



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:55 AM BST

PDB ID : 2LE4
Title : Solution structure of the HMG box DNA-binding domain of human stem cell transcription factor Sox2
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Deposited on : 2011-06-06

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

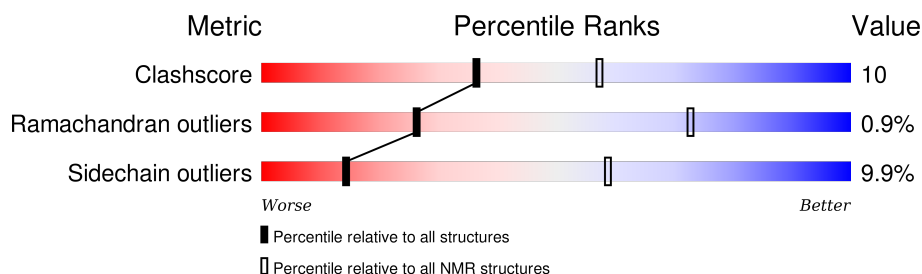
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	81	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:64 (58)	0.57	16

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1415 atoms, of which 721 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription factor SOX-2.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1415	431	721	141	117	5	

There is a discrepancy between the modelled and reference sequences:

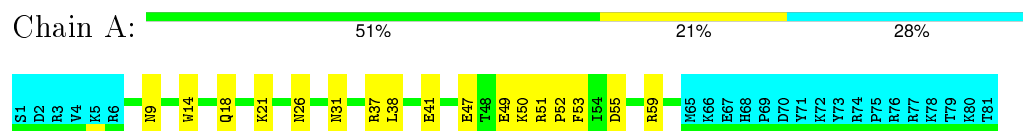
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP P48431

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 factor SOX-2

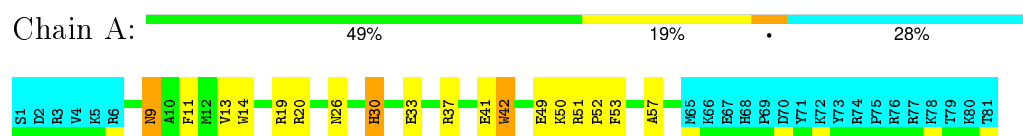


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

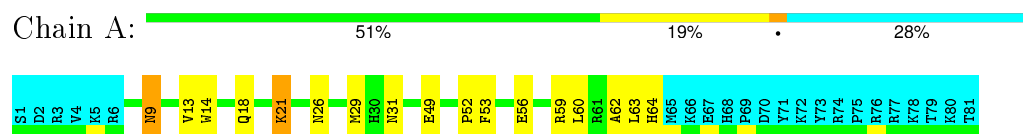
4.2.1 Score per residue for model 1

- Molecule 1: Transcription factor SOX-2



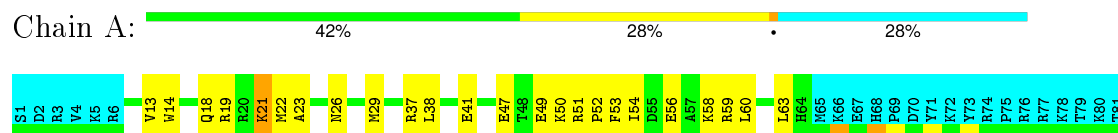
4.2.2 Score per residue for model 2

- Molecule 1: Transcription factor SOX-2



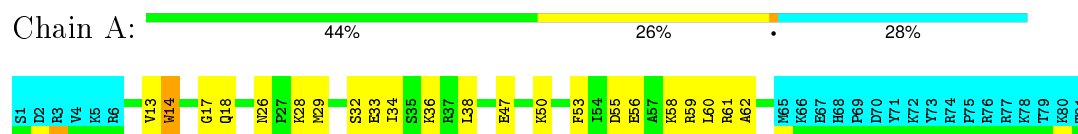
4.2.3 Score per residue for model 3

- Molecule 1: Transcription factor SOX-2



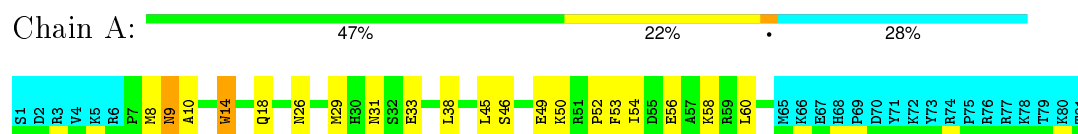
4.2.4 Score per residue for model 4

- Molecule 1: Transcription factor SOX-2



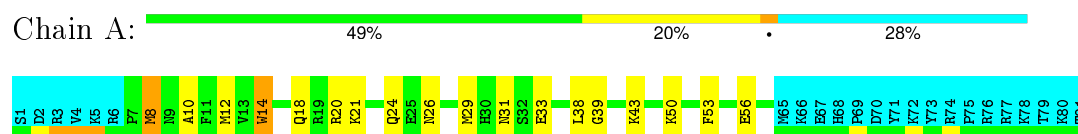
4.2.5 Score per residue for model 5

- Molecule 1: Transcription factor SOX-2



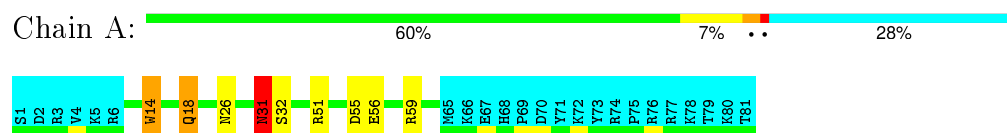
4.2.6 Score per residue for model 6

- Molecule 1: Transcription factor SOX-2



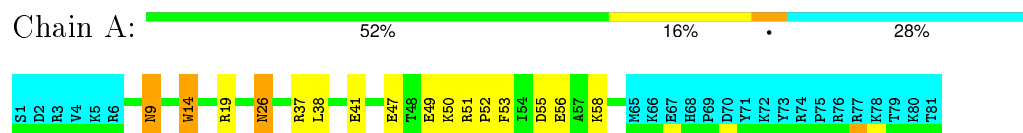
4.2.7 Score per residue for model 7

- Molecule 1: Transcription factor SOX-2



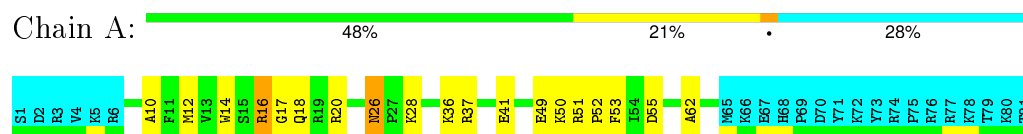
4.2.8 Score per residue for model 8

- Molecule 1: Transcription factor SOX-2



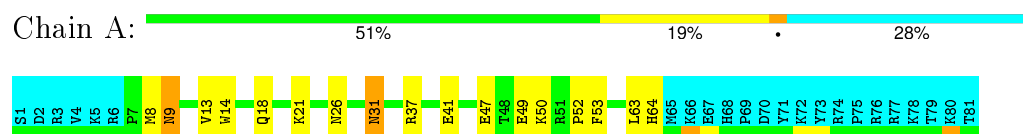
4.2.9 Score per residue for model 9

- Molecule 1: Transcription factor SOX-2



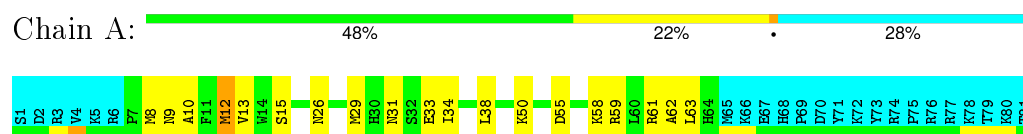
4.2.10 Score per residue for model 10

- Molecule 1: Transcription factor SOX-2



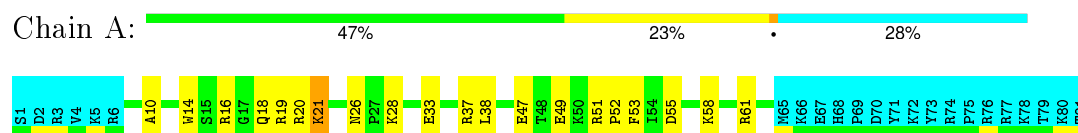
4.2.11 Score per residue for model 11

- Molecule 1: Transcription factor SOX-2



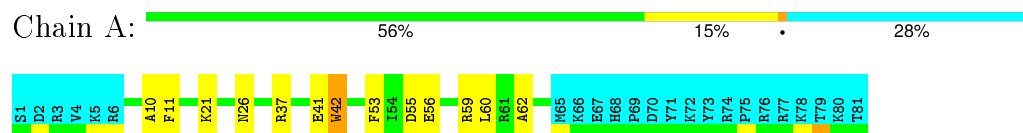
4.2.12 Score per residue for model 12

- Molecule 1: Transcription factor SOX-2



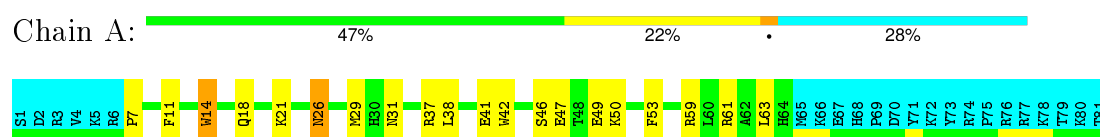
4.2.13 Score per residue for model 13

- Molecule 1: Transcription factor SOX-2



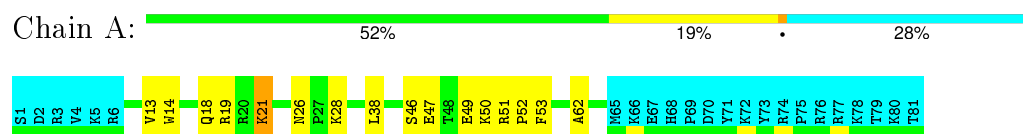
4.2.14 Score per residue for model 14

- Molecule 1: Transcription factor SOX-2



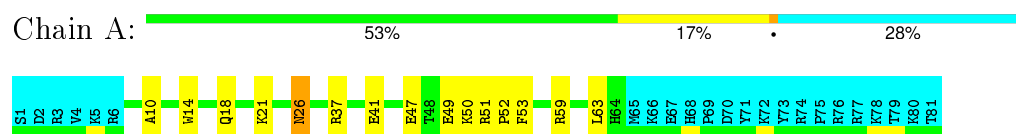
4.2.15 Score per residue for model 15

- Molecule 1: Transcription factor SOX-2



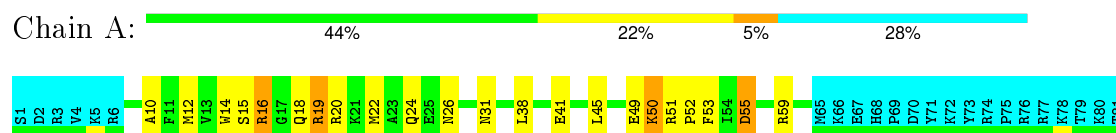
4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: Transcription factor SOX-2



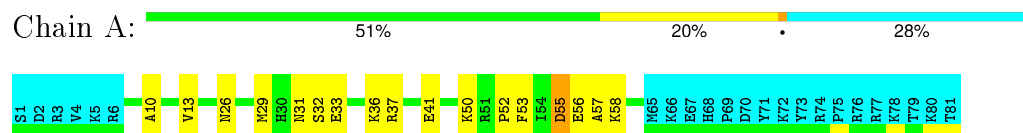
4.2.17 Score per residue for model 17

- Molecule 1: Transcription factor SOX-2



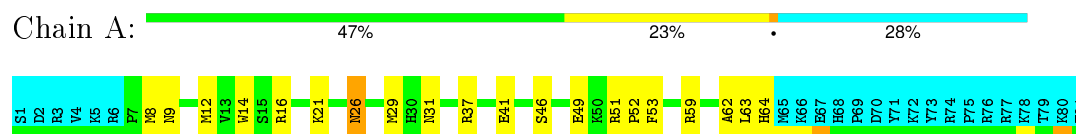
4.2.18 Score per residue for model 18

- Molecule 1: Transcription factor SOX-2



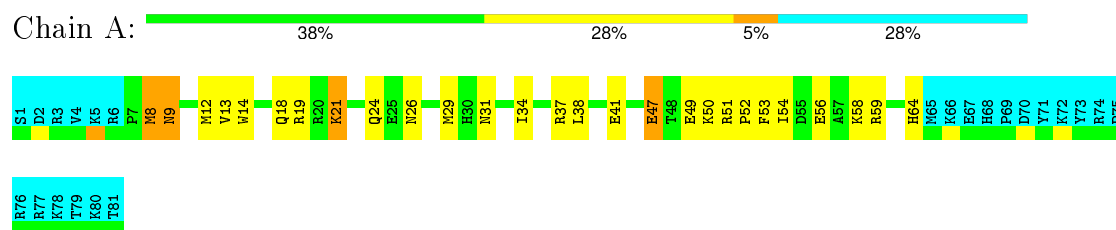
4.2.19 Score per residue for model 19

- Molecule 1: Transcription factor SOX-2



4.2.20 Score per residue for model 20

- Molecule 1: Transcription factor SOX-2



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CNS	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)	2le4_cs.str
Number of chemical shift lists	1
Total number of shifts	982
Number of shifts mapped to atoms	0
Number of unparsed shifts	982
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	485	498	496	10±3
All	All	9700	9960	9920	198

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:ARG:HG3	1:A:52:PRO:HD3	0.97	1.36	1	1
1:A:8:MET:HG3	1:A:12:MET:HB2	0.71	1.61	6	2
1:A:47:GLU:HG3	1:A:50:LYS:HD2	0.69	1.63	10	1
1:A:47:GLU:O	1:A:50:LYS:HG3	0.68	1.87	20	1
1:A:10:ALA:HB1	1:A:53:PHE:HB3	0.64	1.69	16	7
1:A:31:ASN:HD22	1:A:32:SER:N	0.64	1.90	7	1
1:A:14:TRP:O	1:A:18:GLN:HB2	0.63	1.93	7	2
1:A:55:ASP:HA	1:A:58:LYS:HD2	0.63	1.68	8	1
1:A:13:VAL:HG11	1:A:53:PHE:O	0.61	1.96	2	6
1:A:10:ALA:HA	1:A:13:VAL:HG22	0.61	1.73	11	1
1:A:11:PHE:HA	1:A:42:TRP:CZ2	0.60	2.31	1	3
1:A:14:TRP:CE3	1:A:38:LEU:HG	0.60	2.32	4	9
1:A:50:LYS:HA	1:A:53:PHE:CD1	0.60	2.31	9	3
1:A:37:ARG:O	1:A:41:GLU:HG2	0.60	1.95	13	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:SER:HB2	1:A:49:GLU:OE1	0.59	1.97	19	3
1:A:49:GLU:O	1:A:52:PRO:HD2	0.59	1.97	1	11
1:A:12:MET:O	1:A:16:ARG:HD3	0.58	1.97	9	1
1:A:10:ALA:HA	1:A:13:VAL:CG2	0.58	2.28	11	1
1:A:18:GLN:O	1:A:22:MET:HB2	0.58	1.99	3	2
1:A:50:LYS:O	1:A:53:PHE:HB2	0.56	2.01	9	8
1:A:52:PRO:O	1:A:56:GLU:HG2	0.55	2.01	18	2
1:A:28:LYS:HD3	1:A:28:LYS:O	0.55	2.02	12	2
1:A:50:LYS:O	1:A:50:LYS:HD2	0.55	2.02	17	1
1:A:14:TRP:O	1:A:18:GLN:HB3	0.54	2.02	6	4
1:A:19:ARG:HG2	1:A:34:ILE:HD12	0.54	1.80	20	1
1:A:56:GLU:OE1	1:A:59:ARG:HD3	0.54	2.03	13	1
1:A:39:GLY:O	1:A:43:LYS:HG3	0.54	2.03	6	1
1:A:59:ARG:O	1:A:63:LEU:HG	0.54	2.01	3	5
1:A:51:ARG:CG	1:A:52:PRO:HD3	0.54	2.24	1	1
1:A:10:ALA:HB1	1:A:53:PHE:CD2	0.53	2.38	6	2
1:A:51:ARG:HG3	1:A:52:PRO:CD	0.53	2.24	1	1
1:A:12:MET:O	1:A:16:ARG:HD2	0.53	2.04	17	1
1:A:55:ASP:O	1:A:59:ARG:HG2	0.52	2.05	7	1
1:A:56:GLU:O	1:A:60:LEU:HG	0.52	2.05	4	5
1:A:14:TRP:CZ3	1:A:38:LEU:HG	0.52	2.39	17	10
1:A:14:TRP:CD1	1:A:18:GLN:HB2	0.51	2.40	4	1
1:A:14:TRP:HB2	1:A:53:PHE:CD2	0.51	2.40	3	7
1:A:50:LYS:HA	1:A:53:PHE:HD1	0.51	1.66	9	1
1:A:32:SER:O	1:A:36:LYS:HG2	0.51	2.05	4	2
1:A:14:TRP:HB2	1:A:53:PHE:CE2	0.50	2.41	15	2
1:A:26:ASN:N	1:A:26:ASN:HD22	0.50	2.03	16	2
1:A:31:ASN:HA	1:A:34:ILE:HD12	0.50	1.84	11	1
1:A:18:GLN:HA	1:A:21:LYS:HG2	0.49	1.82	14	4
1:A:17:GLY:HA2	1:A:20:ARG:NH1	0.49	2.22	9	1
1:A:55:ASP:HA	1:A:58:LYS:CD	0.48	2.39	8	1
1:A:49:GLU:C	1:A:52:PRO:HD2	0.48	2.28	1	2
1:A:50:LYS:HA	1:A:53:PHE:CD2	0.48	2.43	1	1
1:A:47:GLU:O	1:A:50:LYS:HB2	0.48	2.08	4	1
1:A:21:LYS:HA	1:A:24:GLN:HG2	0.48	1.86	20	1
1:A:17:GLY:HA2	1:A:60:LEU:HD21	0.47	1.86	4	1
1:A:13:VAL:HG21	1:A:57:ALA:HB2	0.47	1.85	1	1
1:A:52:PRO:HA	1:A:55:ASP:HB3	0.47	1.86	9	1
1:A:8:MET:HG2	1:A:12:MET:SD	0.46	2.50	19	1
1:A:55:ASP:O	1:A:59:ARG:HD2	0.46	2.10	13	1
1:A:8:MET:HB3	1:A:12:MET:HB3	0.46	1.86	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:ASN:HD22	1:A:26:ASN:N	0.46	2.08	14	3
1:A:10:ALA:CA	1:A:13:VAL:HG22	0.46	2.40	11	1
1:A:18:GLN:OE1	1:A:21:LYS:HD2	0.45	2.12	15	2
1:A:50:LYS:HA	1:A:53:PHE:HD2	0.45	1.71	1	1
1:A:19:ARG:HH12	1:A:23:ALA:HB2	0.45	1.71	3	1
1:A:50:LYS:O	1:A:50:LYS:HD3	0.45	2.11	18	1
1:A:51:ARG:HB3	1:A:52:PRO:HD3	0.45	1.89	9	6
1:A:15:SER:HA	1:A:38:LEU:HD11	0.45	1.88	11	1
1:A:16:ARG:HA	1:A:19:ARG:HD2	0.44	1.88	12	1
1:A:15:SER:O	1:A:19:ARG:HB2	0.44	2.13	17	1
1:A:54:ILE:O	1:A:58:LYS:HG2	0.44	2.13	5	2
1:A:20:ARG:O	1:A:24:GLN:HG2	0.44	2.12	17	1
1:A:54:ILE:O	1:A:58:LYS:HG3	0.44	2.13	3	1
1:A:56:GLU:OE1	1:A:59:ARG:HD2	0.44	2.13	20	1
1:A:55:ASP:HA	1:A:58:LYS:HE2	0.43	1.90	4	2
1:A:9:ASN:HD22	1:A:9:ASN:C	0.43	2.17	5	3
1:A:55:ASP:O	1:A:59:ARG:HG3	0.43	2.14	4	2
1:A:45:LEU:HD12	1:A:49:GLU:HB2	0.43	1.91	5	1
1:A:58:LYS:O	1:A:61:ARG:HG2	0.42	2.14	11	1
1:A:41:GLU:O	1:A:45:LEU:HB3	0.42	2.14	17	1
1:A:47:GLU:HG2	1:A:51:ARG:NH1	0.42	2.29	16	1
1:A:16:ARG:HA	1:A:19:ARG:CD	0.42	2.43	12	1
1:A:55:ASP:HA	1:A:58:LYS:CE	0.42	2.44	18	1
1:A:9:ASN:O	1:A:13:VAL:HG23	0.42	2.14	1	3
1:A:13:VAL:HG11	1:A:57:ALA:N	0.42	2.30	18	1
1:A:29:MET:SD	1:A:29:MET:N	0.42	2.93	2	1
1:A:51:ARG:HH12	1:A:55:ASP:HB2	0.41	1.74	17	1
1:A:7:PRO:HG3	1:A:61:ARG:HG3	0.41	1.92	14	1
1:A:33:GLU:O	1:A:37:ARG:HD3	0.41	2.15	12	1
1:A:14:TRP:HH2	1:A:41:GLU:HB2	0.41	1.76	19	1
1:A:18:GLN:OE1	1:A:21:LYS:HD3	0.40	2.16	10	1
1:A:18:GLN:HA	1:A:18:GLN:OE1	0.40	2.16	9	1
1:A:33:GLU:H	1:A:33:GLU:CD	0.40	2.20	5	1
1:A:18:GLN:O	1:A:21:LYS:HG2	0.40	2.16	16	1
1:A:37:ARG:O	1:A:41:GLU:HG3	0.40	2.16	19	1
1:A:17:GLY:HA2	1:A:20:ARG:HH11	0.40	1.77	9	1
1:A:29:MET:HB2	1:A:33:GLU:HB2	0.40	1.92	4	1
1:A:34:ILE:O	1:A:38:LEU:HD13	0.40	2.16	4	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	58/81 (72%)	56±1 (96±2%)	2±1 (3±2%)	1±1 (1±1%)	26	73
All	All	1160/1620 (72%)	1110 (96%)	40 (3%)	10 (1%)	26	73

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	31	ASN	9
1	A	30	HIS	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	51/74 (69%)	46±2 (90±4%)	5±2 (10±4%)	14	59
All	All	1020/1480 (69%)	919 (90%)	101 (10%)	14	59

All 26 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	26	ASN	20
1	A	14	TRP	9
1	A	9	ASN	8
1	A	21	LYS	8
1	A	29	MET	8
1	A	47	GLU	6
1	A	8	MET	4
1	A	19	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	33	GLU	4
1	A	56	GLU	3
1	A	31	ASN	3
1	A	16	ARG	3
1	A	20	ARG	3
1	A	42	TRP	2
1	A	50	LYS	2
1	A	55	ASP	2
1	A	28	LYS	2
1	A	51	ARG	2
1	A	61	ARG	1
1	A	59	ARG	1
1	A	24	GLN	1
1	A	12	MET	1
1	A	18	GLN	1
1	A	36	LYS	1
1	A	30	HIS	1
1	A	46	SER	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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: 2le4_cs.str

Chemical shift list name: *sox2A_{sn}*

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	982
Number of shifts mapped to atoms	0
Number of unparsed shifts	982
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. All 982 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	.	1	SER	HA	4.510	0.020	1
2	.	1	SER	HB2	3.875	0.020	2
3	.	1	SER	HB3	3.870	0.020	2
4	.	1	SER	CA	57.159	0.400	1
5	.	1	SER	CB	69.697	0.400	1
6	.	2	ASP	HA	4.651	0.020	1
7	.	2	ASP	HB2	2.592	0.020	2
8	.	2	ASP	HB3	2.694	0.020	2
9	.	2	ASP	C	175.913	0.400	1
10	.	2	ASP	CA	54.239	0.400	1
11	.	2	ASP	CB	41.055	0.400	1
12	.	2	ASP	N	118.843	0.400	1
13	.	3	ARG	HA	4.278	0.020	1
14	.	3	ARG	HB2	1.740	0.020	2
15	.	3	ARG	HB3	1.794	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	.	3	ARG	HG2	1.573	0.020	2
17	.	3	ARG	HG3	1.609	0.020	2
18	.	3	ARG	HD2	3.188	0.020	2
19	.	3	ARG	HD3	3.147	0.020	2
20	.	3	ARG	C	176.171	0.400	1
21	.	3	ARG	CA	56.148	0.400	1
22	.	3	ARG	CB	30.596	0.400	1
23	.	3	ARG	CG	27.087	0.400	1
24	.	3	ARG	CD	43.028	0.400	1
25	.	3	ARG	N	121.675	0.400	1
26	.	4	VAL	HA	4.001	0.020	1
27	.	4	VAL	HB	1.974	0.020	1
28	.	4	VAL	HG11	0.860	0.020	2
29	.	4	VAL	HG12	0.860	0.020	2
30	.	4	VAL	HG13	0.860	0.020	2
31	.	4	VAL	HG21	0.877	0.020	2
32	.	4	VAL	HG22	0.877	0.020	2
33	.	4	VAL	HG23	0.877	0.020	2
34	.	4	VAL	C	175.866	0.400	1
35	.	4	VAL	CA	62.301	0.400	1
36	.	4	VAL	CB	32.516	0.400	1
37	.	4	VAL	CG1	20.690	0.400	1
38	.	4	VAL	CG2	20.848	0.400	1
39	.	4	VAL	N	121.849	0.400	1
40	.	5	LYS	HA	4.282	0.020	1
41	.	5	LYS	HB2	1.718	0.020	2
42	.	5	LYS	HB3	1.749	0.020	2
43	.	5	LYS	HG2	1.411	0.020	2
44	.	5	LYS	HG3	1.650	0.020	2
45	.	5	LYS	HD2	1.615	0.020	2
46	.	5	LYS	HD3	1.610	0.020	2
47	.	5	LYS	HE2	2.971	0.020	2
48	.	5	LYS	HE3	2.930	0.020	2
49	.	5	LYS	C	176.233	0.400	1
50	.	5	LYS	CA	56.115	0.400	1
51	.	5	LYS	CB	32.650	0.400	1
52	.	5	LYS	CG	24.865	0.400	1
53	.	5	LYS	CD	29.559	0.400	1
54	.	5	LYS	CE	41.893	0.400	1
55	.	5	LYS	N	126.382	0.400	1
56	.	6	ARG	HA	3.994	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	.	6	ARG	HB2	1.617	0.020	2
58	.	6	ARG	HB3	1.758	0.020	2
59	.	6	ARG	HG2	1.596	0.020	2
60	.	6	ARG	HG3	1.580	0.020	2
61	.	6	ARG	HD2	3.142	0.020	2
62	.	6	ARG	HD3	3.094	0.020	2
63	.	6	ARG	CA	53.568	0.400	1
64	.	6	ARG	CB	30.020	0.400	1
65	.	6	ARG	CG	27.169	0.400	1
66	.	6	ARG	CD	43.614	0.400	1
67	.	6	ARG	N	123.296	0.400	1
68	.	7	PRO	HA	4.324	0.020	1
69	.	7	PRO	HB2	2.070	0.020	2
70	.	7	PRO	HB3	1.780	0.020	2
71	.	7	PRO	HG2	1.953	0.020	2
72	.	7	PRO	HG3	1.968	0.020	2
73	.	7	PRO	HD2	3.549	0.020	2
74	.	7	PRO	HD3	3.352	0.020	2
75	.	7	PRO	C	176.264	0.400	1
76	.	7	PRO	CA	62.453	0.400	1
77	.	7	PRO	CB	31.557	0.400	1
78	.	7	PRO	CG	27.144	0.400	1
79	.	7	PRO	CD	49.976	0.400	1
80	.	8	MET	HA	4.471	0.020	1
81	.	8	MET	HB2	1.888	0.020	2
82	.	8	MET	HB3	1.975	0.020	2
83	.	8	MET	HG2	2.603	0.020	2
84	.	8	MET	HG3	2.534	0.020	2
85	.	8	MET	HE1	2.098	0.020	1
86	.	8	MET	HE2	2.098	0.020	1
87	.	8	MET	HE3	2.098	0.020	1
88	.	8	MET	C	175.348	0.400	1
89	.	8	MET	CA	55.786	0.400	1
90	.	8	MET	CB	32.465	0.400	1
91	.	8	MET	CG	32.393	0.400	1
92	.	8	MET	CE	17.109	0.400	1
93	.	8	MET	N	120.952	0.400	1
94	.	9	ASN	HA	4.777	0.020	1
95	.	9	ASN	HB2	2.932	0.020	2
96	.	9	ASN	HB3	3.397	0.020	2
97	.	9	ASN	HD21	7.534	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	.	9	ASN	HD22	6.993	0.020	1
99	.	9	ASN	C	174.710	0.400	1
100	.	9	ASN	CA	51.094	0.400	1
101	.	9	ASN	CB	39.793	0.400	1
102	.	9	ASN	N	119.985	0.400	1
103	.	9	ASN	ND2	111.227	0.400	1
104	.	10	ALA	HA	3.923	0.020	1
105	.	10	ALA	HB1	1.680	0.020	1
106	.	10	ALA	HB2	1.680	0.020	1
107	.	10	ALA	HB3	1.680	0.020	1
108	.	10	ALA	C	177.482	0.400	1
109	.	10	ALA	CA	55.910	0.400	1
110	.	10	ALA	CB	19.580	0.400	1
111	.	10	ALA	N	121.997	0.400	1
112	.	11	PHE	HA	4.333	0.020	1
113	.	11	PHE	HB2	2.765	0.020	2
114	.	11	PHE	HB3	2.725	0.020	2
115	.	11	PHE	HD1	6.407	0.020	1
116	.	11	PHE	HD2	6.407	0.020	1
117	.	11	PHE	HE1	7.227	0.020	1
118	.	11	PHE	HE2	7.227	0.020	1
119	.	11	PHE	HZ	7.219	0.020	1
120	.	11	PHE	C	178.569	0.400	1
121	.	11	PHE	CA	59.799	0.400	1
122	.	11	PHE	CB	38.000	0.400	1
123	.	11	PHE	CD1	131.882	0.400	1
124	.	11	PHE	CE1	130.880	0.400	1
125	.	11	PHE	CZ	129.210	0.400	1
126	.	11	PHE	N	118.296	0.400	1
127	.	12	MET	HA	3.637	0.020	1
128	.	12	MET	HB2	2.162	0.020	2
129	.	12	MET	HB3	2.109	0.020	2
130	.	12	MET	HG2	2.628	0.020	2
131	.	12	MET	HG3	2.830	0.020	2
132	.	12	MET	HE1	1.759	0.020	1
133	.	12	MET	HE2	1.759	0.020	1
134	.	12	MET	HE3	1.759	0.020	1
135	.	12	MET	C	178.582	0.400	1
136	.	12	MET	CA	58.695	0.400	1
137	.	12	MET	CB	33.013	0.400	1
138	.	12	MET	CG	32.433	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	.	12	MET	CE	16.629	0.400	1
140	.	12	MET	N	121.709	0.400	1
141	.	13	VAL	HA	3.563	0.020	1
142	.	13	VAL	HB	2.472	0.020	1
143	.	13	VAL	HG11	1.248	0.020	2
144	.	13	VAL	HG12	1.248	0.020	2
145	.	13	VAL	HG13	1.248	0.020	2
146	.	13	VAL	HG21	1.066	0.020	2
147	.	13	VAL	HG22	1.066	0.020	2
148	.	13	VAL	HG23	1.066	0.020	2
149	.	13	VAL	CA	66.518	0.400	1
150	.	13	VAL	CB	32.170	0.400	1
151	.	13	VAL	CG1	22.297	0.400	1
152	.	13	VAL	CG2	23.027	0.400	1
153	.	13	VAL	N	119.989	0.400	1
154	.	14	TRP	HA	3.620	0.020	1
155	.	14	TRP	HB2	2.285	0.020	2
156	.	14	TRP	HB3	2.709	0.020	2
157	.	14	TRP	HD1	7.160	0.020	1
158	.	14	TRP	HE3	6.947	0.020	1
159	.	14	TRP	HZ2	7.140	0.020	1
160	.	14	TRP	HZ3	7.181	0.020	1
161	.	14	TRP	HH2	7.423	0.020	1
162	.	14	TRP	C	178.314	0.400	1
163	.	14	TRP	CA	61.149	0.400	1
164	.	14	TRP	CB	29.354	0.400	1
165	.	14	TRP	CD1	127.680	0.400	1
166	.	14	TRP	CE3	120.335	0.400	1
167	.	14	TRP	CZ2	114.213	0.400	1
168	.	14	TRP	CZ3	122.405	0.400	1
169	.	14	TRP	CH2	124.316	0.400	1
170	.	14	TRP	N	122.034	0.400	1
171	.	15	SER	HA	3.008	0.020	1
172	.	15	SER	HB2	3.170	0.020	2
173	.	15	SER	HB3	3.426	0.020	2
174	.	15	SER	C	175.106	0.400	1
175	.	15	SER	CA	61.527	0.400	1
176	.	15	SER	CB	62.842	0.400	1
177	.	15	SER	N	113.240	0.400	1
178	.	16	ARG	HA	3.880	0.020	1
179	.	16	ARG	HB2	1.954	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	.	16	ARG	HB3	1.798	0.020	2
181	.	16	ARG	HG2	1.657	0.020	2
182	.	16	ARG	HG3	1.566	0.020	2
183	.	16	ARG	HD2	3.117	0.020	2
184	.	16	ARG	HD3	3.164	0.020	2
185	.	16	ARG	C	178.769	0.400	1
186	.	16	ARG	CA	59.555	0.400	1
187	.	16	ARG	CB	29.618	0.400	1
188	.	16	ARG	CG	26.573	0.400	1
189	.	16	ARG	CD	43.100	0.400	1
190	.	16	ARG	N	122.033	0.400	1
191	.	17	GLY	HA2	3.891	0.020	1
192	.	17	GLY	C	176.252	0.400	1
193	.	17	GLY	CA	46.024	0.400	1
194	.	17	GLY	N	105.042	0.400	1
195	.	18	GLN	HA	3.825	0.020	1
196	.	18	GLN	HB2	1.265	0.020	2
197	.	18	GLN	HB3	0.788	0.020	2
198	.	18	GLN	HG2	0.984	0.020	2
199	.	18	GLN	HG3	1.373	0.020	2
200	.	18	GLN	HE21	7.159	0.020	2
201	.	18	GLN	HE22	6.668	0.020	2
202	.	18	GLN	C	177.801	0.400	1
203	.	18	GLN	CA	57.116	0.400	1
204	.	18	GLN	CB	28.482	0.400	1
205	.	18	GLN	CG	31.177	0.400	1
206	.	18	GLN	N	120.707	0.400	1
207	.	18	GLN	NE2	111.899	0.400	1
208	.	19	ARG	HA	3.636	0.020	1
209	.	19	ARG	HB2	1.736	0.020	2
210	.	19	ARG	HB3	1.672	0.020	2
211	.	19	ARG	HG2	1.557	0.020	2
212	.	19	ARG	HG3	1.586	0.020	2
213	.	19	ARG	HD2	3.151	0.020	2
214	.	19	ARG	HD3	3.130	0.020	2
215	.	19	ARG	C	177.426	0.400	1
216	.	19	ARG	CA	59.783	0.400	1
217	.	19	ARG	CB	29.609	0.400	1
218	.	19	ARG	CG	27.025	0.400	1
219	.	19	ARG	CD	42.106	0.400	1
220	.	19	ARG	N	119.689	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	.	20	ARG	HA	4.010	0.020	1
222	.	20	ARG	HB2	1.822	0.020	2
223	.	20	ARG	HB3	1.788	0.020	2
224	.	20	ARG	HG2	1.641	0.020	2
225	.	20	ARG	HG3	1.558	0.020	2
226	.	20	ARG	HD2	3.176	0.020	2
227	.	20	ARG	HD3	3.119	0.020	2
228	.	20	ARG	C	178.365	0.400	1
229	.	20	ARG	CA	59.070	0.400	1
230	.	20	ARG	CB	29.590	0.400	1
231	.	20	ARG	CG	27.503	0.400	1
232	.	20	ARG	CD	43.159	0.400	1
233	.	20	ARG	N	117.193	0.400	1
234	.	21	LYS	HA	4.010	0.020	1
235	.	21	LYS	HB2	1.759	0.020	2
236	.	21	LYS	HB3	1.699	0.020	2
237	.	21	LYS	HG2	1.244	0.020	2
238	.	21	LYS	HG3	1.381	0.020	2
239	.	21	LYS	HD2	1.582	0.020	2
240	.	21	LYS	HD3	1.610	0.020	2
241	.	21	LYS	HE2	2.936	0.020	2
242	.	21	LYS	HE3	2.912	0.020	2
243	.	21	LYS	CA	59.172	0.400	1
244	.	21	LYS	CB	32.689	0.400	1
245	.	21	LYS	CG	24.606	0.400	1
246	.	21	LYS	CD	29.149	0.400	1
247	.	21	LYS	CE	41.910	0.400	1
248	.	21	LYS	N	119.705	0.400	1
249	.	22	MET	HA	4.031	0.020	1
250	.	22	MET	HB2	2.582	0.020	2
251	.	22	MET	HB3	2.463	0.020	2
252	.	22	MET	HG2	1.827	0.020	2
253	.	22	MET	HG3	2.118	0.020	2
254	.	22	MET	HE1	2.011	0.020	1
255	.	22	MET	HE2	2.011	0.020	1
256	.	22	MET	HE3	2.011	0.020	1
257	.	22	MET	C	178.572	0.400	1
258	.	22	MET	CA	59.255	0.400	1
259	.	22	MET	CB	32.220	0.400	1
260	.	22	MET	CG	32.788	0.400	1
261	.	22	MET	CE	17.255	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	.	22	MET	N	118.108	0.400	1
263	.	23	ALA	HA	4.058	0.020	1
264	.	23	ALA	HB1	1.390	0.020	1
265	.	23	ALA	HB2	1.390	0.020	1
266	.	23	ALA	HB3	1.390	0.020	1
267	.	23	ALA	C	179.539	0.400	1
268	.	23	ALA	CA	54.403	0.400	1
269	.	23	ALA	CB	18.150	0.400	1
270	.	23	ALA	N	120.771	0.400	1
271	.	24	GLN	HA	3.992	0.020	1
272	.	24	GLN	HB2	2.154	0.020	2
273	.	24	GLN	HB3	2.087	0.020	2
274	.	24	GLN	HG2	2.462	0.020	2
275	.	24	GLN	HG3	2.374	0.020	2
276	.	24	GLN	HE21	7.174	0.020	2
277	.	24	GLN	HE22	7.138	0.020	2
278	.	24	GLN	C	178.077	0.400	1
279	.	24	GLN	CA	57.930	0.400	1
280	.	24	GLN	CB	28.619	0.400	1
281	.	24	GLN	CG	33.874	0.400	1
282	.	24	GLN	N	116.217	0.400	1
283	.	24	GLN	NE2	111.668	0.400	1
284	.	25	GLU	HA	4.084	0.020	1
285	.	25	GLU	HB2	2.006	0.020	1
286	.	25	GLU	HB3	1.948	0.020	1
287	.	25	GLU	HG2	2.483	0.020	2
288	.	25	GLU	HG3	2.235	0.020	2
289	.	25	GLU	C	176.439	0.400	1
290	.	25	GLU	CA	57.383	0.400	1
291	.	25	GLU	CB	30.420	0.400	1
292	.	25	GLU	CG	36.464	0.400	1
293	.	25	GLU	N	116.566	0.400	1
294	.	26	ASN	HA	5.159	0.020	1
295	.	26	ASN	HB2	2.913	0.020	2
296	.	26	ASN	HB3	2.580	0.020	2
297	.	26	ASN	HD21	7.678	0.020	1
298	.	26	ASN	HD22	7.519	0.020	1
299	.	26	ASN	CA	50.875	0.400	1
300	.	26	ASN	CB	40.083	0.400	1
301	.	26	ASN	N	114.776	0.400	1
302	.	26	ASN	ND2	116.063	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	.	27	PRO	HA	4.541	0.020	1
304	.	27	PRO	HB2	1.975	0.020	2
305	.	27	PRO	HB3	1.867	0.020	2
306	.	27	PRO	HG2	1.940	0.020	2
307	.	27	PRO	HG3	2.020	0.020	2
308	.	27	PRO	HD2	3.399	0.020	2
309	.	27	PRO	HD3	3.671	0.020	2
310	.	27	PRO	C	177.520	0.400	1
311	.	27	PRO	CA	64.560	0.400	1
312	.	27	PRO	CB	32.088	0.400	1
313	.	27	PRO	CG	27.183	0.400	1
314	.	27	PRO	CD	50.276	0.400	1
315	.	28	LYS	HA	4.302	0.020	1
316	.	28	LYS	HB2	1.745	0.020	2
317	.	28	LYS	HB3	1.946	0.020	2
318	.	28	LYS	HG2	1.480	0.020	2
319	.	28	LYS	HG3	1.371	0.020	2
320	.	28	LYS	HD2	1.663	0.020	2
321	.	28	LYS	HD3	1.594	0.020	2
322	.	28	LYS	HE2	2.981	0.020	2
323	.	28	LYS	HE3	2.930	0.020	2
324	.	28	LYS	C	176.853	0.400	1
325	.	28	LYS	CA	55.599	0.400	1
326	.	28	LYS	CB	31.972	0.400	1
327	.	28	LYS	CG	25.229	0.400	1
328	.	28	LYS	CD	28.795	0.400	1
329	.	28	LYS	CE	41.955	0.400	1
330	.	28	LYS	N	116.066	0.400	1
331	.	29	MET	HA	4.116	0.020	1
332	.	29	MET	HB2	1.979	0.020	2
333	.	29	MET	HB3	1.986	0.020	2
334	.	29	MET	HG2	1.629	0.020	2
335	.	29	MET	HG3	2.553	0.020	2
336	.	29	MET	HE1	1.980	0.020	1
337	.	29	MET	HE2	1.980	0.020	1
338	.	29	MET	HE3	1.980	0.020	1
339	.	29	MET	C	175.852	0.400	1
340	.	29	MET	CA	56.586	0.400	1
341	.	29	MET	CB	34.353	0.400	1
342	.	29	MET	CG	32.447	0.400	1
343	.	29	MET	CE	16.960	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	.	29	MET	N	121.363	0.400	1
345	.	30	HIS	HA	4.314	0.020	1
346	.	30	HIS	HB2	1.761	0.020	2
347	.	30	HIS	HB3	1.771	0.020	2
348	.	30	HIS	HD2	7.260	0.020	1
349	.	30	HIS	HE1	8.080	0.020	1
350	.	30	HIS	C	176.054	0.400	1
351	.	30	HIS	CA	55.546	0.400	1
352	.	30	HIS	CB	30.434	0.400	1
353	.	30	HIS	CD2	119.840	0.400	1
354	.	30	HIS	CE1	136.050	0.400	1
355	.	30	HIS	N	125.035	0.400	1
356	.	31	ASN	HA	4.270	0.020	1
357	.	31	ASN	HB2	2.800	0.020	2
358	.	31	ASN	HB3	2.725	0.020	2
359	.	31	ASN	HD21	7.507	0.020	1
360	.	31	ASN	HD22	7.262	0.020	1
361	.	31	ASN	C	176.580	0.400	1
362	.	31	ASN	CA	56.029	0.400	1
363	.	31	ASN	CB	32.241	0.400	1
364	.	31	ASN	N	123.880	0.400	1
365	.	31	ASN	ND2	114.908	0.400	1
366	.	32	SER	HA	4.247	0.020	1
367	.	32	SER	HB2	4.004	0.020	2
368	.	32	SER	HB3	3.944	0.020	2
369	.	32	SER	C	176.838	0.400	1
370	.	32	SER	CA	61.606	0.400	1
371	.	32	SER	CB	69.767	0.400	1
372	.	32	SER	N	116.760	0.400	1
373	.	33	GLU	HA	4.220	0.020	1
374	.	33	GLU	HB2	2.234	0.020	2
375	.	33	GLU	HB3	2.182	0.020	2
376	.	33	GLU	HG2	2.408	0.020	2
377	.	33	GLU	HG3	3.235	0.020	2
378	.	33	GLU	C	178.675	0.400	1
379	.	33	GLU	CA	58.491	0.400	1
380	.	33	GLU	CB	29.355	0.400	1
381	.	33	GLU	CG	36.124	0.400	1
382	.	33	GLU	N	124.395	0.400	1
383	.	34	ILE	HA	3.679	0.020	1
384	.	34	ILE	HB	2.012	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	.	34	ILE	HG12	1.008	0.020	2
386	.	34	ILE	HG13	1.605	0.020	2
387	.	34	ILE	HG21	0.956	0.020	1
388	.	34	ILE	HG22	0.956	0.020	1
389	.	34	ILE	HG23	0.956	0.020	1
390	.	34	ILE	HD11	0.815	0.020	1
391	.	34	ILE	HD12	0.815	0.020	1
392	.	34	ILE	HD13	0.815	0.020	1
393	.	34	ILE	C	177.895	0.400	1
394	.	34	ILE	CA	65.752	0.400	1
395	.	34	ILE	CB	37.506	0.400	1
396	.	34	ILE	CG1	28.771	0.400	1
397	.	34	ILE	CG2	17.196	0.400	1
398	.	34	ILE	CD1	12.603	0.400	1
399	.	34	ILE	N	121.456	0.400	1
400	.	35	SER	HA	4.176	0.020	1
401	.	35	SER	HB2	4.019	0.020	2
402	.	35	SER	HB3	4.073	0.020	2
403	.	35	SER	C	176.977	0.400	1
404	.	35	SER	CA	62.515	0.400	1
405	.	35	SER	CB	62.422	0.400	1
406	.	35	SER	N	114.162	0.400	1
407	.	36	LYS	HA	4.085	0.020	1
408	.	36	LYS	HB2	1.978	0.020	2
409	.	36	LYS	HB3	1.583	0.020	2
410	.	36	LYS	HG2	1.425	0.020	2
411	.	36	LYS	HG3	1.652	0.020	2
412	.	36	LYS	HD2	1.612	0.020	2
413	.	36	LYS	HD3	1.610	0.020	2
414	.	36	LYS	HE2	2.924	0.020	2
415	.	36	LYS	HE3	2.939	0.020	2
416	.	36	LYS	C	179.331	0.400	1
417	.	36	LYS	CA	59.431	0.400	1
418	.	36	LYS	CB	32.601	0.400	1
419	.	36	LYS	CG	25.145	0.400	1
420	.	36	LYS	CD	28.780	0.400	1
421	.	36	LYS	CE	41.780	0.400	1
422	.	36	LYS	N	122.601	0.400	1
423	.	37	ARG	HA	4.220	0.020	1
424	.	37	ARG	HB2	1.976	0.020	2
425	.	37	ARG	HB3	1.706	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	.	37	ARG	HG2	1.736	0.020	2
427	.	37	ARG	HG3	1.807	0.020	2
428	.	37	ARG	HD2	3.194	0.020	2
429	.	37	ARG	HD3	3.223	0.020	2
430	.	37	ARG	C	179.087	0.400	1
431	.	37	ARG	CA	59.128	0.400	1
432	.	37	ARG	CB	29.904	0.400	1
433	.	37	ARG	CG	27.681	0.400	1
434	.	37	ARG	CD	43.112	0.400	1
435	.	37	ARG	N	120.938	0.400	1
436	.	38	LEU	HA	4.411	0.020	1
437	.	38	LEU	HB2	2.204	0.020	2
438	.	38	LEU	HB3	1.722	0.020	2
439	.	38	LEU	HG	2.422	0.020	1
440	.	38	LEU	HD11	0.684	0.020	2
441	.	38	LEU	HD12	0.684	0.020	2
442	.	38	LEU	HD13	0.684	0.020	2
443	.	38	LEU	HD21	0.590	0.020	2
444	.	38	LEU	HD22	0.590	0.020	2
445	.	38	LEU	HD23	0.590	0.020	2
446	.	38	LEU	C	179.548	0.400	1
447	.	38	LEU	CA	58.137	0.400	1
448	.	38	LEU	CB	41.701	0.400	1
449	.	38	LEU	CG	29.687	0.400	1
450	.	38	LEU	CD1	26.680	0.400	1
451	.	38	LEU	CD2	23.806	0.400	1
452	.	38	LEU	N	119.257	0.400	1
453	.	39	GLY	HA2	3.968	0.020	1
454	.	39	GLY	C	176.038	0.400	1
455	.	39	GLY	CA	47.495	0.400	1
456	.	39	GLY	N	104.849	0.400	1
457	.	40	ALA	HA	4.188	0.020	1
458	.	40	ALA	HB1	1.567	0.020	1
459	.	40	ALA	HB2	1.567	0.020	1
460	.	40	ALA	HB3	1.567	0.020	1
461	.	40	ALA	C	180.431	0.400	1
462	.	40	ALA	CA	54.604	0.400	1
463	.	40	ALA	CB	18.442	0.400	1
464	.	40	ALA	N	123.616	0.400	1
465	.	41	GLU	HA	4.051	0.020	1
466	.	41	GLU	HB2	1.841	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	.	41	GLU	HB3	1.750	0.020	2
468	.	41	GLU	HG2	2.415	0.020	2
469	.	41	GLU	HG3	2.636	0.020	2
470	.	41	GLU	CA	59.279	0.400	1
471	.	41	GLU	CB	29.278	0.400	1
472	.	41	GLU	CG	36.552	0.400	1
473	.	41	GLU	N	118.594	0.400	1
474	.	42	TRP	HA	3.595	0.020	1
475	.	42	TRP	HB2	3.059	0.020	2
476	.	42	TRP	HB3	3.336	0.020	2
477	.	42	TRP	HD1	7.250	0.020	1
478	.	42	TRP	HE3	5.565	0.020	1
479	.	42	TRP	HZ2	7.140	0.020	1
480	.	42	TRP	HZ3	6.067	0.020	1
481	.	42	TRP	HH2	6.932	0.020	1
482	.	42	TRP	C	177.529	0.400	1
483	.	42	TRP	CA	59.221	0.400	1
484	.	42	TRP	CB	30.220	0.400	1
485	.	42	TRP	CD1	130.845	0.400	1
486	.	42	TRP	CE3	122.432	0.400	1
487	.	42	TRP	CZ2	112.815	0.400	1
488	.	42	TRP	CZ3	121.423	0.400	1
489	.	42	TRP	CH2	127.062	0.400	1
490	.	42	TRP	N	121.111	0.400	1
491	.	43	LYS	HA	3.769	0.020	1
492	.	43	LYS	HB2	1.847	0.020	2
493	.	43	LYS	HB3	1.780	0.020	2
494	.	43	LYS	HG2	1.657	0.020	2
495	.	43	LYS	HG3	1.447	0.020	2
496	.	43	LYS	HD2	1.566	0.020	2
497	.	43	LYS	HD3	1.697	0.020	2
498	.	43	LYS	HE2	2.909	0.020	2
499	.	43	LYS	HE3	2.946	0.020	2
500	.	43	LYS	C	177.387	0.400	1
501	.	43	LYS	CA	58.347	0.400	1
502	.	43	LYS	CB	32.631	0.400	1
503	.	43	LYS	CG	25.341	0.400	1
504	.	43	LYS	CD	29.252	0.400	1
505	.	43	LYS	CE	42.120	0.400	1
506	.	43	LYS	N	114.076	0.400	1
507	.	44	LEU	HA	4.126	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
508	.	44	LEU	HB2	1.756	0.020	2
509	.	44	LEU	HB3	1.583	0.020	2
510	.	44	LEU	HG	1.576	0.020	1
511	.	44	LEU	HD11	0.900	0.020	2
512	.	44	LEU	HD12	0.900	0.020	2
513	.	44	LEU	HD13	0.900	0.020	2
514	.	44	LEU	HD21	0.803	0.020	2
515	.	44	LEU	HD22	0.803	0.020	2
516	.	44	LEU	HD23	0.803	0.020	2
517	.	44	LEU	C	177.529	0.400	1
518	.	44	LEU	CA	54.796	0.400	1
519	.	44	LEU	CB	42.385	0.400	1
520	.	44	LEU	CG	26.113	0.400	1
521	.	44	LEU	CD1	25.380	0.400	1
522	.	44	LEU	CD2	22.241	0.400	1
523	.	44	LEU	N	115.991	0.400	1
524	.	45	LEU	HA	4.121	0.020	1
525	.	45	LEU	HB2	1.042	0.020	2
526	.	45	LEU	HB3	1.064	0.020	2
527	.	45	LEU	HG	1.621	0.020	1
528	.	45	LEU	HD11	0.590	0.020	2
529	.	45	LEU	HD12	0.590	0.020	2
530	.	45	LEU	HD13	0.590	0.020	2
531	.	45	LEU	HD21	0.377	0.020	2
532	.	45	LEU	HD22	0.377	0.020	2
533	.	45	LEU	HD23	0.377	0.020	2
534	.	45	LEU	C	177.285	0.400	1
535	.	45	LEU	CA	55.198	0.400	1
536	.	45	LEU	CB	42.592	0.400	1
537	.	45	LEU	CG	26.770	0.400	1
538	.	45	LEU	CD1	23.388	0.400	1
539	.	45	LEU	CD2	25.254	0.400	1
540	.	45	LEU	N	121.326	0.400	1
541	.	46	SER	HA	4.314	0.020	1
542	.	46	SER	HB2	4.022	0.020	2
543	.	46	SER	HB3	3.968	0.020	2
544	.	46	SER	C	174.737	0.400	1
545	.	46	SER	CA	57.245	0.400	1
546	.	46	SER	CB	65.048	0.400	1
547	.	46	SER	N	120.111	0.400	1
548	.	47	GLU	HA	3.786	0.020	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
549	.	47	GLU	HB2	2.027	0.020	2
550	.	47	GLU	HB3	2.046	0.020	2
551	.	47	GLU	HG2	2.330	0.020	2
552	.	47	GLU	HG3	2.257	0.020	2
553	.	47	GLU	C	179.464	0.400	1
554	.	47	GLU	CA	59.854	0.400	1
555	.	47	GLU	CB	28.943	0.400	1
556	.	47	GLU	CG	36.103	0.400	1
557	.	47	GLU	N	120.571	0.400	1
558	.	48	THR	HA	3.207	0.020	1
559	.	48	THR	HB	3.676	0.020	1
560	.	48	THR	HG21	1.218	0.020	1
561	.	48	THR	HG22	1.218	0.020	1
562	.	48	THR	HG23	1.218	0.020	1
563	.	48	THR	C	176.740	0.400	1
564	.	48	THR	CA	66.061	0.400	1
565	.	48	THR	CB	68.502	0.400	1
566	.	48	THR	CG2	21.636	0.400	1
567	.	48	THR	N	113.289	0.400	1
568	.	49	GLU	HA	4.095	0.020	1
569	.	49	GLU	HB2	2.168	0.020	2
570	.	49	GLU	HB3	2.036	0.020	2
571	.	49	GLU	HG2	2.286	0.020	2
572	.	49	GLU	HG3	2.310	0.020	2
573	.	49	GLU	C	178.383	0.400	1
574	.	49	GLU	CA	58.511	0.400	1
575	.	49	GLU	CB	30.476	0.400	1
576	.	49	GLU	CG	37.855	0.400	1
577	.	49	GLU	N	121.759	0.400	1
578	.	50	LYS	HA	4.003	0.020	1
579	.	50	LYS	HB2	1.555	0.020	2
580	.	50	LYS	HB3	1.629	0.020	2
581	.	50	LYS	HG2	1.062	0.020	2
582	.	50	LYS	HG3	-0.059	0.020	2
583	.	50	LYS	HD2	0.878	0.020	2
584	.	50	LYS	HD3	1.017	0.020	2
585	.	50	LYS	HE2	1.720	0.020	2
586	.	50	LYS	HE3	1.666	0.020	2
587	.	50	LYS	CA	58.923	0.400	1
588	.	50	LYS	CB	34.008	0.400	1
589	.	50	LYS	CG	26.885	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
590	.	50	LYS	CD	29.354	0.400	1
591	.	50	LYS	CE	41.864	0.400	1
592	.	50	LYS	N	115.605	0.400	1
593	.	51	ARG	HA	4.032	0.020	1
594	.	51	ARG	HB2	2.054	0.020	2
595	.	51	ARG	HB3	2.084	0.020	2
596	.	51	ARG	HG2	1.741	0.020	2
597	.	51	ARG	HG3	1.608	0.020	2
598	.	51	ARG	HD2	3.240	0.020	2
599	.	51	ARG	HD3	3.180	0.020	2
600	.	51	ARG	CA	60.709	0.400	1
601	.	51	ARG	CB	27.114	0.400	1
602	.	51	ARG	CG	26.852	0.400	1
603	.	51	ARG	CD	42.739	0.400	1
604	.	51	ARG	N	119.570	0.400	1
605	.	52	PRO	HA	4.301	0.020	1
606	.	52	PRO	HB2	2.107	0.020	2
607	.	52	PRO	HB3	1.034	0.020	2
608	.	52	PRO	HG2	1.888	0.020	2
609	.	52	PRO	HG3	1.776	0.020	2
610	.	52	PRO	HD2	3.705	0.020	2
611	.	52	PRO	HD3	3.591	0.020	2
612	.	52	PRO	C	179.426	0.400	1
613	.	52	PRO	CA	65.548	0.400	1
614	.	52	PRO	CB	30.695	0.400	1
615	.	52	PRO	CG	28.386	0.400	1
616	.	52	PRO	CD	49.343	0.400	1
617	.	53	PHE	HA	4.162	0.020	1
618	.	53	PHE	HB2	3.294	0.020	2
619	.	53	PHE	HB3	2.103	0.020	2
620	.	53	PHE	HD1	7.479	0.020	1
621	.	53	PHE	HD2	7.494	0.020	1
622	.	53	PHE	HE1	7.685	0.020	1
623	.	53	PHE	HE2	7.712	0.020	1
624	.	53	PHE	HZ	7.704	0.020	1
625	.	53	PHE	C	177.466	0.400	1
626	.	53	PHE	CA	60.739	0.400	1
627	.	53	PHE	CB	36.987	0.400	1
628	.	53	PHE	CD1	131.669	0.400	1
629	.	53	PHE	CD2	131.329	0.400	1
630	.	53	PHE	CE1	133.002	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
631	.	53	PHE	CE2	131.102	0.400	1
632	.	53	PHE	CZ	131.492	0.400	1
633	.	53	PHE	N	117.668	0.400	1
634	.	54	ILE	HA	3.740	0.020	1
635	.	54	ILE	HB	1.984	0.020	1
636	.	54	ILE	HG12	1.090	0.020	2
637	.	54	ILE	HG13	1.512	0.020	2
638	.	54	ILE	HG21	0.876	0.020	1
639	.	54	ILE	HG22	0.876	0.020	1
640	.	54	ILE	HG23	0.876	0.020	1
641	.	54	ILE	HD11	0.682	0.020	1
642	.	54	ILE	HD12	0.682	0.020	1
643	.	54	ILE	HD13	0.682	0.020	1
644	.	54	ILE	C	179.408	0.400	1
645	.	54	ILE	CA	65.302	0.400	1
646	.	54	ILE	CB	38.145	0.400	1
647	.	54	ILE	CG1	28.509	0.400	1
648	.	54	ILE	CG2	16.782	0.400	1
649	.	54	ILE	CD1	15.932	0.400	1
650	.	54	ILE	N	123.179	0.400	1
651	.	55	ASP	HA	4.443	0.020	1
652	.	55	ASP	HB2	2.696	0.020	2
653	.	55	ASP	HB3	2.631	0.020	2
654	.	55	ASP	CA	57.654	0.400	1
655	.	55	ASP	CB	39.500	0.400	1
656	.	55	ASP	N	120.986	0.400	1
657	.	56	GLU	HA	4.609	0.020	1
658	.	56	GLU	HB2	2.197	0.020	2
659	.	56	GLU	HB3	1.980	0.020	2
660	.	56	GLU	HG2	2.462	0.020	2
661	.	56	GLU	HG3	2.221	0.020	2
662	.	56	GLU	C	177.905	0.400	1
663	.	56	GLU	CA	58.289	0.400	1
664	.	56	GLU	CB	28.913	0.400	1
665	.	56	GLU	CG	34.350	0.400	1
666	.	56	GLU	N	122.696	0.400	1
667	.	57	ALA	HA	4.009	0.020	1
668	.	57	ALA	HB1	1.449	0.020	1
669	.	57	ALA	HB2	1.449	0.020	1
670	.	57	ALA	HB3	1.449	0.020	1
671	.	57	ALA	C	179.937	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
672	.	57	ALA	CA	55.645	0.400	1
673	.	57	ALA	CB	16.998	0.400	1
674	.	57	ALA	N	121.271	0.400	1
675	.	58	LYS	HA	4.042	0.020	1
676	.	58	LYS	HB2	1.975	0.020	2
677	.	58	LYS	HB3	2.009	0.020	2
678	.	58	LYS	HG2	1.441	0.020	2
679	.	58	LYS	HG3	1.729	0.020	2
680	.	58	LYS	HD2	1.758	0.020	2
681	.	58	LYS	HD3	1.610	0.020	2
682	.	58	LYS	HE2	2.987	0.020	2
683	.	58	LYS	HE3	2.930	0.020	2
684	.	58	LYS	CA	60.082	0.400	1
685	.	58	LYS	CB	32.440	0.400	1
686	.	58	LYS	CG	25.502	0.400	1
687	.	58	LYS	CD	29.468	0.400	1
688	.	58	LYS	CE	42.133	0.400	1
689	.	58	LYS	N	118.389	0.400	1
690	.	59	ARG	HA	4.040	0.020	1
691	.	59	ARG	HB2	2.110	0.020	2
692	.	59	ARG	HB3	1.923	0.020	2
693	.	59	ARG	HG2	1.389	0.020	2
694	.	59	ARG	HG3	1.706	0.020	2
695	.	59	ARG	HD2	3.041	0.020	2
696	.	59	ARG	HD3	3.372	0.020	2
697	.	59	ARG	HE	8.320	0.020	1
698	.	59	ARG	C	179.586	0.400	1
699	.	59	ARG	CA	59.590	0.400	1
700	.	59	ARG	CB	30.411	0.400	1
701	.	59	ARG	CG	28.057	0.400	1
702	.	59	ARG	CD	42.854	0.400	1
703	.	59	ARG	N	122.704	0.400	1
704	.	60	LEU	HA	4.037	0.020	1
705	.	60	LEU	HB2	1.438	0.020	2
706	.	60	LEU	HB3	1.954	0.020	2
707	.	60	LEU	HG	1.540	0.020	1
708	.	60	LEU	HD11	0.938	0.020	2
709	.	60	LEU	HD12	0.938	0.020	2
710	.	60	LEU	HD13	0.938	0.020	2
711	.	60	LEU	HD21	0.872	0.020	2
712	.	60	LEU	HD22	0.872	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
713	.	60	LEU	HD23	0.872	0.020	2
714	.	60	LEU	C	180.103	0.400	1
715	.	60	LEU	CA	57.525	0.400	1
716	.	60	LEU	CB	41.877	0.400	1
717	.	60	LEU	CG	26.770	0.400	1
718	.	60	LEU	CD1	25.958	0.400	1
719	.	60	LEU	CD2	22.253	0.400	1
720	.	60	LEU	N	119.412	0.400	1
721	.	61	ARG	HA	4.045	0.020	1
722	.	61	ARG	HB2	1.790	0.020	2
723	.	61	ARG	HB3	1.938	0.020	2
724	.	61	ARG	HG2	1.661	0.020	2
725	.	61	ARG	HG3	1.580	0.020	2
726	.	61	ARG	HD2	3.254	0.020	2
727	.	61	ARG	HD3	3.328	0.020	2
728	.	61	ARG	C	178.186	0.400	1
729	.	61	ARG	CA	59.451	0.400	1
730	.	61	ARG	CB	29.848	0.400	1
731	.	61	ARG	CG	27.310	0.400	1
732	.	61	ARG	CD	43.600	0.400	1
733	.	61	ARG	N	120.696	0.400	1
734	.	62	ALA	HA	4.203	0.020	1
735	.	62	ALA	HB1	1.506	0.020	1
736	.	62	ALA	HB2	1.506	0.020	1
737	.	62	ALA	HB3	1.506	0.020	1
738	.	62	ALA	C	180.023	0.400	1
739	.	62	ALA	CA	54.447	0.400	1
740	.	62	ALA	CB	17.922	0.400	1
741	.	62	ALA	N	121.309	0.400	1
742	.	63	LEU	HA	4.091	0.020	1
743	.	63	LEU	HB2	1.796	0.020	1
744	.	63	LEU	HB3	1.612	0.020	1
745	.	63	LEU	HG	1.705	0.020	1
746	.	63	LEU	HD11	0.869	0.020	2
747	.	63	LEU	HD12	0.869	0.020	2
748	.	63	LEU	HD13	0.869	0.020	2
749	.	63	LEU	HD21	0.760	0.020	2
750	.	63	LEU	HD22	0.760	0.020	2
751	.	63	LEU	HD23	0.760	0.020	2
752	.	63	LEU	C	178.543	0.400	1
753	.	63	LEU	CA	57.172	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
754	.	63	LEU	CB	42.000	0.400	1
755	.	63	LEU	CG	26.715	0.400	1
756	.	63	LEU	CD1	23.939	0.400	1
757	.	63	LEU	CD2	24.100	0.400	1
758	.	63	LEU	N	119.205	0.400	1
759	.	64	HIS	HA	4.456	0.020	1
760	.	64	HIS	HB2	3.182	0.020	2
761	.	64	HIS	HB3	3.304	0.020	2
762	.	64	HIS	HD2	6.999	0.020	1
763	.	64	HIS	HE1	7.995	0.020	1
764	.	64	HIS	C	176.684	0.400	1
765	.	64	HIS	CA	58.117	0.400	1
766	.	64	HIS	CB	29.981	0.400	1
767	.	64	HIS	CD2	117.385	0.400	1
768	.	64	HIS	CE1	138.202	0.400	1
769	.	64	HIS	N	118.668	0.400	1
770	.	65	MET	HA	4.098	0.020	1
771	.	65	MET	HB2	1.825	0.020	2
772	.	65	MET	HB3	1.877	0.020	2
773	.	65	MET	HG2	2.717	0.020	2
774	.	65	MET	HG3	2.409	0.020	2
775	.	65	MET	HE1	2.089	0.020	1
776	.	65	MET	HE2	2.089	0.020	1
777	.	65	MET	HE3	2.089	0.020	1
778	.	65	MET	C	175.782	0.400	1
779	.	65	MET	CA	56.954	0.400	1
780	.	65	MET	CB	32.235	0.400	1
781	.	65	MET	CG	32.185	0.400	1
782	.	65	MET	CE	17.239	0.400	1
783	.	65	MET	N	117.960	0.400	1
784	.	66	LYS	HA	4.280	0.020	1
785	.	66	LYS	HB2	1.851	0.020	2
786	.	66	LYS	HB3	1.780	0.020	2
787	.	66	LYS	HG2	1.545	0.020	2
788	.	66	LYS	HG3	1.419	0.020	2
789	.	66	LYS	HD2	1.660	0.020	2
790	.	66	LYS	HD3	1.610	0.020	2
791	.	66	LYS	HE2	2.973	0.020	2
792	.	66	LYS	HE3	2.930	0.020	2
793	.	66	LYS	C	179.120	0.400	1
794	.	66	LYS	CA	56.840	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
795	.	66	LYS	CB	32.623	0.400	1
796	.	66	LYS	CG	24.730	0.400	1
797	.	66	LYS	CD	28.780	0.400	1
798	.	66	LYS	CE	41.780	0.400	1
799	.	66	LYS	N	118.339	0.400	1
800	.	67	GLU	HA	4.242	0.020	1
801	.	67	GLU	HB2	2.040	0.020	2
802	.	67	GLU	HB3	1.425	0.020	2
803	.	67	GLU	HG2	2.250	0.020	2
804	.	67	GLU	HG3	2.419	0.020	2
805	.	67	GLU	C	175.923	0.400	1
806	.	67	GLU	CA	57.420	0.400	1
807	.	67	GLU	CB	32.769	0.400	1
808	.	67	GLU	CG	36.369	0.400	1
809	.	67	GLU	N	117.686	0.400	1
810	.	68	HIS	HA	4.460	0.020	1
811	.	68	HIS	HB2	1.625	0.020	2
812	.	68	HIS	HB3	1.751	0.020	2
813	.	68	HIS	HD1	7.963	0.020	1
814	.	68	HIS	HD2	7.080	0.020	1
815	.	68	HIS	HE1	8.080	0.020	1
816	.	68	HIS	CA	53.604	0.400	1
817	.	68	HIS	CB	30.267	0.400	1
818	.	68	HIS	CD2	121.616	0.400	1
819	.	68	HIS	CE1	136.050	0.400	1
820	.	68	HIS	N	123.010	0.400	1
821	.	69	PRO	HA	4.418	0.020	1
822	.	69	PRO	HB2	2.235	0.020	2
823	.	69	PRO	HB3	1.765	0.020	2
824	.	69	PRO	HG2	1.948	0.020	2
825	.	69	PRO	HG3	1.912	0.020	2
826	.	69	PRO	HD2	3.345	0.020	2
827	.	69	PRO	HD3	3.613	0.020	2
828	.	69	PRO	C	176.656	0.400	1
829	.	69	PRO	CA	63.703	0.400	1
830	.	69	PRO	CB	31.944	0.400	1
831	.	69	PRO	CG	27.216	0.400	1
832	.	69	PRO	CD	50.152	0.400	1
833	.	70	ASP	HA	4.571	0.020	1
834	.	70	ASP	HB2	2.670	0.020	2
835	.	70	ASP	HB3	2.627	0.020	2

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
836	.	70	ASP	C	176.289	0.400	1
837	.	70	ASP	CA	53.996	0.400	1
838	.	70	ASP	CB	40.806	0.400	1
839	.	70	ASP	N	119.377	0.400	1
840	.	71	TYR	HA	4.448	0.020	1
841	.	71	TYR	HB2	3.021	0.020	2
842	.	71	TYR	HB3	2.963	0.020	2
843	.	71	TYR	HD1	7.062	0.020	1
844	.	71	TYR	HD2	7.062	0.020	1
845	.	71	TYR	HE1	6.693	0.020	1
846	.	71	TYR	HE2	6.705	0.020	1
847	.	71	TYR	C	175.806	0.400	1
848	.	71	TYR	CA	58.121	0.400	1
849	.	71	TYR	CB	38.284	0.400	1
850	.	71	TYR	CE1	117.922	0.400	1
851	.	71	TYR	CE2	117.907	0.400	1
852	.	71	TYR	N	121.385	0.400	1
853	.	72	LYS	HA	4.133	0.020	1
854	.	72	LYS	HB2	1.588	0.020	2
855	.	72	LYS	HB3	1.562	0.020	2
856	.	72	LYS	HG2	1.332	0.020	2
857	.	72	LYS	HG3	1.173	0.020	2
858	.	72	LYS	HD2	1.665	0.020	2
859	.	72	LYS	HD3	1.610	0.020	2
860	.	72	LYS	HE2	2.950	0.020	2
861	.	72	LYS	HE3	2.930	0.020	2
862	.	72	LYS	C	175.650	0.400	1
863	.	72	LYS	CA	56.324	0.400	1
864	.	72	LYS	CB	32.839	0.400	1
865	.	72	LYS	CG	24.179	0.400	1
866	.	72	LYS	CD	28.780	0.400	1
867	.	72	LYS	CE	41.780	0.400	1
868	.	72	LYS	N	122.710	0.400	1
869	.	73	TYR	HA	4.437	0.020	1
870	.	73	TYR	HB2	2.957	0.020	2
871	.	73	TYR	HB3	2.910	0.020	2
872	.	73	TYR	HD1	7.094	0.020	1
873	.	73	TYR	HD2	7.078	0.020	1
874	.	73	TYR	HE1	6.772	0.020	1
875	.	73	TYR	HE2	6.754	0.020	1
876	.	73	TYR	C	175.162	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
877	.	73	TYR	CA	57.815	0.400	1
878	.	73	TYR	CB	38.417	0.400	1
879	.	73	TYR	CD1	133.003	0.400	1
880	.	73	TYR	CD2	132.260	0.400	1
881	.	73	TYR	CE1	118.000	0.400	1
882	.	73	TYR	CE2	117.910	0.400	1
883	.	73	TYR	N	121.080	0.400	1
884	.	74	ARG	HA	4.513	0.020	1
885	.	74	ARG	HB2	1.944	0.020	2
886	.	74	ARG	HB3	1.628	0.020	2
887	.	74	ARG	HG2	1.401	0.020	2
888	.	74	ARG	HG3	1.478	0.020	2
889	.	74	ARG	HD2	3.126	0.020	2
890	.	74	ARG	HD3	3.152	0.020	2
891	.	74	ARG	CA	53.376	0.400	1
892	.	74	ARG	CB	30.325	0.400	1
893	.	74	ARG	CG	26.760	0.400	1
894	.	74	ARG	CD	43.393	0.400	1
895	.	74	ARG	N	125.248	0.400	1
896	.	75	PRO	HA	4.330	0.020	1
897	.	75	PRO	HB2	2.251	0.020	2
898	.	75	PRO	HB3	1.844	0.020	2
899	.	75	PRO	HG2	1.518	0.020	2
900	.	75	PRO	HG3	1.949	0.020	2
901	.	75	PRO	HD2	3.640	0.020	2
902	.	75	PRO	HD3	3.630	0.020	2
903	.	75	PRO	C	177.116	0.400	1
904	.	75	PRO	CA	62.382	0.400	1
905	.	75	PRO	CB	31.683	0.400	1
906	.	75	PRO	CG	26.936	0.400	1
907	.	75	PRO	CD	50.280	0.400	1
908	.	76	ARG	HA	4.269	0.020	1
909	.	76	ARG	HB2	2.139	0.020	2
910	.	76	ARG	HB3	1.780	0.020	2
911	.	76	ARG	HG2	1.642	0.020	2
912	.	76	ARG	HG3	1.573	0.020	2
913	.	76	ARG	HD2	3.405	0.020	2
914	.	76	ARG	HD3	3.034	0.020	2
915	.	76	ARG	C	177.167	0.400	1
916	.	76	ARG	CA	56.559	0.400	1
917	.	76	ARG	CB	30.660	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
918	.	76	ARG	CG	24.239	0.400	1
919	.	76	ARG	CD	43.100	0.400	1
920	.	76	ARG	N	121.158	0.400	1
921	.	77	ARG	HA	4.270	0.020	1
922	.	77	ARG	HB2	1.798	0.020	2
923	.	77	ARG	HB3	2.251	0.020	2
924	.	77	ARG	HG2	1.636	0.020	2
925	.	77	ARG	HG3	1.580	0.020	2
926	.	77	ARG	HD2	3.215	0.020	2
927	.	77	ARG	HD3	3.117	0.020	2
928	.	77	ARG	C	175.892	0.400	1
929	.	77	ARG	CA	56.950	0.400	1
930	.	77	ARG	CB	32.639	0.400	1
931	.	77	ARG	CG	27.310	0.400	1
932	.	77	ARG	CD	41.852	0.400	1
933	.	77	ARG	N	119.622	0.400	1
934	.	78	LYS	HA	4.345	0.020	1
935	.	78	LYS	HB2	1.822	0.020	2
936	.	78	LYS	HB3	1.780	0.020	2
937	.	78	LYS	HG2	1.456	0.020	2
938	.	78	LYS	HG3	1.560	0.020	2
939	.	78	LYS	HD2	1.758	0.020	2
940	.	78	LYS	HD3	1.610	0.020	2
941	.	78	LYS	HE2	3.092	0.020	2
942	.	78	LYS	HE3	2.930	0.020	2
943	.	78	LYS	C	178.459	0.400	1
944	.	78	LYS	CA	56.322	0.400	1
945	.	78	LYS	CB	32.830	0.400	1
946	.	78	LYS	CG	24.910	0.400	1
947	.	78	LYS	CD	28.780	0.400	1
948	.	78	LYS	CE	41.780	0.400	1
949	.	78	LYS	N	124.167	0.400	1
950	.	79	THR	HA	4.311	0.020	1
951	.	79	THR	HB	4.181	0.020	1
952	.	79	THR	HG21	1.178	0.020	1
953	.	79	THR	HG22	1.178	0.020	1
954	.	79	THR	HG23	1.178	0.020	1
955	.	79	THR	CA	61.647	0.400	1
956	.	79	THR	CB	69.955	0.400	1
957	.	79	THR	CG2	21.678	0.400	1
958	.	79	THR	N	116.350	0.400	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
959	.	80	LYS	HA	4.368	0.020	1
960	.	80	LYS	HB2	1.790	0.020	2
961	.	80	LYS	HB3	1.761	0.020	2
962	.	80	LYS	HG2	1.463	0.020	2
963	.	80	LYS	HG3	1.370	0.020	2
964	.	80	LYS	HD2	1.760	0.020	2
965	.	80	LYS	HD3	1.610	0.020	2
966	.	80	LYS	HE2	3.022	0.020	2
967	.	80	LYS	HE3	2.930	0.020	2
968	.	80	LYS	CA	56.589	0.400	1
969	.	80	LYS	CB	32.830	0.400	1
970	.	80	LYS	CG	24.910	0.400	1
971	.	80	LYS	CD	28.780	0.400	1
972	.	80	LYS	CE	41.780	0.400	1
973	.	80	LYS	N	124.353	0.400	1
974	.	81	THR	HA	4.314	0.020	1
975	.	81	THR	HB	4.206	0.020	1
976	.	81	THR	HG21	1.180	0.020	1
977	.	81	THR	HG22	1.180	0.020	1
978	.	81	THR	HG23	1.180	0.020	1
979	.	81	THR	CA	63.275	0.400	1
980	.	81	THR	CB	70.158	0.400	1
981	.	81	THR	CG2	21.839	0.400	1
982	.	81	THR	N	121.147	0.400	1

7.1.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 805. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/284 (0%)	0/113 (0%)	0/116 (0%)	0/55 (0%)
Sidechain	0/463 (0%)	0/278 (0%)	0/153 (0%)	0/32 (0%)
Aromatic	0/58 (0%)	0/30 (0%)	0/22 (0%)	0/6 (0%)
Overall	0/805 (0%)	0/421 (0%)	0/291 (0%)	0/93 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1162. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/395 (0%)	0/157 (0%)	0/162 (0%)	0/76 (0%)
Sidechain	0/685 (0%)	0/413 (0%)	0/220 (0%)	0/52 (0%)
Aromatic	0/82 (0%)	0/42 (0%)	0/32 (0%)	0/8 (0%)
Overall	0/1162 (0%)	0/612 (0%)	0/414 (0%)	0/136 (0%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (sox2Asn). RCI is only applicable to proteins.