



Full wwPDB NMR Structure Validation Report ⓘ

Apr 20, 2024 – 03:47 PM EDT

PDB ID : 2MU1
BMRB ID : 25127
Title : NMR structure of the core domain of NP_346487.1, a putative phosphoglycolate phosphatase from *Streptococcus pneumoniae* TIGR4
Authors : Jaudzems, K.; Serrano, P.; Pedrini, B.; Geralt, M.; Wuthrich, K.; Joint Center for Structural Genomics (JCSG)
Deposited on : 2014-09-03

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A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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

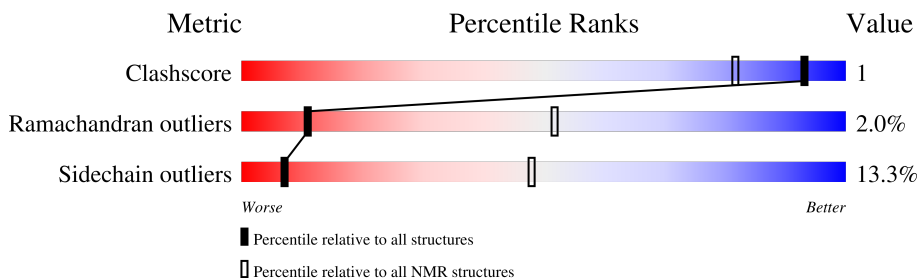
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 77%.

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	208	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:10, A:89-A:204 (126)	0.75	1

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

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

The models can be grouped into 2 clusters and 6 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2146 atoms, of which 1050 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Hydrolase, haloacid dehalogenase-like family.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	137	2146	697	1050	181	216	2	0

There are 2 discrepancies between the modelled and reference sequences:

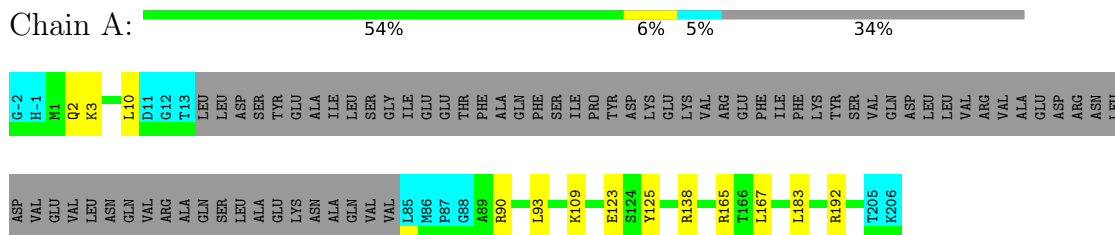
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q97NG6
A	-1	HIS	-	expression tag	UNP Q97NG6

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: Hydrolase, haloacid dehalogenase-like family

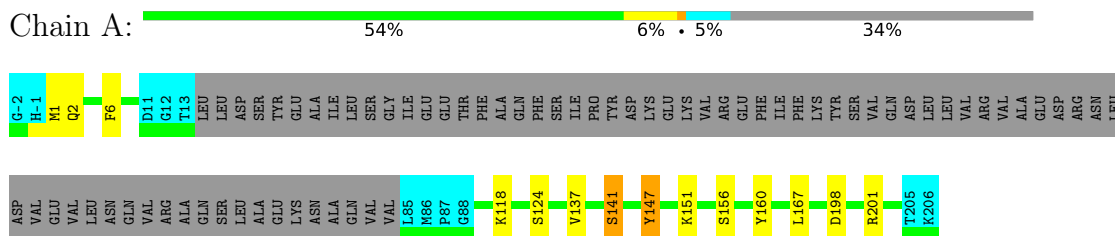


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

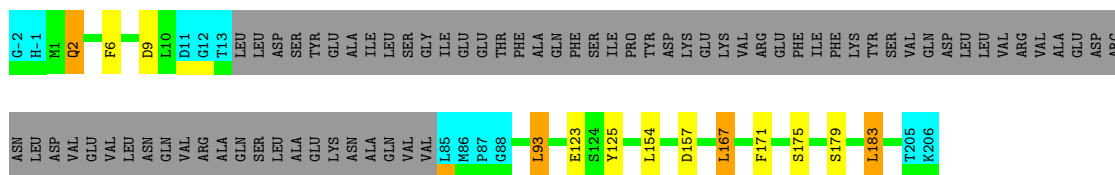
- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.2 Score per residue for model 2

- Molecule 1: Hydrolase, haloacid dehalogenase-like family

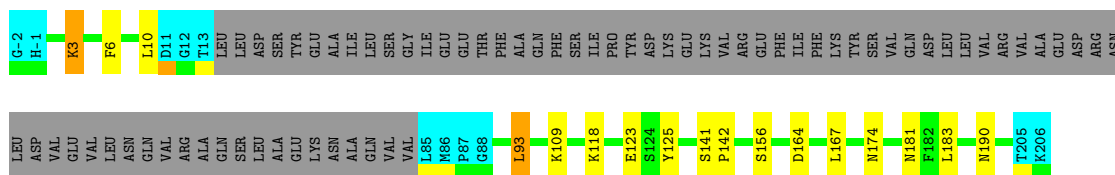




4.2.3 Score per residue for model 3

- Molecule 1: Hydrolase, haloacid dehalogenase-like family

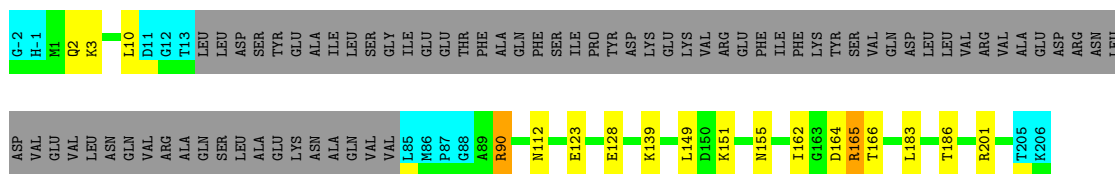
Chain A: 52% 7% 5% 34%



4.2.4 Score per residue for model 4

- Molecule 1: Hydrolase, haloacid dehalogenase-like family

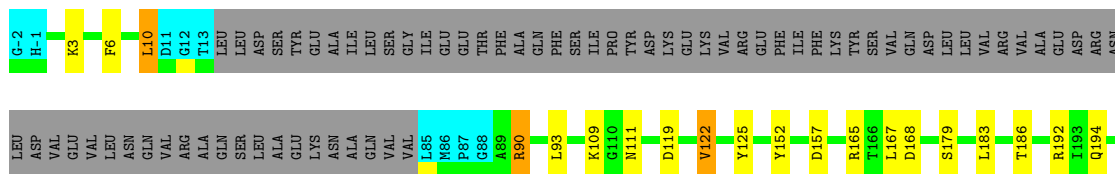
Chain A: 52% 8% 5% 34%



4.2.5 Score per residue for model 5

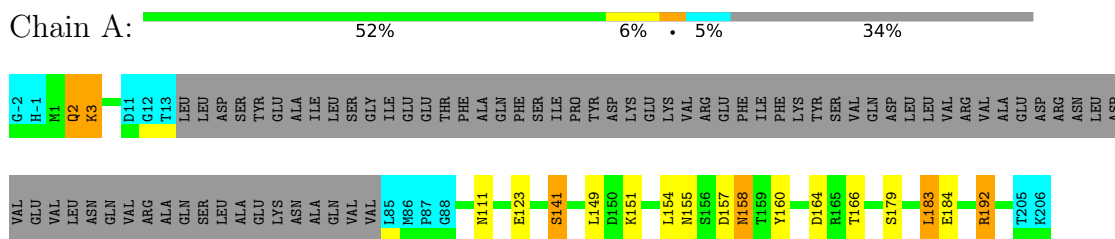
- Molecule 1: Hydrolase, haloacid dehalogenase-like family

Chain A: 50% 9% 5% 34%



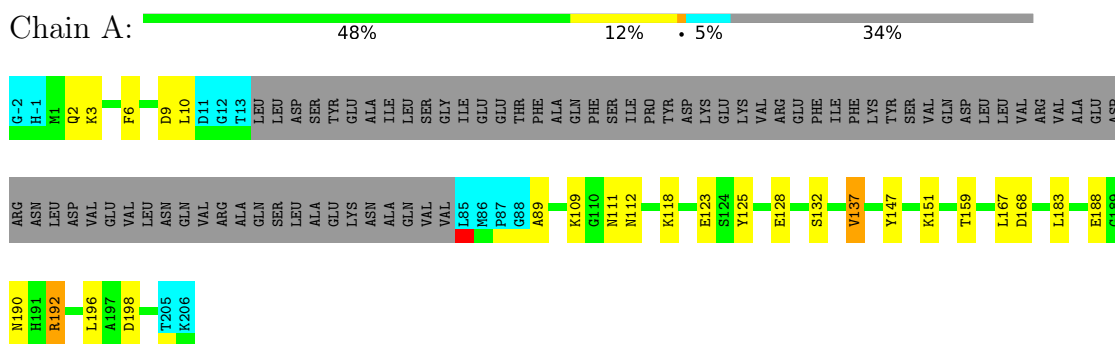
4.2.6 Score per residue for model 6

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



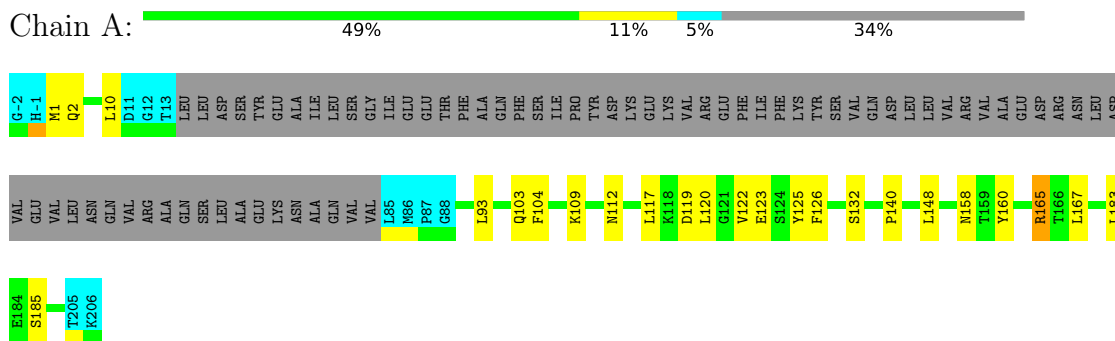
4.2.7 Score per residue for model 7

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.8 Score per residue for model 8

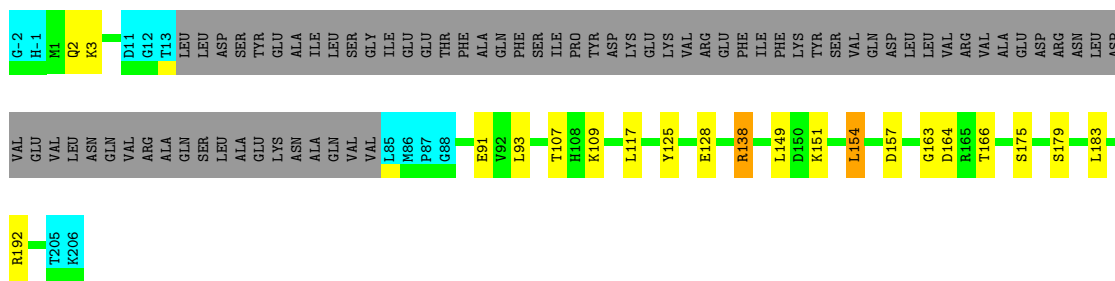
- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.9 Score per residue for model 9

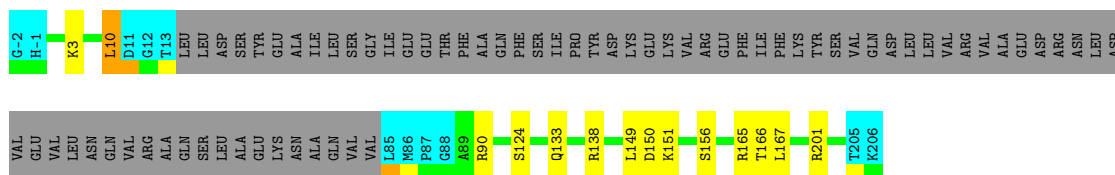
- Molecule 1: Hydrolase, haloacid dehalogenase-like family





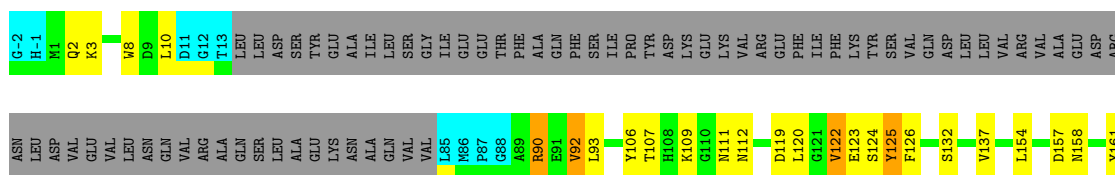
4.2.10 Score per residue for model 10

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



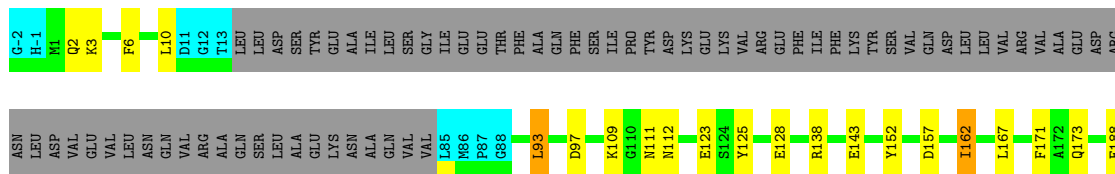
4.2.11 Score per residue for model 11

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.12 Score per residue for model 12

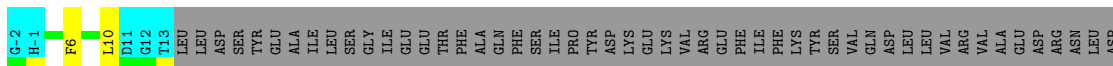
- Molecule 1: Hydrolase, haloacid dehalogenase-like family





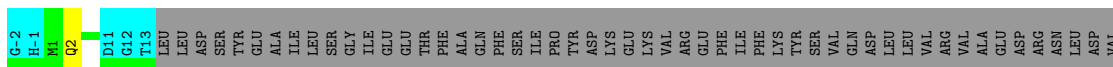
4.2.13 Score per residue for model 13

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



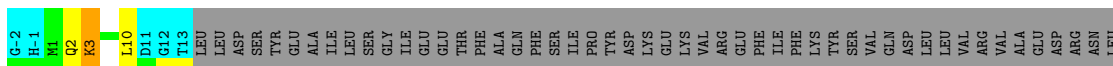
4.2.14 Score per residue for model 14

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.15 Score per residue for model 15

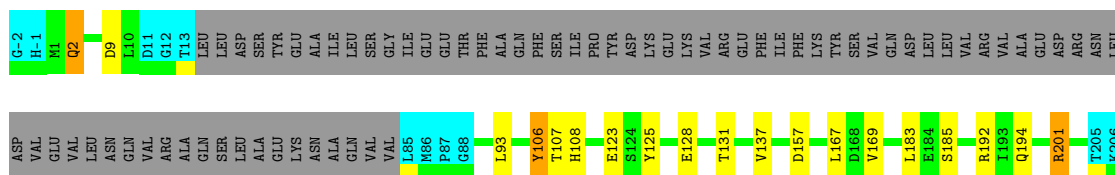
- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.16 Score per residue for model 16

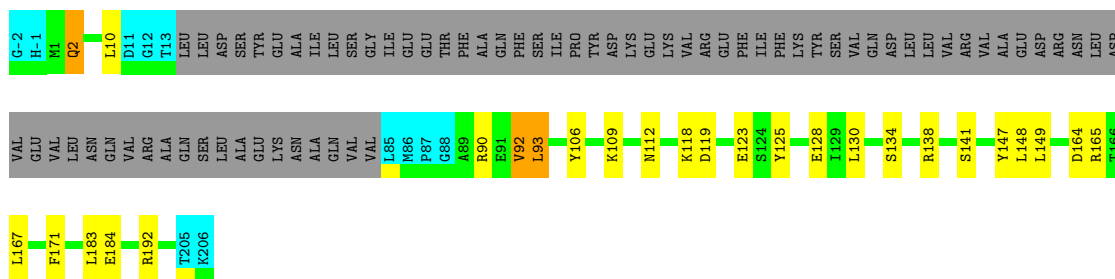
- Molecule 1: Hydrolase, haloacid dehalogenase-like family





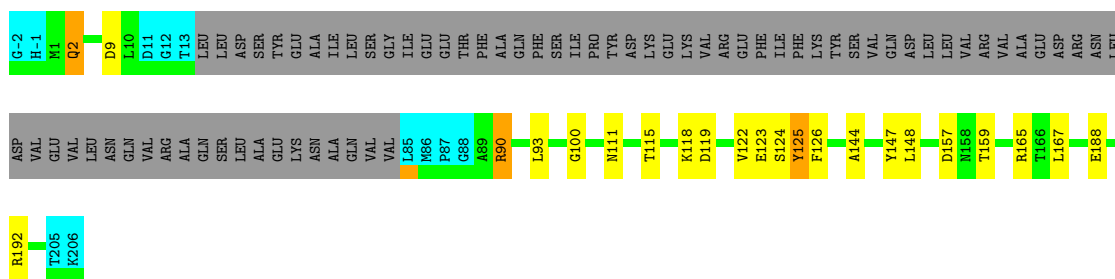
4.2.17 Score per residue for model 17

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



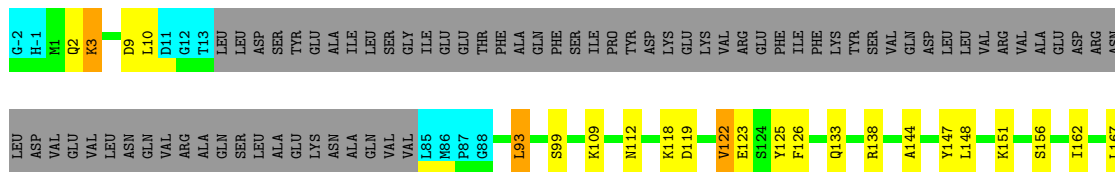
4.2.18 Score per residue for model 18

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



4.2.19 Score per residue for model 19

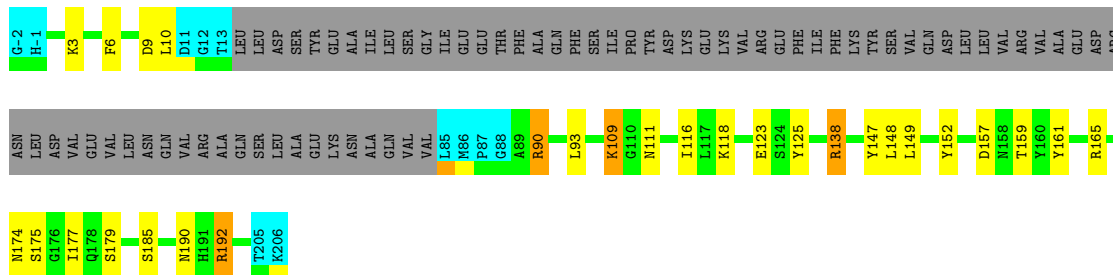
- Molecule 1: Hydrolase, haloacid dehalogenase-like family





4.2.20 Score per residue for model 20

- Molecule 1: Hydrolase, haloacid dehalogenase-like family



5 Refinement protocol and experimental data overview

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

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
CYANA	structure solution	3.0
OPAL	refinement	
UNIO-ATNOS/CANDID	structure solution	
CYANA	refinement	3.0

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	2213
Number of shifts mapped to atoms	1415
Number of unparsed shifts	0
Number of shifts with mapping errors	798
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality i

6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.65±0.01	0±0/1043 (0.0± 0.0%)	1.04±0.04	2±1/1415 (0.1± 0.1%)
All	All	0.65	0/20860 (0.0%)	1.04	40/28300 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.4±1.1
All	All	0	29

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	122	VAL	CA-CB-CG2	7.67	122.41	110.90	18	2
1	A	92	VAL	CA-CB-CG1	6.98	121.37	110.90	11	2
1	A	192	ARG	NE-CZ-NH2	-6.74	116.93	120.30	15	3
1	A	120	LEU	CB-CG-CD2	6.72	122.43	111.00	8	1
1	A	93	LEU	CB-CG-CD1	6.71	122.40	111.00	17	8
1	A	159	THR	CA-CB-CG2	6.34	121.28	112.40	7	2
1	A	148	LEU	CB-CG-CD1	6.29	121.70	111.00	20	3
1	A	165	ARG	NE-CZ-NH1	6.06	123.33	120.30	8	1
1	A	106	TYR	C-N-CA	6.05	136.82	121.70	16	1
1	A	122	VAL	CG1-CB-CG2	-5.86	101.53	110.90	18	1
1	A	192	ARG	CD-NE-CZ	5.66	131.53	123.60	20	1
1	A	138	ARG	NE-CZ-NH2	-5.63	117.48	120.30	15	4
1	A	154	LEU	CB-CG-CD2	-5.38	101.86	111.00	11	1
1	A	183	LEU	C-N-CA	5.32	135.00	121.70	6	1
1	A	125	TYR	CB-CG-CD1	-5.31	117.81	121.00	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	6	PHE	CB-CG-CD2	-5.27	117.11	120.80	20	2
1	A	134	SER	CB-CA-C	5.26	120.09	110.10	13	1
1	A	122	VAL	CB-CA-C	5.23	121.34	111.40	18	1
1	A	90	ARG	NE-CZ-NH2	-5.16	117.72	120.30	4	1
1	A	192	ARG	NE-CZ-NH1	5.09	122.84	120.30	6	1
1	A	154	LEU	CA-CB-CG	5.02	126.84	115.30	9	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	147	TYR	Sidechain	5
1	A	201	ARG	Sidechain	4
1	A	160	TYR	Sidechain	3
1	A	192	ARG	Sidechain	3
1	A	125	TYR	Sidechain	3
1	A	106	TYR	Sidechain	2
1	A	161	TYR	Sidechain	2
1	A	165	ARG	Sidechain	1
1	A	138	ARG	Sidechain	1
1	A	120	LEU	Peptide	1
1	A	171	PHE	Sidechain	1
1	A	90	ARG	Sidechain	1
1	A	100	GLY	Peptide	1
1	A	187	TYR	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1020	976	976	3±2
All	All	20400	19520	19520	52

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:LEU:HD23	1:A:125:TYR:CD2	0.81	2.09	20	7
1:A:122:VAL:HG23	1:A:125:TYR:CD2	0.66	2.25	11	3
1:A:137:VAL:HG23	1:A:141:SER:HB2	0.62	1.71	1	1
1:A:167:LEU:HD12	1:A:171:PHE:CE1	0.62	2.30	2	1
1:A:130:LEU:HD12	1:A:134:SER:CB	0.61	2.25	14	2
1:A:137:VAL:HG23	1:A:141:SER:CB	0.61	2.26	1	1
1:A:183:LEU:HD22	1:A:183:LEU:N	0.58	2.13	2	1
1:A:130:LEU:HD12	1:A:134:SER:HB3	0.57	1.76	17	2
1:A:144:ALA:O	1:A:148:LEU:HD13	0.55	2.00	18	2
1:A:183:LEU:HD22	1:A:183:LEU:H	0.55	1.62	2	1
1:A:193:ILE:HD12	1:A:195:ALA:O	0.52	2.04	11	1
1:A:122:VAL:HG23	1:A:125:TYR:HD2	0.52	1.63	19	2
1:A:93:LEU:HD13	1:A:122:VAL:HG21	0.52	1.80	11	1
1:A:6:PHE:CD2	1:A:162:ILE:HD11	0.51	2.40	12	1
1:A:159:THR:HG23	1:A:177:ILE:HB	0.51	1.81	20	1
1:A:90:ARG:HA	1:A:93:LEU:HD12	0.51	1.81	11	2
1:A:93:LEU:HD23	1:A:125:TYR:CG	0.50	2.41	18	1
1:A:137:VAL:HG12	1:A:138:ARG:H	0.50	1.66	14	1
1:A:147:TYR:HD1	1:A:148:LEU:HD12	0.49	1.67	19	2
1:A:141:SER:H	1:A:171:PHE:HB3	0.47	1.69	17	1
1:A:93:LEU:HD13	1:A:122:VAL:CG2	0.47	2.38	11	1
1:A:8:TRP:CD2	1:A:162:ILE:HD13	0.47	2.44	11	1
1:A:147:TYR:CZ	1:A:151:LYS:HE3	0.47	2.45	1	1
1:A:122:VAL:HG22	1:A:126:PHE:CE2	0.46	2.45	19	2
1:A:107:THR:HG23	1:A:109:LYS:H	0.45	1.71	9	2
1:A:93:LEU:CD2	1:A:125:TYR:CD2	0.45	2.98	18	1
1:A:155:ASN:ND2	1:A:158:ASN:HD21	0.45	2.09	6	1
1:A:106:TYR:O	1:A:107:THR:HG22	0.44	2.12	16	1
1:A:104:PHE:CD2	1:A:148:LEU:HD22	0.43	2.48	8	1
1:A:93:LEU:HD21	1:A:126:PHE:CE1	0.43	2.48	8	1
1:A:169:VAL:HG21	1:A:185:SER:HB2	0.42	1.90	16	1
1:A:89:ALA:N	1:A:196:LEU:HD11	0.42	2.29	7	1
1:A:93:LEU:HD21	1:A:126:PHE:CZ	0.42	2.50	18	2
1:A:183:LEU:HD13	1:A:183:LEU:N	0.41	2.29	19	1
1:A:109:LYS:HE2	1:A:116:ILE:CD1	0.41	2.45	20	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	126/208 (61%)	111±3 (88±3%)	12±3 (10±2%)	3±1 (2±1%)	11	52
All	All	2520/4160 (61%)	2222 (88%)	247 (10%)	51 (2%)	11	52

All 19 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	3	LYS	10
1	A	2	GLN	8
1	A	137	VAL	5
1	A	10	LEU	4
1	A	162	ILE	3
1	A	166	THR	3
1	A	1	MET	2
1	A	141	SER	2
1	A	163	GLY	2
1	A	122	VAL	2
1	A	136	PHE	2
1	A	142	PRO	1
1	A	186	THR	1
1	A	184	GLU	1
1	A	140	PRO	1
1	A	139	LYS	1
1	A	188	GLU	1
1	A	167	LEU	1
1	A	138	ARG	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	109/181 (60%)	94±4 (87±4%)	14±4 (13±4%)	7	48
All	All	2180/3620 (60%)	1890 (87%)	290 (13%)	7	48

All 63 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	167	LEU	16
1	A	123	GLU	16
1	A	183	LEU	13
1	A	2	GLN	12
1	A	157	ASP	10
1	A	10	LEU	10
1	A	165	ARG	10
1	A	179	SER	9
1	A	109	LYS	9
1	A	192	ARG	9
1	A	118	LYS	8
1	A	190	ASN	8
1	A	90	ARG	8
1	A	112	ASN	8
1	A	111	ASN	7
1	A	119	ASP	7
1	A	9	ASP	6
1	A	3	LYS	6
1	A	164	ASP	6
1	A	128	GLU	6
1	A	149	LEU	6
1	A	151	LYS	6
1	A	156	SER	5
1	A	6	PHE	5
1	A	168	ASP	5
1	A	124	SER	4
1	A	152	TYR	4
1	A	132	SER	4
1	A	188	GLU	4
1	A	185	SER	4
1	A	138	ARG	4
1	A	198	ASP	3
1	A	154	LEU	3
1	A	175	SER	3
1	A	166	THR	3
1	A	158	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	117	LEU	3
1	A	141	SER	2
1	A	174	ASN	2
1	A	181	ASN	2
1	A	139	LYS	2
1	A	155	ASN	2
1	A	186	THR	2
1	A	194	GLN	2
1	A	137	VAL	2
1	A	133	GLN	2
1	A	92	VAL	2
1	A	171	PHE	2
1	A	103	GLN	1
1	A	91	GLU	1
1	A	150	ASP	1
1	A	201	ARG	1
1	A	97	ASP	1
1	A	143	GLU	1
1	A	173	GLN	1
1	A	134	SER	1
1	A	170	GLU	1
1	A	108	HIS	1
1	A	131	THR	1
1	A	184	GLU	1
1	A	115	THR	1
1	A	93	LEU	1
1	A	99	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 monosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation i

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 76% 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 i

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2213
Number of shifts mapped to atoms	1415
Number of unparsed shifts	0
Number of shifts with mapping errors	798
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

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

- No matching atom found in the structure. All 798 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	LEU	CA	55.551	0.3	1
1	A	14	LEU	CB	45.022	0.3	1
1	A	14	LEU	CG	26.685	0.3	1
1	A	14	LEU	CD1	25.061	0.3	1
1	A	14	LEU	CD2	22.897	0.3	1
1	A	14	LEU	HA	4.319	0.020	1
1	A	14	LEU	HB2	0.968	0.020	2
1	A	14	LEU	HB3	1.591	0.020	2
1	A	14	LEU	HG	1.562	0.020	1
1	A	14	LEU	N	115.127	0.3	1
1	A	14	LEU	HD11	0.133	0.020	1
1	A	14	LEU	HD12	0.133	0.020	1
1	A	14	LEU	HD13	0.133	0.020	1
1	A	14	LEU	HD21	-0.142	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	14	LEU	HD22	-0.142	0.020	1
1	A	14	LEU	HD23	-0.142	0.020	1
1	A	15	LEU	CA	52.747	0.3	1
1	A	15	LEU	CB	43.387	0.3	1
1	A	15	LEU	CG	26.188	0.3	1
1	A	15	LEU	CD1	25.632	0.3	1
1	A	15	LEU	CD2	22.292	0.3	1
1	A	15	LEU	HA	4.555	0.020	1
1	A	15	LEU	HB2	1.14	0.020	2
1	A	15	LEU	HB3	1.677	0.020	2
1	A	15	LEU	HG	1.286	0.020	1
1	A	15	LEU	N	114.497	0.3	1
1	A	15	LEU	HD11	0.609	0.020	1
1	A	15	LEU	HD12	0.609	0.020	1
1	A	15	LEU	HD13	0.609	0.020	1
1	A	15	LEU	HD21	0.417	0.020	1
1	A	15	LEU	HD22	0.417	0.020	1
1	A	15	LEU	HD23	0.417	0.020	1
1	A	16	ASP	CA	52.322	0.3	1
1	A	16	ASP	CB	39.475	0.3	1
1	A	16	ASP	HA	4.981	0.020	1
1	A	16	ASP	HB2	2.275	0.020	2
1	A	16	ASP	HB3	2.916	0.020	2
1	A	16	ASP	N	124.003	0.3	1
1	A	17	SER	CA	57.39	0.3	1
1	A	17	SER	CB	63.756	0.3	1
1	A	17	SER	HA	4.745	0.020	1
1	A	17	SER	HB2	3.337	0.020	2
1	A	17	SER	HB3	3.926	0.020	2
1	A	17	SER	N	114.347	0.3	1
1	A	18	TYR	CA	63.037	0.3	1
1	A	18	TYR	CB	36.913	0.3	1
1	A	18	TYR	CD1	131.783	0.3	1
1	A	18	TYR	CE1	118.09	0.3	1
1	A	18	TYR	HA	4.213	0.020	1
1	A	18	TYR	HB2	2.861	0.020	2
1	A	18	TYR	HB3	3.132	0.020	2
1	A	18	TYR	HD1	7.014	0.020	1
1	A	18	TYR	HD2	7.014	0.020	1
1	A	18	TYR	HE1	6.614	0.020	1
1	A	18	TYR	HE2	6.614	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	TYR	N	122.052	0.3	1
1	A	19	GLU	CA	59.617	0.3	1
1	A	19	GLU	CB	28.225	0.3	1
1	A	19	GLU	CG	35.997	0.3	1
1	A	19	GLU	HA	4.022	0.020	1
1	A	19	GLU	HB2	1.953	0.020	2
1	A	19	GLU	HB3	1.993	0.020	2
1	A	19	GLU	HG2	2.261	0.020	1
1	A	19	GLU	HG3	2.261	0.020	1
1	A	19	GLU	N	118.11	0.3	1
1	A	20	ALA	CA	55.197	0.3	1
1	A	20	ALA	CB	18.324	0.3	1
1	A	20	ALA	HA	3.855	0.020	1
1	A	20	ALA	N	123.891	0.3	1
1	A	20	ALA	HB1	1.344	0.020	1
1	A	20	ALA	HB2	1.344	0.020	1
1	A	20	ALA	HB3	1.344	0.020	1
1	A	21	ILE	CA	64.297	0.3	1
1	A	21	ILE	CB	38.337	0.3	1
1	A	21	ILE	CG1	28.722	0.3	1
1	A	21	ILE	CG2	16.855	0.3	1
1	A	21	ILE	CD1	12.801	0.3	1
1	A	21	ILE	HA	3.585	0.020	1
1	A	21	ILE	HB	1.838	0.020	1
1	A	21	ILE	HG12	0.929	0.020	2
1	A	21	ILE	HG13	1.577	0.020	2
1	A	21	ILE	N	119.273	0.3	1
1	A	21	ILE	HG21	0.777	0.020	1
1	A	21	ILE	HG22	0.777	0.020	1
1	A	21	ILE	HG23	0.777	0.020	1
1	A	21	ILE	HD11	0.506	0.020	1
1	A	21	ILE	HD12	0.506	0.020	1
1	A	21	ILE	HD13	0.506	0.020	1
1	A	22	LEU	CA	58.47	0.3	1
1	A	22	LEU	CB	39.871	0.3	1
1	A	22	LEU	CG	27.264	0.3	1
1	A	22	LEU	CD1	25.955	0.3	1
1	A	22	LEU	CD2	23.469	0.3	1
1	A	22	LEU	HA	3.875	0.020	1
1	A	22	LEU	HB2	1.653	0.020	2
1	A	22	LEU	HB3	1.922	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	22	LEU	HG	1.818	0.020	1
1	A	22	LEU	N	121.307	0.3	1
1	A	22	LEU	HD11	0.739	0.020	1
1	A	22	LEU	HD12	0.739	0.020	1
1	A	22	LEU	HD13	0.739	0.020	1
1	A	22	LEU	HD21	0.788	0.020	1
1	A	22	LEU	HD22	0.788	0.020	1
1	A	22	LEU	HD23	0.788	0.020	1
1	A	23	SER	CA	62.551	0.3	1
1	A	23	SER	CB	62.334	0.3	1
1	A	23	SER	HA	4.085	0.020	1
1	A	23	SER	HB2	3.678	0.020	2
1	A	23	SER	HB3	3.894	0.020	2
1	A	23	SER	N	116.237	0.3	1
1	A	24	GLY	CA	46.744	0.3	1
1	A	24	GLY	HA2	4.08	0.020	1
1	A	24	GLY	N	109.813	0.3	1
1	A	25	ILE	CA	65.163	0.3	1
1	A	25	ILE	CB	36.781	0.3	1
1	A	25	ILE	CG1	28.766	0.3	1
1	A	25	ILE	CG2	17.304	0.3	1
1	A	25	ILE	CD1	13.811	0.3	1
1	A	25	ILE	HA	3.208	0.020	1
1	A	25	ILE	HB	1.867	0.020	1
1	A	25	ILE	HG12	0.712	0.020	2
1	A	25	ILE	HG13	1.674	0.020	2
1	A	25	ILE	N	125.721	0.3	1
1	A	25	ILE	HG21	0.073	0.020	1
1	A	25	ILE	HG22	0.073	0.020	1
1	A	25	ILE	HG23	0.073	0.020	1
1	A	25	ILE	HD11	0.714	0.020	1
1	A	25	ILE	HD12	0.714	0.020	1
1	A	25	ILE	HD13	0.714	0.020	1
1	A	26	GLU	CA	59.967	0.3	1
1	A	26	GLU	CB	28.857	0.3	1
1	A	26	GLU	CG	35.25	0.3	1
1	A	26	GLU	HA	2.424	0.020	1
1	A	26	GLU	HB2	1.054	0.020	2
1	A	26	GLU	HB3	1.743	0.020	2
1	A	26	GLU	HG2	1.423	0.020	2
1	A	26	GLU	HG3	1.658	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	26	GLU	N	122.409	0.3	1
1	A	27	GLU	CA	59.39	0.3	1
1	A	27	GLU	CB	29.837	0.3	1
1	A	27	GLU	CG	36.175	0.3	1
1	A	27	GLU	HA	3.916	0.020	1
1	A	27	GLU	HB2	1.97	0.020	2
1	A	27	GLU	HB3	2.01	0.020	2
1	A	27	GLU	HG2	2.277	0.020	1
1	A	27	GLU	HG3	2.277	0.020	1
1	A	27	GLU	N	118.448	0.3	1
1	A	28	THR	CA	67.418	0.3	1
1	A	28	THR	CB	68.057	0.3	1
1	A	28	THR	CG2	20.738	0.3	1
1	A	28	THR	HA	3.778	0.020	1
1	A	28	THR	HB	4.371	0.020	1
1	A	28	THR	N	117.81	0.3	1
1	A	28	THR	HG21	1.272	0.020	1
1	A	28	THR	HG22	1.272	0.020	1
1	A	28	THR	HG23	1.272	0.020	1
1	A	29	PHE	CA	59.329	0.3	1
1	A	29	PHE	CB	34.988	0.3	1
1	A	29	PHE	CD1	130.24	0.3	1
1	A	29	PHE	CE1	130.313	0.3	1
1	A	29	PHE	CZ	128.616	0.3	1
1	A	29	PHE	HA	4.223	0.020	1
1	A	29	PHE	HB2	3.127	0.020	2
1	A	29	PHE	HB3	3.713	0.020	2
1	A	29	PHE	HD1	7.0	0.020	1
1	A	29	PHE	HD2	7.0	0.020	1
1	A	29	PHE	HE1	7.043	0.020	1
1	A	29	PHE	HE2	7.043	0.020	1
1	A	29	PHE	HZ	6.832	0.020	1
1	A	29	PHE	N	121.353	0.3	1
1	A	30	ALA	CA	55.066	0.3	1
1	A	30	ALA	CB	17.523	0.3	1
1	A	30	ALA	HA	4.19	0.020	1
1	A	30	ALA	N	121.612	0.3	1
1	A	30	ALA	HB1	1.475	0.020	1
1	A	30	ALA	HB2	1.475	0.020	1
1	A	30	ALA	HB3	1.475	0.020	1
1	A	31	GLN	CA	58.169	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	GLN	CB	27.732	0.3	1
1	A	31	GLN	CG	33.621	0.3	1
1	A	31	GLN	HA	3.85	0.020	1
1	A	31	GLN	HB2	1.816	0.020	2
1	A	31	GLN	HB3	2.028	0.020	2
1	A	31	GLN	HG2	1.903	0.020	2
1	A	31	GLN	HG3	2.047	0.020	2
1	A	31	GLN	HE21	6.706	0.020	1
1	A	31	GLN	HE22	7.03	0.020	1
1	A	31	GLN	N	117.11	0.3	1
1	A	31	GLN	NE2	111.661	0.3	1
1	A	32	PHE	CA	57.54	0.3	1
1	A	32	PHE	CB	40.387	0.3	1
1	A	32	PHE	CD1	132.462	0.3	1
1	A	32	PHE	CE1	130.515	0.3	1
1	A	32	PHE	CZ	129.555	0.3	1
1	A	32	PHE	HA	4.551	0.020	1
1	A	32	PHE	HB2	2.29	0.020	2
1	A	32	PHE	HB3	3.371	0.020	2
1	A	32	PHE	HD1	7.399	0.020	1
1	A	32	PHE	HD2	7.399	0.020	1
1	A	32	PHE	HE1	7.154	0.020	1
1	A	32	PHE	HE2	7.154	0.020	1
1	A	32	PHE	HZ	7.097	0.020	1
1	A	32	PHE	N	114.473	0.3	1
1	A	33	SER	CA	58.846	0.3	1
1	A	33	SER	CB	61.052	0.3	1
1	A	33	SER	HA	3.925	0.020	1
1	A	33	SER	HB2	3.974	0.020	1
1	A	33	SER	HB3	3.974	0.020	1
1	A	33	SER	N	113.652	0.3	1
1	A	34	ILE	CA	58.227	0.3	1
1	A	34	ILE	CB	39.02	0.3	1
1	A	34	ILE	CG1	27.189	0.3	1
1	A	34	ILE	CG2	16.486	0.3	1
1	A	34	ILE	CD1	13.617	0.3	1
1	A	34	ILE	HA	3.97	0.020	1
1	A	34	ILE	HB	1.01	0.020	1
1	A	34	ILE	HG12	0.395	0.020	2
1	A	34	ILE	HG13	1.388	0.020	2
1	A	34	ILE	N	122.257	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	34	ILE	HG21	0.002	0.020	1
1	A	34	ILE	HG22	0.002	0.020	1
1	A	34	ILE	HG23	0.002	0.020	1
1	A	34	ILE	HD11	0.209	0.020	1
1	A	34	ILE	HD12	0.209	0.020	1
1	A	34	ILE	HD13	0.209	0.020	1
1	A	35	PRO	CA	63.986	0.3	1
1	A	35	PRO	CB	31.901	0.3	1
1	A	35	PRO	CG	27.609	0.3	1
1	A	35	PRO	CD	50.761	0.3	1
1	A	35	PRO	HA	4.158	0.020	1
1	A	35	PRO	HB2	1.755	0.020	2
1	A	35	PRO	HB3	2.196	0.020	2
1	A	35	PRO	HG2	1.838	0.020	2
1	A	35	PRO	HG3	1.984	0.020	2
1	A	35	PRO	HD2	3.347	0.020	2
1	A	35	PRO	HD3	3.88	0.020	2
1	A	36	TYR	CA	57.238	0.3	1
1	A	36	TYR	CB	41.453	0.3	1
1	A	36	TYR	CD1	132.834	0.3	1
1	A	36	TYR	CE1	118.787	0.3	1
1	A	36	TYR	HA	4.652	0.020	1
1	A	36	TYR	HB2	3.012	0.020	1
1	A	36	TYR	HB3	3.012	0.020	1
1	A	36	TYR	HD1	6.779	0.020	1
1	A	36	TYR	HD2	6.779	0.020	1
1	A	36	TYR	HE1	6.341	0.020	1
1	A	36	TYR	HE2	6.341	0.020	1
1	A	36	TYR	N	125.28	0.3	1
1	A	37	ASP	CA	51.992	0.3	1
1	A	37	ASP	CB	42.016	0.3	1
1	A	37	ASP	HA	4.441	0.020	1
1	A	37	ASP	HB2	2.233	0.020	2
1	A	37	ASP	HB3	2.634	0.020	2
1	A	37	ASP	N	130.12	0.3	1
1	A	38	LYS	CA	60.355	0.3	1
1	A	38	LYS	CB	33.554	0.3	1
1	A	38	LYS	CG	24.98	0.3	1
1	A	38	LYS	CD	29.996	0.3	1
1	A	38	LYS	CE	42.284	0.3	1
1	A	38	LYS	HA	3.144	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	38	LYS	HB2	1.595	0.020	2
1	A	38	LYS	HB3	1.72	0.020	2
1	A	38	LYS	HG2	1.448	0.020	2
1	A	38	LYS	HG3	1.102	0.020	2
1	A	38	LYS	HD2	1.645	0.020	2
1	A	38	LYS	HD3	1.726	0.020	2
1	A	38	LYS	HE2	2.831	0.020	1
1	A	38	LYS	HE3	2.831	0.020	1
1	A	38	LYS	N	125.978	0.3	1
1	A	39	GLU	CA	58.622	0.3	1
1	A	39	GLU	CB	28.674	0.3	1
1	A	39	GLU	CG	36.011	0.3	1
1	A	39	GLU	HA	3.944	0.020	1
1	A	39	GLU	HB2	1.894	0.020	2
1	A	39	GLU	HB3	1.949	0.020	2
1	A	39	GLU	HG2	2.187	0.020	2
1	A	39	GLU	HG3	2.269	0.020	2
1	A	39	GLU	N	114.411	0.3	1
1	A	40	LYS	CA	58.647	0.3	1
1	A	40	LYS	CB	32.272	0.3	1
1	A	40	LYS	CG	25.169	0.3	1
1	A	40	LYS	CD	28.695	0.3	1
1	A	40	LYS	CE	41.945	0.3	1
1	A	40	LYS	HA	4.037	0.020	1
1	A	40	LYS	HB2	1.738	0.020	1
1	A	40	LYS	HB3	1.738	0.020	1
1	A	40	LYS	HG2	1.292	0.020	2
1	A	40	LYS	HG3	1.432	0.020	2
1	A	40	LYS	HD2	1.516	0.020	2
1	A	40	LYS	HD3	1.599	0.020	2
1	A	40	LYS	HE2	2.895	0.020	1
1	A	40	LYS	HE3	2.895	0.020	1
1	A	40	LYS	N	120.252	0.3	1
1	A	41	VAL	CA	67.209	0.3	1
1	A	41	VAL	CB	30.955	0.3	1
1	A	41	VAL	CG1	22.726	0.3	1
1	A	41	VAL	CG2	23.432	0.3	1
1	A	41	VAL	HA	3.477	0.020	1
1	A	41	VAL	HB	1.823	0.020	1
1	A	41	VAL	N	122.149	0.3	1
1	A	41	VAL	HG11	0.813	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	VAL	HG12	0.813	0.020	1
1	A	41	VAL	HG13	0.813	0.020	1
1	A	41	VAL	HG21	0.87	0.020	1
1	A	41	VAL	HG22	0.87	0.020	1
1	A	41	VAL	HG23	0.87	0.020	1
1	A	42	ARG	CA	60.002	0.3	1
1	A	42	ARG	CB	29.92	0.3	1
1	A	42	ARG	CG	26.733	0.3	1
1	A	42	ARG	CD	43.0	0.3	1
1	A	42	ARG	HA	3.528	0.020	1
1	A	42	ARG	HB2	1.687	0.020	2
1	A	42	ARG	HB3	1.769	0.020	2
1	A	42	ARG	HG2	1.069	0.020	2
1	A	42	ARG	HG3	1.179	0.020	2
1	A	42	ARG	HD2	2.915	0.020	2
1	A	42	ARG	HD3	3.021	0.020	2
1	A	42	ARG	HE	7.748	0.020	1
1	A	42	ARG	N	120.182	0.3	1
1	A	42	ARG	NE	83.246	0.3	1
1	A	43	GLU	CA	59.047	0.3	1
1	A	43	GLU	CB	29.688	0.3	1
1	A	43	GLU	CG	36.12	0.3	1
1	A	43	GLU	HA	3.85	0.020	1
1	A	43	GLU	HB2	2.028	0.020	1
1	A	43	GLU	HB3	2.028	0.020	1
1	A	43	GLU	HG2	2.158	0.020	2
1	A	43	GLU	HG3	2.336	0.020	2
1	A	43	GLU	N	115.453	0.3	1
1	A	44	PHE	CA	62.113	0.3	1
1	A	44	PHE	CB	39.815	0.3	1
1	A	44	PHE	CD1	132.34	0.3	1
1	A	44	PHE	CE1	131.247	0.3	1
1	A	44	PHE	CZ	129.394	0.3	1
1	A	44	PHE	HA	4.131	0.020	1
1	A	44	PHE	HB2	3.213	0.020	2
1	A	44	PHE	HB3	3.322	0.020	2
1	A	44	PHE	HD1	7.185	0.020	1
1	A	44	PHE	HD2	7.185	0.020	1
1	A	44	PHE	HE1	7.186	0.020	1
1	A	44	PHE	HE2	7.186	0.020	1
1	A	44	PHE	HZ	6.833	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	44	PHE	N	119.694	0.3	1
1	A	45	ILE	CA	64.764	0.3	1
1	A	45	ILE	CB	37.783	0.3	1
1	A	45	ILE	CG1	26.165	0.3	1
1	A	45	ILE	CG2	19.028	0.3	1
1	A	45	ILE	CD1	14.398	0.3	1
1	A	45	ILE	HA	3.892	0.020	1
1	A	45	ILE	HB	1.964	0.020	1
1	A	45	ILE	HG12	1.387	0.020	2
1	A	45	ILE	HG13	1.511	0.020	2
1	A	45	ILE	N	113.389	0.3	1
1	A	45	ILE	HG21	1.023	0.020	1
1	A	45	ILE	HG22	1.023	0.020	1
1	A	45	ILE	HG23	1.023	0.020	1
1	A	45	ILE	HD11	0.687	0.020	1
1	A	45	ILE	HD12	0.687	0.020	1
1	A	45	ILE	HD13	0.687	0.020	1
1	A	46	PHE	CA	59.203	0.3	1
1	A	46	PHE	CB	38.529	0.3	1
1	A	46	PHE	CD1	130.658	0.3	1
1	A	46	PHE	CE1	130.717	0.3	1
1	A	46	PHE	HA	4.249	0.020	1
1	A	46	PHE	HB2	2.954	0.020	2
1	A	46	PHE	HB3	3.028	0.020	2
1	A	46	PHE	HD1	7.012	0.020	1
1	A	46	PHE	HD2	7.012	0.020	1
1	A	46	PHE	HE1	6.841	0.020	1
1	A	46	PHE	HE2	6.841	0.020	1
1	A	46	PHE	N	119.349	0.3	1
1	A	47	LYS	CA	58.171	0.3	1
1	A	47	LYS	CB	33.615	0.3	1
1	A	47	LYS	CG	24.907	0.3	1
1	A	47	LYS	CD	29.185	0.3	1
1	A	47	LYS	CE	41.849	0.3	1
1	A	47	LYS	HA	3.793	0.020	1
1	A	47	LYS	HB2	0.972	0.020	2
1	A	47	LYS	HB3	1.32	0.020	2
1	A	47	LYS	HG2	0.505	0.020	2
1	A	47	LYS	HG3	0.979	0.020	2
1	A	47	LYS	HD2	1.332	0.020	2
1	A	47	LYS	HD3	1.373	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	LYS	HE2	2.731	0.020	2
1	A	47	LYS	HE3	2.752	0.020	2
1	A	47	LYS	N	119.458	0.3	1
1	A	48	TYR	CA	56.263	0.3	1
1	A	48	TYR	CB	36.947	0.3	1
1	A	48	TYR	CD1	133.681	0.3	1
1	A	48	TYR	CE1	117.165	0.3	1
1	A	48	TYR	HA	4.64	0.020	1
1	A	48	TYR	HB2	2.291	0.020	2
1	A	48	TYR	HB3	3.139	0.020	2
1	A	48	TYR	HD1	6.264	0.020	1
1	A	48	TYR	HD2	6.264	0.020	1
1	A	48	TYR	HE1	6.49	0.020	1
1	A	48	TYR	HE2	6.49	0.020	1
1	A	48	TYR	N	119.211	0.3	1
1	A	49	SER	CA	57.955	0.3	1
1	A	49	SER	CB	65.271	0.3	1
1	A	49	SER	HA	4.79	0.020	1
1	A	49	SER	HB2	4.281	0.020	2
1	A	49	SER	HB3	4.366	0.020	2
1	A	49	SER	N	110.613	0.3	1
1	A	50	VAL	CA	66.71	0.3	1
1	A	50	VAL	CB	31.236	0.3	1
1	A	50	VAL	CG1	20.952	0.3	1
1	A	50	VAL	CG2	23.451	0.3	1
1	A	50	VAL	HA	3.689	0.020	1
1	A	50	VAL	HB	2.187	0.020	1
1	A	50	VAL	HG11	0.804	0.020	1
1	A	50	VAL	HG12	0.804	0.020	1
1	A	50	VAL	HG13	0.804	0.020	1
1	A	50	VAL	HG21	1.08	0.020	1
1	A	50	VAL	HG22	1.08	0.020	1
1	A	50	VAL	HG23	1.08	0.020	1
1	A	51	GLN	CA	59.509	0.3	1
1	A	51	GLN	CB	27.36	0.3	1
1	A	51	GLN	CG	33.219	0.3	1
1	A	51	GLN	HA	3.907	0.020	1
1	A	51	GLN	HB2	1.857	0.020	2
1	A	51	GLN	HB3	2.061	0.020	2
1	A	51	GLN	HG2	2.243	0.020	2
1	A	51	GLN	HG3	2.316	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	GLN	HE21	6.916	0.020	1
1	A	51	GLN	HE22	7.288	0.020	1
1	A	51	GLN	N	120.02	0.3	1
1	A	51	GLN	NE2	111.077	0.3	1
1	A	52	ASP	CA	57.493	0.3	1
1	A	52	ASP	CB	40.877	0.3	1
1	A	52	ASP	HA	4.307	0.020	1
1	A	52	ASP	HB2	2.704	0.020	2
1	A	52	ASP	HB3	2.785	0.020	2
1	A	52	ASP	N	116.384	0.3	1
1	A	53	LEU	CA	57.677	0.3	1
1	A	53	LEU	CB	40.864	0.3	1
1	A	53	LEU	CG	27.139	0.3	1
1	A	53	LEU	CD1	21.883	0.3	1
1	A	53	LEU	CD2	28.201	0.3	1
1	A	53	LEU	HA	3.636	0.020	1
1	A	53	LEU	HB2	1.569	0.020	2
1	A	53	LEU	HB3	2.329	0.020	2
1	A	53	LEU	HG	1.447	0.020	1
1	A	53	LEU	N	121.833	0.3	1
1	A	53	LEU	HD11	0.428	0.020	1
1	A	53	LEU	HD12	0.428	0.020	1
1	A	53	LEU	HD13	0.428	0.020	1
1	A	53	LEU	HD21	0.91	0.020	1
1	A	53	LEU	HD22	0.91	0.020	1
1	A	53	LEU	HD23	0.91	0.020	1
1	A	54	LEU	CA	57.851	0.3	1
1	A	54	LEU	CB	40.004	0.3	1
1	A	54	LEU	CG	26.969	0.3	1
1	A	54	LEU	CD1	22.014	0.3	1
1	A	54	LEU	CD2	25.576	0.3	1
1	A	54	LEU	HA	3.877	0.020	1
1	A	54	LEU	HB2	1.221	0.020	2
1	A	54	LEU	HB3	1.836	0.020	2
1	A	54	LEU	HG	1.925	0.020	1
1	A	54	LEU	N	117.282	0.3	1
1	A	54	LEU	HD11	0.749	0.020	1
1	A	54	LEU	HD12	0.749	0.020	1
1	A	54	LEU	HD13	0.749	0.020	1
1	A	54	LEU	HD21	0.77	0.020	1
1	A	54	LEU	HD22	0.77	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	54	LEU	HD23	0.77	0.020	1
1	A	55	VAL	CA	66.618	0.3	1
1	A	55	VAL	CB	31.999	0.3	1
1	A	55	VAL	CG1	20.92	0.3	1
1	A	55	VAL	CG2	23.396	0.3	1
1	A	55	VAL	HA	3.436	0.020	1
1	A	55	VAL	HB	2.041	0.020	1
1	A	55	VAL	N	118.307	0.3	1
1	A	55	VAL	HG11	0.853	0.020	1
1	A	55	VAL	HG12	0.853	0.020	1
1	A	55	VAL	HG13	0.853	0.020	1
1	A	55	VAL	HG21	1.037	0.020	1
1	A	55	VAL	HG22	1.037	0.020	1
1	A	55	VAL	HG23	1.037	0.020	1
1	A	56	ARG	CA	58.609	0.3	1
1	A	56	ARG	CB	29.933	0.3	1
1	A	56	ARG	CG	26.467	0.3	1
1	A	56	ARG	CD	43.096	0.3	1
1	A	56	ARG	HA	3.982	0.020	1
1	A	56	ARG	HB2	1.847	0.020	1
1	A	56	ARG	HB3	1.847	0.020	1
1	A	56	ARG	HG2	1.523	0.020	2
1	A	56	ARG	HG3	1.59	0.020	2
1	A	56	ARG	HD2	3.07	0.020	1
1	A	56	ARG	HD3	3.07	0.020	1
1	A	56	ARG	HE	7.286	0.020	1
1	A	56	ARG	N	119.881	0.3	1
1	A	56	ARG	NE	85.31	0.3	1
1	A	57	VAL	CA	64.976	0.3	1
1	A	57	VAL	CB	31.216	0.3	1
1	A	57	VAL	CG1	21.228	0.3	1
1	A	57	VAL	CG2	21.535	0.3	1
1	A	57	VAL	HA	3.73	0.020	1
1	A	57	VAL	HB	1.78	0.020	1
1	A	57	VAL	N	115.815	0.3	1
1	A	57	VAL	HG11	0.797	0.020	1
1	A	57	VAL	HG12	0.797	0.020	1
1	A	57	VAL	HG13	0.797	0.020	1
1	A	57	VAL	HG21	0.591	0.020	1
1	A	57	VAL	HG22	0.591	0.020	1
1	A	57	VAL	HG23	0.591	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	58	ALA	CA	55.345	0.3	1
1	A	58	ALA	CB	17.556	0.3	1
1	A	58	ALA	HA	3.64	0.020	1
1	A	58	ALA	N	122.132	0.3	1
1	A	58	ALA	HB1	1.294	0.020	1
1	A	58	ALA	HB2	1.294	0.020	1
1	A	58	ALA	HB3	1.294	0.020	1
1	A	59	GLU	CA	58.871	0.3	1
1	A	59	GLU	CB	29.244	0.3	1
1	A	59	GLU	CG	36.236	0.3	1
1	A	59	GLU	HA	4.004	0.020	1
1	A	59	GLU	HB2	1.983	0.020	2
1	A	59	GLU	HB3	2.105	0.020	2
1	A	59	GLU	HG2	2.182	0.020	2
1	A	59	GLU	HG3	2.364	0.020	2
1	A	59	GLU	N	117.496	0.3	1
1	A	60	ASP	CA	56.881	0.3	1
1	A	60	ASP	CB	41.121	0.3	1
1	A	60	ASP	HA	4.298	0.020	1
1	A	60	ASP	HB2	2.54	0.020	2
1	A	60	ASP	HB3	2.649	0.020	2
1	A	60	ASP	N	118.807	0.3	1
1	A	61	ARG	CA	54.13	0.3	1
1	A	61	ARG	CB	29.993	0.3	1
1	A	61	ARG	CG	27.372	0.3	1
1	A	61	ARG	CD	42.322	0.3	1
1	A	61	ARG	HA	4.312	0.020	1
1	A	61	ARG	HB2	1.38	0.020	2
1	A	61	ARG	HB3	1.951	0.020	2
1	A	61	ARG	HG2	1.447	0.020	2
1	A	61	ARG	HG3	1.523	0.020	2
1	A	61	ARG	HD2	2.978	0.020	1
1	A	61	ARG	HD3	2.978	0.020	1
1	A	61	ARG	HE	7.525	0.020	1
1	A	61	ARG	N	114.261	0.3	1
1	A	61	ARG	NE	83.709	0.3	1
1	A	62	ASN	CA	54.228	0.3	1
1	A	62	ASN	CB	36.795	0.3	1
1	A	62	ASN	HA	4.329	0.020	1
1	A	62	ASN	HB2	2.659	0.020	2
1	A	62	ASN	HB3	3.023	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	ASN	HD21	7.41	0.020	1
1	A	62	ASN	HD22	6.704	0.020	1
1	A	62	ASN	N	117.542	0.3	1
1	A	62	ASN	ND2	111.835	0.3	1
1	A	63	LEU	CA	52.588	0.3	1
1	A	63	LEU	CB	45.196	0.3	1
1	A	63	LEU	CG	26.13	0.3	1
1	A	63	LEU	CD1	26.101	0.3	1
1	A	63	LEU	CD2	22.582	0.3	1
1	A	63	LEU	HA	4.536	0.020	1
1	A	63	LEU	HB2	1.059	0.020	1
1	A	63	LEU	HB3	1.059	0.020	1
1	A	63	LEU	HG	1.336	0.020	1
1	A	63	LEU	N	117.915	0.3	1
1	A	63	LEU	HD11	0.426	0.020	1
1	A	63	LEU	HD12	0.426	0.020	1
1	A	63	LEU	HD13	0.426	0.020	1
1	A	63	LEU	HD21	0.729	0.020	1
1	A	63	LEU	HD22	0.729	0.020	1
1	A	63	LEU	HD23	0.729	0.020	1
1	A	64	ASP	CA	52.711	0.3	1
1	A	64	ASP	CB	41.699	0.3	1
1	A	64	ASP	HA	4.585	0.020	1
1	A	64	ASP	HB2	2.46	0.020	2
1	A	64	ASP	HB3	2.715	0.020	2
1	A	64	ASP	N	120.276	0.3	1
1	A	65	VAL	CA	65.238	0.3	1
1	A	65	VAL	CB	31.564	0.3	1
1	A	65	VAL	CG1	19.812	0.3	1
1	A	65	VAL	CG2	22.669	0.3	1
1	A	65	VAL	HA	3.408	0.020	1
1	A	65	VAL	HB	1.922	0.020	1
1	A	65	VAL	N	128.221	0.3	1
1	A	65	VAL	HG11	0.85	0.020	1
1	A	65	VAL	HG12	0.85	0.020	1
1	A	65	VAL	HG13	0.85	0.020	1
1	A	65	VAL	HG21	0.833	0.020	1
1	A	65	VAL	HG22	0.833	0.020	1
1	A	65	VAL	HG23	0.833	0.020	1
1	A	66	GLU	CA	58.74	0.3	1
1	A	66	GLU	CB	28.611	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	66	GLU	CG	35.864	0.3	1
1	A	66	GLU	HA	4.119	0.020	1
1	A	66	GLU	HB2	1.946	0.020	1
1	A	66	GLU	HB3	1.946	0.020	1
1	A	66	GLU	HG2	2.19	0.020	2
1	A	66	GLU	HG3	2.277	0.020	2
1	A	66	GLU	N	120.317	0.3	1
1	A	67	VAL	CA	65.671	0.3	1
1	A	67	VAL	CB	31.416	0.3	1
1	A	67	VAL	CG1	22.266	0.3	1
1	A	67	VAL	CG2	21.17	0.3	1
1	A	67	VAL	HA	3.704	0.020	1
1	A	67	VAL	HB	2.189	0.020	1
1	A	67	VAL	N	120.128	0.3	1
1	A	67	VAL	HG11	0.976	0.020	1
1	A	67	VAL	HG12	0.976	0.020	1
1	A	67	VAL	HG13	0.976	0.020	1
1	A	67	VAL	HG21	0.991	0.020	1
1	A	67	VAL	HG22	0.991	0.020	1
1	A	67	VAL	HG23	0.991	0.020	1
1	A	68	LEU	CA	58.337	0.3	1
1	A	68	LEU	CB	41.701	0.3	1
1	A	68	LEU	CG	27.057	0.3	1
1	A	68	LEU	CD1	23.427	0.3	1
1	A	68	LEU	CD2	26.214	0.3	1
1	A	68	LEU	HA	3.72	0.020	1
1	A	68	LEU	HB2	1.139	0.020	2
1	A	68	LEU	HB3	1.744	0.020	2
1	A	68	LEU	HG	1.204	0.020	1
1	A	68	LEU	N	118.223	0.3	1
1	A	68	LEU	HD11	0.11	0.020	1
1	A	68	LEU	HD12	0.11	0.020	1
1	A	68	LEU	HD13	0.11	0.020	1
1	A	68	LEU	HD21	0.43	0.020	1
1	A	68	LEU	HD22	0.43	0.020	1
1	A	68	LEU	HD23	0.43	0.020	1
1	A	69	ASN	CA	55.971	0.3	1
1	A	69	ASN	CB	38.425	0.3	1
1	A	69	ASN	HA	4.258	0.020	1
1	A	69	ASN	HB2	2.669	0.020	2
1	A	69	ASN	HB3	2.763	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	69	ASN	HD21	7.363	0.020	1
1	A	69	ASN	HD22	6.928	0.020	1
1	A	69	ASN	N	115.822	0.3	1
1	A	69	ASN	ND2	112.222	0.3	1
1	A	70	GLN	CA	58.849	0.3	1
1	A	70	GLN	CB	28.149	0.3	1
1	A	70	GLN	CG	33.612	0.3	1
1	A	70	GLN	HA	4.012	0.020	1
1	A	70	GLN	HB2	2.12	0.020	2
1	A	70	GLN	HB3	2.191	0.020	2
1	A	70	GLN	HG2	2.341	0.020	2
1	A	70	GLN	HG3	2.47	0.020	2
1	A	70	GLN	HE21	7.422	0.020	1
1	A	70	GLN	HE22	6.694	0.020	1
1	A	70	GLN	N	121.411	0.3	1
1	A	70	GLN	NE2	111.273	0.3	1
1	A	71	VAL	CA	66.367	0.3	1
1	A	71	VAL	CB	31.585	0.3	1
1	A	71	VAL	CG1	22.339	0.3	1
1	A	71	VAL	CG2	23.375	0.3	1
1	A	71	VAL	HA	3.613	0.020	1
1	A	71	VAL	HB	2.227	0.020	1
1	A	71	VAL	N	120.434	0.3	1
1	A	71	VAL	HG11	1.033	0.020	1
1	A	71	VAL	HG12	1.033	0.020	1
1	A	71	VAL	HG13	1.033	0.020	1
1	A	71	VAL	HG21	1.21	0.020	1
1	A	71	VAL	HG22	1.21	0.020	1
1	A	71	VAL	HG23	1.21	0.020	1
1	A	72	ARG	CA	59.718	0.3	1
1	A	72	ARG	CB	30.068	0.3	1
1	A	72	ARG	CG	27.894	0.3	1
1	A	72	ARG	CD	43.785	0.3	1
1	A	72	ARG	HA	3.834	0.020	1
1	A	72	ARG	HB2	1.856	0.020	1
1	A	72	ARG	HB3	1.856	0.020	1
1	A	72	ARG	HG2	1.322	0.020	2
1	A	72	ARG	HG3	1.42	0.020	2
1	A	72	ARG	HD2	2.792	0.020	2
1	A	72	ARG	HD3	3.159	0.020	2
1	A	72	ARG	HE	7.627	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	72	ARG	N	122.174	0.3	1
1	A	72	ARG	NE	82.911	0.3	1
1	A	73	ALA	CA	54.381	0.3	1
1	A	73	ALA	CB	18.135	0.3	1
1	A	73	ALA	HA	3.953	0.020	1
1	A	73	ALA	N	120.614	0.3	1
1	A	73	ALA	HB1	1.445	0.020	1
1	A	73	ALA	HB2	1.445	0.020	1
1	A	73	ALA	HB3	1.445	0.020	1
1	A	74	GLN	CA	54.842	0.3	1
1	A	74	GLN	CB	28.863	0.3	1
1	A	74	GLN	CG	33.596	0.3	1
1	A	74	GLN	HA	4.275	0.020	1
1	A	74	GLN	HB2	1.999	0.020	2
1	A	74	GLN	HB3	2.225	0.020	2
1	A	74	GLN	HG2	2.365	0.020	2
1	A	74	GLN	HG3	2.472	0.020	2
1	A	74	GLN	HE21	7.397	0.020	1
1	A	74	GLN	HE22	6.779	0.020	1
1	A	74	GLN	N	114.424	0.3	1
1	A	74	GLN	NE2	111.725	0.3	1
1	A	75	SER	CA	58.931	0.3	1
1	A	75	SER	CB	63.641	0.3	1
1	A	75	SER	HA	4.222	0.020	1
1	A	75	SER	HB2	3.85	0.020	2
1	A	75	SER	HB3	4.109	0.020	2
1	A	75	SER	N	113.737	0.3	1
1	A	76	LEU	CA	56.992	0.3	1
1	A	76	LEU	CB	41.652	0.3	1
1	A	76	LEU	CG	26.844	0.3	1
1	A	76	LEU	CD1	23.465	0.3	1
1	A	76	LEU	CD2	24.692	0.3	1
1	A	76	LEU	HA	4.049	0.020	1
1	A	76	LEU	HB2	1.482	0.020	2
1	A	76	LEU	HB3	1.744	0.020	2
1	A	76	LEU	HG	1.71	0.020	1
1	A	76	LEU	N	132.236	0.3	1
1	A	76	LEU	HD11	0.793	0.020	1
1	A	76	LEU	HD12	0.793	0.020	1
1	A	76	LEU	HD13	0.793	0.020	1
1	A	76	LEU	HD21	0.848	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	76	LEU	HD22	0.848	0.020	1
1	A	76	LEU	HD23	0.848	0.020	1
1	A	77	ALA	CA	54.677	0.3	1
1	A	77	ALA	CB	18.3	0.3	1
1	A	77	ALA	HA	3.905	0.020	1
1	A	77	ALA	N	122.734	0.3	1
1	A	77	ALA	HB1	1.167	0.020	1
1	A	77	ALA	HB2	1.167	0.020	1
1	A	77	ALA	HB3	1.167	0.020	1
1	A	78	GLU	CA	58.714	0.3	1
1	A	78	GLU	CB	29.12	0.3	1
1	A	78	GLU	CG	36.045	0.3	1
1	A	78	GLU	HA	3.849	0.020	1
1	A	78	GLU	HB2	1.775	0.020	1
1	A	78	GLU	HB3	1.775	0.020	1
1	A	78	GLU	HG2	1.913	0.020	2
1	A	78	GLU	HG3	1.964	0.020	2
1	A	78	GLU	N	116.091	0.3	1
1	A	79	LYS	CA	58.657	0.3	1
1	A	79	LYS	CB	32.541	0.3	1
1	A	79	LYS	CG	24.652	0.3	1
1	A	79	LYS	CD	28.92	0.3	1
1	A	79	LYS	CE	41.98	0.3	1
1	A	79	LYS	HA	3.94	0.020	1
1	A	79	LYS	HB2	1.776	0.020	2
1	A	79	LYS	HB3	1.81	0.020	2
1	A	79	LYS	HG2	1.357	0.020	2
1	A	79	LYS	HG3	1.43	0.020	2
1	A	79	LYS	HD2	1.557	0.020	1
1	A	79	LYS	HD3	1.557	0.020	1
1	A	79	LYS	HE2	2.868	0.020	1
1	A	79	LYS	HE3	2.868	0.020	1
1	A	79	LYS	N	119.239	0.3	1
1	A	80	ASN	CA	52.937	0.3	1
1	A	80	ASN	CB	38.585	0.3	1
1	A	80	ASN	HA	4.577	0.020	1
1	A	80	ASN	HB2	2.63	0.020	2
1	A	80	ASN	HB3	2.793	0.020	2
1	A	80	ASN	HD21	7.438	0.020	1
1	A	80	ASN	HD22	6.814	0.020	1
1	A	80	ASN	N	114.534	0.3	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	ASN	ND2	111.676	0.3	1
1	A	81	ALA	CA	52.384	0.3	1
1	A	81	ALA	CB	19.065	0.3	1
1	A	81	ALA	HA	4.126	0.020	1
1	A	81	ALA	N	123.795	0.3	1
1	A	81	ALA	HB1	1.346	0.020	1
1	A	81	ALA	HB2	1.346	0.020	1
1	A	81	ALA	HB3	1.346	0.020	1
1	A	82	GLN	CA	55.792	0.3	1
1	A	82	GLN	CB	28.931	0.3	1
1	A	82	GLN	CG	33.885	0.3	1
1	A	82	GLN	HA	4.246	0.020	1
1	A	82	GLN	HB2	1.898	0.020	2
1	A	82	GLN	HB3	1.938	0.020	2
1	A	82	GLN	HG2	2.191	0.020	2
1	A	82	GLN	HG3	2.248	0.020	2
1	A	82	GLN	HE21	6.766	0.020	1
1	A	82	GLN	HE22	7.421	0.020	1
1	A	82	GLN	N	120.773	0.3	1
1	A	82	GLN	NE2	112.419	0.3	1
1	A	83	VAL	CA	61.998	0.3	1
1	A	83	VAL	CB	33.163	0.3	1
1	A	83	VAL	CG1	22.929	0.3	1
1	A	83	VAL	CG2	21.286	0.3	1
1	A	83	VAL	HA	4.179	0.020	1
1	A	83	VAL	HB	1.84	0.020	1
1	A	83	VAL	N	124.751	0.3	1
1	A	83	VAL	HG11	0.722	0.020	1
1	A	83	VAL	HG12	0.722	0.020	1
1	A	83	VAL	HG13	0.722	0.020	1
1	A	83	VAL	HG21	0.793	0.020	1
1	A	83	VAL	HG22	0.793	0.020	1
1	A	83	VAL	HG23	0.793	0.020	1
1	A	84	VAL	CA	58.712	0.3	1
1	A	84	VAL	CB	35.158	0.3	1
1	A	84	VAL	CG1	21.394	0.3	1
1	A	84	VAL	CG2	18.566	0.3	1
1	A	84	VAL	HA	4.637	0.020	1
1	A	84	VAL	HB	2.3	0.020	1
1	A	84	VAL	N	117.432	0.3	1
1	A	84	VAL	HG11	0.851	0.020	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	VAL	HG12	0.851	0.020	1
1	A	84	VAL	HG13	0.851	0.020	1
1	A	84	VAL	HG21	0.87	0.020	1
1	A	84	VAL	HG22	0.87	0.020	1
1	A	84	VAL	HG23	0.87	0.020	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	205	-0.12 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	196	0.41 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	196	0.23 ± 0.42	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 1325 atoms were assigned a chemical shift out of a possible 1728. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	367/633 (58%)	124/257 (48%)	123/252 (49%)	120/124 (97%)
Sidechain	830/914 (91%)	564/592 (95%)	246/287 (86%)	20/35 (57%)
Aromatic	128/181 (71%)	78/88 (89%)	48/89 (54%)	2/4 (50%)
Overall	1325/1728 (77%)	766/937 (82%)	417/628 (66%)	142/163 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1415 atoms were assigned a chemical shift out of a possible 1855. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	397/689 (58%)	136/281 (48%)	134/274 (49%)	127/134 (95%)
Sidechain	886/978 (91%)	602/634 (95%)	264/308 (86%)	20/36 (56%)
Aromatic	132/188 (70%)	80/92 (87%)	50/91 (55%)	2/5 (40%)
Overall	1415/1855 (76%)	818/1007 (81%)	448/673 (67%)	149/175 (85%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	162	ILE	HD11	-1.47	-0.72 – 2.09	-7.7
1	A	162	ILE	HD12	-1.47	-0.72 – 2.09	-7.7
1	A	162	ILE	HD13	-1.47	-0.72 – 2.09	-7.7
1	A	151	LYS	HG2	-0.37	0.13 – 2.61	-7.0
1	A	200	SER	HB2	2.12	2.61 – 5.13	-7.0
1	A	173	GLN	HB2	0.59	0.80 – 3.29	-5.9
1	A	93	LEU	HB2	-0.14	-0.07 – 3.30	-5.2

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. 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:

