wwPDB NMR Structure Validation Summary Report

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BMRB ID	:	20074
Title	:	Protein Fibril
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Deposited on	:	2009-05-01

This is a wwPDB NMR Structure Validation Summary 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

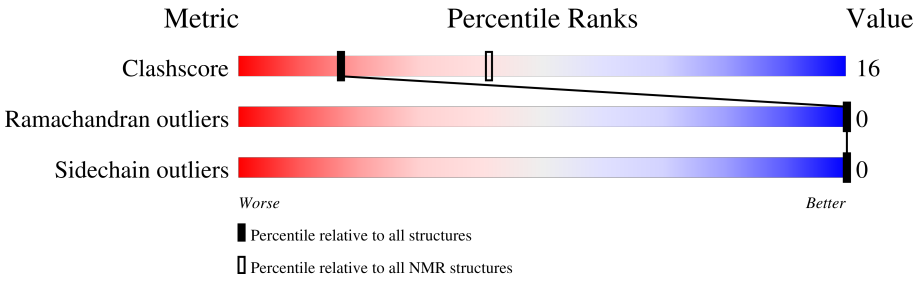
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 39%.

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	7	57% 43%
1	B	7	86% 14%
1	C	7	100%
1	D	7	86% 14%
1	E	7	71% 29%
1	F	7	86% 14%
1	G	7	86% 14%
1	H	7	86% 14%

2 Ensemble composition and analysis

This entry contains 10 models. Model 4 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:1-A:7, B:1-B:7, C:1-C:7, D:1-D:7, E:1-E:7, F:1-F:7, G:1-G:7, H:1-H:7 (56)	0.50	4

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. No single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 5, 6
2	7, 9, 10
3	2, 8

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 824 atoms, of which 416 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NFGAIL segment from human islet amyloid polypeptide.

Mol	Chain	Residues	Atoms					Trace
1	A	7	Total	C	H	N	O	0
			103	33	52	8	10	
1	B	7	Total	C	H	N	O	0
			103	33	52	8	10	
1	C	7	Total	C	H	N	O	0
			103	33	52	8	10	
1	D	7	Total	C	H	N	O	0
			103	33	52	8	10	
1	E	7	Total	C	H	N	O	0
			103	33	52	8	10	
1	F	7	Total	C	H	N	O	0
			103	33	52	8	10	
1	G	7	Total	C	H	N	O	0
			103	33	52	8	10	
1	H	7	Total	C	H	N	O	0
			103	33	52	8	10	

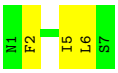
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: NFGAIL segment from human islet amyloid polypeptide

Chain A:

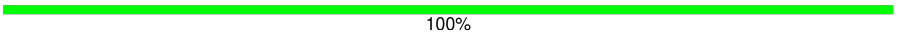


• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain B:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain C:



There are no outlier residues in this chain.

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain D:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain E:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain F:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain G:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

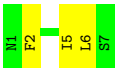
Chain H:

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain A:

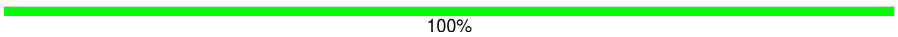


• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain B:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain C:



There are no outlier residues in this chain.

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain D:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain E:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain F:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain G:

• Molecule 1: NFGAIL segment from human islet amyloid polypeptide

Chain H:

5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 10 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	refinement	2.18

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1152
Number of shifts mapped to atoms	1152
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	39%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	51	52	52	5±1
1	E	51	52	52	4±2
1	G	51	52	52	2±1
1	B	51	52	52	3±3
1	D	51	52	52	2±2
1	F	51	52	52	2±2
1	H	51	52	52	2±2
1	C	51	52	52	1±1
All	All	4080	4160	4160	128

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 16.

5 of 57 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:2:PHE:CD2	1:D:1:ASN:ND2	0.62	2.68	2	1
1:A:2:PHE:CZ	1:B:1:ASN:ND2	0.62	2.67	6	1
1:E:2:PHE:CD2	1:F:1:ASN:ND2	0.62	2.67	2	1
1:A:2:PHE:CE1	1:B:1:ASN:ND2	0.62	2.68	6	1
1:A:6:LEU:HD22	1:E:2:PHE:CD2	0.59	2.33	4	8

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	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	B	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	C	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	D	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	E	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	F	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	G	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
1	H	5/7 (71%)	5±0 (100±0%)	0±0 (0±0%)	0±0 (0±0%)	100	100
All	All	400/560 (71%)	400 (100%)	0 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100
1	B	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100
1	C	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100
1	D	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100
1	E	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100
1	F	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100
1	G	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100
1	H	5/5 (100%)	5±0 (100±0%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	400/400 (100%)	400 (100%)	0 (0%)	100 100

There are no protein residues with a non-rotameric sidechain to report.

6.3.3 RNA

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 39% for the well-defined parts and 39% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	1152
Number of shifts mapped to atoms	1152
Number of unparsed shifts	0
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.

- Chemical shift has been reported more than once. First 5 (of 0) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	ASN	C	172.41	0.05	1
1	C	1	ASN	C	172.41	0.05	1
1	B	1	ASN	C	172.41	0.05	1
1	E	1	ASN	C	172.41	0.05	1
1	D	1	ASN	C	172.41	0.05	1
1	G	1	ASN	C	172.41	0.05	1
1	F	1	ASN	C	172.41	0.05	1
1	H	1	ASN	C	172.41	0.05	1
1	A	1	ASN	CA	52.10	0.05	1
1	C	1	ASN	CA	52.10	0.05	1
1	B	1	ASN	CA	52.10	0.05	1
1	E	1	ASN	CA	52.10	0.05	1
1	D	1	ASN	CA	52.10	0.05	1
1	G	1	ASN	CA	52.10	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	F	1	ASN	CA	52.10	0.05	1
1	H	1	ASN	CA	52.10	0.05	1
1	A	1	ASN	CB	41.84	0.05	1
1	C	1	ASN	CB	41.84	0.05	1
1	B	1	ASN	CB	41.84	0.05	1
1	E	1	ASN	CB	41.84	0.05	1
1	D	1	ASN	CB	41.84	0.05	1
1	G	1	ASN	CB	41.84	0.05	1
1	F	1	ASN	CB	41.84	0.05	1
1	H	1	ASN	CB	41.84	0.05	1
1	A	1	ASN	CG	175.11	0.05	1
1	C	1	ASN	CG	175.11	0.05	1
1	B	1	ASN	CG	175.11	0.05	1
1	E	1	ASN	CG	175.11	0.05	1
1	D	1	ASN	CG	175.11	0.05	1
1	G	1	ASN	CG	175.11	0.05	1
1	F	1	ASN	CG	175.11	0.05	1
1	H	1	ASN	CG	175.11	0.05	1
1	A	1	ASN	N	120.42	0.05	1
1	C	1	ASN	N	120.42	0.05	1
1	B	1	ASN	N	120.42	0.05	1
1	E	1	ASN	N	120.42	0.05	1
1	D	1	ASN	N	120.42	0.05	1
1	G	1	ASN	N	120.42	0.05	1
1	F	1	ASN	N	120.42	0.05	1
1	H	1	ASN	N	120.42	0.05	1
1	A	2	PHE	C	173.20	0.05	1
1	C	2	PHE	C	173.20	0.05	1
1	B	2	PHE	C	173.20	0.05	1
1	E	2	PHE	C	173.20	0.05	1
1	D	2	PHE	C	173.20	0.05	1
1	G	2	PHE	C	173.20	0.05	1
1	F	2	PHE	C	173.20	0.05	1
1	H	2	PHE	C	173.20	0.05	1
1	A	2	PHE	CA	56.26	0.05	1
1	C	2	PHE	CA	56.26	0.05	1
1	B	2	PHE	CA	56.26	0.05	1
1	E	2	PHE	CA	56.26	0.05	1
1	D	2	PHE	CA	56.26	0.05	1
1	G	2	PHE	CA	56.26	0.05	1
1	F	2	PHE	CA	56.26	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	H	2	PHE	CA	56.26	0.05	1
1	A	2	PHE	CB	44.42	0.05	1
1	C	2	PHE	CB	44.42	0.05	1
1	B	2	PHE	CB	44.42	0.05	1
1	E	2	PHE	CB	44.42	0.05	1
1	D	2	PHE	CB	44.42	0.05	1
1	G	2	PHE	CB	44.42	0.05	1
1	F	2	PHE	CB	44.42	0.05	1
1	H	2	PHE	CB	44.42	0.05	1
1	A	2	PHE	CD1	131.25	0.05	4
1	C	2	PHE	CD1	131.25	0.05	4
1	B	2	PHE	CD1	131.25	0.05	4
1	E	2	PHE	CD1	131.25	0.05	4
1	D	2	PHE	CD1	131.25	0.05	4
1	G	2	PHE	CD1	131.25	0.05	4
1	F	2	PHE	CD1	131.25	0.05	4
1	H	2	PHE	CD1	131.25	0.05	4
1	A	2	PHE	CD2	132.60	0.05	4
1	C	2	PHE	CD2	132.60	0.05	4
1	B	2	PHE	CD2	132.60	0.05	4
1	E	2	PHE	CD2	132.60	0.05	4
1	D	2	PHE	CD2	132.60	0.05	4
1	G	2	PHE	CD2	132.60	0.05	4
1	F	2	PHE	CD2	132.60	0.05	4
1	H	2	PHE	CD2	132.60	0.05	4
1	A	2	PHE	CE1	130.62	0.05	4
1	C	2	PHE	CE1	130.62	0.05	4
1	B	2	PHE	CE1	130.62	0.05	4
1	E	2	PHE	CE1	130.62	0.05	4
1	D	2	PHE	CE1	130.62	0.05	4
1	G	2	PHE	CE1	130.62	0.05	4
1	F	2	PHE	CE1	130.62	0.05	4
1	H	2	PHE	CE1	130.62	0.05	4
1	A	2	PHE	CE2	130.62	0.05	4
1	C	2	PHE	CE2	130.62	0.05	4
1	B	2	PHE	CE2	130.62	0.05	4
1	E	2	PHE	CE2	130.62	0.05	4
1	D	2	PHE	CE2	130.62	0.05	4
1	G	2	PHE	CE2	130.62	0.05	4
1	F	2	PHE	CE2	130.62	0.05	4
1	H	2	PHE	CE2	130.62	0.05	4

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	PHE	CG	137.79	0.05	1
1	C	2	PHE	CG	137.79	0.05	1
1	B	2	PHE	CG	137.79	0.05	1
1	E	2	PHE	CG	137.79	0.05	1
1	D	2	PHE	CG	137.79	0.05	1
1	G	2	PHE	CG	137.79	0.05	1
1	F	2	PHE	CG	137.79	0.05	1
1	H	2	PHE	CG	137.79	0.05	1
1	A	2	PHE	CZ	131.78	0.05	4
1	C	2	PHE	CZ	131.78	0.05	4
1	B	2	PHE	CZ	131.78	0.05	4
1	E	2	PHE	CZ	131.78	0.05	4
1	D	2	PHE	CZ	131.78	0.05	4
1	G	2	PHE	CZ	131.78	0.05	4
1	F	2	PHE	CZ	131.78	0.05	4
1	H	2	PHE	CZ	131.78	0.05	4
1	A	2	PHE	N	125.95	0.05	1
1	C	2	PHE	N	125.95	0.05	1
1	B	2	PHE	N	125.95	0.05	1
1	E	2	PHE	N	125.95	0.05	1
1	D	2	PHE	N	125.95	0.05	1
1	G	2	PHE	N	125.95	0.05	1
1	F	2	PHE	N	125.95	0.05	1
1	H	2	PHE	N	125.95	0.05	1
1	A	3	GLY	C	171.41	0.05	1
1	C	3	GLY	C	171.41	0.05	1
1	B	3	GLY	C	171.41	0.05	1
1	E	3	GLY	C	171.41	0.05	1
1	D	3	GLY	C	171.41	0.05	1
1	G	3	GLY	C	171.41	0.05	1
1	F	3	GLY	C	171.41	0.05	1
1	H	3	GLY	C	171.41	0.05	1
1	A	3	GLY	CA	44.30	0.05	1
1	C	3	GLY	CA	44.30	0.05	1
1	B	3	GLY	CA	44.30	0.05	1
1	E	3	GLY	CA	44.30	0.05	1
1	D	3	GLY	CA	44.30	0.05	1
1	G	3	GLY	CA	44.30	0.05	1
1	F	3	GLY	CA	44.30	0.05	1
1	H	3	GLY	CA	44.30	0.05	1
1	A	3	GLY	N	113.20	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	3	GLY	N	113.20	0.05	1
1	B	3	GLY	N	113.20	0.05	1
1	E	3	GLY	N	113.20	0.05	1
1	D	3	GLY	N	113.20	0.05	1
1	G	3	GLY	N	113.20	0.05	1
1	F	3	GLY	N	113.20	0.05	1
1	H	3	GLY	N	113.20	0.05	1
1	A	4	ALA	C	175.18	0.05	1
1	C	4	ALA	C	175.18	0.05	1
1	B	4	ALA	C	175.18	0.05	1
1	E	4	ALA	C	175.18	0.05	1
1	D	4	ALA	C	175.18	0.05	1
1	G	4	ALA	C	175.18	0.05	1
1	F	4	ALA	C	175.18	0.05	1
1	H	4	ALA	C	175.18	0.05	1
1	A	4	ALA	CA	50.07	0.05	1
1	C	4	ALA	CA	50.07	0.05	1
1	B	4	ALA	CA	50.07	0.05	1
1	E	4	ALA	CA	50.07	0.05	1
1	D	4	ALA	CA	50.07	0.05	1
1	G	4	ALA	CA	50.07	0.05	1
1	F	4	ALA	CA	50.07	0.05	1
1	H	4	ALA	CA	50.07	0.05	1
1	A	4	ALA	CB	21.91	0.05	1
1	C	4	ALA	CB	21.91	0.05	1
1	B	4	ALA	CB	21.91	0.05	1
1	E	4	ALA	CB	21.91	0.05	1
1	D	4	ALA	CB	21.91	0.05	1
1	G	4	ALA	CB	21.91	0.05	1
1	F	4	ALA	CB	21.91	0.05	1
1	H	4	ALA	CB	21.91	0.05	1
1	A	4	ALA	N	120.41	0.05	1
1	C	4	ALA	N	120.41	0.05	1
1	B	4	ALA	N	120.41	0.05	1
1	E	4	ALA	N	120.41	0.05	1
1	D	4	ALA	N	120.41	0.05	1
1	G	4	ALA	N	120.41	0.05	1
1	F	4	ALA	N	120.41	0.05	1
1	H	4	ALA	N	120.41	0.05	1
1	A	5	ILE	C	172.34	0.05	1
1	C	5	ILE	C	172.34	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	5	ILE	C	172.34	0.05	1
1	E	5	ILE	C	172.34	0.05	1
1	D	5	ILE	C	172.34	0.05	1
1	G	5	ILE	C	172.34	0.05	1
1	F	5	ILE	C	172.34	0.05	1
1	H	5	ILE	C	172.34	0.05	1
1	A	5	ILE	CA	59.28	0.05	1
1	C	5	ILE	CA	59.28	0.05	1
1	B	5	ILE	CA	59.28	0.05	1
1	E	5	ILE	CA	59.28	0.05	1
1	D	5	ILE	CA	59.28	0.05	1
1	G	5	ILE	CA	59.28	0.05	1
1	F	5	ILE	CA	59.28	0.05	1
1	H	5	ILE	CA	59.28	0.05	1
1	A	5	ILE	CB	43.98	0.05	1
1	C	5	ILE	CB	43.98	0.05	1
1	B	5	ILE	CB	43.98	0.05	1
1	E	5	ILE	CB	43.98	0.05	1
1	D	5	ILE	CB	43.98	0.05	1
1	G	5	ILE	CB	43.98	0.05	1
1	F	5	ILE	CB	43.98	0.05	1
1	H	5	ILE	CB	43.98	0.05	1
1	A	5	ILE	CD1	15.19	0.05	1
1	C	5	ILE	CD1	15.19	0.05	1
1	B	5	ILE	CD1	15.19	0.05	1
1	E	5	ILE	CD1	15.19	0.05	1
1	D	5	ILE	CD1	15.19	0.05	1
1	G	5	ILE	CD1	15.19	0.05	1
1	F	5	ILE	CD1	15.19	0.05	1
1	H	5	ILE	CD1	15.19	0.05	1
1	A	5	ILE	CG1	28.73	0.05	1
1	C	5	ILE	CG1	28.73	0.05	1
1	B	5	ILE	CG1	28.73	0.05	1
1	E	5	ILE	CG1	28.73	0.05	1
1	D	5	ILE	CG1	28.73	0.05	1
1	G	5	ILE	CG1	28.73	0.05	1
1	F	5	ILE	CG1	28.73	0.05	1
1	H	5	ILE	CG1	28.73	0.05	1
1	A	5	ILE	CG2	16.30	0.05	1
1	C	5	ILE	CG2	16.30	0.05	1
1	B	5	ILE	CG2	16.30	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	E	5	ILE	CG2	16.30	0.05	1
1	D	5	ILE	CG2	16.30	0.05	1
1	G	5	ILE	CG2	16.30	0.05	1
1	F	5	ILE	CG2	16.30	0.05	1
1	H	5	ILE	CG2	16.30	0.05	1
1	A	5	ILE	N	118.22	0.05	1
1	C	5	ILE	N	118.22	0.05	1
1	B	5	ILE	N	118.22	0.05	1
1	E	5	ILE	N	118.22	0.05	1
1	D	5	ILE	N	118.22	0.05	1
1	G	5	ILE	N	118.22	0.05	1
1	F	5	ILE	N	118.22	0.05	1
1	H	5	ILE	N	118.22	0.05	1
1	A	6	LEU	C	174.39	0.05	1
1	C	6	LEU	C	174.39	0.05	1
1	B	6	LEU	C	174.39	0.05	1
1	E	6	LEU	C	174.39	0.05	1
1	D	6	LEU	C	174.39	0.05	1
1	G	6	LEU	C	174.39	0.05	1
1	F	6	LEU	C	174.39	0.05	1
1	H	6	LEU	C	174.39	0.05	1
1	A	6	LEU	CA	53.97	0.05	1
1	C	6	LEU	CA	53.97	0.05	1
1	B	6	LEU	CA	53.97	0.05	1
1	E	6	LEU	CA	53.97	0.05	1
1	D	6	LEU	CA	53.97	0.05	1
1	G	6	LEU	CA	53.97	0.05	1
1	F	6	LEU	CA	53.97	0.05	1
1	H	6	LEU	CA	53.97	0.05	1
1	A	6	LEU	CB	45.22	0.05	1
1	C	6	LEU	CB	45.22	0.05	1
1	B	6	LEU	CB	45.22	0.05	1
1	E	6	LEU	CB	45.22	0.05	1
1	D	6	LEU	CB	45.22	0.05	1
1	G	6	LEU	CB	45.22	0.05	1
1	F	6	LEU	CB	45.22	0.05	1
1	H	6	LEU	CB	45.22	0.05	1
1	A	6	LEU	CD1	27.33	0.05	1
1	C	6	LEU	CD1	27.33	0.05	1
1	B	6	LEU	CD1	27.33	0.05	1
1	E	6	LEU	CD1	27.33	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	D	6	LEU	CD1	27.33	0.05	1
1	G	6	LEU	CD1	27.33	0.05	1
1	F	6	LEU	CD1	27.33	0.05	1
1	H	6	LEU	CD1	27.33	0.05	1
1	A	6	LEU	CD2	23.55	0.05	1
1	C	6	LEU	CD2	23.55	0.05	1
1	B	6	LEU	CD2	23.55	0.05	1
1	E	6	LEU	CD2	23.55	0.05	1
1	D	6	LEU	CD2	23.55	0.05	1
1	G	6	LEU	CD2	23.55	0.05	1
1	F	6	LEU	CD2	23.55	0.05	1
1	H	6	LEU	CD2	23.55	0.05	1
1	A	6	LEU	CG	29.13	0.05	1
1	C	6	LEU	CG	29.13	0.05	1
1	B	6	LEU	CG	29.13	0.05	1
1	E	6	LEU	CG	29.13	0.05	1
1	D	6	LEU	CG	29.13	0.05	1
1	G	6	LEU	CG	29.13	0.05	1
1	F	6	LEU	CG	29.13	0.05	1
1	H	6	LEU	CG	29.13	0.05	1
1	A	6	LEU	N	128.53	0.05	1
1	C	6	LEU	N	128.53	0.05	1
1	B	6	LEU	N	128.53	0.05	1
1	E	6	LEU	N	128.53	0.05	1
1	D	6	LEU	N	128.53	0.05	1
1	G	6	LEU	N	128.53	0.05	1
1	F	6	LEU	N	128.53	0.05	1
1	H	6	LEU	N	128.53	0.05	1
1	A	1	ASN	C	171.67	0.05	1
1	C	1	ASN	C	171.67	0.05	1
1	B	1	ASN	C	171.67	0.05	1
1	E	1	ASN	C	171.67	0.05	1
1	D	1	ASN	C	171.67	0.05	1
1	G	1	ASN	C	171.67	0.05	1
1	F	1	ASN	C	171.67	0.05	1
1	H	1	ASN	C	171.67	0.05	1
1	A	1	ASN	CA	51.95	0.05	1
1	C	1	ASN	CA	51.95	0.05	1
1	B	1	ASN	CA	51.95	0.05	1
1	E	1	ASN	CA	51.95	0.05	1
1	D	1	ASN	CA	51.95	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	G	1	ASN	CA	51.95	0.05	1
1	F	1	ASN	CA	51.95	0.05	1
1	H	1	ASN	CA	51.95	0.05	1
1	A	1	ASN	CB	41.62	0.05	1
1	C	1	ASN	CB	41.62	0.05	1
1	B	1	ASN	CB	41.62	0.05	1
1	E	1	ASN	CB	41.62	0.05	1
1	D	1	ASN	CB	41.62	0.05	1
1	G	1	ASN	CB	41.62	0.05	1
1	F	1	ASN	CB	41.62	0.05	1
1	H	1	ASN	CB	41.62	0.05	1
1	A	1	ASN	CG	174.78	0.05	1
1	C	1	ASN	CG	174.78	0.05	1
1	B	1	ASN	CG	174.78	0.05	1
1	E	1	ASN	CG	174.78	0.05	1
1	D	1	ASN	CG	174.78	0.05	1
1	G	1	ASN	CG	174.78	0.05	1
1	F	1	ASN	CG	174.78	0.05	1
1	H	1	ASN	CG	174.78	0.05	1
1	A	1	ASN	N	119.69	0.05	1
1	C	1	ASN	N	119.69	0.05	1
1	B	1	ASN	N	119.69	0.05	1
1	E	1	ASN	N	119.69	0.05	1
1	D	1	ASN	N	119.69	0.05	1
1	G	1	ASN	N	119.69	0.05	1
1	F	1	ASN	N	119.69	0.05	1
1	H	1	ASN	N	119.69	0.05	1
1	A	2	PHE	C	175.27	0.05	1
1	C	2	PHE	C	175.27	0.05	1
1	B	2	PHE	C	175.27	0.05	1
1	E	2	PHE	C	175.27	0.05	1
1	D	2	PHE	C	175.27	0.05	1
1	G	2	PHE	C	175.27	0.05	1
1	F	2	PHE	C	175.27	0.05	1
1	H	2	PHE	C	175.27	0.05	1
1	A	2	PHE	CA	55.56	0.05	1
1	C	2	PHE	CA	55.56	0.05	1
1	B	2	PHE	CA	55.56	0.05	1
1	E	2	PHE	CA	55.56	0.05	1
1	D	2	PHE	CA	55.56	0.05	1
1	G	2	PHE	CA	55.56	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	F	2	PHE	CA	55.56	0.05	1
1	H	2	PHE	CA	55.56	0.05	1
1	A	2	PHE	CB	42.79	0.05	1
1	C	2	PHE	CB	42.79	0.05	1
1	B	2	PHE	CB	42.79	0.05	1
1	E	2	PHE	CB	42.79	0.05	1
1	D	2	PHE	CB	42.79	0.05	1
1	G	2	PHE	CB	42.79	0.05	1
1	F	2	PHE	CB	42.79	0.05	1
1	H	2	PHE	CB	42.79	0.05	1
1	A	2	PHE	CD1	131.27	0.05	4
1	C	2	PHE	CD1	131.27	0.05	4
1	B	2	PHE	CD1	131.27	0.05	4
1	E	2	PHE	CD1	131.27	0.05	4
1	D	2	PHE	CD1	131.27	0.05	4
1	G	2	PHE	CD1	131.27	0.05	4
1	F	2	PHE	CD1	131.27	0.05	4
1	H	2	PHE	CD1	131.27	0.05	4
1	A	2	PHE	CD2	131.27	0.05	4
1	C	2	PHE	CD2	131.27	0.05	4
1	B	2	PHE	CD2	131.27	0.05	4
1	E	2	PHE	CD2	131.27	0.05	4
1	D	2	PHE	CD2	131.27	0.05	4
1	G	2	PHE	CD2	131.27	0.05	4
1	F	2	PHE	CD2	131.27	0.05	4
1	H	2	PHE	CD2	131.27	0.05	4
1	A	2	PHE	CE1	132.60	0.05	4
1	C	2	PHE	CE1	132.60	0.05	4
1	B	2	PHE	CE1	132.60	0.05	4
1	E	2	PHE	CE1	132.60	0.05	4
1	D	2	PHE	CE1	132.60	0.05	4
1	G	2	PHE	CE1	132.60	0.05	4
1	F	2	PHE	CE1	132.60	0.05	4
1	H	2	PHE	CE1	132.60	0.05	4
1	A	2	PHE	CE2	132.60	0.05	4
1	C	2	PHE	CE2	132.60	0.05	4
1	B	2	PHE	CE2	132.60	0.05	4
1	E	2	PHE	CE2	132.60	0.05	4
1	D	2	PHE	CE2	132.60	0.05	4
1	G	2	PHE	CE2	132.60	0.05	4
1	F	2	PHE	CE2	132.60	0.05	4

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	H	2	PHE	CE2	132.60	0.05	4
1	A	2	PHE	CG	137.04	0.05	1
1	C	2	PHE	CG	137.04	0.05	1
1	B	2	PHE	CG	137.04	0.05	1
1	E	2	PHE	CG	137.04	0.05	1
1	D	2	PHE	CG	137.04	0.05	1
1	G	2	PHE	CG	137.04	0.05	1
1	F	2	PHE	CG	137.04	0.05	1
1	H	2	PHE	CG	137.04	0.05	1
1	A	2	PHE	CZ	131.72	0.05	4
1	C	2	PHE	CZ	131.72	0.05	4
1	B	2	PHE	CZ	131.72	0.05	4
1	E	2	PHE	CZ	131.72	0.05	4
1	D	2	PHE	CZ	131.72	0.05	4
1	G	2	PHE	CZ	131.72	0.05	4
1	F	2	PHE	CZ	131.72	0.05	4
1	H	2	PHE	CZ	131.72	0.05	4
1	A	2	PHE	N	120.36	0.05	1
1	C	2	PHE	N	120.36	0.05	1
1	B	2	PHE	N	120.36	0.05	1
1	E	2	PHE	N	120.36	0.05	1
1	D	2	PHE	N	120.36	0.05	1
1	G	2	PHE	N	120.36	0.05	1
1	F	2	PHE	N	120.36	0.05	1
1	H	2	PHE	N	120.36	0.05	1
1	A	3	GLY	C	168.74	0.05	1
1	C	3	GLY	C	168.74	0.05	1
1	B	3	GLY	C	168.74	0.05	1
1	E	3	GLY	C	168.74	0.05	1
1	D	3	GLY	C	168.74	0.05	1
1	G	3	GLY	C	168.74	0.05	1
1	F	3	GLY	C	168.74	0.05	1
1	H	3	GLY	C	168.74	0.05	1
1	A	3	GLY	CA	48.06	0.05	1
1	C	3	GLY	CA	48.06	0.05	1
1	B	3	GLY	CA	48.06	0.05	1
1	E	3	GLY	CA	48.06	0.05	1
1	D	3	GLY	CA	48.06	0.05	1
1	G	3	GLY	CA	48.06	0.05	1
1	F	3	GLY	CA	48.06	0.05	1
1	H	3	GLY	CA	48.06	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	GLY	N	115.53	0.05	1
1	C	3	GLY	N	115.53	0.05	1
1	B	3	GLY	N	115.53	0.05	1
1	E	3	GLY	N	115.53	0.05	1
1	D	3	GLY	N	115.53	0.05	1
1	G	3	GLY	N	115.53	0.05	1
1	F	3	GLY	N	115.53	0.05	1
1	H	3	GLY	N	115.53	0.05	1
1	A	4	ALA	C	174.31	0.05	1
1	C	4	ALA	C	174.31	0.05	1
1	B	4	ALA	C	174.31	0.05	1
1	E	4	ALA	C	174.31	0.05	1
1	D	4	ALA	C	174.31	0.05	1
1	G	4	ALA	C	174.31	0.05	1
1	F	4	ALA	C	174.31	0.05	1
1	H	4	ALA	C	174.31	0.05	1
1	A	4	ALA	CA	49.51	0.05	1
1	C	4	ALA	CA	49.51	0.05	1
1	B	4	ALA	CA	49.51	0.05	1
1	E	4	ALA	CA	49.51	0.05	1
1	D	4	ALA	CA	49.51	0.05	1
1	G	4	ALA	CA	49.51	0.05	1
1	F	4	ALA	CA	49.51	0.05	1
1	H	4	ALA	CA	49.51	0.05	1
1	A	4	ALA	CB	21.09	0.05	1
1	C	4	ALA	CB	21.09	0.05	1
1	B	4	ALA	CB	21.09	0.05	1
1	E	4	ALA	CB	21.09	0.05	1
1	D	4	ALA	CB	21.09	0.05	1
1	G	4	ALA	CB	21.09	0.05	1
1	F	4	ALA	CB	21.09	0.05	1
1	H	4	ALA	CB	21.09	0.05	1
1	A	4	ALA	N	127.05	0.05	1
1	C	4	ALA	N	127.05	0.05	1
1	B	4	ALA	N	127.05	0.05	1
1	E	4	ALA	N	127.05	0.05	1
1	D	4	ALA	N	127.05	0.05	1
1	G	4	ALA	N	127.05	0.05	1
1	F	4	ALA	N	127.05	0.05	1
1	H	4	ALA	N	127.05	0.05	1
1	A	5	ILE	C	173.57	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	5	ILE	C	173.57	0.05	1
1	B	5	ILE	C	173.57	0.05	1
1	E	5	ILE	C	173.57	0.05	1
1	D	5	ILE	C	173.57	0.05	1
1	G	5	ILE	C	173.57	0.05	1
1	F	5	ILE	C	173.57	0.05	1
1	H	5	ILE	C	173.57	0.05	1
1	A	5	ILE	CA	59.89	0.05	1
1	C	5	ILE	CA	59.89	0.05	1
1	B	5	ILE	CA	59.89	0.05	1
1	E	5	ILE	CA	59.89	0.05	1
1	D	5	ILE	CA	59.89	0.05	1
1	G	5	ILE	CA	59.89	0.05	1
1	F	5	ILE	CA	59.89	0.05	1
1	H	5	ILE	CA	59.89	0.05	1
1	A	5	ILE	CB	41.33	0.05	1
1	C	5	ILE	CB	41.33	0.05	1
1	B	5	ILE	CB	41.33	0.05	1
1	E	5	ILE	CB	41.33	0.05	1
1	D	5	ILE	CB	41.33	0.05	1
1	G	5	ILE	CB	41.33	0.05	1
1	F	5	ILE	CB	41.33	0.05	1
1	H	5	ILE	CB	41.33	0.05	1
1	A	5	ILE	CD1	15.25	0.05	1
1	C	5	ILE	CD1	15.25	0.05	1
1	B	5	ILE	CD1	15.25	0.05	1
1	E	5	ILE	CD1	15.25	0.05	1
1	D	5	ILE	CD1	15.25	0.05	1
1	G	5	ILE	CD1	15.25	0.05	1
1	F	5	ILE	CD1	15.25	0.05	1
1	H	5	ILE	CD1	15.25	0.05	1
1	A	5	ILE	CG1	28.09	0.05	1
1	C	5	ILE	CG1	28.09	0.05	1
1	B	5	ILE	CG1	28.09	0.05	1
1	E	5	ILE	CG1	28.09	0.05	1
1	D	5	ILE	CG1	28.09	0.05	1
1	G	5	ILE	CG1	28.09	0.05	1
1	F	5	ILE	CG1	28.09	0.05	1
1	H	5	ILE	CG1	28.09	0.05	1
1	A	5	ILE	CG2	16.65	0.05	1
1	C	5	ILE	CG2	16.65	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	5	ILE	CG2	16.65	0.05	1
1	E	5	ILE	CG2	16.65	0.05	1
1	D	5	ILE	CG2	16.65	0.05	1
1	G	5	ILE	CG2	16.65	0.05	1
1	F	5	ILE	CG2	16.65	0.05	1
1	H	5	ILE	CG2	16.65	0.05	1
1	A	5	ILE	N	119.52	0.05	1
1	C	5	ILE	N	119.52	0.05	1
1	B	5	ILE	N	119.52	0.05	1
1	E	5	ILE	N	119.52	0.05	1
1	D	5	ILE	N	119.52	0.05	1
1	G	5	ILE	N	119.52	0.05	1
1	F	5	ILE	N	119.52	0.05	1
1	H	5	ILE	N	119.52	0.05	1
1	A	6	LEU	C	175.01	0.05	1
1	C	6	LEU	C	175.01	0.05	1
1	B	6	LEU	C	175.01	0.05	1
1	E	6	LEU	C	175.01	0.05	1
1	D	6	LEU	C	175.01	0.05	1
1	G	6	LEU	C	175.01	0.05	1
1	F	6	LEU	C	175.01	0.05	1
1	H	6	LEU	C	175.01	0.05	1
1	A	6	LEU	CA	54.47	0.05	1
1	C	6	LEU	CA	54.47	0.05	1
1	B	6	LEU	CA	54.47	0.05	1
1	E	6	LEU	CA	54.47	0.05	1
1	D	6	LEU	CA	54.47	0.05	1
1	G	6	LEU	CA	54.47	0.05	1
1	F	6	LEU	CA	54.47	0.05	1
1	H	6	LEU	CA	54.47	0.05	1
1	A	6	LEU	CB	44.11	0.05	1
1	C	6	LEU	CB	44.11	0.05	1
1	B	6	LEU	CB	44.11	0.05	1
1	E	6	LEU	CB	44.11	0.05	1
1	D	6	LEU	CB	44.11	0.05	1
1	G	6	LEU	CB	44.11	0.05	1
1	F	6	LEU	CB	44.11	0.05	1
1	H	6	LEU	CB	44.11	0.05	1
1	A	6	LEU	CD1	25.87	0.05	1
1	C	6	LEU	CD1	25.87	0.05	1
1	B	6	LEU	CD1	25.87	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	E	6	LEU	CD1	25.87	0.05	1
1	D	6	LEU	CD1	25.87	0.05	1
1	G	6	LEU	CD1	25.87	0.05	1
1	F	6	LEU	CD1	25.87	0.05	1
1	H	6	LEU	CD1	25.87	0.05	1
1	A	6	LEU	CD2	23.20	0.05	1
1	C	6	LEU	CD2	23.20	0.05	1
1	B	6	LEU	CD2	23.20	0.05	1
1	E	6	LEU	CD2	23.20	0.05	1
1	D	6	LEU	CD2	23.20	0.05	1
1	G	6	LEU	CD2	23.20	0.05	1
1	F	6	LEU	CD2	23.20	0.05	1
1	H	6	LEU	CD2	23.20	0.05	1
1	A	6	LEU	CG	29.33	0.05	1
1	C	6	LEU	CG	29.33	0.05	1
1	B	6	LEU	CG	29.33	0.05	1
1	E	6	LEU	CG	29.33	0.05	1
1	D	6	LEU	CG	29.33	0.05	1
1	G	6	LEU	CG	29.33	0.05	1
1	F	6	LEU	CG	29.33	0.05	1
1	H	6	LEU	CG	29.33	0.05	1
1	A	6	LEU	N	126.79	0.05	1
1	C	6	LEU	N	126.79	0.05	1
1	B	6	LEU	N	126.79	0.05	1
1	E	6	LEU	N	126.79	0.05	1
1	D	6	LEU	N	126.79	0.05	1
1	G	6	LEU	N	126.79	0.05	1
1	F	6	LEU	N	126.79	0.05	1
1	H	6	LEU	N	126.79	0.05	1
1	A	1	ASN	C	171.67	0.05	1
1	C	1	ASN	C	171.67	0.05	1
1	B	1	ASN	C	171.67	0.05	1
1	E	1	ASN	C	171.67	0.05	1
1	D	1	ASN	C	171.67	0.05	1
1	G	1	ASN	C	171.67	0.05	1
1	F	1	ASN	C	171.67	0.05	1
1	H	1	ASN	C	171.67	0.05	1
1	A	1	ASN	CA	51.95	0.05	1
1	C	1	ASN	CA	51.95	0.05	1
1	B	1	ASN	CA	51.95	0.05	1
1	E	1	ASN	CA	51.95	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	D	1	ASN	CA	51.95	0.05	1
1	G	1	ASN	CA	51.95	0.05	1
1	F	1	ASN	CA	51.95	0.05	1
1	H	1	ASN	CA	51.95	0.05	1
1	A	1	ASN	CB	41.62	0.05	1
1	C	1	ASN	CB	41.62	0.05	1
1	B	1	ASN	CB	41.62	0.05	1
1	E	1	ASN	CB	41.62	0.05	1
1	D	1	ASN	CB	41.62	0.05	1
1	G	1	ASN	CB	41.62	0.05	1
1	F	1	ASN	CB	41.62	0.05	1
1	H	1	ASN	CB	41.62	0.05	1
1	A	1	ASN	CG	174.78	0.05	1
1	C	1	ASN	CG	174.78	0.05	1
1	B	1	ASN	CG	174.78	0.05	1
1	E	1	ASN	CG	174.78	0.05	1
1	D	1	ASN	CG	174.78	0.05	1
1	G	1	ASN	CG	174.78	0.05	1
1	F	1	ASN	CG	174.78	0.05	1
1	H	1	ASN	CG	174.78	0.05	1
1	A	1	ASN	N	119.69	0.05	1
1	C	1	ASN	N	119.69	0.05	1
1	B	1	ASN	N	119.69	0.05	1
1	E	1	ASN	N	119.69	0.05	1
1	D	1	ASN	N	119.69	0.05	1
1	G	1	ASN	N	119.69	0.05	1
1	F	1	ASN	N	119.69	0.05	1
1	H	1	ASN	N	119.69	0.05	1
1	A	2	PHE	C	175.27	0.05	1
1	C	2	PHE	C	175.27	0.05	1
1	B	2	PHE	C	175.27	0.05	1
1	E	2	PHE	C	175.27	0.05	1
1	D	2	PHE	C	175.27	0.05	1
1	G	2	PHE	C	175.27	0.05	1
1	F	2	PHE	C	175.27	0.05	1
1	H	2	PHE	C	175.27	0.05	1
1	A	2	PHE	CA	55.56	0.05	1
1	C	2	PHE	CA	55.56	0.05	1
1	B	2	PHE	CA	55.56	0.05	1
1	E	2	PHE	CA	55.56	0.05	1
1	D	2	PHE	CA	55.56	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	G	2	PHE	CA	55.56	0.05	1
1	F	2	PHE	CA	55.56	0.05	1
1	H	2	PHE	CA	55.56	0.05	1
1	A	2	PHE	CB	42.79	0.05	1
1	C	2	PHE	CB	42.79	0.05	1
1	B	2	PHE	CB	42.79	0.05	1
1	E	2	PHE	CB	42.79	0.05	1
1	D	2	PHE	CB	42.79	0.05	1
1	G	2	PHE	CB	42.79	0.05	1
1	F	2	PHE	CB	42.79	0.05	1
1	H	2	PHE	CB	42.79	0.05	1
1	A	2	PHE	CD1	131.27	0.05	4
1	C	2	PHE	CD1	131.27	0.05	4
1	B	2	PHE	CD1	131.27	0.05	4
1	E	2	PHE	CD1	131.27	0.05	4
1	D	2	PHE	CD1	131.27	0.05	4
1	G	2	PHE	CD1	131.27	0.05	4
1	F	2	PHE	CD1	131.27	0.05	4
1	H	2	PHE	CD1	131.27	0.05	4
1	A	2	PHE	CD2	131.27	0.05	4
1	C	2	PHE	CD2	131.27	0.05	4
1	B	2	PHE	CD2	131.27	0.05	4
1	E	2	PHE	CD2	131.27	0.05	4
1	D	2	PHE	CD2	131.27	0.05	4
1	G	2	PHE	CD2	131.27	0.05	4
1	F	2	PHE	CD2	131.27	0.05	4
1	H	2	PHE	CD2	131.27	0.05	4
1	A	2	PHE	CE1	132.60	0.05	4
1	C	2	PHE	CE1	132.60	0.05	4
1	B	2	PHE	CE1	132.60	0.05	4
1	E	2	PHE	CE1	132.60	0.05	4
1	D	2	PHE	CE1	132.60	0.05	4
1	G	2	PHE	CE1	132.60	0.05	4
1	F	2	PHE	CE1	132.60	0.05	4
1	H	2	PHE	CE1	132.60	0.05	4
1	A	2	PHE	CE2	132.60	0.05	4
1	C	2	PHE	CE2	132.60	0.05	4
1	B	2	PHE	CE2	132.60	0.05	4
1	E	2	PHE	CE2	132.60	0.05	4
1	D	2	PHE	CE2	132.60	0.05	4
1	G	2	PHE	CE2	132.60	0.05	4

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	F	2	PHE	CE2	132.60	0.05	4
1	H	2	PHE	CE2	132.60	0.05	4
1	A	2	PHE	CG	137.04	0.05	1
1	C	2	PHE	CG	137.04	0.05	1
1	B	2	PHE	CG	137.04	0.05	1
1	E	2	PHE	CG	137.04	0.05	1
1	D	2	PHE	CG	137.04	0.05	1
1	G	2	PHE	CG	137.04	0.05	1
1	F	2	PHE	CG	137.04	0.05	1
1	H	2	PHE	CG	137.04	0.05	1
1	A	2	PHE	CZ	131.72	0.05	4
1	C	2	PHE	CZ	131.72	0.05	4
1	B	2	PHE	CZ	131.72	0.05	4
1	E	2	PHE	CZ	131.72	0.05	4
1	D	2	PHE	CZ	131.72	0.05	4
1	G	2	PHE	CZ	131.72	0.05	4
1	F	2	PHE	CZ	131.72	0.05	4
1	H	2	PHE	CZ	131.72	0.05	4
1	A	2	PHE	N	120.36	0.05	1
1	C	2	PHE	N	120.36	0.05	1
1	B	2	PHE	N	120.36	0.05	1
1	E	2	PHE	N	120.36	0.05	1
1	D	2	PHE	N	120.36	0.05	1
1	G	2	PHE	N	120.36	0.05	1
1	F	2	PHE	N	120.36	0.05	1
1	H	2	PHE	N	120.36	0.05	1
1	A	3	GLY	C	168.97	0.05	1
1	C	3	GLY	C	168.97	0.05	1
1	B	3	GLY	C	168.97	0.05	1
1	E	3	GLY	C	168.97	0.05	1
1	D	3	GLY	C	168.97	0.05	1
1	G	3	GLY	C	168.97	0.05	1
1	F	3	GLY	C	168.97	0.05	1
1	H	3	GLY	C	168.97	0.05	1
1	A	3	GLY	CA	48.06	0.05	1
1	C	3	GLY	CA	48.06	0.05	1
1	B	3	GLY	CA	48.06	0.05	1
1	E	3	GLY	CA	48.06	0.05	1
1	D	3	GLY	CA	48.06	0.05	1
1	G	3	GLY	CA	48.06	0.05	1
1	F	3	GLY	CA	48.06	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	H	3	GLY	CA	48.06	0.05	1
1	A	3	GLY	N	115.53	0.05	1
1	C	3	GLY	N	115.53	0.05	1
1	B	3	GLY	N	115.53	0.05	1
1	E	3	GLY	N	115.53	0.05	1
1	D	3	GLY	N	115.53	0.05	1
1	G	3	GLY	N	115.53	0.05	1
1	F	3	GLY	N	115.53	0.05	1
1	H	3	GLY	N	115.53	0.05	1
1	A	4	ALA	C	174.31	0.05	1
1	C	4	ALA	C	174.31	0.05	1
1	B	4	ALA	C	174.31	0.05	1
1	E	4	ALA	C	174.31	0.05	1
1	D	4	ALA	C	174.31	0.05	1
1	G	4	ALA	C	174.31	0.05	1
1	F	4	ALA	C	174.31	0.05	1
1	H	4	ALA	C	174.31	0.05	1
1	A	4	ALA	CA	49.51	0.05	1
1	C	4	ALA	CA	49.51	0.05	1
1	B	4	ALA	CA	49.51	0.05	1
1	E	4	ALA	CA	49.51	0.05	1
1	D	4	ALA	CA	49.51	0.05	1
1	G	4	ALA	CA	49.51	0.05	1
1	F	4	ALA	CA	49.51	0.05	1
1	H	4	ALA	CA	49.51	0.05	1
1	A	4	ALA	CB	21.09	0.05	1
1	C	4	ALA	CB	21.09	0.05	1
1	B	4	ALA	CB	21.09	0.05	1
1	E	4	ALA	CB	21.09	0.05	1
1	D	4	ALA	CB	21.09	0.05	1
1	G	4	ALA	CB	21.09	0.05	1
1	F	4	ALA	CB	21.09	0.05	1
1	H	4	ALA	CB	21.09	0.05	1
1	A	4	ALA	N	127.76	0.05	1
1	C	4	ALA	N	127.76	0.05	1
1	B	4	ALA	N	127.76	0.05	1
1	E	4	ALA	N	127.76	0.05	1
1	D	4	ALA	N	127.76	0.05	1
1	G	4	ALA	N	127.76	0.05	1
1	F	4	ALA	N	127.76	0.05	1
1	H	4	ALA	N	127.76	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	ILE	C	173.57	0.05	1
1	C	5	ILE	C	173.57	0.05	1
1	B	5	ILE	C	173.57	0.05	1
1	E	5	ILE	C	173.57	0.05	1
1	D	5	ILE	C	173.57	0.05	1
1	G	5	ILE	C	173.57	0.05	1
1	F	5	ILE	C	173.57	0.05	1
1	H	5	ILE	C	173.57	0.05	1
1	A	5	ILE	CA	59.85	0.05	1
1	C	5	ILE	CA	59.85	0.05	1
1	B	5	ILE	CA	59.85	0.05	1
1	E	5	ILE	CA	59.85	0.05	1
1	D	5	ILE	CA	59.85	0.05	1
1	G	5	ILE	CA	59.85	0.05	1
1	F	5	ILE	CA	59.85	0.05	1
1	H	5	ILE	CA	59.85	0.05	1
1	A	5	ILE	CB	41.97	0.05	1
1	C	5	ILE	CB	41.97	0.05	1
1	B	5	ILE	CB	41.97	0.05	1
1	E	5	ILE	CB	41.97	0.05	1
1	D	5	ILE	CB	41.97	0.05	1
1	G	5	ILE	CB	41.97	0.05	1
1	F	5	ILE	CB	41.97	0.05	1
1	H	5	ILE	CB	41.97	0.05	1
1	A	5	ILE	CD1	15.13	0.05	1
1	C	5	ILE	CD1	15.13	0.05	1
1	B	5	ILE	CD1	15.13	0.05	1
1	E	5	ILE	CD1	15.13	0.05	1
1	D	5	ILE	CD1	15.13	0.05	1
1	G	5	ILE	CD1	15.13	0.05	1
1	F	5	ILE	CD1	15.13	0.05	1
1	H	5	ILE	CD1	15.13	0.05	1
1	A	5	ILE	CG1	28.13	0.05	1
1	C	5	ILE	CG1	28.13	0.05	1
1	B	5	ILE	CG1	28.13	0.05	1
1	E	5	ILE	CG1	28.13	0.05	1
1	D	5	ILE	CG1	28.13	0.05	1
1	G	5	ILE	CG1	28.13	0.05	1
1	F	5	ILE	CG1	28.13	0.05	1
1	H	5	ILE	CG1	28.13	0.05	1
1	A	5	ILE	CG2	16.60	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	C	5	ILE	CG2	16.60	0.05	1
1	B	5	ILE	CG2	16.60	0.05	1
1	E	5	ILE	CG2	16.60	0.05	1
1	D	5	ILE	CG2	16.60	0.05	1
1	G	5	ILE	CG2	16.60	0.05	1
1	F	5	ILE	CG2	16.60	0.05	1
1	H	5	ILE	CG2	16.60	0.05	1
1	A	5	ILE	N	119.52	0.05	1
1	C	5	ILE	N	119.52	0.05	1
1	B	5	ILE	N	119.52	0.05	1
1	E	5	ILE	N	119.52	0.05	1
1	D	5	ILE	N	119.52	0.05	1
1	G	5	ILE	N	119.52	0.05	1
1	F	5	ILE	N	119.52	0.05	1
1	H	5	ILE	N	119.52	0.05	1
1	A	6	LEU	C	175.01	0.05	1
1	C	6	LEU	C	175.01	0.05	1
1	B	6	LEU	C	175.01	0.05	1
1	E	6	LEU	C	175.01	0.05	1
1	D	6	LEU	C	175.01	0.05	1
1	G	6	LEU	C	175.01	0.05	1
1	F	6	LEU	C	175.01	0.05	1
1	H	6	LEU	C	175.01	0.05	1
1	A	6	LEU	CA	54.47	0.05	1
1	C	6	LEU	CA	54.47	0.05	1
1	B	6	LEU	CA	54.47	0.05	1
1	E	6	LEU	CA	54.47	0.05	1
1	D	6	LEU	CA	54.47	0.05	1
1	G	6	LEU	CA	54.47	0.05	1
1	F	6	LEU	CA	54.47	0.05	1
1	H	6	LEU	CA	54.47	0.05	1
1	A	6	LEU	CB	44.11	0.05	1
1	C	6	LEU	CB	44.11	0.05	1
1	B	6	LEU	CB	44.11	0.05	1
1	E	6	LEU	CB	44.11	0.05	1
1	D	6	LEU	CB	44.11	0.05	1
1	G	6	LEU	CB	44.11	0.05	1
1	F	6	LEU	CB	44.11	0.05	1
1	H	6	LEU	CB	44.11	0.05	1
1	A	6	LEU	CD1	25.87	0.05	1
1	C	6	LEU	CD1	25.87	0.05	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	6	LEU	CD1	25.87	0.05	1
1	E	6	LEU	CD1	25.87	0.05	1
1	D	6	LEU	CD1	25.87	0.05	1
1	G	6	LEU	CD1	25.87	0.05	1
1	F	6	LEU	CD1	25.87	0.05	1
1	H	6	LEU	CD1	25.87	0.05	1
1	A	6	LEU	CD2	23.20	0.05	1
1	C	6	LEU	CD2	23.20	0.05	1
1	B	6	LEU	CD2	23.20	0.05	1
1	E	6	LEU	CD2	23.20	0.05	1
1	D	6	LEU	CD2	23.20	0.05	1
1	G	6	LEU	CD2	23.20	0.05	1
1	F	6	LEU	CD2	23.20	0.05	1
1	H	6	LEU	CD2	23.20	0.05	1
1	A	6	LEU	CG	29.33	0.05	1
1	C	6	LEU	CG	29.33	0.05	1
1	B	6	LEU	CG	29.33	0.05	1
1	E	6	LEU	CG	29.33	0.05	1
1	D	6	LEU	CG	29.33	0.05	1
1	G	6	LEU	CG	29.33	0.05	1
1	F	6	LEU	CG	29.33	0.05	1
1	H	6	LEU	CG	29.33	0.05	1
1	A	6	LEU	N	126.79	0.05	1
1	C	6	LEU	N	126.79	0.05	1
1	B	6	LEU	N	126.79	0.05	1
1	E	6	LEU	N	126.79	0.05	1
1	D	6	LEU	N	126.79	0.05	1
1	G	6	LEU	N	126.79	0.05	1
1	F	6	LEU	N	126.79	0.05	1
1	H	6	LEU	N	126.79	0.05	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	48	0.53 ± 0.08	Should be checked
$^{13}C_{\beta}$	40	-2.14 ± 0.29	Should be checked
$^{13}C'$	48	1.79 ± 0.14	Should be applied
^{15}N	48	-0.97 ± 0.66	None needed (imprecise)

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 39%, i.e. 280 atoms were assigned a chemical shift out of a possible 712. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	144/288 (50%)	0/120 (0%)	96/112 (86%)	48/56 (86%)
Sidechain	96/344 (28%)	0/232 (0%)	96/104 (92%)	0/8 (0%)
Aromatic	40/80 (50%)	0/40 (0%)	40/40 (100%)	0/0 (—%)
Overall	280/712 (39%)	0/392 (0%)	232/256 (91%)	48/64 (75%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

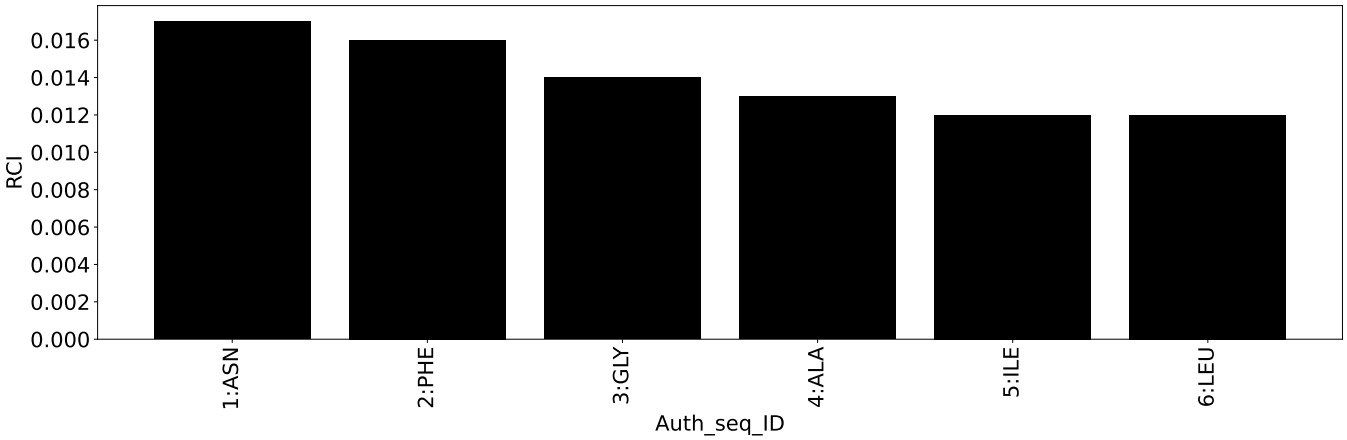
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

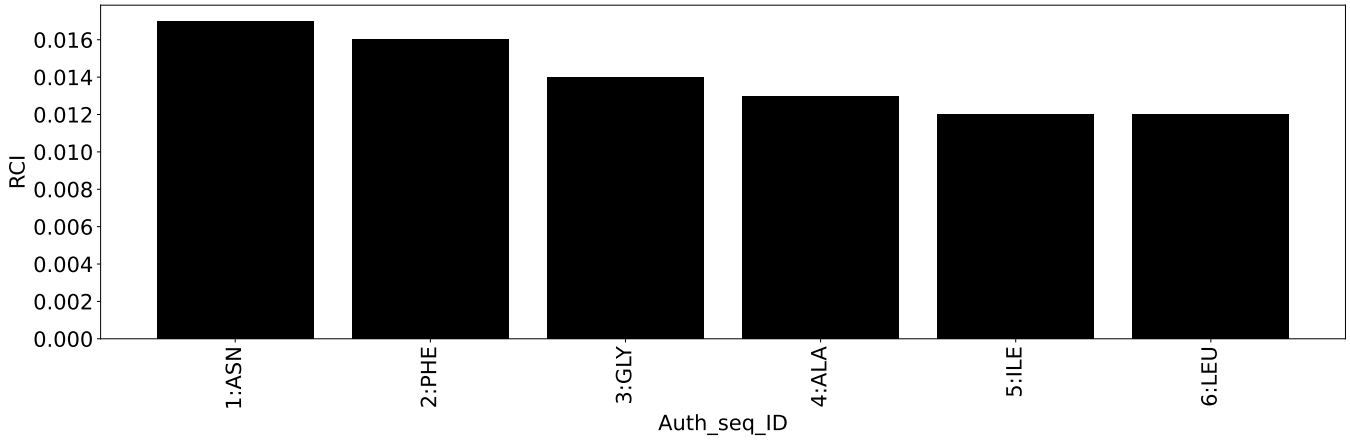
7.1.5 Random Coil Index (RCI) plots

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

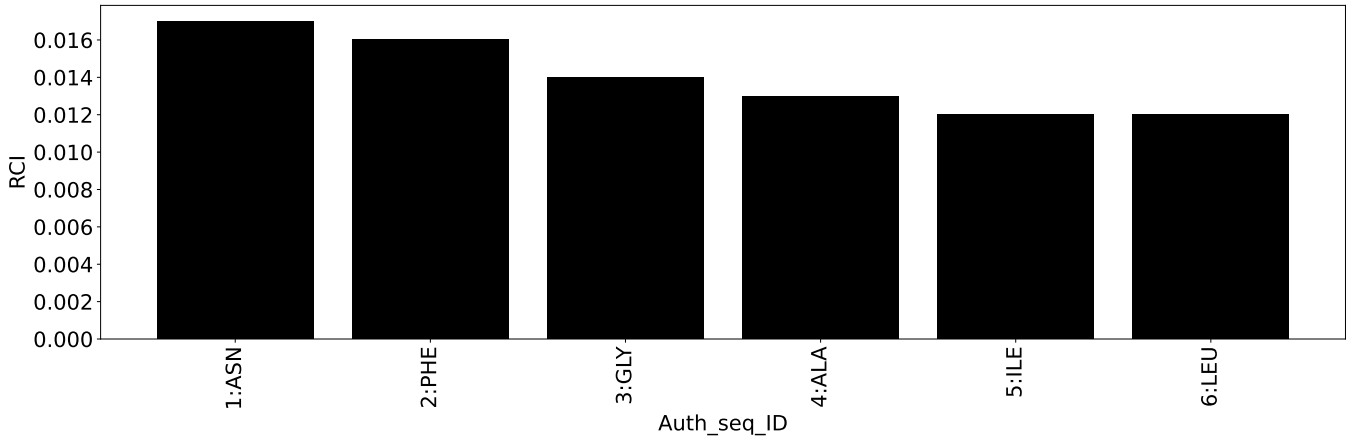
Random coil index (RCI) for chain A:



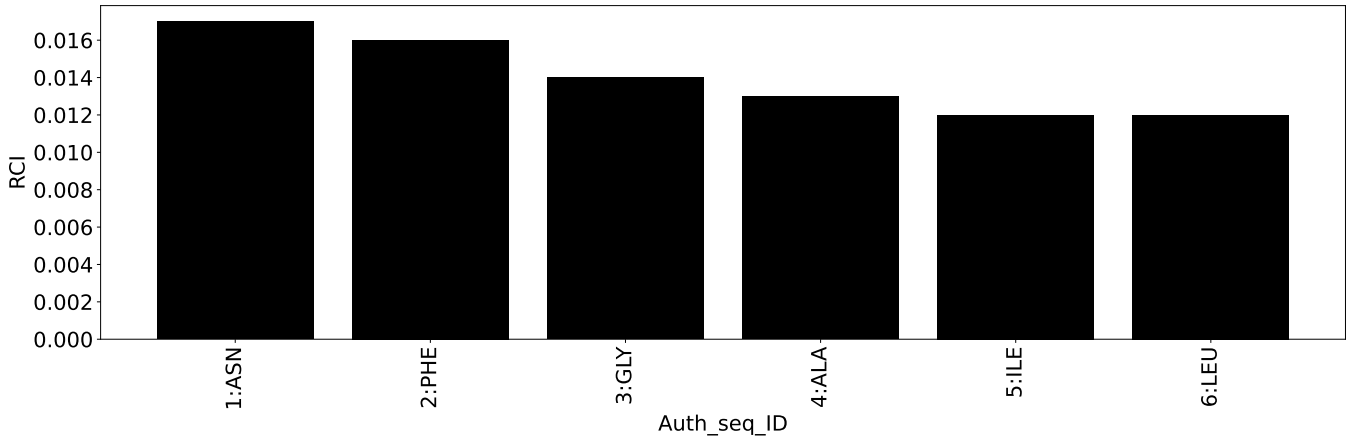
Random coil index (RCI) for chain B:



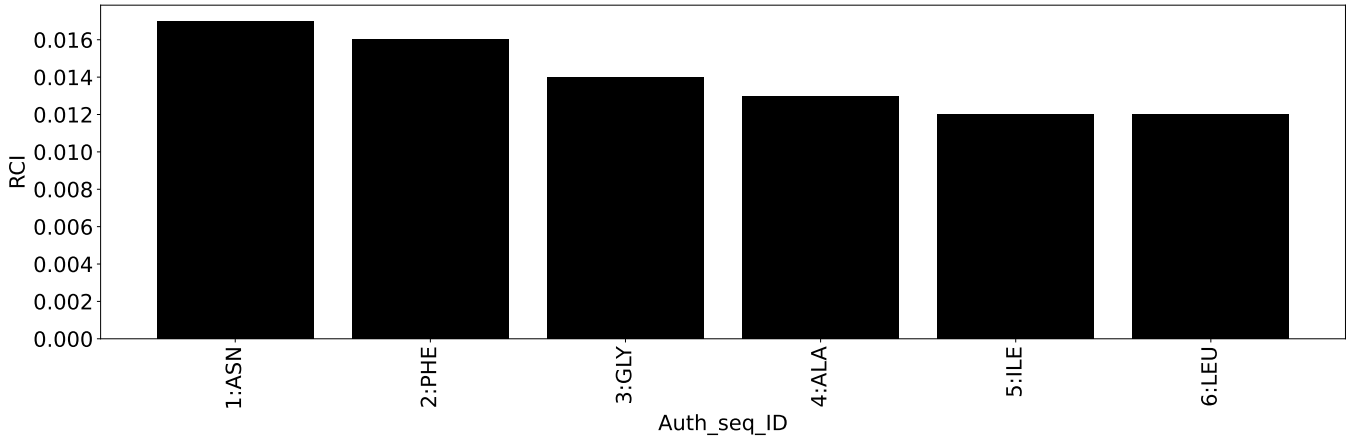
Random coil index (RCI) for chain C:



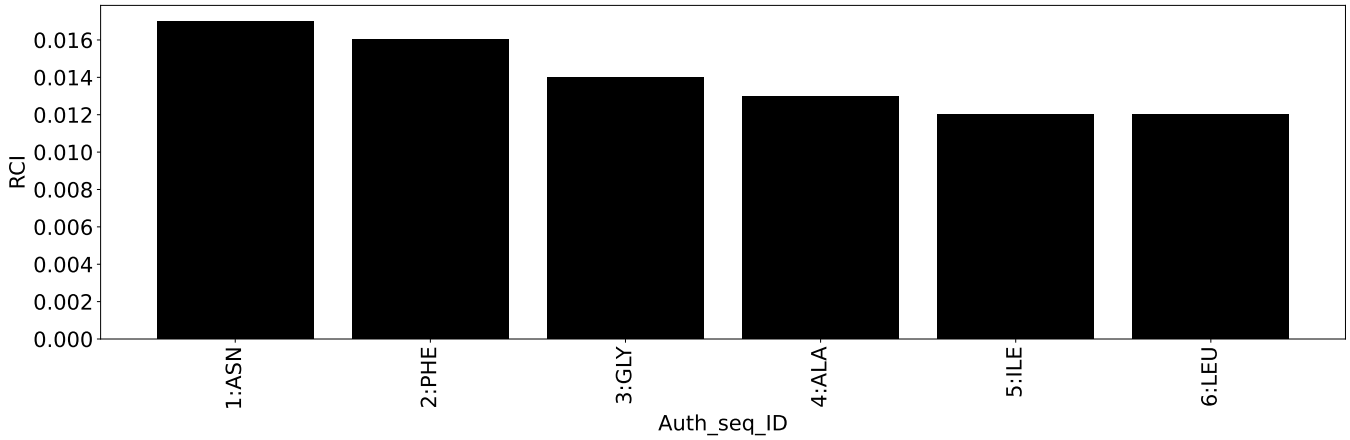
Random coil index (RCI) for chain D:



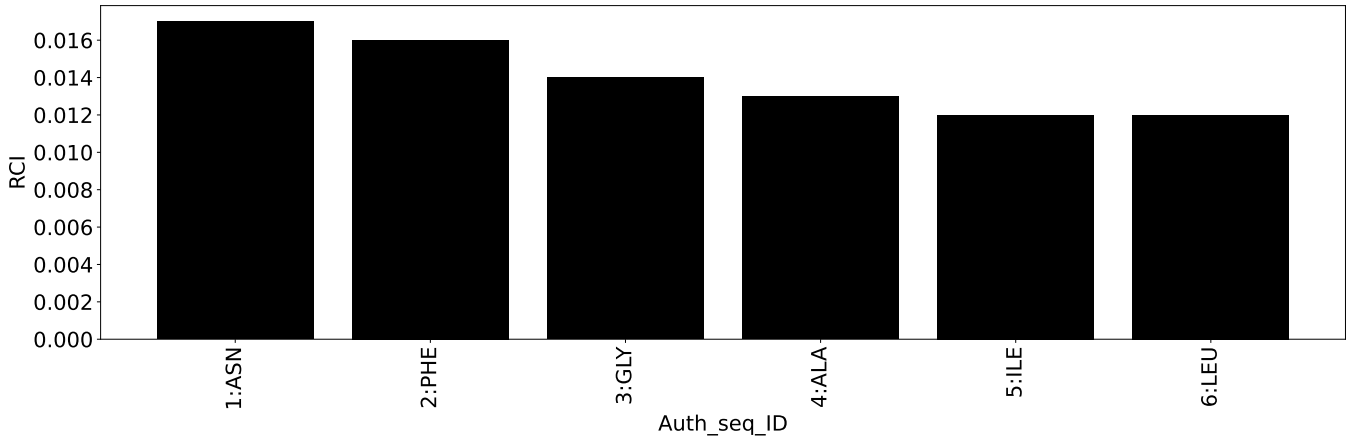
Random coil index (RCI) for chain E:



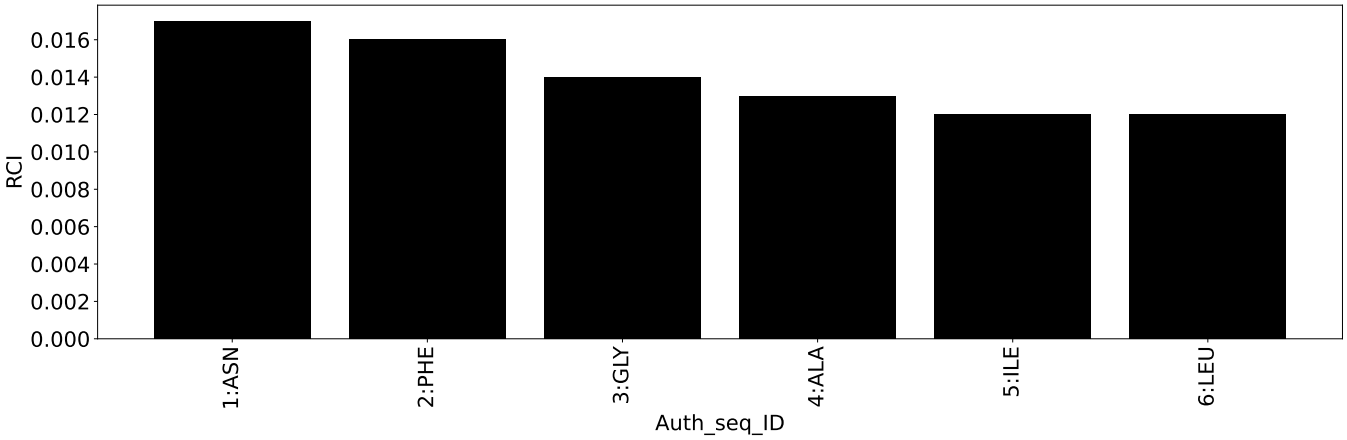
Random coil index (RCI) for chain F:



Random coil index (RCI) for chain G:



Random coil index (RCI) for chain H:


RCI
0.016
0.014
0.012
0.010
0.008
0.006
0.004
0.002
0.000
1:ASN
2:PHE
3:GLY
4:ALA
5:ILE
6:LEU
Auth_seq_ID