



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:07 AM BST

PDB ID : 2KYG  
Title : Structure of the AML1-ETO Nery Domain - PKA(RIIa) complex and its contribution to AML1-ETO activity  
Authors : Corpora, T.A.; Cierpecki, T.; Bushweller, J.  
Deposited on : 2010-05-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

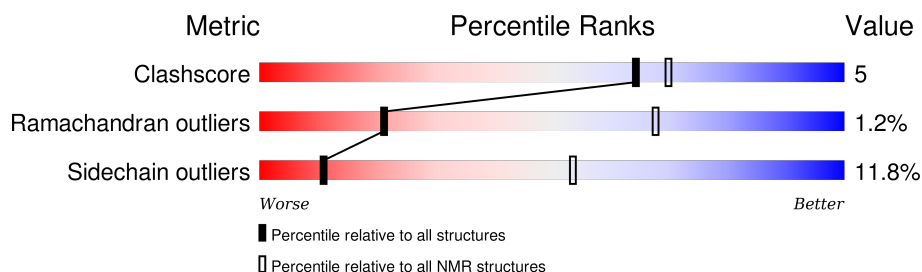
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 91%.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	50	
1	B	50	
2	C	38	

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 5 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:4-A:40, B:7-B:40, C:591-C:613 (94)	0.25	5

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2167 atoms, of which 1085 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called cAMP-dependent protein kinase type II-alpha regulatory sub-unit.

Mol	Chain	Residues	Atoms						Trace
1	A	50	Total	C	H	N	O	S	0
			792	251	397	68	74	2	
1	B	50	Total	C	H	N	O	S	0
			792	251	397	68	74	2	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	EXPRESSION TAG	UNP P13861
A	-6	ALA	-	EXPRESSION TAG	UNP P13861
A	-5	MET	-	EXPRESSION TAG	UNP P13861
A	-4	GLY	-	EXPRESSION TAG	UNP P13861
A	-3	SER	-	EXPRESSION TAG	UNP P13861
B	-7	GLY	-	EXPRESSION TAG	UNP P13861
B	-6	ALA	-	EXPRESSION TAG	UNP P13861
B	-5	MET	-	EXPRESSION TAG	UNP P13861
B	-4	GLY	-	EXPRESSION TAG	UNP P13861
B	-3	SER	-	EXPRESSION TAG	UNP P13861

- Molecule 2 is a protein called Protein CBFA2T1.

Mol	Chain	Residues	Atoms						Trace
2	C	38	Total	C	H	N	O	S	0
			583	181	291	49	60	2	

There are 7 discrepancies between the modelled and reference sequences:

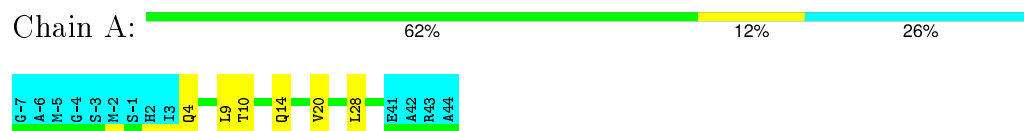
Chain	Residue	Modelled	Actual	Comment	Reference
C	578	ALA	-	EXPRESSION TAG	UNP Q06455
C	579	MET	-	EXPRESSION TAG	UNP Q06455
C	580	ALA	-	EXPRESSION TAG	UNP Q06455
C	581	ASP	-	EXPRESSION TAG	UNP Q06455
C	582	ILE	-	EXPRESSION TAG	UNP Q06455
C	583	GLY	-	EXPRESSION TAG	UNP Q06455
C	584	SER	-	EXPRESSION TAG	UNP Q06455

## 4 Residue-property plots

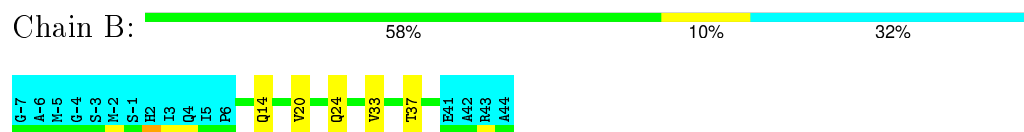
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

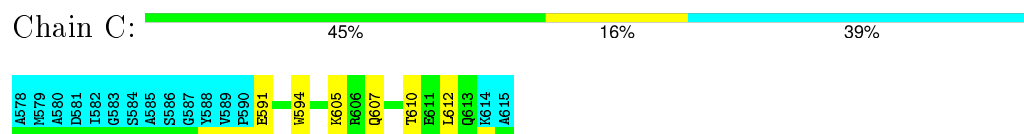
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1

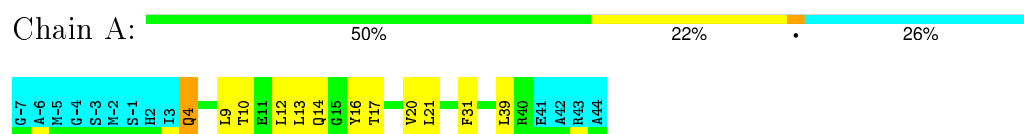


### 4.2 Scores per residue for each member of the ensemble

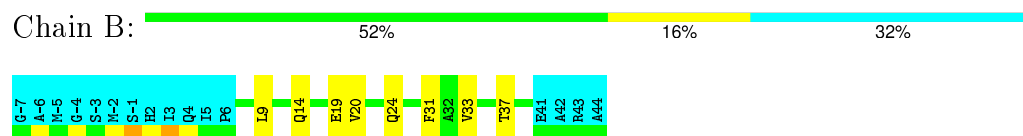
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

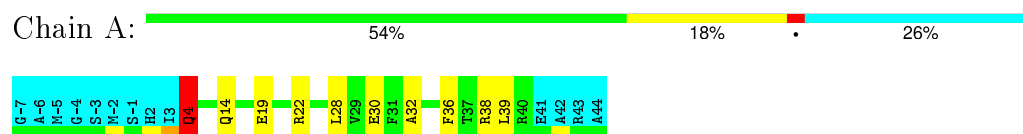


- Molecule 2: Protein CBFA2T1

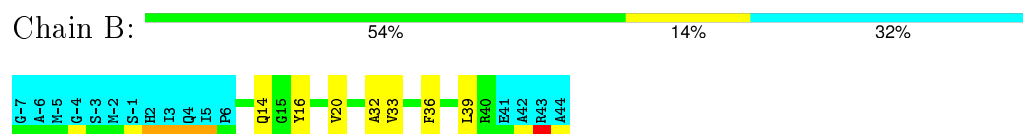


#### 4.2.2 Score per residue for model 2

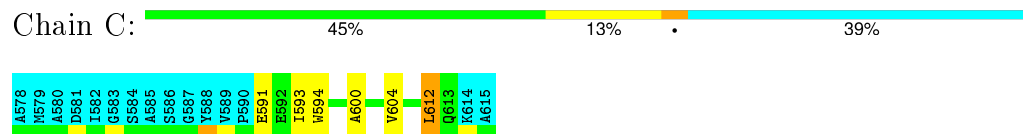
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1



#### 4.2.3 Score per residue for model 3

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

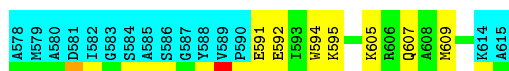


- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



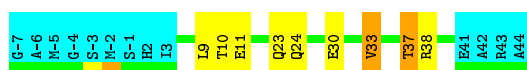


- Molecule 2: Protein CBFA2T1

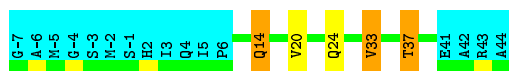


#### 4.2.4 Score per residue for model 4

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1



#### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

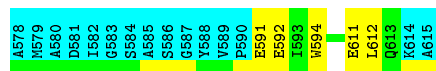


- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1

Chain C: 



#### 4.2.6 Score per residue for model 6

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain A: 



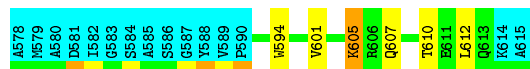
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain B: 



- Molecule 2: Protein CBFA2T1

Chain C: 



#### 4.2.7 Score per residue for model 7

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

Chain A: 



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

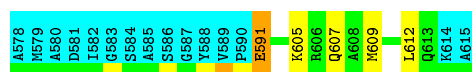
Chain B: 



- Molecule 2: Protein CBFA2T1

Chain C: 





#### 4.2.8 Score per residue for model 8

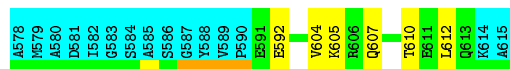
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1



#### 4.2.9 Score per residue for model 9

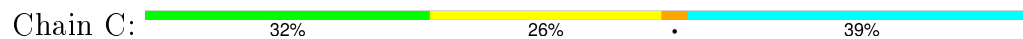
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

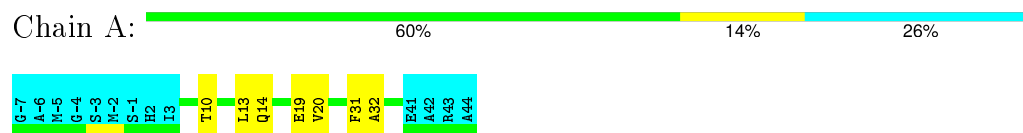


- Molecule 2: Protein CBFA2T1

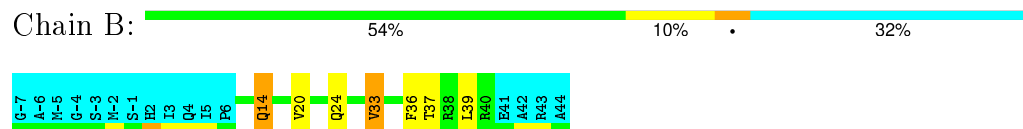


#### 4.2.10 Score per residue for model 10

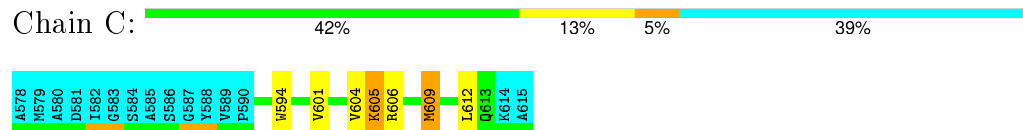
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1

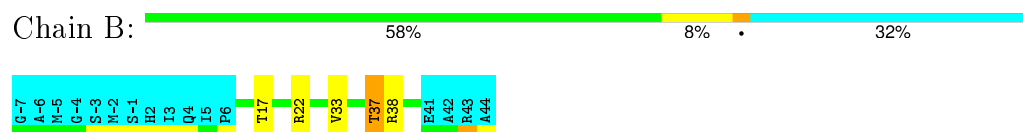


#### 4.2.11 Score per residue for model 11

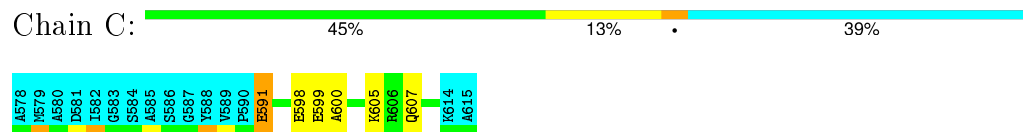
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

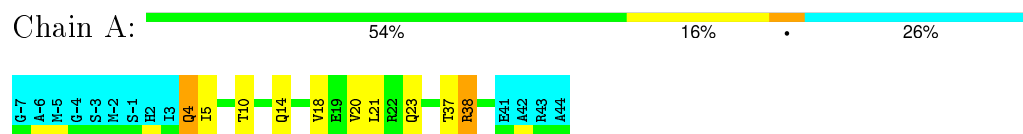


- Molecule 2: Protein CBFA2T1

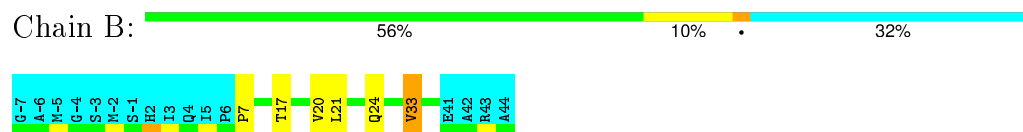


#### 4.2.12 Score per residue for model 12

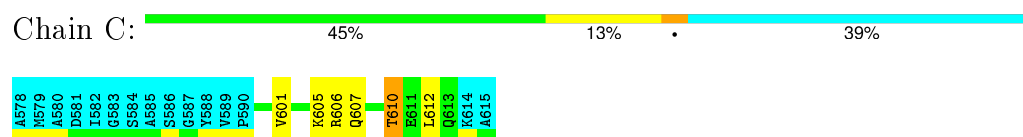
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

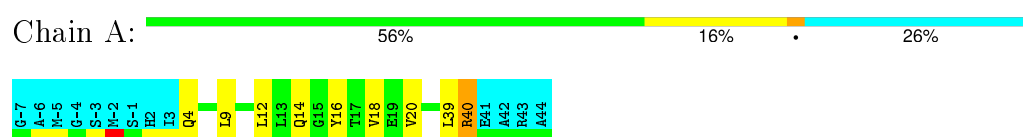


- Molecule 2: Protein CBFA2T1

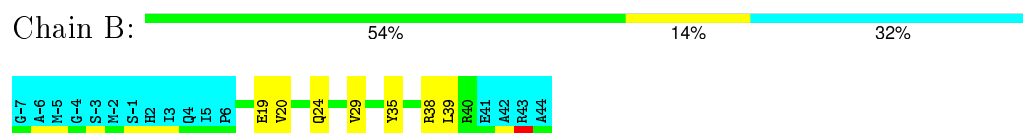


#### 4.2.13 Score per residue for model 13

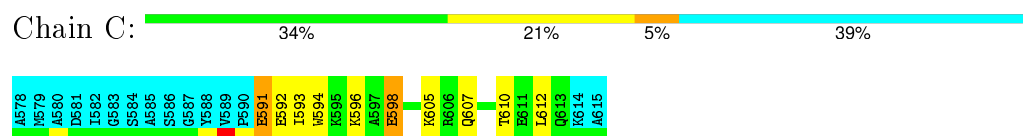
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



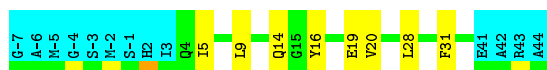
- Molecule 2: Protein CBFA2T1



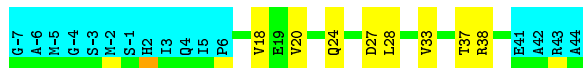
#### 4.2.14 Score per residue for model 14

- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit

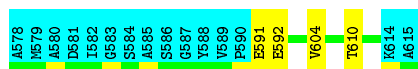




- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1



#### 4.2.15 Score per residue for model 15

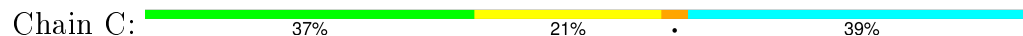
- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 1: cAMP-dependent protein kinase type II-alpha regulatory subunit



- Molecule 2: Protein CBFA2T1



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 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
TALOS	structure solution	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 16954
Number of chemical shift lists	1
Total number of shifts	2543
Number of shifts mapped to atoms	1701
Number of unparsed shifts	842
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	305	308	308	4±2
1	B	281	282	282	5±2
2	C	192	191	191	3±2
All	All	11670	11715	11715	121

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:600:ALA:O	2:C:604:VAL:HG13	0.79	1.76	4	1
2:C:607:GLN:O	2:C:610:THR:HG22	0.77	1.78	6	1
1:B:33:VAL:O	1:B:37:THR:HG23	0.76	1.80	1	6
1:A:14:GLN:O	1:A:18:VAL:HG22	0.72	1.85	9	3
1:A:16:TYR:O	1:A:20:VAL:HG23	0.71	1.85	14	4
1:A:10:THR:HG23	2:C:604:VAL:HG12	0.70	1.63	4	1
1:B:17:THR:HG21	2:C:600:ALA:HB3	0.64	1.70	9	3
1:A:9:LEU:HD12	1:B:28:LEU:HD11	0.63	1.69	15	1
1:A:17:THR:O	1:A:21:LEU:HD12	0.61	1.96	1	1
1:B:16:TYR:O	1:B:20:VAL:HG23	0.59	1.96	2	2
1:B:33:VAL:O	1:B:37:THR:OG1	0.56	2.14	11	2
1:B:20:VAL:O	1:B:24:GLN:N	0.56	2.38	3	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:LEU:HB2	2:C:604:VAL:HG21	0.56	1.78	1	3
1:A:28:LEU:HD22	1:B:9:LEU:HD23	0.55	1.77	5	1
1:A:9:LEU:HD12	1:B:28:LEU:CD2	0.53	2.32	6	1
2:C:594:TRP:CD2	2:C:598:GLU:OE2	0.53	2.61	13	1
1:A:33:VAL:O	1:A:37:THR:HG23	0.52	2.05	15	2
1:A:33:VAL:HG13	1:A:37:THR:OG1	0.51	2.05	3	1
2:C:598:GLU:OE1	2:C:598:GLU:N	0.49	2.45	13	1
1:B:14:GLN:NE2	2:C:594:TRP:CH2	0.49	2.81	15	1
1:A:28:LEU:N	1:A:28:LEU:HD22	0.48	2.23	2	3
1:A:5:ILE:HD13	1:B:21:LEU:HD11	0.48	1.85	15	1
1:A:14:GLN:N	2:C:604:VAL:HG21	0.48	2.24	15	2
1:A:28:LEU:HD22	1:A:28:LEU:N	0.48	2.22	8	1
1:B:9:LEU:HD23	1:B:9:LEU:O	0.48	2.08	8	1
2:C:600:ALA:O	2:C:604:VAL:HG12	0.48	2.08	2	1
1:A:32:ALA:CB	1:B:36:PHE:CE1	0.47	2.97	15	1
1:A:33:VAL:HG11	1:B:37:THR:HG23	0.47	1.87	4	1
1:A:9:LEU:HD12	1:B:28:LEU:HD22	0.46	1.87	6	1
1:A:40:ARG:HG2	1:B:29:VAL:CG1	0.46	2.41	13	1
2:C:607:GLN:O	2:C:610:THR:OG1	0.46	2.28	9	4
2:C:609:MET:HA	2:C:612:LEU:HD12	0.46	1.88	9	1
1:A:4:GLN:CG	1:A:4:GLN:O	0.45	2.63	2	1
1:A:28:LEU:HD12	1:A:28:LEU:N	0.45	2.27	6	1
1:B:14:GLN:OE1	2:C:594:TRP:CH2	0.44	2.70	9	5
1:B:14:GLN:OE1	2:C:594:TRP:CE2	0.44	2.71	6	3
1:A:36:PHE:CE1	1:B:32:ALA:CB	0.44	3.01	2	2
1:B:19:GLU:OE1	1:B:31:PHE:CE2	0.44	2.70	1	1
1:B:9:LEU:HD23	1:B:9:LEU:C	0.44	2.33	8	1
2:C:601:VAL:O	2:C:605:LYS:HB2	0.44	2.12	12	2
1:A:33:VAL:O	1:A:37:THR:OG1	0.43	2.27	4	1
1:B:14:GLN:OE1	2:C:594:TRP:CZ2	0.43	2.71	9	3
1:A:32:ALA:CB	1:B:36:PHE:CD1	0.43	3.01	10	4
1:B:17:THR:HG22	1:B:21:LEU:HD23	0.43	1.90	12	1
1:B:22:ARG:O	1:B:22:ARG:NE	0.43	2.52	8	1
1:A:16:TYR:CE1	1:A:31:PHE:CD2	0.43	3.07	1	1
1:B:28:LEU:N	1:B:28:LEU:CD2	0.43	2.82	14	2
1:A:13:LEU:HB3	2:C:604:VAL:HG11	0.43	1.91	10	1
1:B:19:GLU:OE1	1:B:31:PHE:CZ	0.42	2.72	1	1
1:A:20:VAL:O	1:A:24:GLN:N	0.42	2.52	6	2
1:A:33:VAL:CG1	1:B:37:THR:HG23	0.42	2.43	4	1
1:A:9:LEU:HD22	1:B:17:THR:HG23	0.42	1.90	6	1
1:A:9:LEU:O	1:A:9:LEU:HD23	0.42	2.13	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLN:N	2:C:604:VAL:CG2	0.42	2.83	8	2
2:C:601:VAL:O	2:C:605:LYS:CB	0.42	2.67	10	1
1:A:29:VAL:HG12	1:B:40:ARG:HG2	0.42	1.90	6	1
1:A:13:LEU:CB	2:C:604:VAL:HG21	0.41	2.45	1	1
1:B:29:VAL:HG13	1:B:30:GLU:N	0.41	2.30	3	1
1:B:19:GLU:OE2	1:B:35:TYR:CD1	0.41	2.73	13	2
1:B:27:ASP:OD1	1:B:29:VAL:HG22	0.41	2.16	8	1
1:B:14:GLN:OE1	2:C:594:TRP:CD2	0.41	2.74	6	1
1:B:17:THR:HG21	2:C:600:ALA:CB	0.41	2.42	9	1
1:B:14:GLN:OE1	2:C:594:TRP:CZ3	0.41	2.74	9	1
1:A:28:LEU:CD2	1:A:28:LEU:N	0.41	2.84	14	1
1:A:9:LEU:CD1	1:B:28:LEU:HD11	0.41	2.43	15	1
1:A:29:VAL:HG13	1:A:30:GLU:N	0.41	2.31	7	2
1:A:13:LEU:HG	1:B:13:LEU:HD22	0.41	1.92	5	1
1:A:32:ALA:HB1	1:B:36:PHE:CG	0.41	2.50	10	1
1:A:19:GLU:OE1	1:A:31:PHE:CZ	0.41	2.73	14	1
1:A:37:THR:HG22	1:B:33:VAL:CG1	0.40	2.47	12	1
1:A:21:LEU:O	1:A:24:GLN:NE2	0.40	2.54	5	1
2:C:594:TRP:CG	2:C:598:GLU:OE2	0.40	2.74	13	1
1:B:17:THR:O	1:B:20:VAL:HG12	0.40	2.15	5	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	37/50 (74%)	34±1 (91±2%)	3±1 (8±2%)	0±0 (1±1%)	26	73
1	B	34/50 (68%)	32±1 (95±2%)	1±1 (4±3%)	0±0 (0±1%)	43	81
2	C	23/38 (61%)	21±1 (93±3%)	1±0 (4±2%)	1±0 (3±2%)	9	43
All	All	1410/2070 (68%)	1315 (93%)	78 (6%)	17 (1%)	21	68

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.



Mol	Chain	Res	Type	Models (Total)
2	C	591	GLU	10
1	A	4	GLN	3
1	A	24	GLN	2
1	B	7	PRO	1
1	B	24	GLN	1

### 6.3.2 Protein sidechains ⓘ

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	34/42 (81%)	29±2 (86±5%)	5±2 (14±5%)	9 49
1	B	31/42 (74%)	29±1 (93±2%)	2±1 (7±2%)	23 68
2	C	20/29 (69%)	17±1 (84±6%)	3±1 (16±6%)	7 45
All	All	1275/1695 (75%)	1125 (88%)	150 (12%)	11 53

All 53 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	10	THR	8
2	C	605	LYS	8
1	A	14	GLN	7
2	C	610	THR	7
1	A	9	LEU	7
2	C	612	LEU	7
1	B	33	VAL	6
2	C	607	GLN	6
1	A	40	ARG	6
1	A	20	VAL	5
1	B	14	GLN	5
1	A	12	LEU	5
1	A	38	ARG	4
2	C	606	ARG	4
1	A	39	LEU	4
1	A	4	GLN	4
1	B	39	LEU	3
1	A	33	VAL	3

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Mol	Chain	Res	Type	Models (Total)
1	B	38	ARG	3
1	A	23	GLN	3
2	C	609	MET	3
2	C	591	GLU	2
1	A	30	GLU	2
1	B	40	ARG	2
1	A	5	ILE	2
1	A	11	GLU	2
1	B	20	VAL	2
2	C	598	GLU	2
1	B	27	ASP	2
1	B	37	THR	2
1	A	19	GLU	2
2	C	603	GLU	1
2	C	596	LYS	1
2	C	595	LYS	1
1	B	18	VAL	1
2	C	611	GLU	1
2	C	592	GLU	1
1	B	12	LEU	1
1	A	22	ARG	1
1	B	29	VAL	1
1	A	34	GLU	1
1	B	9	LEU	1
1	A	28	LEU	1
1	B	21	LEU	1
1	B	23	GLN	1
1	B	17	THR	1
2	C	593	ILE	1
1	A	31	PHE	1
1	B	22	ARG	1
2	C	599	GLU	1
1	A	21	LEU	1
1	A	37	THR	1
2	C	604	VAL	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 89% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 16954

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	2543
Number of shifts mapped to atoms	1701
Number of unparsed shifts	842
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- Chemical shift has been reported more than once. All 842 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1141	A	-6	ALA	H	8.505	0.08	6
1142	B	-6	ALA	H	8.505	0.08	6
1145	A	-6	ALA	HB1	1.376	0.08	6
1146	B	-6	ALA	HB1	1.376	0.08	6
1147	A	-6	ALA	HB2	1.376	0.08	6
1148	B	-6	ALA	HB2	1.376	0.08	6
1149	A	-6	ALA	HB3	1.376	0.08	6
1150	B	-6	ALA	HB3	1.376	0.08	6
1153	A	-2	MET	H	8.476	0.08	6
1154	B	-2	MET	H	8.476	0.08	6
1155	A	-2	MET	N	122.074	0.22	6
1156	B	-2	MET	N	122.074	0.22	6
1157	A	2	HIS	H	8.464	0.08	6
1158	B	2	HIS	H	8.464	0.08	6
1159	A	2	HIS	HA	4.708	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1160	B	2	HIS	HA	4.708	0.08	6
1161	A	2	HIS	HB2	3.239	0.08	6
1162	B	2	HIS	HB2	3.239	0.08	6
1163	A	2	HIS	HB3	3.070	0.08	6
1164	B	2	HIS	HB3	3.070	0.08	6
1165	A	2	HIS	C	173.944	0.42	6
1166	B	2	HIS	C	173.944	0.42	6
1167	A	2	HIS	CA	55.149	0.42	6
1168	B	2	HIS	CA	55.149	0.42	6
1169	A	2	HIS	CB	29.006	0.42	6
1170	B	2	HIS	CB	29.006	0.42	6
1171	A	2	HIS	N	120.326	0.22	6
1172	B	2	HIS	N	120.326	0.22	6
1173	A	3	ILE	H	8.073	0.08	6
1174	B	3	ILE	H	8.073	0.08	6
1175	A	3	ILE	HA	4.042	0.08	6
1176	B	3	ILE	HA	4.042	0.08	6
1177	A	3	ILE	HB	1.699	0.08	6
1178	B	3	ILE	HB	1.699	0.08	6
1179	A	3	ILE	HD11	0.702	0.08	6
1180	B	3	ILE	HD11	0.702	0.08	6
1181	A	3	ILE	HD12	0.702	0.08	6
1182	B	3	ILE	HD12	0.702	0.08	6
1183	A	3	ILE	HD13	0.702	0.08	6
1184	B	3	ILE	HD13	0.702	0.08	6
1185	A	3	ILE	HG12	1.267	0.08	6
1186	B	3	ILE	HG12	1.267	0.08	6
1187	A	3	ILE	HG13	1.105	0.08	6
1188	B	3	ILE	HG13	1.105	0.08	6
1189	A	3	ILE	HG21	0.725	0.08	6
1190	B	3	ILE	HG21	0.725	0.08	6
1191	A	3	ILE	HG22	0.725	0.08	6
1192	B	3	ILE	HG22	0.725	0.08	6
1193	A	3	ILE	HG23	0.725	0.08	6
1194	B	3	ILE	HG23	0.725	0.08	6
1195	A	3	ILE	CA	60.615	0.42	6
1196	B	3	ILE	CA	60.615	0.42	6
1197	A	3	ILE	CB	38.055	0.42	6
1198	B	3	ILE	CB	38.055	0.42	6
1199	A	3	ILE	CD1	12.735	0.42	6
1200	B	3	ILE	CD1	12.735	0.42	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1201	A	3	ILE	CG1	27.324	0.42	6
1202	B	3	ILE	CG1	27.324	0.42	6
1203	A	3	ILE	CG2	18.295	0.42	6
1204	B	3	ILE	CG2	18.295	0.42	6
1205	A	3	ILE	N	122.061	0.22	6
1206	B	3	ILE	N	122.061	0.22	6
1207	A	4	GLN	H	8.173	0.08	6
1208	B	4	GLN	H	8.173	0.08	6
1209	A	4	GLN	HA	4.446	0.08	6
1210	B	4	GLN	HA	4.446	0.08	6
1211	A	4	GLN	HB2	1.927	0.08	6
1212	B	4	GLN	HB2	1.927	0.08	6
1213	A	4	GLN	HB3	1.784	0.08	6
1214	B	4	GLN	HB3	1.784	0.08	6
1215	A	4	GLN	HG2	2.210	0.08	6
1216	B	4	GLN	HG2	2.210	0.08	6
1217	A	4	GLN	HG3	2.210	0.08	6
1218	B	4	GLN	HG3	2.210	0.08	6
1219	A	4	GLN	C	174.871	0.42	6
1220	B	4	GLN	C	174.871	0.42	6
1221	A	4	GLN	CA	53.989	0.42	6
1222	B	4	GLN	CA	53.989	0.42	6
1223	A	4	GLN	N	124.996	0.22	6
1224	B	4	GLN	N	124.996	0.22	6
1225	A	5	ILE	H	8.552	0.08	6
1226	B	5	ILE	H	8.552	0.08	6
1227	A	5	ILE	HA	4.119	0.08	6
1228	B	5	ILE	HA	4.119	0.08	6
1229	A	5	ILE	HB	1.941	0.08	6
1230	B	5	ILE	HB	1.941	0.08	6
1231	A	5	ILE	HD11	0.720	0.08	6
1232	B	5	ILE	HD11	0.720	0.08	6
1233	A	5	ILE	HD12	0.720	0.08	6
1234	B	5	ILE	HD12	0.720	0.08	6
1235	A	5	ILE	HD13	0.720	0.08	6
1236	B	5	ILE	HD13	0.720	0.08	6
1237	A	5	ILE	HG12	1.518	0.08	6
1238	B	5	ILE	HG12	1.518	0.08	6
1239	A	5	ILE	HG13	1.209	0.08	6
1240	B	5	ILE	HG13	1.209	0.08	6
1241	A	5	ILE	HG21	0.934	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1242	B	5	ILE	HG21	0.934	0.08	6
1243	A	5	ILE	HG22	0.934	0.08	6
1244	B	5	ILE	HG22	0.934	0.08	6
1245	A	5	ILE	HG23	0.934	0.08	6
1246	B	5	ILE	HG23	0.934	0.08	6
1247	A	5	ILE	CB	37.132	0.42	6
1248	B	5	ILE	CB	37.132	0.42	6
1249	A	5	ILE	CD1	11.852	0.42	6
1250	B	5	ILE	CD1	11.852	0.42	6
1251	A	5	ILE	CG1	27.032	0.42	6
1252	B	5	ILE	CG1	27.032	0.42	6
1253	A	5	ILE	CG2	17.781	0.42	6
1254	B	5	ILE	CG2	17.781	0.42	6
1255	A	5	ILE	N	124.116	0.22	6
1256	B	5	ILE	N	124.116	0.22	6
1257	A	6	PRO	HD3	3.361	0.08	6
1258	B	6	PRO	HD3	3.361	0.08	6
1259	A	6	PRO	CD	50.877	0.42	6
1260	B	6	PRO	CD	50.877	0.42	6
1261	A	7	PRO	HA	4.346	0.08	6
1262	B	7	PRO	HA	4.346	0.08	6
1263	A	7	PRO	HB2	2.332	0.08	6
1264	B	7	PRO	HB2	2.332	0.08	6
1265	A	7	PRO	HB3	1.921	0.08	6
1266	B	7	PRO	HB3	1.921	0.08	6
1267	A	7	PRO	HD2	3.871	0.08	6
1268	B	7	PRO	HD2	3.871	0.08	6
1269	A	7	PRO	HD3	3.662	0.08	6
1270	B	7	PRO	HD3	3.662	0.08	6
1271	A	7	PRO	HG2	2.033	0.08	6
1272	B	7	PRO	HG2	2.033	0.08	6
1273	A	7	PRO	HG3	2.033	0.08	6
1274	B	7	PRO	HG3	2.033	0.08	6
1275	A	7	PRO	C	177.329	0.42	6
1276	B	7	PRO	C	177.329	0.42	6
1277	A	7	PRO	CA	63.904	0.42	6
1278	B	7	PRO	CA	63.904	0.42	6
1279	A	7	PRO	CB	31.682	0.42	6
1280	B	7	PRO	CB	31.682	0.42	6
1281	A	7	PRO	CG	27.640	0.42	6
1282	B	7	PRO	CG	27.640	0.42	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1283	A	8	GLY	H	8.758	0.08	6
1284	B	8	GLY	H	8.758	0.08	6
1285	A	8	GLY	HA2	4.200	0.08	6
1286	B	8	GLY	HA2	4.200	0.08	6
1287	A	8	GLY	HA3	3.920	0.08	6
1288	B	8	GLY	HA3	3.920	0.08	6
1289	A	8	GLY	C	175.538	0.42	6
1290	B	8	GLY	C	175.538	0.42	6
1291	A	8	GLY	CA	45.463	0.42	6
1292	B	8	GLY	CA	45.463	0.42	6
1293	A	8	GLY	N	110.218	0.22	6
1294	B	8	GLY	N	110.218	0.22	6
1295	A	9	LEU	H	7.486	0.08	6
1296	B	9	LEU	H	7.486	0.08	6
1297	A	9	LEU	HA	4.115	0.08	6
1298	B	9	LEU	HA	4.115	0.08	6
1299	A	9	LEU	HB2	1.808	0.08	6
1300	B	9	LEU	HB2	1.808	0.08	6
1301	A	9	LEU	HD11	1.092	0.08	6
1302	B	9	LEU	HD11	1.092	0.08	6
1303	A	9	LEU	HD12	1.092	0.08	6
1304	B	9	LEU	HD12	1.092	0.08	6
1305	A	9	LEU	HD13	1.092	0.08	6
1306	B	9	LEU	HD13	1.092	0.08	6
1307	A	9	LEU	HD21	0.943	0.08	6
1308	B	9	LEU	HD21	0.943	0.08	6
1309	A	9	LEU	HD22	0.943	0.08	6
1310	B	9	LEU	HD22	0.943	0.08	6
1311	A	9	LEU	HD23	0.943	0.08	6
1312	B	9	LEU	HD23	0.943	0.08	6
1313	A	9	LEU	C	177.747	0.42	6
1314	B	9	LEU	C	177.747	0.42	6
1315	A	9	LEU	CA	58.397	0.42	6
1316	B	9	LEU	CA	58.397	0.42	6
1317	A	9	LEU	CD1	24.387	0.42	6
1318	B	9	LEU	CD1	24.387	0.42	6
1319	A	9	LEU	CD2	25.879	0.42	6
1320	B	9	LEU	CD2	25.879	0.42	6
1321	A	9	LEU	N	121.269	0.22	6
1322	B	9	LEU	N	121.269	0.22	6
1323	A	10	THR	H	8.560	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1324	B	10	THR	H	8.560	0.08	6
1325	A	10	THR	HA	4.100	0.08	6
1326	B	10	THR	HA	4.100	0.08	6
1327	A	10	THR	HB	3.482	0.08	6
1328	B	10	THR	HB	3.482	0.08	6
1329	A	10	THR	HG21	1.175	0.08	6
1330	B	10	THR	HG21	1.175	0.08	6
1331	A	10	THR	HG22	1.175	0.08	6
1332	B	10	THR	HG22	1.175	0.08	6
1333	A	10	THR	HG23	1.175	0.08	6
1334	B	10	THR	HG23	1.175	0.08	6
1335	A	10	THR	C	175.248	0.42	6
1336	B	10	THR	C	175.248	0.42	6
1337	A	10	THR	CA	68.355	0.42	6
1338	B	10	THR	CA	68.355	0.42	6
1339	A	10	THR	CB	68.438	0.42	6
1340	B	10	THR	CB	68.438	0.42	6
1341	A	10	THR	CG2	21.802	0.42	6
1342	B	10	THR	CG2	21.802	0.42	6
1343	A	10	THR	N	115.641	0.22	6
1344	B	10	THR	N	115.641	0.22	6
1345	A	11	GLU	H	9.271	0.08	6
1346	B	11	GLU	H	9.271	0.08	6
1347	A	11	GLU	HA	4.015	0.08	6
1348	B	11	GLU	HA	4.015	0.08	6
1349	A	11	GLU	HB2	2.148	0.08	6
1350	B	11	GLU	HB2	2.148	0.08	6
1351	A	11	GLU	HB3	2.004	0.08	6
1352	B	11	GLU	HB3	2.004	0.08	6
1353	A	11	GLU	HG2	2.574	0.08	6
1354	B	11	GLU	HG2	2.574	0.08	6
1355	A	11	GLU	C	179.669	0.42	6
1356	B	11	GLU	C	179.669	0.42	6
1357	A	11	GLU	CA	60.667	0.42	6
1358	B	11	GLU	CA	60.667	0.42	6
1359	A	11	GLU	CB	28.651	0.42	6
1360	B	11	GLU	CB	28.651	0.42	6
1361	A	11	GLU	N	121.061	0.22	6
1362	B	11	GLU	N	121.061	0.22	6
1363	A	12	LEU	H	7.827	0.08	6
1364	B	12	LEU	H	7.827	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1365	A	12	LEU	HA	4.372	0.08	6
1366	B	12	LEU	HA	4.372	0.08	6
1367	A	12	LEU	HB2	2.141	0.08	6
1368	B	12	LEU	HB2	2.141	0.08	6
1369	A	12	LEU	HB3	1.944	0.08	6
1370	B	12	LEU	HB3	1.944	0.08	6
1371	A	12	LEU	HD11	1.056	0.08	6
1372	B	12	LEU	HD11	1.056	0.08	6
1373	A	12	LEU	HD12	1.056	0.08	6
1374	B	12	LEU	HD12	1.056	0.08	6
1375	A	12	LEU	HD13	1.056	0.08	6
1376	B	12	LEU	HD13	1.056	0.08	6
1377	A	12	LEU	HD21	0.975	0.08	6
1378	B	12	LEU	HD21	0.975	0.08	6
1379	A	12	LEU	HD22	0.975	0.08	6
1380	B	12	LEU	HD22	0.975	0.08	6
1381	A	12	LEU	HD23	0.975	0.08	6
1382	B	12	LEU	HD23	0.975	0.08	6
1383	A	12	LEU	HG	1.968	0.08	6
1384	B	12	LEU	HG	1.968	0.08	6
1385	A	12	LEU	C	179.816	0.42	6
1386	B	12	LEU	C	179.816	0.42	6
1387	A	12	LEU	CA	57.863	0.42	6
1388	B	12	LEU	CA	57.863	0.42	6
1389	A	12	LEU	CB	42.687	0.42	6
1390	B	12	LEU	CB	42.687	0.42	6
1391	A	12	LEU	CD1	26.848	0.42	6
1392	B	12	LEU	CD1	26.848	0.42	6
1393	A	12	LEU	CD2	25.537	0.42	6
1394	B	12	LEU	CD2	25.537	0.42	6
1397	A	12	LEU	N	121.451	0.22	6
1398	B	12	LEU	N	121.451	0.22	6
1399	A	13	LEU	H	8.312	0.08	6
1400	B	13	LEU	H	8.312	0.08	6
1401	A	13	LEU	HA	4.136	0.08	6
1402	B	13	LEU	HA	4.136	0.08	6
1403	A	13	LEU	HD11	1.016	0.08	6
1404	B	13	LEU	HD11	1.016	0.08	6
1405	A	13	LEU	HD12	1.016	0.08	6
1406	B	13	LEU	HD12	1.016	0.08	6
1407	A	13	LEU	HD13	1.016	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1408	B	13	LEU	HD13	1.016	0.08	6
1409	A	13	LEU	HD21	0.960	0.08	6
1410	B	13	LEU	HD21	0.960	0.08	6
1411	A	13	LEU	HD22	0.960	0.08	6
1412	B	13	LEU	HD22	0.960	0.08	6
1413	A	13	LEU	HD23	0.960	0.08	6
1414	B	13	LEU	HD23	0.960	0.08	6
1415	A	13	LEU	C	180.174	0.42	6
1416	B	13	LEU	C	180.174	0.42	6
1417	A	13	LEU	CA	57.967	0.42	6
1418	B	13	LEU	CA	57.967	0.42	6
1419	A	13	LEU	CD1	22.589	0.42	6
1420	B	13	LEU	CD1	22.589	0.42	6
1421	A	13	LEU	CD2	25.955	0.42	6
1422	B	13	LEU	CD2	25.955	0.42	6
1423	A	13	LEU	N	116.979	0.22	6
1424	B	13	LEU	N	116.979	0.22	6
1425	A	14	GLN	H	9.116	0.08	6
1426	B	14	GLN	H	9.116	0.08	6
1427	A	14	GLN	HA	3.712	0.08	6
1428	B	14	GLN	HA	3.712	0.08	6
1429	A	14	GLN	HB2	2.255	0.08	6
1430	B	14	GLN	HB2	2.255	0.08	6
1431	A	14	GLN	HB3	1.930	0.08	6
1432	B	14	GLN	HB3	1.930	0.08	6
1433	A	14	GLN	HG2	1.978	0.08	6
1434	B	14	GLN	HG2	1.978	0.08	6
1435	A	14	GLN	HG3	1.941	0.08	6
1436	B	14	GLN	HG3	1.941	0.08	6
1437	A	14	GLN	C	177.444	0.42	6
1438	B	14	GLN	C	177.444	0.42	6
1439	A	14	GLN	CA	59.669	0.42	6
1440	B	14	GLN	CA	59.669	0.42	6
1441	A	14	GLN	CB	27.706	0.42	6
1442	B	14	GLN	CB	27.706	0.42	6
1443	A	14	GLN	CG	32.654	0.42	6
1444	B	14	GLN	CG	32.654	0.42	6
1445	A	14	GLN	N	122.704	0.22	6
1446	B	14	GLN	N	122.704	0.22	6
1447	A	15	GLY	H	8.168	0.08	6
1448	B	15	GLY	H	8.168	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1449	A	15	GLY	HA2	4.072	0.08	6
1450	B	15	GLY	HA2	4.072	0.08	6
1451	A	15	GLY	HA3	3.694	0.08	6
1452	B	15	GLY	HA3	3.694	0.08	6
1453	A	15	GLY	C	175.830	0.42	6
1454	B	15	GLY	C	175.830	0.42	6
1455	A	15	GLY	CA	47.847	0.42	6
1456	B	15	GLY	CA	47.847	0.42	6
1457	A	15	GLY	N	105.825	0.22	6
1458	B	15	GLY	N	105.825	0.22	6
1459	A	16	TYR	H	7.256	0.08	6
1460	B	16	TYR	H	7.256	0.08	6
1461	A	16	TYR	HA	2.776	0.08	6
1462	B	16	TYR	HA	2.776	0.08	6
1463	A	16	TYR	HB2	2.756	0.08	6
1464	B	16	TYR	HB2	2.756	0.08	6
1465	A	16	TYR	HB3	2.626	0.08	6
1466	B	16	TYR	HB3	2.626	0.08	6
1467	A	16	TYR	HD1	6.391	0.08	6
1468	B	16	TYR	HD1	6.391	0.08	6
1469	A	16	TYR	HD2	6.391	0.08	6
1470	B	16	TYR	HD2	6.391	0.08	6
1471	A	16	TYR	HE1	6.259	0.08	6
1472	B	16	TYR	HE1	6.259	0.08	6
1473	A	16	TYR	HE2	6.259	0.08	6
1474	B	16	TYR	HE2	6.259	0.08	6
1475	A	16	TYR	C	175.622	0.42	6
1476	B	16	TYR	C	175.622	0.42	6
1477	A	16	TYR	CA	60.719	0.42	6
1478	B	16	TYR	CA	60.719	0.42	6
1479	A	16	TYR	CD1	132.499	0.42	6
1480	B	16	TYR	CD1	132.499	0.42	6
1481	A	16	TYR	CD2	132.499	0.42	6
1482	B	16	TYR	CD2	132.499	0.42	6
1483	A	16	TYR	CE1	117.728	0.42	6
1484	B	16	TYR	CE1	117.728	0.42	6
1485	A	16	TYR	CE2	117.728	0.42	6
1486	B	16	TYR	CE2	117.728	0.42	6
1487	A	16	TYR	N	119.860	0.22	6
1488	B	16	TYR	N	119.860	0.22	6
1489	A	17	THR	H	7.866	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1490	B	17	THR	H	7.866	0.08	6
1491	A	17	THR	HA	3.180	0.08	6
1492	B	17	THR	HA	3.180	0.08	6
1493	A	17	THR	HB	3.948	0.08	6
1494	B	17	THR	HB	3.948	0.08	6
1495	A	17	THR	HG21	1.026	0.08	6
1496	B	17	THR	HG21	1.026	0.08	6
1497	A	17	THR	HG22	1.026	0.08	6
1498	B	17	THR	HG22	1.026	0.08	6
1499	A	17	THR	HG23	1.026	0.08	6
1500	B	17	THR	HG23	1.026	0.08	6
1501	A	17	THR	C	176.073	0.42	6
1502	B	17	THR	C	176.073	0.42	6
1503	A	17	THR	CA	68.496	0.42	6
1504	B	17	THR	CA	68.496	0.42	6
1507	A	17	THR	CG2	21.804	0.42	6
1508	B	17	THR	CG2	21.804	0.42	6
1509	A	17	THR	N	115.938	0.22	6
1510	B	17	THR	N	115.938	0.22	6
1511	A	18	VAL	H	8.536	0.08	6
1512	B	18	VAL	H	8.536	0.08	6
1513	A	18	VAL	HA	3.131	0.08	6
1514	B	18	VAL	HA	3.131	0.08	6
1515	A	18	VAL	HB	2.076	0.08	6
1516	B	18	VAL	HB	2.076	0.08	6
1517	A	18	VAL	HG11	0.785	0.08	6
1518	B	18	VAL	HG11	0.785	0.08	6
1519	A	18	VAL	HG12	0.785	0.08	6
1520	B	18	VAL	HG12	0.785	0.08	6
1521	A	18	VAL	HG13	0.785	0.08	6
1522	B	18	VAL	HG13	0.785	0.08	6
1523	A	18	VAL	HG21	0.746	0.08	6
1524	B	18	VAL	HG21	0.746	0.08	6
1525	A	18	VAL	HG22	0.746	0.08	6
1526	B	18	VAL	HG22	0.746	0.08	6
1527	A	18	VAL	HG23	0.746	0.08	6
1528	B	18	VAL	HG23	0.746	0.08	6
1529	A	18	VAL	C	177.275	0.42	6
1530	B	18	VAL	C	177.275	0.42	6
1531	A	18	VAL	CA	67.575	0.42	6
1532	B	18	VAL	CA	67.575	0.42	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1533	A	18	VAL	CG1	21.812	0.42	6
1534	B	18	VAL	CG1	21.812	0.42	6
1535	A	18	VAL	CG2	24.310	0.42	6
1536	B	18	VAL	CG2	24.310	0.42	6
1537	A	18	VAL	N	120.679	0.22	6
1538	B	18	VAL	N	120.679	0.22	6
1539	A	19	GLU	H	7.185	0.08	6
1540	B	19	GLU	H	7.185	0.08	6
1541	A	19	GLU	HA	4.193	0.08	6
1542	B	19	GLU	HA	4.193	0.08	6
1543	A	19	GLU	HB2	2.140	0.08	6
1544	B	19	GLU	HB2	2.140	0.08	6
1545	A	19	GLU	HB3	1.906	0.08	6
1546	B	19	GLU	HB3	1.906	0.08	6
1547	A	19	GLU	HG2	2.534	0.08	6
1548	B	19	GLU	HG2	2.534	0.08	6
1549	A	19	GLU	HG3	2.534	0.08	6
1550	B	19	GLU	HG3	2.534	0.08	6
1551	A	19	GLU	C	178.980	0.42	6
1552	B	19	GLU	C	178.980	0.42	6
1555	A	19	GLU	CB	28.299	0.42	6
1556	B	19	GLU	CB	28.299	0.42	6
1559	A	19	GLU	N	116.841	0.22	6
1560	B	19	GLU	N	116.841	0.22	6
1561	A	20	VAL	H	8.159	0.08	6
1562	B	20	VAL	H	8.159	0.08	6
1563	A	20	VAL	HA	2.696	0.08	6
1564	B	20	VAL	HA	2.696	0.08	6
1565	A	20	VAL	HB	1.839	0.08	6
1566	B	20	VAL	HB	1.839	0.08	6
1567	A	20	VAL	HG11	0.564	0.08	6
1568	B	20	VAL	HG11	0.564	0.08	6
1569	A	20	VAL	HG12	0.564	0.08	6
1570	B	20	VAL	HG12	0.564	0.08	6
1571	A	20	VAL	HG13	0.564	0.08	6
1572	B	20	VAL	HG13	0.564	0.08	6
1573	A	20	VAL	HG21	0.210	0.08	6
1574	B	20	VAL	HG21	0.210	0.08	6
1575	A	20	VAL	HG22	0.210	0.08	6
1576	B	20	VAL	HG22	0.210	0.08	6
1577	A	20	VAL	HG23	0.210	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1578	B	20	VAL	HG23	0.210	0.08	6
1579	A	20	VAL	C	178.746	0.42	6
1580	B	20	VAL	C	178.746	0.42	6
1587	A	20	VAL	CG2	23.567	0.42	6
1588	B	20	VAL	CG2	23.567	0.42	6
1589	A	20	VAL	N	120.642	0.22	6
1590	B	20	VAL	N	120.642	0.22	6
1591	A	21	LEU	H	8.032	0.08	6
1592	B	21	LEU	H	8.032	0.08	6
1593	A	21	LEU	HA	3.861	0.08	6
1594	B	21	LEU	HA	3.861	0.08	6
1595	A	21	LEU	HB2	1.902	0.08	6
1596	B	21	LEU	HB2	1.902	0.08	6
1597	A	21	LEU	HB3	1.189	0.08	6
1598	B	21	LEU	HB3	1.189	0.08	6
1599	A	21	LEU	HD11	0.668	0.08	6
1600	B	21	LEU	HD11	0.668	0.08	6
1601	A	21	LEU	HD12	0.668	0.08	6
1602	B	21	LEU	HD12	0.668	0.08	6
1603	A	21	LEU	HD13	0.668	0.08	6
1604	B	21	LEU	HD13	0.668	0.08	6
1605	A	21	LEU	HD21	0.683	0.08	6
1606	B	21	LEU	HD21	0.683	0.08	6
1607	A	21	LEU	HD22	0.683	0.08	6
1608	B	21	LEU	HD22	0.683	0.08	6
1609	A	21	LEU	HD23	0.683	0.08	6
1610	B	21	LEU	HD23	0.683	0.08	6
1611	A	21	LEU	HG	1.159	0.08	6
1612	B	21	LEU	HG	1.159	0.08	6
1613	A	21	LEU	C	178.840	0.42	6
1614	B	21	LEU	C	178.840	0.42	6
1617	A	21	LEU	CB	41.244	0.42	6
1618	B	21	LEU	CB	41.244	0.42	6
1619	A	21	LEU	CD1	26.254	0.42	6
1620	B	21	LEU	CD1	26.254	0.42	6
1621	A	21	LEU	CD2	23.141	0.42	6
1622	B	21	LEU	CD2	23.141	0.42	6
1623	A	21	LEU	N	119.632	0.22	6
1624	B	21	LEU	N	119.632	0.22	6
1625	A	22	ARG	H	8.209	0.08	6
1626	B	22	ARG	H	8.209	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1627	A	22	ARG	HA	4.014	0.08	6
1628	B	22	ARG	HA	4.014	0.08	6
1629	A	22	ARG	HB2	1.819	0.08	6
1630	B	22	ARG	HB2	1.819	0.08	6
1631	A	22	ARG	HB3	1.819	0.08	6
1632	B	22	ARG	HB3	1.819	0.08	6
1633	A	22	ARG	HD2	3.083	0.08	6
1634	B	22	ARG	HD2	3.083	0.08	6
1635	A	22	ARG	HD3	3.083	0.08	6
1636	B	22	ARG	HD3	3.083	0.08	6
1637	A	22	ARG	HE	7.558	0.08	6
1638	B	22	ARG	HE	7.558	0.08	6
1639	A	22	ARG	HG2	1.494	0.08	6
1640	B	22	ARG	HG2	1.494	0.08	6
1641	A	22	ARG	HG3	1.504	0.08	6
1642	B	22	ARG	HG3	1.504	0.08	6
1643	A	22	ARG	C	178.285	0.42	6
1644	B	22	ARG	C	178.285	0.42	6
1645	A	22	ARG	CA	59.270	0.42	6
1646	B	22	ARG	CA	59.270	0.42	6
1647	A	22	ARG	CB	31.931	0.42	6
1648	B	22	ARG	CB	31.931	0.42	6
1649	A	22	ARG	CD	43.838	0.42	6
1650	B	22	ARG	CD	43.838	0.42	6
1651	A	22	ARG	CG	27.590	0.42	6
1652	B	22	ARG	CG	27.590	0.42	6
1653	A	22	ARG	N	116.446	0.22	6
1654	B	22	ARG	N	116.446	0.22	6
1655	A	22	ARG	NE	83.634	0.22	6
1656	B	22	ARG	NE	83.634	0.22	6
1657	A	23	GLN	H	8.496	0.08	6
1658	B	23	GLN	H	8.496	0.08	6
1659	A	23	GLN	HA	4.160	0.08	6
1660	B	23	GLN	HA	4.160	0.08	6
1661	A	23	GLN	HB2	1.960	0.08	6
1662	B	23	GLN	HB2	1.960	0.08	6
1663	A	23	GLN	HB3	1.479	0.08	6
1664	B	23	GLN	HB3	1.479	0.08	6
1665	A	23	GLN	HE21	8.152	0.08	6
1666	B	23	GLN	HE21	8.152	0.08	6
1667	A	23	GLN	HE22	6.876	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1668	B	23	GLN	HE22	6.876	0.08	6
1669	A	23	GLN	HG2	2.490	0.08	6
1670	B	23	GLN	HG2	2.490	0.08	6
1671	A	23	GLN	HG3	2.224	0.08	6
1672	B	23	GLN	HG3	2.224	0.08	6
1673	A	23	GLN	C	175.785	0.42	6
1674	B	23	GLN	C	175.785	0.42	6
1675	A	23	GLN	N	114.939	0.22	6
1676	B	23	GLN	N	114.939	0.22	6
1677	A	23	GLN	NE2	113.142	0.22	6
1678	B	23	GLN	NE2	113.142	0.22	6
1679	A	24	GLN	H	8.111	0.08	6
1680	B	24	GLN	H	8.111	0.08	6
1681	A	24	GLN	HA	3.767	0.08	6
1682	B	24	GLN	HA	3.767	0.08	6
1683	A	24	GLN	HB2	2.126	0.08	6
1684	B	24	GLN	HB2	2.126	0.08	6
1687	A	24	GLN	HE21	7.599	0.08	6
1688	B	24	GLN	HE21	7.599	0.08	6
1689	A	24	GLN	HE22	6.891	0.08	6
1690	B	24	GLN	HE22	6.891	0.08	6
1693	A	24	GLN	N	114.018	0.22	6
1694	B	24	GLN	N	114.018	0.22	6
1695	A	24	GLN	NE2	112.255	0.22	6
1696	B	24	GLN	NE2	112.255	0.22	6
1697	A	25	PRO	HA	4.548	0.08	6
1698	B	25	PRO	HA	4.548	0.08	6
1701	A	25	PRO	HB3	1.675	0.08	6
1702	B	25	PRO	HB3	1.675	0.08	6
1703	A	25	PRO	HD2	3.385	0.08	6
1704	B	25	PRO	HD2	3.385	0.08	6
1705	A	25	PRO	HD3	2.804	0.08	6
1706	B	25	PRO	HD3	2.804	0.08	6
1707	A	25	PRO	HG2	1.418	0.08	6
1708	B	25	PRO	HG2	1.418	0.08	6
1709	A	25	PRO	HG3	1.418	0.08	6
1710	B	25	PRO	HG3	1.418	0.08	6
1715	A	25	PRO	CD	50.720	0.42	6
1716	B	25	PRO	CD	50.720	0.42	6
1719	A	26	PRO	HA	4.339	0.08	6
1720	B	26	PRO	HA	4.339	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1721	A	26	PRO	HB2	2.277	0.08	6
1722	B	26	PRO	HB2	2.277	0.08	6
1743	A	27	ASP	H	7.472	0.08	6
1744	B	27	ASP	H	7.472	0.08	6
1745	A	27	ASP	HA	4.942	0.08	6
1746	B	27	ASP	HA	4.942	0.08	6
1747	A	27	ASP	HB2	2.894	0.08	6
1748	B	27	ASP	HB2	2.894	0.08	6
1749	A	27	ASP	HB3	2.501	0.08	6
1750	B	27	ASP	HB3	2.501	0.08	6
1753	A	27	ASP	CB	42.434	0.42	6
1754	B	27	ASP	CB	42.434	0.42	6
1755	A	27	ASP	N	115.990	0.22	6
1756	B	27	ASP	N	115.990	0.22	6
1757	A	28	LEU	H	9.020	0.08	6
1758	B	28	LEU	H	9.020	0.08	6
1765	A	28	LEU	HD11	0.816	0.08	6
1766	B	28	LEU	HD11	0.816	0.08	6
1767	A	28	LEU	HD12	0.816	0.08	6
1768	B	28	LEU	HD12	0.816	0.08	6
1769	A	28	LEU	HD13	0.816	0.08	6
1770	B	28	LEU	HD13	0.816	0.08	6
1771	A	28	LEU	HD21	0.745	0.08	6
1772	B	28	LEU	HD21	0.745	0.08	6
1773	A	28	LEU	HD22	0.745	0.08	6
1774	B	28	LEU	HD22	0.745	0.08	6
1775	A	28	LEU	HD23	0.745	0.08	6
1776	B	28	LEU	HD23	0.745	0.08	6
1783	A	28	LEU	CD1	25.856	0.42	6
1784	B	28	LEU	CD1	25.856	0.42	6
1785	A	28	LEU	CD2	23.725	0.42	6
1786	B	28	LEU	CD2	23.725	0.42	6
1789	A	28	LEU	N	125.823	0.22	6
1790	B	28	LEU	N	125.823	0.22	6
1791	A	29	VAL	H	8.153	0.08	6
1792	B	29	VAL	H	8.153	0.08	6
1793	A	29	VAL	HA	3.572	0.08	6
1794	B	29	VAL	HA	3.572	0.08	6
1797	A	29	VAL	HG11	1.140	0.08	6
1798	B	29	VAL	HG11	1.140	0.08	6
1799	A	29	VAL	HG12	1.140	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1800	B	29	VAL	HG12	1.140	0.08	6
1801	A	29	VAL	HG13	1.140	0.08	6
1802	B	29	VAL	HG13	1.140	0.08	6
1803	A	29	VAL	HG21	0.974	0.08	6
1804	B	29	VAL	HG21	0.974	0.08	6
1805	A	29	VAL	HG22	0.974	0.08	6
1806	B	29	VAL	HG22	0.974	0.08	6
1807	A	29	VAL	HG23	0.974	0.08	6
1808	B	29	VAL	HG23	0.974	0.08	6
1809	A	29	VAL	C	177.450	0.42	6
1810	B	29	VAL	C	177.450	0.42	6
1811	A	29	VAL	CA	66.863	0.42	6
1812	B	29	VAL	CA	66.863	0.42	6
1815	A	29	VAL	CG2	24.094	0.42	6
1816	B	29	VAL	CG2	24.094	0.42	6
1817	A	29	VAL	N	121.256	0.22	6
1818	B	29	VAL	N	121.256	0.22	6
1819	A	30	GLU	H	8.144	0.08	6
1820	B	30	GLU	H	8.144	0.08	6
1821	A	30	GLU	HA	3.954	0.08	6
1822	B	30	GLU	HA	3.954	0.08	6
1823	A	30	GLU	HB2	2.071	0.08	6
1824	B	30	GLU	HB2	2.071	0.08	6
1825	A	30	GLU	HB3	1.828	0.08	6
1826	B	30	GLU	HB3	1.828	0.08	6
1831	A	30	GLU	CA	58.703	0.42	6
1832	B	30	GLU	CA	58.703	0.42	6
1837	A	30	GLU	N	120.617	0.22	6
1838	B	30	GLU	N	120.617	0.22	6
1839	A	31	PHE	H	8.126	0.08	6
1840	B	31	PHE	H	8.126	0.08	6
1841	A	31	PHE	HA	4.211	0.08	6
1842	B	31	PHE	HA	4.211	0.08	6
1843	A	31	PHE	HB2	3.203	0.08	6
1844	B	31	PHE	HB2	3.203	0.08	6
1845	A	31	PHE	HB3	2.775	0.08	6
1846	B	31	PHE	HB3	2.775	0.08	6
1847	A	31	PHE	HD1	7.090	0.08	6
1848	B	31	PHE	HD1	7.090	0.08	6
1849	A	31	PHE	HD2	7.090	0.08	6
1850	B	31	PHE	HD2	7.090	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1851	A	31	PHE	HE1	6.975	0.08	6
1852	B	31	PHE	HE1	6.975	0.08	6
1853	A	31	PHE	HE2	6.975	0.08	6
1854	B	31	PHE	HE2	6.975	0.08	6
1855	A	31	PHE	HZ	7.057	0.08	6
1856	B	31	PHE	HZ	7.057	0.08	6
1865	A	31	PHE	CE1	130.673	0.42	6
1866	B	31	PHE	CE1	130.673	0.42	6
1867	A	31	PHE	CE2	130.673	0.42	6
1868	B	31	PHE	CE2	130.673	0.42	6
1869	A	31	PHE	CZ	129.678	0.42	6
1870	B	31	PHE	CZ	129.678	0.42	6
1871	A	32	ALA	H	7.885	0.08	6
1872	B	32	ALA	H	7.885	0.08	6
1873	A	32	ALA	HA	3.744	0.08	6
1874	B	32	ALA	HA	3.744	0.08	6
1875	A	32	ALA	HB1	0.590	0.08	6
1876	B	32	ALA	HB1	0.590	0.08	6
1877	A	32	ALA	HB2	0.590	0.08	6
1878	B	32	ALA	HB2	0.590	0.08	6
1879	A	32	ALA	HB3	0.590	0.08	6
1880	B	32	ALA	HB3	0.590	0.08	6
1881	A	32	ALA	C	178.861	0.42	6
1882	B	32	ALA	C	178.861	0.42	6
1883	A	32	ALA	CA	55.829	0.42	6
1884	B	32	ALA	CA	55.829	0.42	6
1885	A	32	ALA	CB	16.187	0.42	6
1886	B	32	ALA	CB	16.187	0.42	6
1887	A	32	ALA	N	120.501	0.22	6
1888	B	32	ALA	N	120.501	0.22	6
1889	A	33	VAL	H	8.106	0.08	6
1890	B	33	VAL	H	8.106	0.08	6
1891	A	33	VAL	HA	3.343	0.08	6
1892	B	33	VAL	HA	3.343	0.08	6
1893	A	33	VAL	HB	2.202	0.08	6
1894	B	33	VAL	HB	2.202	0.08	6
1895	A	33	VAL	HG11	0.962	0.08	6
1896	B	33	VAL	HG11	0.962	0.08	6
1897	A	33	VAL	HG12	0.962	0.08	6
1898	B	33	VAL	HG12	0.962	0.08	6
1899	A	33	VAL	HG13	0.962	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1900	B	33	VAL	HG13	0.962	0.08	6
1901	A	33	VAL	HG21	0.864	0.08	6
1902	B	33	VAL	HG21	0.864	0.08	6
1903	A	33	VAL	HG22	0.864	0.08	6
1904	B	33	VAL	HG22	0.864	0.08	6
1905	A	33	VAL	HG23	0.864	0.08	6
1906	B	33	VAL	HG23	0.864	0.08	6
1907	A	33	VAL	C	179.434	0.42	6
1908	B	33	VAL	C	179.434	0.42	6
1909	A	33	VAL	CA	68.846	0.42	6
1910	B	33	VAL	CA	68.846	0.42	6
1915	A	33	VAL	CG2	21.630	0.42	6
1916	B	33	VAL	CG2	21.630	0.42	6
1917	A	33	VAL	N	117.689	0.22	6
1918	B	33	VAL	N	117.689	0.22	6
1919	A	34	GLU	H	7.933	0.08	6
1920	B	34	GLU	H	7.933	0.08	6
1921	A	34	GLU	HA	3.834	0.08	6
1922	B	34	GLU	HA	3.834	0.08	6
1923	A	34	GLU	HB2	1.926	0.08	6
1924	B	34	GLU	HB2	1.926	0.08	6
1925	A	34	GLU	HB3	1.926	0.08	6
1926	B	34	GLU	HB3	1.926	0.08	6
1927	A	34	GLU	HG2	2.493	0.08	6
1928	B	34	GLU	HG2	2.493	0.08	6
1931	A	34	GLU	C	177.872	0.42	6
1932	B	34	GLU	C	177.872	0.42	6
1933	A	34	GLU	CA	59.798	0.42	6
1934	B	34	GLU	CA	59.798	0.42	6
1937	A	34	GLU	N	120.695	0.22	6
1938	B	34	GLU	N	120.695	0.22	6
1939	A	35	TYR	H	8.955	0.08	6
1940	B	35	TYR	H	8.955	0.08	6
1941	A	35	TYR	HA	3.553	0.08	6
1942	B	35	TYR	HA	3.553	0.08	6
1943	A	35	TYR	HB2	2.230	0.08	6
1944	B	35	TYR	HB2	2.230	0.08	6
1945	A	35	TYR	HB3	2.159	0.08	6
1946	B	35	TYR	HB3	2.159	0.08	6
1947	A	35	TYR	HD1	5.814	0.08	6
1948	B	35	TYR	HD1	5.814	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1949	A	35	TYR	HD2	5.814	0.08	6
1950	B	35	TYR	HD2	5.814	0.08	6
1951	A	35	TYR	HE1	6.421	0.08	6
1952	B	35	TYR	HE1	6.421	0.08	6
1953	A	35	TYR	HE2	6.421	0.08	6
1954	B	35	TYR	HE2	6.421	0.08	6
1955	A	35	TYR	C	177.743	0.42	6
1956	B	35	TYR	C	177.743	0.42	6
1957	A	35	TYR	CA	61.853	0.42	6
1958	B	35	TYR	CA	61.853	0.42	6
1961	A	35	TYR	N	120.973	0.22	6
1962	B	35	TYR	N	120.973	0.22	6
1963	A	36	PHE	H	8.617	0.08	6
1964	B	36	PHE	H	8.617	0.08	6
1965	A	36	PHE	HA	4.074	0.08	6
1966	B	36	PHE	HA	4.074	0.08	6
1967	A	36	PHE	HB2	3.144	0.08	6
1968	B	36	PHE	HB2	3.144	0.08	6
1969	A	36	PHE	HB3	2.722	0.08	6
1970	B	36	PHE	HB3	2.722	0.08	6
1971	A	36	PHE	HD1	7.292	0.08	6
1972	B	36	PHE	HD1	7.292	0.08	6
1973	A	36	PHE	HD2	7.292	0.08	6
1974	B	36	PHE	HD2	7.292	0.08	6
1975	A	36	PHE	HE1	6.612	0.08	6
1976	B	36	PHE	HE1	6.612	0.08	6
1977	A	36	PHE	HE2	6.612	0.08	6
1978	B	36	PHE	HE2	6.612	0.08	6
1979	A	36	PHE	HZ	6.690	0.08	6
1980	B	36	PHE	HZ	6.690	0.08	6
1981	A	36	PHE	CA	62.765	0.42	6
1982	B	36	PHE	CA	62.765	0.42	6
1983	A	36	PHE	CB	37.930	0.42	6
1984	B	36	PHE	CB	37.930	0.42	6
1985	A	36	PHE	CD1	131.999	0.42	6
1986	B	36	PHE	CD1	131.999	0.42	6
1987	A	36	PHE	CD2	131.999	0.42	6
1988	B	36	PHE	CD2	131.999	0.42	6
1989	A	36	PHE	CE1	128.562	0.42	6
1990	B	36	PHE	CE1	128.562	0.42	6
1991	A	36	PHE	CE2	128.562	0.42	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1992	B	36	PHE	CE2	128.562	0.42	6
1993	A	36	PHE	CZ	130.851	0.42	6
1994	B	36	PHE	CZ	130.851	0.42	6
1995	A	36	PHE	N	115.284	0.22	6
1996	B	36	PHE	N	115.284	0.22	6
1997	A	37	THR	H	7.982	0.08	6
1998	B	37	THR	H	7.982	0.08	6
1999	A	37	THR	HA	4.207	0.08	6
2000	B	37	THR	HA	4.207	0.08	6
2001	A	37	THR	HB	3.715	0.08	6
2002	B	37	THR	HB	3.715	0.08	6
2003	A	37	THR	HG21	1.149	0.08	6
2004	B	37	THR	HG21	1.149	0.08	6
2005	A	37	THR	HG22	1.149	0.08	6
2006	B	37	THR	HG22	1.149	0.08	6
2007	A	37	THR	HG23	1.149	0.08	6
2008	B	37	THR	HG23	1.149	0.08	6
2009	A	37	THR	C	176.218	0.42	6
2010	B	37	THR	C	176.218	0.42	6
2015	A	37	THR	N	116.925	0.22	6
2016	B	37	THR	N	116.925	0.22	6
2017	A	38	ARG	H	7.706	0.08	6
2018	B	38	ARG	H	7.706	0.08	6
2019	A	38	ARG	HA	3.902	0.08	6
2020	B	38	ARG	HA	3.902	0.08	6
2021	A	38	ARG	HD2	3.572	0.08	6
2022	B	38	ARG	HD2	3.572	0.08	6
2023	A	38	ARG	HD3	3.051	0.08	6
2024	B	38	ARG	HD3	3.051	0.08	6
2025	A	38	ARG	C	179.228	0.42	6
2026	B	38	ARG	C	179.228	0.42	6
2027	A	38	ARG	CA	59.293	0.42	6
2028	B	38	ARG	CA	59.293	0.42	6
2029	A	38	ARG	N	121.818	0.22	6
2030	B	38	ARG	N	121.818	0.22	6
2031	A	39	LEU	H	7.402	0.08	6
2032	B	39	LEU	H	7.402	0.08	6
2033	A	39	LEU	HA	3.885	0.08	6
2034	B	39	LEU	HA	3.885	0.08	6
2035	A	39	LEU	HB2	1.540	0.08	6
2036	B	39	LEU	HB2	1.540	0.08	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2037	A	39	LEU	HB3	1.507	0.08	6
2038	B	39	LEU	HB3	1.507	0.08	6
2039	A	39	LEU	HD11	0.975	0.08	6
2040	B	39	LEU	HD11	0.975	0.08	6
2041	A	39	LEU	HD12	0.975	0.08	6
2042	B	39	LEU	HD12	0.975	0.08	6
2043	A	39	LEU	HD13	0.975	0.08	6
2044	B	39	LEU	HD13	0.975	0.08	6
2045	A	39	LEU	HD21	0.717	0.08	6
2046	B	39	LEU	HD21	0.717	0.08	6
2047	A	39	LEU	HD22	0.717	0.08	6
2048	B	39	LEU	HD22	0.717	0.08	6
2049	A	39	LEU	HD23	0.717	0.08	6
2050	B	39	LEU	HD23	0.717	0.08	6
2051	A	39	LEU	HG	1.349	0.08	6
2052	B	39	LEU	HG	1.349	0.08	6
2053	A	39	LEU	CA	57.645	0.42	6
2054	B	39	LEU	CA	57.645	0.42	6
2055	A	39	LEU	N	119.207	0.22	6
2056	B	39	LEU	N	119.207	0.22	6
2057	A	40	ARG	H	7.876	0.08	6
2058	B	40	ARG	H	7.876	0.08	6
2059	A	40	ARG	HA	3.865	0.08	6
2060	B	40	ARG	HA	3.865	0.08	6
2061	A	40	ARG	HE	7.203	0.08	6
2062	B	40	ARG	HE	7.203	0.08	6
2063	A	40	ARG	N	119.680	0.22	6
2064	B	40	ARG	N	119.680	0.22	6
2065	A	40	ARG	NE	84.462	0.22	6
2066	B	40	ARG	NE	84.462	0.22	6
2067	A	41	GLU	H	7.952	0.08	6
2068	B	41	GLU	H	7.952	0.08	6
2069	A	41	GLU	N	117.647	0.22	6
2070	B	41	GLU	N	117.647	0.22	6
2071	A	43	ARG	HE	7.706	0.08	6
2072	B	43	ARG	HE	7.706	0.08	6
2073	A	43	ARG	HG2	1.735	0.08	6
2074	B	43	ARG	HG2	1.735	0.08	6
2075	A	43	ARG	HG3	1.735	0.08	6
2076	B	43	ARG	HG3	1.735	0.08	6
2077	A	43	ARG	NE	83.668	0.22	6

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2078	B	43	ARG	NE	83.668	0.22	6
2079	A	44	ALA	HB1	1.311	0.08	6
2080	B	44	ALA	HB1	1.311	0.08	6
2081	A	44	ALA	HB2	1.311	0.08	6
2082	B	44	ALA	HB2	1.311	0.08	6
2083	A	44	ALA	HB3	1.311	0.08	6
2084	B	44	ALA	HB3	1.311	0.08	6

### 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
$^{13}\text{C}_\alpha$	129	$-0.50 \pm 0.11$	Should be applied
$^{13}\text{C}_\beta$	115	$0.24 \pm 0.05$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	125	$-0.28 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	125	$0.19 \pm 0.32$	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 91%, i.e. 1128 atoms were assigned a chemical shift out of a possible 1235. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	452/456 (99%)	181/181 (100%)	184/188 (98%)	87/87 (100%)
Sidechain	596/699 (85%)	372/408 (91%)	207/257 (81%)	17/34 (50%)
Aromatic	80/80 (100%)	42/42 (100%)	37/37 (100%)	1/1 (100%)
Overall	1128/1235 (91%)	595/631 (94%)	428/482 (89%)	105/122 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1515 atoms were assigned a chemical shift out of a possible 1699. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	642/672 (96%)	263/267 (99%)	254/276 (92%)	125/129 (97%)
Sidechain	779/923 (84%)	493/542 (91%)	266/339 (78%)	20/42 (48%)
Aromatic	94/104 (90%)	50/54 (93%)	43/45 (96%)	1/5 (20%)
Overall	1515/1699 (89%)	806/863 (93%)	563/660 (85%)	146/176 (83%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

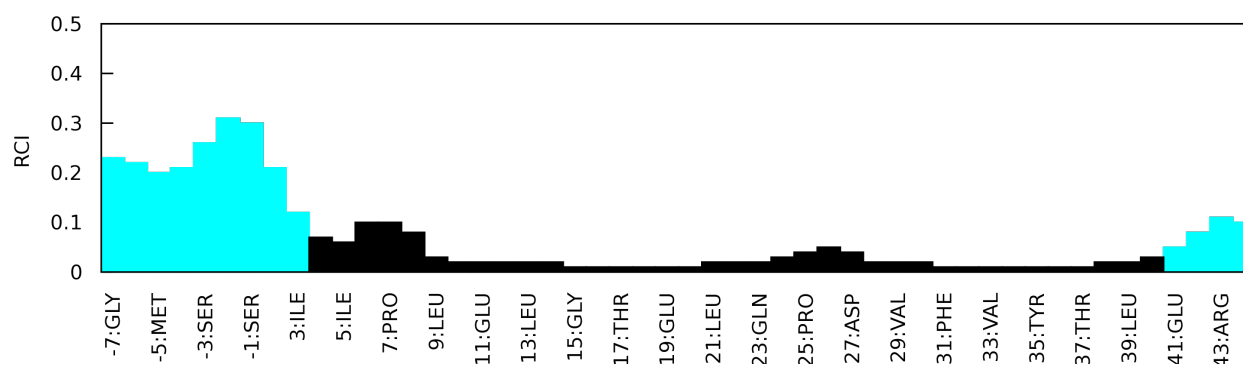
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
2	C	606	ARG	NE	103.71	92.63 – 76.73	12.0

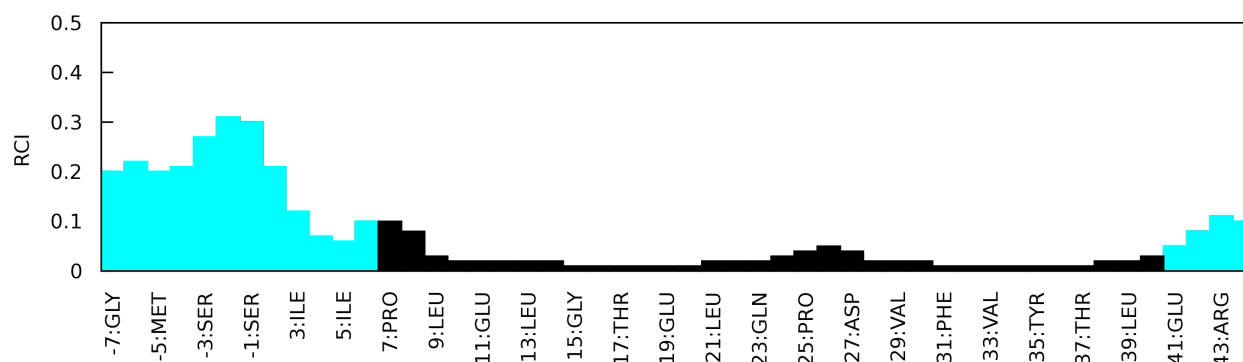
### 7.1.5 Random Coil Index (RCI) plots [i](#)

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

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:

