHE:CG	0.53	2.92	3	4
1:A:96:THR:HG23	1:A:98:ASP:H	0.53	1.63	1	2
1:A:10:TYR:CD1	1:A:75:MET:SD	0.53	3.02	10	2
1:A:73:MET:CE	1:A:79:SER:OG	0.53	2.56	15	1
1:A:29:HIS:CB	1:A:82:LEU:HD21	0.53	2.34	8	1
1:A:86:VAL:O	1:A:89:VAL:CG1	0.53	2.57	19	9
1:A:80:TRP:NE1	1:A:98:ASP:O	0.53	2.42	2	6
1:A:74:VAL:O	1:A:74:VAL:HG23	0.53	2.03	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:VAL:CG2	1:A:88:ARG:O	0.53	2.57	19	2
1:A:73:MET:CG	1:A:74:VAL:N	0.53	2.72	3	8
1:A:38:LEU:CD1	1:A:39:PHE:CD2	0.53	2.92	8	1
1:A:38:LEU:HD22	1:A:74:VAL:CG1	0.53	2.34	16	1
1:A:96:THR:OG1	1:A:97:SER:N	0.53	2.42	19	1
1:A:76:ASN:OD1	1:A:79:SER:N	0.52	2.42	14	12
1:A:43:MET:HE2	1:A:70:LEU:HB2	0.52	1.80	12	1
1:A:19:GLU:OE2	1:A:69:VAL:HG22	0.52	2.04	16	3
1:A:19:GLU:OE2	1:A:69:VAL:CG2	0.52	2.57	2	2
1:A:76:ASN:O	1:A:80:TRP:CB	0.52	2.58	5	4
1:A:75:MET:SD	1:A:100:PRO:CG	0.52	2.98	8	6
1:A:7:LYS:CB	1:A:72:GLN:OE1	0.52	2.57	19	4
1:A:44:VAL:O	1:A:44:VAL:CG1	0.52	2.58	4	1
1:A:76:ASN:ND2	1:A:78:ALA:HB3	0.52	2.19	17	5
1:A:80:TRP:CH2	1:A:84:ARG:CZ	0.52	2.93	5	1
1:A:38:LEU:CB	1:A:74:VAL:HG12	0.52	2.32	7	2
1:A:19:GLU:OE2	1:A:67:GLY:N	0.52	2.43	10	2
1:A:30:ILE:O	1:A:34:ASN:N	0.52	2.43	12	15
1:A:30:ILE:HG13	1:A:82:LEU:HD21	0.52	1.82	13	2
1:A:38:LEU:HD11	1:A:39:PHE:CD2	0.52	2.40	8	1
1:A:19:GLU:CG	1:A:20:GLY:N	0.51	2.72	20	4
1:A:8:ARG:NE	1:A:10:TYR:OH	0.51	2.43	4	2
1:A:35:MET:SD	1:A:82:LEU:CD2	0.51	2.98	15	1
1:A:35:MET:HE1	1:A:38:LEU:CD1	0.51	2.35	2	3
1:A:83:VAL:CG2	1:A:92:PHE:CE2	0.51	2.92	3	3
1:A:80:TRP:CZ2	1:A:84:ARG:HD2	0.51	2.40	13	2
1:A:43:MET:N	1:A:70:LEU:O	0.51	2.43	18	2
1:A:19:GLU:OE2	1:A:68:TYR:N	0.51	2.43	14	1
1:A:31:LYS:CD	1:A:36:GLU:OE2	0.51	2.59	16	1
1:A:9:TRP:NE1	1:A:72:GLN:OE1	0.51	2.44	1	1
1:A:75:MET:CE	1:A:100:PRO:HG2	0.51	2.36	10	15
1:A:68:TYR:OH	1:A:93:ILE:CG2	0.51	2.59	6	3
1:A:75:MET:CE	1:A:100:PRO:HG3	0.51	2.36	16	2
1:A:87:PRO:O	1:A:89:VAL:HG23	0.51	2.05	10	3
1:A:78:ALA:HA	1:A:81:HIS:CE1	0.51	2.40	16	1
1:A:44:VAL:HG12	1:A:44:VAL:O	0.51	2.05	16	1
1:A:26:LEU:HD21	1:A:39:PHE:CE2	0.50	2.41	12	2
1:A:30:ILE:HG12	1:A:39:PHE:CE1	0.50	2.41	6	7
1:A:94:GLY:O	1:A:96:THR:N	0.50	2.44	19	2
1:A:35:MET:HG2	1:A:38:LEU:CD1	0.50	2.37	12	2
1:A:18:PHE:O	1:A:22:VAL:CG2	0.50	2.57	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLN:CG	1:A:90:MET:SD	0.50	2.99	16	2
1:A:13:GLN:O	1:A:89:VAL:HG23	0.50	2.05	12	2
1:A:43:MET:CE	1:A:112:MET:SD	0.50	2.99	5	3
1:A:29:HIS:CD2	1:A:86:VAL:HB	0.50	2.41	10	4
1:A:39:PHE:CD1	1:A:73:MET:HB2	0.50	2.42	8	2
1:A:35:MET:HE3	1:A:78:ALA:HB1	0.50	1.83	8	2
1:A:9:TRP:CZ3	1:A:43:MET:HG2	0.50	2.42	14	5
1:A:80:TRP:CD1	1:A:92:PHE:CE2	0.50	3.00	16	1
1:A:69:VAL:C	1:A:70:LEU:HD12	0.50	2.28	18	3
1:A:73:MET:SD	1:A:79:SER:CB	0.50	3.00	17	2
1:A:86:VAL:HG13	1:A:89:VAL:HG21	0.49	1.83	3	2
1:A:73:MET:HG2	1:A:74:VAL:N	0.49	2.22	3	15
1:A:12:VAL:HG22	1:A:92:PHE:CE1	0.49	2.42	18	2
1:A:38:LEU:CD1	1:A:39:PHE:CE2	0.49	2.94	8	1
1:A:43:MET:CE	1:A:112:MET:CE	0.49	2.89	16	1
1:A:30:ILE:HG12	1:A:39:PHE:CE2	0.49	2.43	9	5
1:A:79:SER:OG	1:A:80:TRP:N	0.49	2.46	1	2
1:A:75:MET:HE1	1:A:92:PHE:CE1	0.49	2.43	14	1
1:A:89:VAL:O	1:A:89:VAL:HG13	0.49	2.07	16	3
1:A:22:VAL:HG13	1:A:86:VAL:CG1	0.49	2.34	20	1
1:A:76:ASN:HD21	1:A:78:ALA:HB3	0.49	1.67	17	1
1:A:43:MET:SD	1:A:108:VAL:CG1	0.49	3.01	5	1
1:A:8:ARG:HB2	1:A:10:TYR:CE1	0.49	2.43	10	2
1:A:68:TYR:CZ	1:A:93:ILE:HG21	0.49	2.43	20	2
1:A:10:TYR:CE2	1:A:75:MET:HG2	0.49	2.43	16	2
1:A:35:MET:CE	1:A:78:ALA:HB1	0.49	2.38	1	3
1:A:19:GLU:HG2	1:A:69:VAL:CG2	0.49	2.37	6	1
1:A:83:VAL:HG12	1:A:89:VAL:HG11	0.49	1.82	10	1
1:A:43:MET:CE	1:A:108:VAL:HG11	0.48	2.38	3	2
1:A:42:VAL:CG2	1:A:71:VAL:HG22	0.48	2.15	7	2
1:A:80:TRP:CD1	1:A:98:ASP:O	0.48	2.67	2	2
1:A:80:TRP:CZ2	1:A:98:ASP:HB3	0.48	2.43	16	1
1:A:43:MET:SD	1:A:108:VAL:HG11	0.48	2.48	5	1
1:A:70:LEU:HD23	1:A:108:VAL:HG22	0.48	1.84	10	1
1:A:33:HIS:NE2	1:A:82:LEU:CD1	0.48	2.77	15	1
1:A:19:GLU:HG3	1:A:20:GLY:N	0.48	2.22	20	3
1:A:30:ILE:CG2	1:A:36:GLU:HA	0.48	2.39	5	3
1:A:13:GLN:OE1	1:A:90:MET:CE	0.48	2.61	9	1
1:A:80:TRP:CH2	1:A:84:ARG:HD2	0.48	2.44	20	1
1:A:10:TYR:CZ	1:A:75:MET:HB2	0.48	2.43	17	1
1:A:43:MET:HE1	1:A:108:VAL:CG1	0.48	2.37	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLN:CG	1:A:93:ILE:CD1	0.48	2.85	18	2
1:A:30:ILE:CG2	1:A:35:MET:C	0.48	2.82	1	2
1:A:43:MET:O	1:A:69:VAL:CG1	0.47	2.60	4	2
1:A:8:ARG:HD3	1:A:102:PRO:CB	0.47	2.39	5	3
1:A:70:LEU:H	1:A:70:LEU:HD22	0.47	1.68	4	1
1:A:10:TYR:CE2	1:A:75:MET:HG3	0.47	2.43	10	2
1:A:43:MET:O	1:A:44:VAL:HG23	0.47	2.10	9	1
1:A:25:SER:OG	1:A:86:VAL:HG13	0.47	2.09	19	1
1:A:29:HIS:NE2	1:A:87:PRO:HD2	0.47	2.25	6	1
1:A:97:SER:O	1:A:98:ASP:OD1	0.47	2.33	5	1
1:A:26:LEU:HD23	1:A:26:LEU:O	0.47	2.09	16	1
1:A:88:ARG:CZ	1:A:88:ARG:HB2	0.47	2.39	13	1
1:A:11:VAL:HG22	1:A:68:TYR:OH	0.47	2.10	17	1
1:A:18:PHE:CG	1:A:88:ARG:HD3	0.47	2.44	8	1
1:A:35:MET:HB3	1:A:39:PHE:CE1	0.47	2.45	15	1
1:A:11:VAL:HG11	1:A:93:ILE:CD1	0.47	2.36	17	1
1:A:42:VAL:HG22	1:A:71:VAL:CG1	0.46	2.30	8	1
1:A:38:LEU:CD2	1:A:76:ASN:ND2	0.46	2.79	6	1
1:A:13:GLN:HG2	1:A:93:ILE:HD11	0.46	1.86	12	2
1:A:43:MET:O	1:A:44:VAL:CG2	0.46	2.64	9	1
1:A:92:PHE:CD1	1:A:100:PRO:HG3	0.46	2.45	15	2
1:A:11:VAL:CG1	1:A:93:ILE:CD1	0.46	2.91	17	2
1:A:30:ILE:HG22	1:A:36:GLU:N	0.46	2.26	19	3
1:A:35:MET:CG	1:A:38:LEU:HD12	0.46	2.40	12	2
1:A:35:MET:CA	1:A:38:LEU:HD12	0.46	2.40	15	1
1:A:13:GLN:CG	1:A:90:MET:HB2	0.46	2.40	7	9
1:A:19:GLU:OE2	1:A:68:TYR:O	0.46	2.34	1	7
1:A:38:LEU:CD1	1:A:73:MET:CG	0.46	2.94	8	1
1:A:33:HIS:NE2	1:A:82:LEU:HD11	0.46	2.26	15	1
1:A:10:TYR:CD1	1:A:75:MET:HE3	0.46	2.45	16	1
1:A:30:ILE:CG1	1:A:82:LEU:HD21	0.46	2.41	18	2
1:A:11:VAL:O	1:A:92:PHE:CD1	0.46	2.68	14	1
1:A:25:SER:OG	1:A:29:HIS:NE2	0.46	2.43	14	1
1:A:73:MET:SD	1:A:79:SER:OG	0.46	2.74	14	2
1:A:68:TYR:CE2	1:A:93:ILE:HD13	0.46	2.45	19	1
1:A:9:TRP:CH2	1:A:43:MET:HG3	0.46	2.45	2	1
1:A:29:HIS:NE2	1:A:86:VAL:HB	0.46	2.26	15	1
1:A:76:ASN:O	1:A:80:TRP:HB2	0.46	2.11	5	4
1:A:35:MET:HB3	1:A:39:PHE:CD1	0.46	2.45	15	1
1:A:73:MET:SD	1:A:74:VAL:O	0.45	2.74	9	4
1:A:76:ASN:OD1	1:A:79:SER:OG	0.45	2.33	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:VAL:CG1	1:A:93:ILE:HB	0.45	2.41	10	4
1:A:9:TRP:CZ2	1:A:72:GLN:NE2	0.45	2.84	2	1
1:A:11:VAL:HG12	1:A:12:VAL:N	0.45	2.26	10	1
1:A:83:VAL:HG11	1:A:92:PHE:CE1	0.45	2.46	16	1
1:A:35:MET:CB	1:A:38:LEU:HD21	0.45	2.40	18	1
1:A:27:ARG:HA	1:A:30:ILE:HD12	0.45	1.88	9	1
1:A:36:GLU:O	1:A:39:PHE:O	0.45	2.34	3	8
1:A:13:GLN:OE1	1:A:90:MET:SD	0.45	2.74	9	1
1:A:73:MET:HE2	1:A:79:SER:HB2	0.45	1.89	17	1
1:A:7:LYS:HB3	1:A:72:GLN:OE1	0.45	2.11	19	3
1:A:11:VAL:CG1	1:A:12:VAL:N	0.45	2.80	10	1
1:A:80:TRP:CD1	1:A:92:PHE:CZ	0.45	3.04	16	1
1:A:35:MET:SD	1:A:38:LEU:CD1	0.45	3.05	19	1
1:A:14:ALA:N	1:A:67:GLY:O	0.45	2.49	4	3
1:A:79:SER:O	1:A:83:VAL:HG23	0.45	2.12	19	2
1:A:25:SER:OG	1:A:86:VAL:CG1	0.45	2.65	19	1
1:A:89:VAL:HG13	1:A:89:VAL:O	0.44	2.11	4	3
1:A:27:ARG:O	1:A:31:LYS:HB2	0.44	2.13	6	1
1:A:13:GLN:NE2	1:A:90:MET:SD	0.44	2.90	1	2
1:A:10:TYR:CE1	1:A:75:MET:SD	0.44	3.11	10	1
1:A:33:HIS:CB	1:A:35:MET:SD	0.44	3.06	12	1
1:A:38:LEU:H	1:A:38:LEU:HD23	0.44	1.72	18	1
1:A:13:GLN:HG3	1:A:93:ILE:CG1	0.44	2.42	19	1
1:A:15:PHE:CD1	1:A:88:ARG:HA	0.44	2.48	17	1
1:A:43:MET:CE	1:A:108:VAL:CG1	0.44	2.95	12	1
1:A:35:MET:CE	1:A:38:LEU:HD12	0.44	2.43	16	1
1:A:30:ILE:CG2	1:A:36:GLU:CA	0.44	2.96	2	3
1:A:75:MET:HA	1:A:75:MET:HE3	0.44	1.89	7	1
1:A:41:GLU:OE1	1:A:41:GLU:N	0.44	2.50	18	1
1:A:73:MET:SD	1:A:79:SER:HB2	0.44	2.53	18	2
1:A:15:PHE:CD2	1:A:18:PHE:CE2	0.44	3.06	4	1
1:A:10:TYR:CE1	1:A:102:PRO:HA	0.44	2.47	8	1
1:A:27:ARG:O	1:A:31:LYS:CB	0.44	2.66	13	2
1:A:30:ILE:CG2	1:A:36:GLU:CD	0.44	2.86	8	1
1:A:78:ALA:HA	1:A:81:HIS:ND1	0.44	2.28	16	1
1:A:26:LEU:HD13	1:A:86:VAL:CG2	0.44	2.43	2	1
1:A:103:ILE:CD1	1:A:108:VAL:HG23	0.44	2.43	12	1
1:A:43:MET:HE2	1:A:70:LEU:CB	0.44	2.43	12	1
1:A:21:ARG:NH2	1:A:88:ARG:HG3	0.44	2.27	14	1
1:A:18:PHE:HB3	1:A:22:VAL:HG23	0.43	1.91	10	1
1:A:11:VAL:HG22	1:A:70:LEU:CD1	0.43	2.43	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:VAL:O	1:A:86:VAL:HG23	0.43	2.13	19	1
1:A:75:MET:HE3	1:A:75:MET:HA	0.43	1.89	20	1
1:A:10:TYR:CZ	1:A:75:MET:SD	0.43	3.12	2	1
1:A:73:MET:CE	1:A:79:SER:HB3	0.43	2.43	13	2
1:A:12:VAL:O	1:A:13:GLN:C	0.43	2.56	10	1
1:A:73:MET:CE	1:A:79:SER:HB2	0.43	2.43	17	1
1:A:80:TRP:CZ2	1:A:98:ASP:HA	0.43	2.48	20	4
1:A:75:MET:SD	1:A:100:PRO:HG2	0.43	2.52	14	3
1:A:9:TRP:CZ3	1:A:43:MET:HE2	0.43	2.49	2	1
1:A:26:LEU:O	1:A:29:HIS:N	0.43	2.52	5	2
1:A:13:GLN:OE1	1:A:68:TYR:CZ	0.43	2.71	7	1
1:A:41:GLU:HG3	1:A:42:VAL:N	0.43	2.29	8	1
1:A:30:ILE:HG23	1:A:35:MET:CA	0.43	2.44	10	1
1:A:13:GLN:CD	1:A:93:ILE:CD1	0.43	2.84	12	1
1:A:98:ASP:C	1:A:98:ASP:OD1	0.43	2.57	15	2
1:A:13:GLN:HG3	1:A:90:MET:SD	0.43	2.54	16	1
1:A:79:SER:O	1:A:80:TRP:C	0.43	2.57	1	6
1:A:11:VAL:HG11	1:A:68:TYR:CE2	0.43	2.49	18	1
1:A:9:TRP:CZ2	1:A:72:GLN:OE1	0.43	2.72	1	1
1:A:9:TRP:CZ3	1:A:43:MET:CE	0.43	3.02	2	1
1:A:38:LEU:HD23	1:A:74:VAL:CG1	0.43	2.43	3	1
1:A:25:SER:HB2	1:A:86:VAL:CG1	0.43	2.44	11	1
1:A:23:ALA:CB	1:A:42:VAL:HG11	0.43	2.32	15	1
1:A:70:LEU:H	1:A:70:LEU:HD12	0.43	1.69	15	1
1:A:13:GLN:CG	1:A:93:ILE:HG12	0.43	2.43	17	1
1:A:38:LEU:HD23	1:A:38:LEU:H	0.43	1.74	7	1
1:A:74:VAL:O	1:A:74:VAL:HG13	0.43	2.13	7	1
1:A:13:GLN:NE2	1:A:67:GLY:O	0.43	2.52	16	1
1:A:98:ASP:OD1	1:A:99:ARG:N	0.43	2.52	18	1
1:A:8:ARG:HB2	1:A:10:TYR:CE2	0.43	2.48	2	1
1:A:26:LEU:O	1:A:27:ARG:C	0.43	2.57	2	6
1:A:13:GLN:OE1	1:A:68:TYR:CE1	0.43	2.72	7	2
1:A:27:ARG:CG	1:A:31:LYS:HE3	0.43	2.44	11	1
1:A:31:LYS:HD3	1:A:36:GLU:OE2	0.43	2.12	16	1
1:A:38:LEU:HD12	1:A:73:MET:HG2	0.43	1.90	8	1
1:A:94:GLY:O	1:A:95:GLY:C	0.43	2.57	6	2
1:A:78:ALA:O	1:A:79:SER:C	0.43	2.56	13	3
1:A:8:ARG:CG	1:A:8:ARG:NH1	0.43	2.82	10	1
1:A:75:MET:SD	1:A:100:PRO:HG3	0.43	2.54	16	1
1:A:10:TYR:CE1	1:A:75:MET:CG	0.42	3.02	2	1
1:A:72:GLN:O	1:A:73:MET:HB2	0.42	2.14	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:GLN:CB	1:A:90:MET:HB2	0.42	2.44	5	5
1:A:80:TRP:CH2	1:A:84:ARG:NE	0.42	2.87	5	1
1:A:14:ALA:O	1:A:90:MET:HG2	0.42	2.14	10	1
1:A:30:ILE:CD1	1:A:39:PHE:CZ	0.42	3.02	15	1
1:A:35:MET:CE	1:A:38:LEU:HD13	0.42	2.44	19	1
1:A:19:GLU:HG3	1:A:69:VAL:HG23	0.42	1.90	6	1
1:A:98:ASP:O	1:A:99:ARG:CG	0.42	2.68	5	2
1:A:21:ARG:O	1:A:22:VAL:C	0.42	2.57	12	3
1:A:7:LYS:HB2	1:A:72:GLN:OE1	0.42	2.14	17	1
1:A:29:HIS:C	1:A:82:LEU:HD11	0.42	2.35	17	1
1:A:33:HIS:HB2	1:A:35:MET:SD	0.42	2.55	12	1
1:A:18:PHE:CD1	1:A:88:ARG:HD3	0.42	2.50	19	2
1:A:42:VAL:HG12	1:A:43:MET:N	0.42	2.29	18	1
1:A:43:MET:CE	1:A:112:MET:HG3	0.42	2.45	19	1
1:A:10:TYR:CD2	1:A:75:MET:CE	0.42	3.02	19	1
1:A:33:HIS:HB3	1:A:35:MET:SD	0.42	2.55	8	1
1:A:22:VAL:HG22	1:A:88:ARG:HB3	0.42	1.91	15	1
1:A:14:ALA:O	1:A:67:GLY:HA3	0.41	2.15	12	1
1:A:96:THR:O	1:A:97:SER:C	0.41	2.57	16	1
1:A:21:ARG:CZ	1:A:88:ARG:HG3	0.41	2.46	14	1
1:A:98:ASP:O	1:A:99:ARG:CD	0.41	2.68	5	1
1:A:43:MET:CE	1:A:70:LEU:HB2	0.41	2.45	12	1
1:A:35:MET:O	1:A:36:GLU:C	0.41	2.58	15	2
1:A:13:GLN:HB3	1:A:90:MET:CE	0.41	2.46	17	2
1:A:27:ARG:CG	1:A:31:LYS:HE2	0.41	2.45	14	1
1:A:96:THR:OG1	1:A:98:ASP:OD1	0.41	2.34	18	1
1:A:28:GLU:O	1:A:32:LEU:CD1	0.41	2.68	17	1
1:A:25:SER:O	1:A:28:GLU:HB3	0.41	2.16	9	1
1:A:95:GLY:O	1:A:96:THR:C	0.41	2.57	16	1
1:A:89:VAL:CG1	1:A:89:VAL:O	0.41	2.68	16	1
1:A:22:VAL:HG22	1:A:88:ARG:HB2	0.41	1.93	2	1
1:A:87:PRO:O	1:A:88:ARG:HB2	0.41	2.16	3	4
1:A:89:VAL:O	1:A:89:VAL:CG1	0.41	2.68	4	1
1:A:15:PHE:CD2	1:A:88:ARG:HA	0.41	2.51	6	1
1:A:94:GLY:O	1:A:95:GLY:O	0.41	2.39	6	2
1:A:13:GLN:CG	1:A:90:MET:CB	0.41	2.98	7	1
1:A:29:HIS:CD2	1:A:86:VAL:CG2	0.41	3.04	10	1
1:A:35:MET:O	1:A:38:LEU:HD12	0.41	2.16	15	1
1:A:38:LEU:CD2	1:A:74:VAL:CG1	0.41	2.98	16	1
1:A:10:TYR:CE2	1:A:75:MET:CE	0.41	3.04	19	1
1:A:13:GLN:HB3	1:A:90:MET:HE2	0.41	1.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ARG:HA	1:A:30:ILE:HG12	0.40	1.93	5	1
1:A:10:TYR:CG	1:A:75:MET:HE3	0.40	2.51	14	1
1:A:97:SER:O	1:A:98:ASP:HB2	0.40	2.15	16	1
1:A:38:LEU:HD23	1:A:74:VAL:CG2	0.40	2.45	1	1
1:A:77:ASP:O	1:A:81:HIS:HB2	0.40	2.17	9	1
1:A:13:GLN:CB	1:A:93:ILE:HD11	0.40	2.43	9	1
1:A:27:ARG:NE	1:A:31:LYS:NZ	0.40	2.69	16	1
1:A:76:ASN:O	1:A:80:TRP:HB3	0.40	2.16	16	1
1:A:38:LEU:CD1	1:A:79:SER:HB3	0.40	2.45	18	1
1:A:33:HIS:O	1:A:34:ASN:HB2	0.40	2.17	17	1
1:A:33:HIS:HB2	1:A:35:MET:HG2	0.40	1.93	5	1
1:A:72:GLN:O	1:A:73:MET:CB	0.40	2.68	16	1
1:A:13:GLN:NE2	1:A:93:ILE:CD1	0.40	2.85	18	1
1:A:35:MET:O	1:A:38:LEU:HG	0.40	2.16	18	1
1:A:38:LEU:HD13	1:A:79:SER:HG	0.40	1.68	12	1
1:A:14:ALA:O	1:A:67:GLY:CA	0.40	2.69	12	1
1:A:26:LEU:O	1:A:30:ILE:HG13	0.40	2.17	13	1
1:A:11:VAL:HG11	1:A:93:ILE:HB	0.40	1.92	17	1
1:A:83:VAL:HG21	1:A:92:PHE:HE2	0.40	1.73	2	1
1:A:69:VAL:C	1:A:70:LEU:HD22	0.40	2.37	9	1
1:A:26:LEU:HD21	1:A:86:VAL:HG21	0.40	1.91	11	1
1:A:12:VAL:N	1:A:69:VAL:O	0.40	2.53	14	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	84/123 (68%)	80±1 (95±2%)	4±1 (5±2%)	0±0 (0±1%)	44	80
All	All	1680/2460 (68%)	1596 (95%)	79 (5%)	5 (0%)	44	80

All 2 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	95	GLY	4
1	A	7	LYS	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	72/107 (67%)	70±1 (97±2%)	2±1 (3±2%)	44	89
All	All	1440/2140 (67%)	1397 (97%)	43 (3%)	44	89

All 9 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	99	ARG	10
1	A	82	LEU	8
1	A	38	LEU	7
1	A	92	PHE	5
1	A	35	MET	4
1	A	68	TYR	4
1	A	75	MET	3
1	A	72	GLN	1
1	A	96	THR	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 carbohydrates 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 88% for the well-defined parts and 80% 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	1410
Number of shifts mapped to atoms	1410
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	121	-0.47 ± 0.10	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	100	0.40 ± 0.11	None needed (< 0.5 ppm)
$^{13}C'$	115	-0.31 ± 0.10	None needed (< 0.5 ppm)
^{15}N	115	-0.22 ± 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 88%, i.e. 918 atoms were assigned a chemical shift out of a possible 1044. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	410/414 (99%)	165/165 (100%)	164/168 (98%)	81/81 (100%)
Sidechain	433/533 (81%)	265/312 (85%)	164/196 (84%)	4/25 (16%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	75/97 (77%)	40/52 (77%)	33/40 (82%)	2/5 (40%)
Overall	918/1044 (88%)	470/529 (89%)	361/404 (89%)	87/111 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1268 atoms were assigned a chemical shift out of a possible 1583. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	587/601 (98%)	236/239 (99%)	236/246 (96%)	115/116 (99%)
Sidechain	593/867 (68%)	367/513 (72%)	221/303 (73%)	5/51 (10%)
Aromatic	88/115 (77%)	47/62 (76%)	39/48 (81%)	2/5 (40%)
Overall	1268/1583 (80%)	650/814 (80%)	496/597 (83%)	122/172 (71%)

7.1.4 Statistically unusual chemical shifts ⓘ

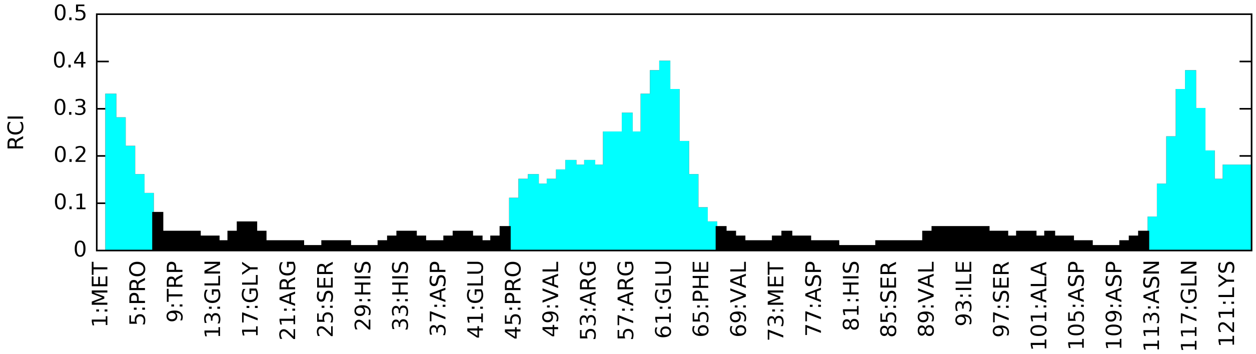
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	72	GLN	HB2	0.08	3.30 – 0.80	-7.9
1	A	39	PHE	CE2	139.70	136.81 – 124.71	7.4
1	A	80	TRP	CE3	131.40	129.06 – 111.96	6.4
1	A	72	GLN	HG3	0.52	3.75 – 0.85	-6.1
1	A	72	GLN	HG2	0.79	3.67 – 0.97	-5.7

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:


0.5
0.4
0.3
0.2
0.1
0
RCI
1:MET
5:PRO
9:TRP
13:GLN
17:GLY
21:ARG
25:SER
29:HIS
33:HIS
37:ASP
41:GLU
45:PRO
49:VAL
53:ARG
57:ARG
61:GLU
65:PHE
69:VAL
73:MET
77:ASP
81:HIS
85:SER
89:VAL
93:ILE
97:SER
101:ALA
105:ASP
109:ASP
113:ASN
117:GLN
121:LYS