



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:02 pm GMT

PDB ID : 2KHS
Title : Solution structure of SNase121:SNase(111-143) complex
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Deposited on : 2009-04-10

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 ⓘ 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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

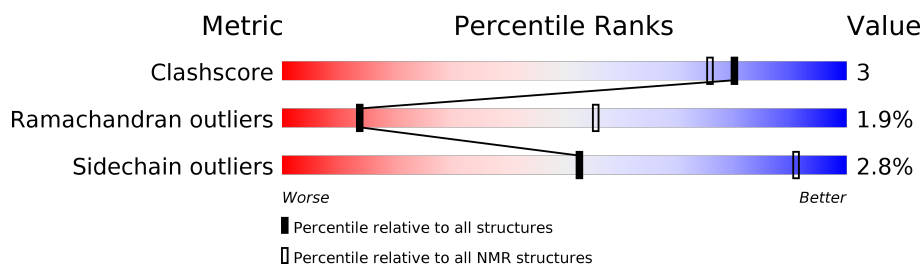
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 63%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	121	
2	B	35	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:8-A:41, A:55-A:82, A:87-A:112, B:134-B:156 (111)	0.52	17

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 5 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2530 atoms, of which 1286 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Thermonuclease.

Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1955	611	999	165	176	4	

- Molecule 2 is a protein called Nuclease.

Mol	Chain	Residues	Atoms					Trace
2	B	35	Total	C	H	N	O	0
			575	180	287	51	57	

There are 2 discrepancies between the modelled and reference sequences:

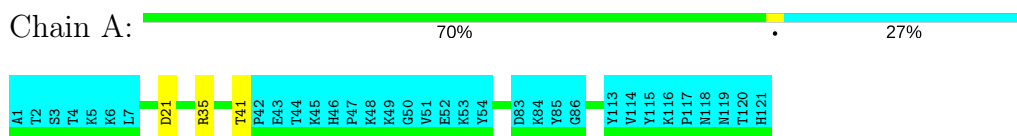
Chain	Residue	Modelled	Actual	Comment	Reference
B	122	GLY	-	EXPRESSION TAG	UNP Q1WCB7
B	123	SER	-	EXPRESSION TAG	UNP Q1WCB7

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: Thermonuclease



- Molecule 2: Nuclease



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: Thermonuclease

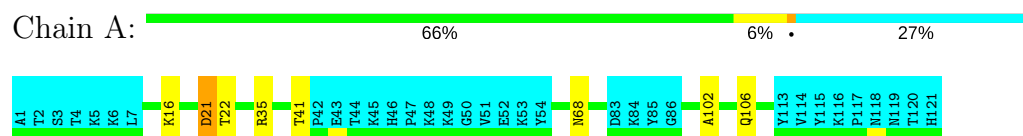


- Molecule 2: Nuclease

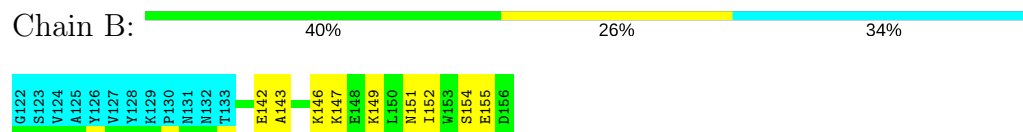


4.2.2 Score per residue for model 2

• Molecule 1: Thermonuclease

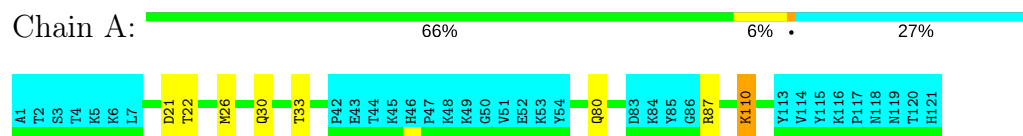


• Molecule 2: Nuclease



4.2.3 Score per residue for model 3

• Molecule 1: Thermonuclease

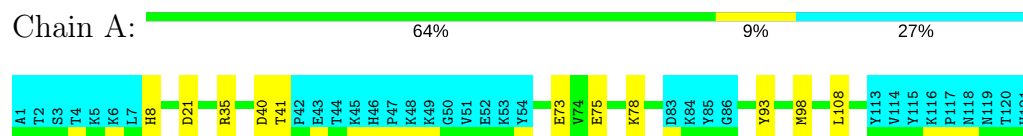


• Molecule 2: Nuclease



4.2.4 Score per residue for model 4

• Molecule 1: Thermonuclease

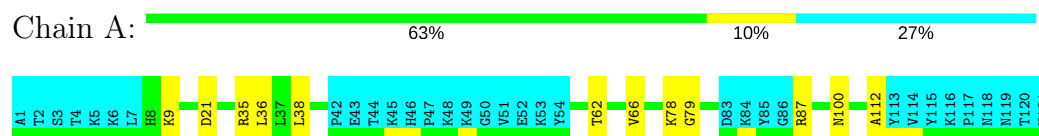


• Molecule 2: Nuclease



4.2.5 Score per residue for model 5

• Molecule 1: Thermonuclease

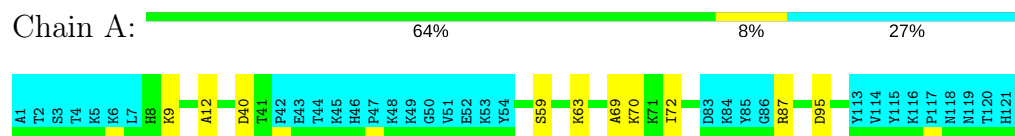


• Molecule 2: Nuclease

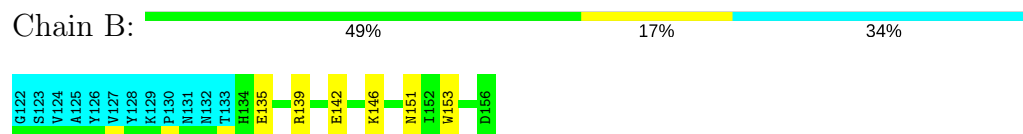


4.2.6 Score per residue for model 6

• Molecule 1: Thermonuclease

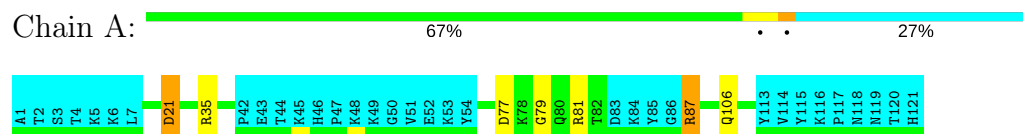


• Molecule 2: Nuclease

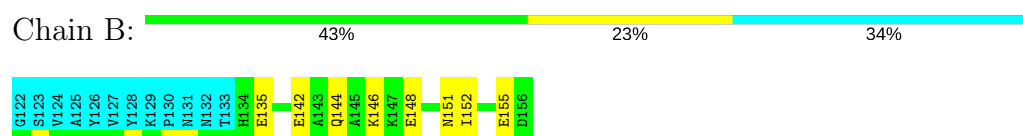


4.2.7 Score per residue for model 7

• Molecule 1: Thermonuclease

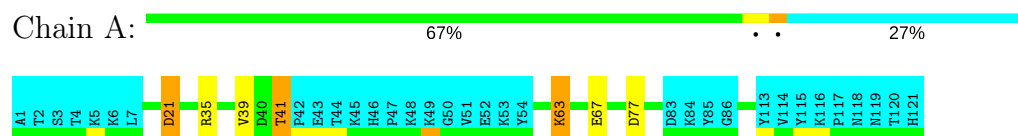


• Molecule 2: Nuclease



4.2.8 Score per residue for model 8

• Molecule 1: Thermonuclease

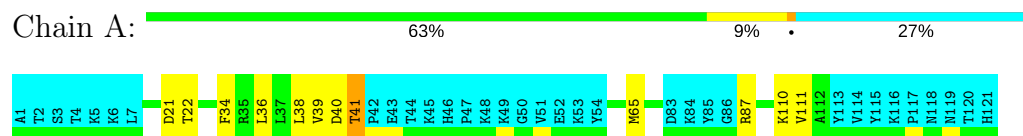


• Molecule 2: Nuclease



4.2.9 Score per residue for model 9

• Molecule 1: Thermonuclease

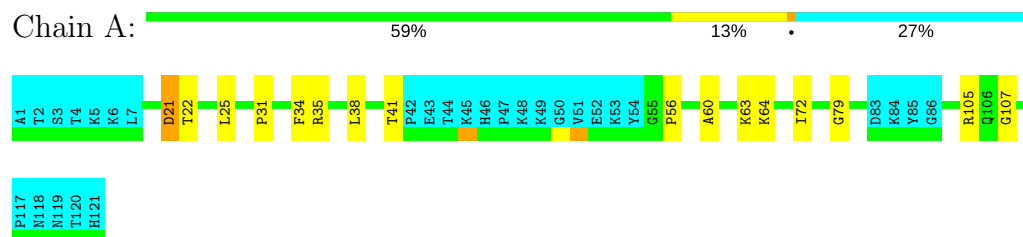


• Molecule 2: Nuclease



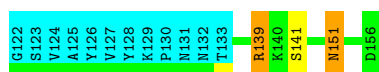
4.2.10 Score per residue for model 10

• Molecule 1: Thermonuclease



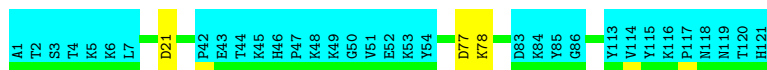
• Molecule 2: Nuclease





4.2.11 Score per residue for model 11

- Molecule 1: Thermonuclease

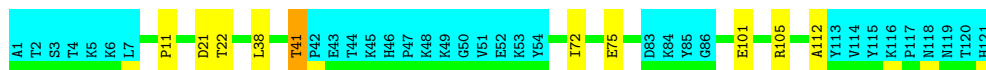


- Molecule 2: Nuclease

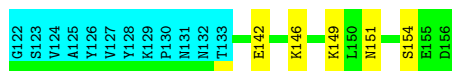


4.2.12 Score per residue for model 12

- Molecule 1: Thermonuclease

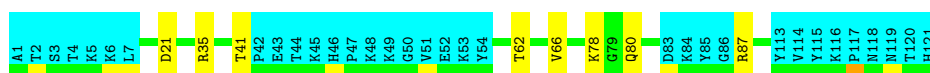


- Molecule 2: Nuclease



4.2.13 Score per residue for model 13

- Molecule 1: Thermonuclease



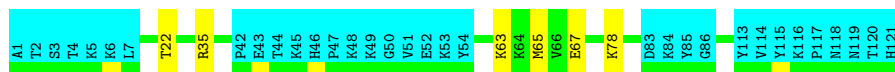
- Molecule 2: Nuclease





4.2.14 Score per residue for model 14

- Molecule 1: Thermonuclease

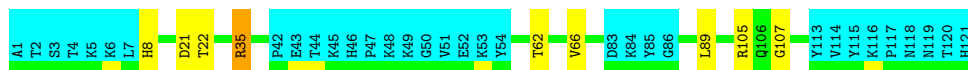


- Molecule 2: Nuclease

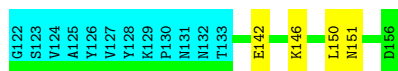


4.2.15 Score per residue for model 15

- Molecule 1: Thermonuclease

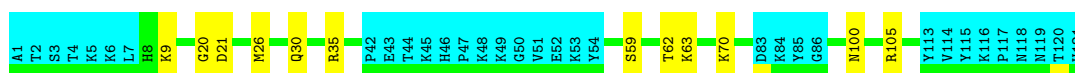


- Molecule 2: Nuclease



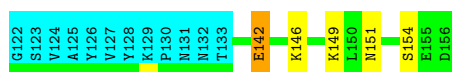
4.2.16 Score per residue for model 16

- Molecule 1: Thermonuclease



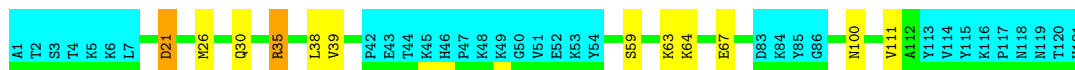
- Molecule 2: Nuclease





4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Thermonuclease

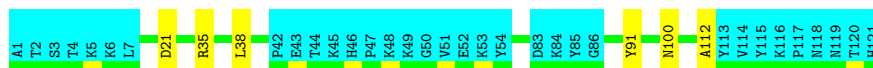


- Molecule 2: Nuclease



4.2.18 Score per residue for model 18

- Molecule 1: Thermonuclease



- Molecule 2: Nuclease



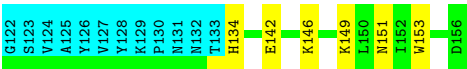
4.2.19 Score per residue for model 19

- Molecule 1: Thermonuclease



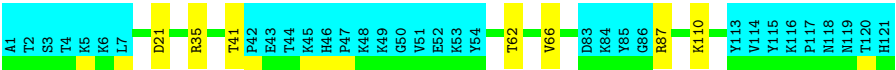
- Molecule 2: Nuclease





4.2.20 Score per residue for model 20

- Molecule 1: Thermonuclease



- Molecule 2: Nuclease



5 Refinement protocol and experimental data overview

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

Of the 200 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
CNS	structure solution	1.2
CNS	refinement	1.2

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 15357
Number of chemical shift lists	1
Total number of shifts	1624
Number of shifts mapped to atoms	1261
Number of unparsed shifts	0
Number of shifts with mapping errors	363
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	63%

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.

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	0.4±0.5
All	All	0	8

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	35	ARG	Sidechain	3
1	A	81	ARG	Sidechain	2
1	A	87	ARG	Sidechain	2
1	A	105	ARG	Sidechain	1

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	683	719	718	3±2
2	B	196	197	196	2±1
All	All	17580	18320	18280	112

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ASP:OD2	1:A:35:ARG:HD2	0.60	1.97	4	1
1:A:21:ASP:OD1	1:A:35:ARG:HD2	0.59	1.97	5	3
1:A:22:THR:HA	1:A:34:PHE:O	0.55	2.00	9	2
2:B:142:GLU:O	2:B:146:LYS:HG3	0.55	2.01	13	14
1:A:101:GLU:O	1:A:105:ARG:HG2	0.55	2.00	12	1
1:A:78:LYS:NZ	1:A:78:LYS:HA	0.55	2.17	5	1
1:A:69:ALA:HB2	1:A:94:ALA:HB1	0.53	1.80	19	1
1:A:38:LEU:HA	1:A:112:ALA:O	0.53	2.03	18	4
1:A:35:ARG:HB2	1:A:87:ARG:NH1	0.52	2.19	7	1
2:B:142:GLU:HG3	2:B:153:TRP:CZ2	0.52	2.39	20	5
1:A:26:MET:HA	1:A:30:GLN:O	0.52	2.05	17	3
2:B:149:LYS:O	2:B:154:SER:HB3	0.52	2.05	16	2
2:B:149:LYS:O	2:B:154:SER:HB2	0.51	2.05	13	6
1:A:21:ASP:O	1:A:35:ARG:HA	0.51	2.05	15	5
1:A:21:ASP:OD1	1:A:35:ARG:HG2	0.49	2.08	1	1
1:A:93:TYR:CE2	1:A:98:MET:HG3	0.49	2.42	4	1
2:B:142:GLU:O	2:B:146:LYS:HG2	0.49	2.07	8	1
1:A:60:ALA:O	1:A:64:LYS:HG3	0.49	2.08	1	2
1:A:40:ASP:HB3	1:A:110:LYS:HB2	0.48	1.84	9	1
1:A:11:PRO:HA	1:A:72:ILE:O	0.47	2.10	12	1
1:A:65:MET:SD	1:A:99:VAL:HG22	0.47	2.48	19	1
1:A:12:ALA:O	1:A:72:ILE:HB	0.47	2.10	6	1
1:A:110:LYS:HG2	2:B:153:TRP:CH2	0.46	2.45	20	1
1:A:8:HIS:O	1:A:75:GLU:HA	0.46	2.11	19	2
2:B:152:ILE:O	2:B:155:GLU:HG2	0.46	2.11	9	4
1:A:25:LEU:O	1:A:31:PRO:HA	0.46	2.11	10	1
1:A:21:ASP:HB3	1:A:41:THR:OG1	0.46	2.11	2	1
1:A:59:SER:O	1:A:63:LYS:HG3	0.45	2.10	16	4
2:B:136:GLN:O	2:B:140:LYS:HG2	0.45	2.11	11	1
1:A:62:THR:O	1:A:66:VAL:HG22	0.45	2.12	15	5
1:A:110:LYS:HG3	2:B:153:TRP:CZ3	0.45	2.45	3	1
1:A:36:LEU:HB2	1:A:39:VAL:HG21	0.45	1.88	9	1
2:B:139:ARG:O	2:B:139:ARG:HD3	0.45	2.11	10	1
2:B:136:GLN:O	2:B:140:LYS:HG3	0.45	2.11	3	1
1:A:102:ALA:O	1:A:106:GLN:HG2	0.45	2.12	2	1
1:A:110:LYS:HA	2:B:153:TRP:CH2	0.44	2.47	3	1
2:B:135:GLU:O	2:B:139:ARG:HG2	0.44	2.12	13	1
1:A:38:LEU:O	1:A:111:VAL:HA	0.44	2.13	17	3
2:B:135:GLU:OE2	2:B:139:ARG:HD2	0.43	2.12	6	1
2:B:143:ALA:O	2:B:147:LYS:HG2	0.43	2.13	2	2
2:B:146:LYS:HA	2:B:153:TRP:CG	0.43	2.48	18	1
1:A:63:LYS:O	1:A:67:GLU:HG2	0.43	2.13	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:GLY:O	2:B:151:ASN:HB2	0.43	2.13	10	1
1:A:107:GLY:HA3	2:B:150:LEU:O	0.43	2.14	15	1
1:A:63:LYS:O	1:A:67:GLU:HG3	0.42	2.14	17	1
1:A:20:GLY:HA2	1:A:62:THR:OG1	0.42	2.14	16	1
1:A:33:THR:O	1:A:87:ARG:HD3	0.42	2.14	3	1
1:A:73:GLU:HB2	1:A:93:TYR:HB2	0.42	1.90	4	1
1:A:69:ALA:HA	1:A:95:ASP:OD1	0.42	2.15	6	1
1:A:105:ARG:CZ	2:B:141:SER:HA	0.41	2.45	10	1
1:A:77:ASP:OD1	1:A:78:LYS:HG2	0.41	2.15	11	1
1:A:36:LEU:HB3	1:A:100:ASN:ND2	0.41	2.30	5	1
1:A:25:LEU:HD11	1:A:72:ILE:HG21	0.41	1.92	10	1
1:A:63:LYS:HE3	1:A:67:GLU:OE1	0.41	2.16	8	1
2:B:144:GLN:HA	2:B:144:GLN:HE21	0.41	1.76	17	1
2:B:140:LYS:HE2	2:B:140:LYS:HA	0.41	1.91	4	1
1:A:21:ASP:OD2	1:A:41:THR:HG22	0.41	2.15	12	1
1:A:39:VAL:HG23	1:A:100:ASN:HD22	0.41	1.76	17	1
1:A:70:LYS:N	1:A:70:LYS:HD2	0.40	2.31	6	1
1:A:70:LYS:HD3	1:A:70:LYS:N	0.40	2.31	19	1
1:A:91:TYR:CZ	1:A:100:ASN:HB2	0.40	2.52	18	1
2:B:144:GLN:O	2:B:148:GLU:HG2	0.40	2.16	7	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	88/121 (73%)	83±2 (95±2%)	4±2 (4±2%)	1±1 (1±1%)	19	65
2	B	22/35 (63%)	20±1 (93±3%)	1±1 (3±3%)	1±0 (5±0%)	5	29
All	All	2200/3120 (71%)	2074 (94%)	84 (4%)	42 (2%)	14	55

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	151	ASN	20

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Mol	Chain	Res	Type	Models (Total)
1	A	21	ASP	12
1	A	41	THR	7
1	A	79	GLY	3

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	71/101 (70%)	69±1 (97±2%)	2±1 (3±2%)	49	89
2	B	21/31 (68%)	21±0 (98±2%)	0±0 (2±2%)	65	94
All	All	1840/2640 (70%)	1788 (97%)	52 (3%)	52	91

All 28 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	22	THR	6
1	A	87	ARG	4
1	A	35	ARG	4
1	A	9	LYS	3
2	B	142	GLU	3
1	A	65	MET	3
1	A	78	LYS	3
1	A	40	ASP	2
1	A	63	LYS	2
1	A	64	LYS	2
2	B	135	GLU	2
1	A	16	LYS	2
2	B	144	GLN	1
1	A	41	THR	1
1	A	68	ASN	1
1	A	105	ARG	1
1	A	80	GLN	1
1	A	110	LYS	1
2	B	139	ARG	1
1	A	70	LYS	1
1	A	81	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	8	HIS	1
1	A	89	LEU	1
2	B	149	LYS	1
1	A	21	ASP	1
1	A	106	GLN	1
1	A	100	ASN	1
1	A	56	PRO	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

The completeness of assignment taking into account all chemical shift lists is 63% for the well-defined parts and 60% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 15357

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	1624
Number of shifts mapped to atoms	1261
Number of unparsed shifts	0
Number of shifts with mapping errors	363
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- Residue not found in structure. All 363 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	153	TRP	C	176.2	0.2	1
A	130	PRO	CB	32.2	0.2	1
A	140	LYS	CD	29.1	0.2	1
A	154	SER	H	8.11	0.02	1
A	139	ARG	HA	4.05	0.02	1
A	146	LYS	C	180.9	0.2	1
A	130	PRO	HA	4.23	0.02	1
A	153	TRP	H	7.9	0.02	1
A	150	LEU	HD22	0.84	0.02	2
A	127	VAL	HG21	0.84	0.02	2
A	138	LEU	N	119.5	0.2	1
A	133	THR	H	10.32	0.02	1
A	135	GLU	CA	61.7	0.2	1
A	125	ALA	C	177.0	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	142	GLU	HG3	2.89	0.02	2
A	145	ALA	HB3	1.76	0.02	1
A	134	HIS	HA	5.41	0.02	1
A	147	LYS	CE	41.6	0.2	1
A	148	GLU	CA	56.6	0.2	1
A	141	SER	HA	4.34	0.02	1
A	154	SER	HB3	4.06	0.02	2
A	150	LEU	HD21	0.84	0.02	2
A	133	THR	HA	3.81	0.02	1
A	138	LEU	HD21	0.92	0.02	1
A	145	ALA	CA	55.8	0.2	1
A	150	LEU	CG	25.2	0.2	1
A	128	TYR	HB3	2.95	0.02	2
A	149	LYS	HB2	1.8	0.02	2
A	135	GLU	N	120.7	0.2	1
A	152	ILE	N	124.6	0.2	1
A	137	LEU	HA	4.11	0.02	1
A	142	GLU	HB2	2.23	0.02	2
A	148	GLU	N	116.4	0.2	1
A	156	ASP	HA	4.44	0.02	1
A	149	LYS	HD2	1.75	0.02	1
A	152	ILE	HB	1.05	0.02	1
A	145	ALA	HA	3.94	0.02	1
A	132	ASN	HB2	2.42	0.02	2
A	130	PRO	HB3	1.97	0.02	2
A	143	ALA	HB3	1.5	0.02	1
A	152	ILE	C	176.7	0.2	1
A	149	LYS	HA	3.57	0.02	1
A	139	ARG	CD	43.0	0.2	1
A	131	ASN	CB	38.6	0.2	1
A	136	GLN	HA	4.03	0.02	1
A	136	GLN	HG3	2.45	0.02	2
A	142	GLU	CA	59.2	0.2	1
A	152	ILE	CA	65.6	0.2	1
A	143	ALA	H	8.02	0.02	1
A	151	ASN	CB	38.7	0.2	1
A	135	GLU	HB3	1.99	0.02	2
A	140	LYS	H	8.13	0.02	1
A	137	LEU	HB2	1.79	0.02	2
A	144	GLN	CA	58.6	0.2	1
A	131	ASN	H	8.47	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	129	LYS	CE	42.0	0.2	1
A	152	ILE	HG23	0.12	0.02	1
A	146	LYS	HA	3.43	0.02	1
A	130	PRO	C	175.2	0.2	1
A	138	LEU	HD13	0.75	0.02	1
A	129	LYS	H	8.21	0.02	1
A	143	ALA	CB	17.5	0.2	1
A	126	TYR	N	120.7	0.2	1
A	153	TRP	HB2	2.85	0.02	2
A	134	HIS	C	174.8	0.2	1
A	136	GLN	N	117.2	0.2	1
A	124	VAL	HG23	0.89	0.02	2
A	127	VAL	HB	1.87	0.02	1
A	129	LYS	CB	33.1	0.2	1
A	147	LYS	H	7.84	0.02	1
A	133	THR	HG23	0.68	0.02	1
A	131	ASN	N	120.9	0.2	1
A	134	HIS	CA	53.9	0.2	1
A	138	LEU	HD11	0.75	0.02	1
A	142	GLU	C	177.4	0.2	1
A	148	GLU	HG3	2.53	0.02	2
A	156	ASP	N	126.8	0.2	1
A	132	ASN	HA	4.99	0.02	1
A	126	TYR	CA	58.1	0.2	1
A	130	PRO	HG2	1.62	0.02	2
A	138	LEU	HB3	1.97	0.02	2
A	147	LYS	CB	32.2	0.2	1
A	139	ARG	CA	60.1	0.2	1
A	130	PRO	HB2	2.19	0.02	2
A	125	ALA	HA	4.3	0.02	1
A	144	GLN	N	118.7	0.2	1
A	149	LYS	CG	24.9	0.2	1
A	142	GLU	CB	31.0	0.2	1
A	155	GLU	HA	4.49	0.02	1
A	143	ALA	N	119.5	0.2	1
A	124	VAL	H	8.28	0.02	1
A	150	LEU	HB2	1.39	0.02	2
A	129	LYS	HA	4.48	0.02	1
A	150	LEU	HB3	1.55	0.02	2
A	146	LYS	H	8.19	0.02	1
A	155	GLU	H	8.07	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	126	TYR	HE1	6.75	0.02	1
A	129	LYS	HG3	1.45	0.02	2
A	138	LEU	CB	41.1	0.2	1
A	143	ALA	CA	54.8	0.2	1
A	156	ASP	CB	42.3	0.2	1
A	146	LYS	CB	32.2	0.2	1
A	129	LYS	HE3	2.99	0.02	2
A	140	LYS	HG2	0.88	0.02	2
A	142	GLU	HA	3.9	0.02	1
A	140	LYS	CE	41.9	0.2	1
A	125	ALA	CB	19.2	0.2	1
A	129	LYS	CA	53.5	0.2	1
A	127	VAL	HG22	0.84	0.02	2
A	154	SER	C	175.3	0.2	1
A	132	ASN	N	117.8	0.2	1
A	153	TRP	HZ2	7.57	0.02	1
A	135	GLU	CB	30.2	0.2	1
A	149	LYS	HE2	3.07	0.02	2
A	145	ALA	HB2	1.76	0.02	1
A	149	LYS	H	7.86	0.02	1
A	148	GLU	CB	30.0	0.2	1
A	154	SER	HB2	4.18	0.02	2
A	129	LYS	HB3	1.6	0.02	2
A	147	LYS	CA	59.5	0.2	1
A	127	VAL	C	174.8	0.2	1
A	139	ARG	CB	29.4	0.2	1
A	135	GLU	H	7.5	0.02	1
A	152	ILE	H	8.42	0.02	1
A	124	VAL	N	122.1	0.2	1
A	126	TYR	HA	4.48	0.02	1
A	128	TYR	HB2	2.87	0.02	2
A	142	GLU	CG	38.6	0.2	1
A	147	LYS	C	178.8	0.2	1
A	142	GLU	HB3	1.94	0.02	2
A	145	ALA	C	179.5	0.2	1
A	151	ASN	N	119.3	0.2	1
A	146	LYS	N	117.2	0.2	1
A	139	ARG	H	8.96	0.02	1
A	126	TYR	H	8.16	0.02	1
A	146	LYS	HG3	0.47	0.02	2
A	143	ALA	HB2	1.5	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	149	LYS	HG3	1.42	0.02	2
A	125	ALA	N	128.2	0.2	1
A	152	ILE	CG2	15.3	0.2	1
A	136	GLN	H	8.87	0.02	1
A	124	VAL	CA	62.1	0.2	1
A	136	GLN	HG2	2.51	0.02	2
A	149	LYS	CB	29.1	0.2	1
A	132	ASN	CB	39.5	0.2	1
A	138	LEU	CA	58.8	0.2	1
A	138	LEU	HA	4.0	0.02	1
A	144	GLN	HG3	2.41	0.02	2
A	125	ALA	HB1	1.31	0.02	1
A	137	LEU	HB3	1.84	0.02	2
A	125	ALA	CA	52.2	0.2	1
A	150	LEU	HD12	1.0	0.02	2
A	129	LYS	CD	29.0	0.2	1
A	153	TRP	HD1	7.02	0.02	1
A	132	ASN	H	7.71	0.02	1
A	133	THR	CA	69.4	0.2	1
A	152	ILE	HG22	0.12	0.02	1
A	150	LEU	N	117.2	0.2	1
A	155	GLU	HB2	1.95	0.02	2
A	135	GLU	CG	35.8	0.2	1
A	145	ALA	HB1	1.76	0.02	1
A	153	TRP	HB3	3.73	0.02	2
A	140	LYS	HD2	1.64	0.02	2
A	148	GLU	CG	37.0	0.2	1
A	133	THR	C	176.3	0.2	1
A	142	GLU	N	125.2	0.2	1
A	150	LEU	HD23	0.84	0.02	2
A	147	LYS	CD	29.1	0.2	1
A	140	LYS	CA	60.0	0.2	1
A	127	VAL	HA	4.0	0.02	1
A	141	SER	CB	62.6	0.2	1
A	154	SER	CB	64.3	0.2	1
A	131	ASN	HB2	2.8	0.02	2
A	148	GLU	HG2	2.28	0.02	2
A	156	ASP	HB3	2.75	0.02	2
A	124	VAL	HA	4.15	0.02	1
A	124	VAL	CG1	20.4	0.2	2
A	138	LEU	HB2	1.51	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	140	LYS	N	122.1	0.2	1
A	152	ILE	CG1	26.0	0.2	1
A	136	GLN	CB	27.4	0.2	1
A	126	TYR	HD1	6.99	0.02	1
A	150	LEU	CA	55.0	0.2	1
A	144	GLN	HB3	2.21	0.02	2
A	147	LYS	HB3	1.95	0.02	2
A	152	ILE	CD1	13.6	0.2	1
A	139	ARG	C	179.7	0.2	1
A	136	GLN	HB2	1.96	0.02	2
A	150	LEU	HD11	1.0	0.02	2
A	127	VAL	CG1	20.7	0.2	2
A	143	ALA	C	181.0	0.2	1
A	147	LYS	CG	24.7	0.2	1
A	130	PRO	HD2	3.58	0.02	2
A	139	ARG	HD2	3.25	0.02	2
A	144	GLN	CG	33.7	0.2	1
A	136	GLN	CG	33.9	0.2	1
A	138	LEU	CD1	23.6	0.2	2
A	149	LYS	HB3	2.08	0.02	2
A	150	LEU	H	7.67	0.02	1
A	139	ARG	HB2	1.95	0.02	2
A	128	TYR	C	174.9	0.2	1
A	138	LEU	HD23	0.92	0.02	1
A	133	THR	CB	67.4	0.2	1
A	141	SER	N	118.5	0.2	1
A	152	ILE	HG21	0.12	0.02	1
A	147	LYS	HA	3.95	0.02	1
A	151	ASN	HA	3.8	0.02	1
A	156	ASP	CA	56.1	0.2	1
A	126	TYR	HB2	2.92	0.02	2
A	151	ASN	H	9.13	0.02	1
A	139	ARG	HG3	1.75	0.02	2
A	131	ASN	HA	4.91	0.02	1
A	140	LYS	CB	31.9	0.2	1
A	128	TYR	N	125.4	0.2	1
A	137	LEU	HG	1.51	0.02	1
A	137	LEU	N	122.5	0.2	1
A	139	ARG	N	119.3	0.2	1
A	137	LEU	HD12	0.72	0.02	1
A	127	VAL	CA	61.8	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	140	LYS	HB3	2.06	0.02	2
A	141	SER	CA	64.0	0.2	1
A	133	THR	HG21	0.68	0.02	1
A	140	LYS	HA	4.18	0.02	1
A	127	VAL	HG23	0.84	0.02	2
A	153	TRP	HZ3	7.11	0.02	1
A	154	SER	HA	4.24	0.02	1
A	125	ALA	H	8.36	0.02	1
A	148	GLU	HB2	2.06	0.02	2
A	133	THR	CG2	21.1	0.2	1
A	134	HIS	HB3	3.23	0.02	2
A	141	SER	C	175.4	0.2	1
A	146	LYS	HD2	1.02	0.02	2
A	129	LYS	HB2	1.71	0.02	2
A	127	VAL	N	124.1	0.2	1
A	149	LYS	N	116.8	0.2	1
A	152	ILE	HG13	0.57	0.02	2
A	144	GLN	HA	4.0	0.02	1
A	150	LEU	HA	4.2	0.02	1
A	138	LEU	C	179.1	0.2	1
A	155	GLU	CA	56.1	0.2	1
A	146	LYS	HG2	0.18	0.02	2
A	143	ALA	HB1	1.5	0.02	1
A	147	LYS	HG2	1.51	0.02	2
A	149	LYS	C	175.0	0.2	1
A	147	LYS	HE2	2.97	0.02	2
A	141	SER	HB3	4.1	0.02	2
A	137	LEU	CD1	24.3	0.2	2
A	145	ALA	N	123.3	0.2	1
A	127	VAL	H	7.83	0.02	1
A	132	ASN	CA	51.4	0.2	1
A	137	LEU	HD21	0.87	0.02	1
A	155	GLU	HG3	2.32	0.02	2
A	153	TRP	CA	54.7	0.2	1
A	137	LEU	HD23	0.87	0.02	1
A	155	GLU	N	121.5	0.2	1
A	144	GLN	C	177.2	0.2	1
A	140	LYS	CG	25.1	0.2	1
A	129	LYS	C	173.5	0.2	1
A	129	LYS	CG	24.5	0.2	1
A	127	VAL	CB	33.3	0.2	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	137	LEU	CA	58.6	0.2	1
A	125	ALA	HB2	1.31	0.02	1
A	154	SER	N	116.2	0.2	1
A	150	LEU	CD1	22.9	0.2	2
A	148	GLU	C	174.5	0.2	1
A	155	GLU	HB3	2.25	0.02	2
A	151	ASN	C	176.3	0.2	1
A	153	TRP	N	120.1	0.2	1
A	153	TRP	HE3	7.74	0.02	1
A	146	LYS	CG	24.3	0.2	1
A	137	LEU	C	179.0	0.2	1
A	153	TRP	HH2	7.16	0.02	1
A	128	TYR	HA	4.49	0.02	1
A	136	GLN	CA	59.7	0.2	1
A	133	THR	HB	3.75	0.02	1
A	142	GLU	H	8.61	0.02	1
A	145	ALA	CB	18.4	0.2	1
A	154	SER	CA	60.1	0.2	1
A	140	LYS	C	179.8	0.2	1
A	156	ASP	HB2	2.63	0.02	2
A	151	ASN	HB2	2.79	0.02	2
A	124	VAL	HB	2.03	0.02	1
A	131	ASN	C	175.1	0.2	1
A	155	GLU	CB	30.5	0.2	1
A	150	LEU	C	178.5	0.2	1
A	132	ASN	HB3	3.45	0.02	2
A	128	TYR	HD2	7.15	0.02	1
A	148	GLU	H	7.68	0.02	1
A	145	ALA	H	7.97	0.02	1
A	140	LYS	HE2	2.97	0.02	2
A	138	LEU	HD22	0.92	0.02	1
A	138	LEU	H	8.17	0.02	1
A	133	THR	N	122.9	0.2	1
A	131	ASN	CA	51.6	0.2	1
A	156	ASP	H	8.01	0.02	1
A	134	HIS	N	113.4	0.2	1
A	149	LYS	CE	42.1	0.2	1
A	138	LEU	CG	26.3	0.2	1
A	137	LEU	H	7.97	0.02	1
A	152	ILE	CB	37.2	0.2	1
A	136	GLN	HB3	2.14	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	136	GLN	C	178.3	0.2	1
A	130	PRO	HD3	3.45	0.02	2
A	135	GLU	HB2	2.21	0.02	2
A	139	ARG	HD3	3.14	0.02	2
A	137	LEU	HD11	0.72	0.02	1
A	140	LYS	HB2	1.71	0.02	2
A	128	TYR	CB	39.2	0.2	1
A	139	ARG	HB3	2.05	0.02	2
A	147	LYS	HG3	1.45	0.02	2
A	137	LEU	CB	42.0	0.2	1
A	146	LYS	CD	29.1	0.2	1
A	144	GLN	HB2	1.96	0.02	2
A	128	TYR	H	8.31	0.02	1
A	139	ARG	HG2	1.72	0.02	2
A	130	PRO	CA	62.3	0.2	1
A	137	LEU	HD13	0.72	0.02	1
A	149	LYS	CA	56.7	0.2	1
A	133	THR	HG22	0.68	0.02	1
A	134	HIS	CB	29.6	0.2	1
A	138	LEU	HD12	0.75	0.02	1
A	124	VAL	CB	32.8	0.2	1
A	150	LEU	HG	1.66	0.02	1
A	126	TYR	CB	39.0	0.2	1
A	148	GLU	HB3	2.14	0.02	2
A	147	LYS	HB2	2.0	0.02	2
A	134	HIS	HB2	2.31	0.02	2
A	146	LYS	HD3	0.82	0.02	2
A	147	LYS	HD2	1.68	0.02	2
A	124	VAL	HG22	0.89	0.02	2
A	134	HIS	H	6.93	0.02	1
A	153	TRP	CB	30.2	0.2	1
A	129	LYS	N	126.2	0.2	1
A	148	GLU	HA	4.03	0.02	1
A	143	ALA	HA	3.84	0.02	1
A	126	TYR	C	175.1	0.2	1
A	137	LEU	HD22	0.87	0.02	1
A	146	LYS	HB2	1.26	0.02	2
A	141	SER	H	7.83	0.02	1
A	124	VAL	HG21	0.89	0.02	2
A	150	LEU	HD13	1.0	0.02	2
A	135	GLU	HG2	2.21	0.02	2

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	135	GLU	HA	3.74	0.02	1
A	129	LYS	HD2	1.5	0.02	2
A	152	ILE	HA	3.38	0.02	1
A	153	TRP	HA	4.95	0.02	1
A	147	LYS	N	122.5	0.2	1
A	144	GLN	H	7.52	0.02	1
A	128	TYR	CA	58.1	0.2	1
A	137	LEU	CG	26.8	0.2	1
A	125	ALA	HB3	1.31	0.02	1
A	141	SER	HB2	3.65	0.02	2
A	129	LYS	HG2	1.37	0.02	2
A	146	LYS	HE2	2.22	0.02	2
A	128	TYR	HE2	6.82	0.02	1
A	155	GLU	HG2	2.41	0.02	2
A	135	GLU	C	177.2	0.2	1
A	151	ASN	CA	56.7	0.2	1
A	146	LYS	CA	59.5	0.2	1
A	150	LEU	CB	44.0	0.2	1
A	140	LYS	HG3	1.45	0.02	2
A	132	ASN	C	177.5	0.2	1
A	144	GLN	CB	28.0	0.2	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	149	-0.06 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	140	0.02 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	139	0.12 ± 0.15	None needed (< 0.5 ppm)
^{15}N	141	-0.09 ± 0.52	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 63%, i.e. 887 atoms were assigned a chemical shift out of a possible 1407. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	416/549 (76%)	164/219 (75%)	170/222 (77%)	82/108 (76%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	455/779 (58%)	284/456 (62%)	171/285 (60%)	0/38 (0%)
Aromatic	16/79 (20%)	14/41 (34%)	2/33 (6%)	0/5 (0%)
Overall	887/1407 (63%)	462/716 (65%)	343/540 (64%)	82/151 (54%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 1180 atoms were assigned a chemical shift out of a possible 1974. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	553/766 (72%)	219/305 (72%)	225/312 (72%)	109/149 (73%)
Sidechain	603/1065 (57%)	377/627 (60%)	226/387 (58%)	0/51 (0%)
Aromatic	24/143 (17%)	20/73 (27%)	4/61 (7%)	0/9 (0%)
Overall	1180/1974 (60%)	616/1005 (61%)	455/760 (60%)	109/209 (52%)

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	120	THR	HG23	4.33	2.29 – -0.01	13.9
1	A	120	THR	HG22	4.33	2.29 – -0.01	13.9
1	A	120	THR	HG21	4.33	2.29 – -0.01	13.9
1	A	44	THR	HG23	3.88	2.29 – -0.01	11.9
1	A	44	THR	HG22	3.88	2.29 – -0.01	11.9
1	A	44	THR	HG21	3.88	2.29 – -0.01	11.9

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:

