

# Full wwPDB NMR Structure Validation Report (i)

Sep 16, 2024 – 10:20 am BST

PDB ID	:	8S8O
BMRB ID	:	34908
Title	:	Solution Structure of cAMP-dependent Protein Kinase RII-alpha Subunit
		Dimerization and Docking Domain Complex with Microtubule Associated Pro-
		tein $2c$ (84-111)
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Deposited on	:	2024-03-06

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $SOLUTION\ NMR$ 

The overall completeness of chemical shifts assignment is 66%.

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.



Matria	Whole archive	NMR archive
Metric	$(\# { m Entries})$	$(\# { m Entries})$
Clashscore	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain		
1	А	52	63%	17%	19%
1	В	52	60%	12%	29%
2	С	28	57%	29%	14%



# 2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 20 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	Vell-defined core Residue range (total) Backbone RMSD (Å) Medoid mod					
1	A:7-A:48, B:10-B:46, C:86-	0.88	20			
	C:109 (103)					

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

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



# 3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2050 atoms, of which 1028 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called cAMP-dependent protein kinase type II-alpha regulatory subunit.

Mol	Chain	Residues		A	Atom	s			Trace
1	Δ	52	Total	С	Η	Ν	Ο	S	0
	I A	52	814	259	408	70	75	2	0
1	р	52	Total	С	Η	Ν	0	S	0
I D	52	812	259	406	70	75	2	0	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLY	-	expression tag	UNP P13861
А	2	ALA	-	expression tag	UNP P13861
А	3	MET	-	expression tag	UNP P13861
А	4	GLY	-	expression tag	UNP P13861
В	1	GLY	-	expression tag	UNP P13861
В	2	ALA	-	expression tag	UNP P13861
В	3	MET	-	expression tag	UNP P13861
В	4	GLY	-	expression tag	UNP P13861

• Molecule 2 is a protein called Isoform 3 of Microtubule-associated protein 2.

Mol	Chain	Residues		At	oms			Trace
0	C	20	Total	С	Η	Ν	0	0
	C	28	424	128	214	37	45	0



# 4 Residue-property plots (i)

# 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: cAMP-dependent protein kinase type II-alpha regulatory subunit



# 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 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	68%	18%	14%
R84 E85 E85 E88 E88 E88 A104 A104 A104 A106 L106 K107 E111 E111			

#### 4.2.2 Score per residue for model 2

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

Chain A:	60%	21%	19%
61 A2 A3 G4 M5 S6 S6 S6 L1 L1 L1 L1 C1 B C1 D	q20           721           T22           V23           V23           V23           V23           V23           V25           V40           F41           F44           A49           A51           S52		

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

Chain B:	50%	19% •	29%
61 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3	114 115 115 118 118 118 118 123 123 123 123 123 123 123 123 124 124 124 124 124 124 124 124 124 124	A47 A49 A49 A50 S52 S52	

• Molecule 2: Isoform 3 of Microtubule-associated protein 2



#### 4.2.3 Score per residue for model 3

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





Chain B:	44%	25%	•	29%
61 42 42 42 43 43 43 43 43 43 43 43 43 43 43 44 44	L14 T15 E16 G20 Y21 Y22 Y22 Y22 Y22 Y23 Y23 Y23 Y23	V34 V38 V38 F41 F41 F45 F46 F47 R48 A47 A47 A47 A47 A47 A47 A47 A47 A47 A47	A51 S52	
• Molecule 2: Iso	oform 3 of Microtul	oule-associated p	protein 2	
Chain C:	54%		32%	14%
R84 E85 E88 V90 V90 I94 E101 E101 A100 V103				
4.2.4 Score p	er residue for mo	odel 4		
• Molecule 1: cA	MP-dependent pro	tein kinase type	II-alpha r	egulatory subuni
Chain A:	62%		17% •	19%
G1 M3 G4 M5 G4 M5 M5 M5 M5 M5 M5 G4 M5 M5 M5 M5 M5 M5 M5 M5 M5 M5 M5 M5 M5	721 722 723 728 728 728 728 728 728 728 740 740 740 740 750	A51 S52		
• Molecule 1: cA	MP-dependent pro	otein kinase type	II-alpha r	egulatory subuni
Chain B:	54%	17%	5	29%
G1 A2 M3 M5 M5 M5 M5 M5 M3 12 11 P11	T15 019 020 020 020 020 020 F36 F36 F36 F36 F36 F36 F36 F36 F36 F36	A49 P50 S52 S52		
• Molecule 2: Iso	oform 3 of Microtul	oule-associated p	protein 2	
Chain C:	61%		25%	14%
R84 E85 V90 194 V98 F101 E101 A102 V103	A104 V1065 1106 A110 B111			
4.2.5 Score p	er residue for mo	odel 5		
• Molecule 1: cA	MP-dependent pro	otein kinase type	II-alpha r	egulatory subuni
Chain A:	69%		12%	19%
61 M3 M5 M5 M5 M5 M5 M5 M2 12 12 122	V25 P30 P30 P30 P30 P30 P30 P50 P50 P51 S52			
• Molecule 1: cA	MP-dependent pro	otein kinase type	II-alpha r	egulatory subuni
Chain B:	56%	13%	, D •	29%



# • Molecule 2: Isoform 3 of Microtubule-associated protein 2



#### 4.2.6 Score per residue for model 6

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



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



• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain	C:	43%	43%	14%
R84 E85 T86 A87	V90 S91 A92 R93 I94 V95	490 E101 A102 V103 V105 L106 L106 C110 E111		

## 4.2.7 Score per residue for model 7

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





• Molecule 2: Isoform 3 of Microtubule-associated protein 2



#### 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

Chain B:	50%	21%	29%
G1 A2 M3 M5 M5 M5 M5 M5 M5 10 10 10 10 10 10 10 10 10 10 10 10 10	P11 P11 114 715 721 722 729 729 729 733 733 733 733 733 733 733 733 733 73	A47 R48 A49 A51 S52 S52	

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	43%	43%	14%
R84 E85 T86 V90 S91 S91 S91 S91 V95 V95 V95	E101 A102 V103 V105 L106 K107 K107 E111		

#### 4.2.9 Score per residue for model 9

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



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



• Molecule 2: Isoform 3 of Microtubule-associated protein 2



Chain C:	46%	39%	14%
R84 E885 136 194 194	199 E101 A102 A103 A103 A104 A106 L106 A110 B111 B111		

#### 4.2.10 Score per residue for model 10

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

Chain A:				60%			21%	19%
G1 M5 M5 S6 S6 S6 S6 S6 S6 S6 S6 S6 S6 S7 S6 S7 S7 S7 S7 S7 S7 S7 S7 S7 S7 S7 S7 S7	Y21 T22	V25 P30	F30 E39 Y40	T42 R43 L44 R45	E46	A49 P50 A51 S52		

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

Chain B:	62%	10%	29%
61 M3 G4 G4 G4 G4 G1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1 C1	114 122 122 122 144 144 144 144 144 144		

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	50%	29%	7%	14%
R84 E85 E85 E85 E85 E85 R93 194 A12 A12 A105 A105 A105 K107 K107	<mark>9110</mark> 81111			

4.2.11 Score per residue for model 11

Chain A:	60%	19%	• 19	9%
G1 A2 M3 M5 S6 L14	L18 019 720 721 722 725 726 726 726 726 726 726 749 749 750 852			
• Molecule	1: cAMP-dependent protein kinase ty	pe II-alpha	regulate	ory subunit
Chain B:	52% 1	9%	29%	
G1 A2 M3 M5 K5 K5 K5 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1 K1	10 11 114 114 115 115 115 115 115			
• Molecule	2: Isoform 3 of Microtubule-associated	d protein 2		
Chain C:	54%	29%	·	14%





#### 4.2.12 Score per residue for model 12

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

Chain A:	58%	21%	•	19%
G1 A2 M3 M5 M5 S6	115 118 118 118 118 120 120 120 120 122 122 124 124 124 124 124 124			

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

Chain B:	56%	12% •	29%
G1 A2 M3 M5 M5 M5 M5 M5 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3	122 123 123 123 144 144 144 144 144 144 144 144 144 14		

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	68%	18%	14%
R84 E85 194 V98 V98 V98 V103 L106			

#### 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

Chain B:	42%	25%	•
G1 A2 M3 G4 M5 M5 H7 13 13 13 10	P11 P12 C14 C14 C20 P21 P25 C24 V25 C24 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20	L33 V34 V34 F35 F35 A37 A37 A37 A37 A37 A47 A47 A47 A47 A47 A43 A43 A43 A43 A43 A43 A43 A43 A43 A43	

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	61%	25%	14%
884 855 855 859 859 194 104 8101 8102 8102 8102			



29%

#### 4.2.14 Score per residue for model 14

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

Chain A:	58%	23%	19%
G1 A2 M3 M5 G4 G4 M5 S6 H7 I8 E16 L17	L18 20 720 722 722 722 723 726 726 726 726 726 726 726 726 726 726		
• Molecule 1:	cAMP-dependent protein kinase	type II-alpha re	egulatory subu

Chain B: 58% 13% 29%

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

R45 A45 A51 A51

Chain C:	57%	29%	14%
R84 E85 194 V97 V98	810 1106 1106 1110 1110		

#### 4.2.15 Score per residue for model 15

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

Chain A:	54%	25%	·	19%
G1 A2 A3 G4 M5 S6 L18	Y21 722 824 V23 V25 126 126 126 F30 F30 F41 F44 F44 F44 F44 F44 F44 F44 F44 F44			

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

Chain B: 56% 13% · 29%

# 

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C: 68% 18% 14%



#### 4.2.16 Score per residue for model 16

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



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

Chain B:	58%	12% ·	29%
61 M3 M3 M5 M5 M5 M5 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3	L14 T15 722 V25 V34 V34 V34 V34 V35 V35 V35 V35 V34 V35 V34 V35 V34 V35 V34 V34 V34 V34 V34 V34 V34 V34 V34 V34		

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	61%	25%	14%
R84 E85 194 194 194 E101 E101	V106 K106 K107 110 1111 E1111		

#### 4.2.17 Score per residue for model 17

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

Chain A:	58%	23%	19%
G1 A2 M3 M5 M5 M5 N4 N5 N1 N1 N1 N1 N1 N1 N1 N1 N1 N1 N1 N1 N1	610 721 722 721 722 726 726 736 736 736 736 736 740 740 740 740 740 740 740 740 740 751 852		

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

Chain B: 50% 19% 29%

• Molecule 2: Isoform 3 of Microtubule-associated protein 2





#### 4.2.18 Score per residue for model 18

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

Chain A:		56%	25%	19%
G1 A2 M3 M5 M5 M5 M5 M5 M5 M5 M5 M5 M5 M5 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3	L17 L18 Q19 Q20 V23 V25 L26 L26 L26 L26	P30 740 144 144 144 144 144 144 144 144 144 1		

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

Chain B:	44%	27%	29%
61 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3 M3	L14 T15 Q19 Q19 V23 V25 V25 Q29 Q28 Q29 P30	L33 L42 R43 R43 R48 R48 R48 R48 A49 A51 S52	
- Malassala 9. Is	абалла Э. аб М: алады		:

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	71%	14%	14%
R84 E86 E86 E86 E101 V105 C108 E109 Q110 Q110 E111			

#### 4.2.19 Score per residue for model 19

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

Chain A:	60%	19%	•	19%
61 M3 64 M5 64 M5 86 86 11 115 620 620	721 722 725 726 726 740 740 740 740 840 850 852			

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

Chain B: 52% 19% 29%

# 

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C: 64% 21% 14%



#### 4.2.20 Score per residue for model 20 (medoid)

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

Chain A:	67%	12%	•	19%
G1 A2 M3 G4 M5 S6 L18	019 721 727 728 728 729 720 740 749 750 851 852			

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

Chain B:				58%	6	12%	•	29%
61 42 42 42 11 10 11 10 11	Q19	T22 V25	<b>Q</b> 29	D32	A47 A49 A51 S52 S52			

• Molecule 2: Isoform 3 of Microtubule-associated protein 2

Chain C:	57%	29%	14%
R84 E85 E85 891 891 896 799 E101 A100 A100 V103	V105 L106 0110 E111		



# 5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure calculation	1.21
SCULPTOR	structure calculation	3.1
CNS	refinement	1.21
SCULPTOR	refinement	3.1

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	1760
Number of shifts mapped to atoms	1217
Number of unparsed shifts	0
Number of shifts with mapping errors	543
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%



# 6 Model quality (i)

# 6.1 Standard geometry (i)

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

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

Mol	Chain	Chirality	Planarity
1	В	$0.0{\pm}0.0$	$0.1 \pm 0.4$
1	А	$0.0{\pm}0.0$	$0.1 \pm 0.4$
All	All	0	6

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	А	45	ARG	Sidechain	2
1	В	45	ARG	Sidechain	2
1	А	43	ARG	Sidechain	1
1	В	43	ARG	Sidechain	1

# 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	А	348	350	350	9±2
1	В	305	306	306	$5\pm3$
2	С	172	181	181	4±2
All	All	16500	16740	16740	329

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.



A 4 1			$\mathbf{D}^{\prime}$	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
2:C:103:VAL:O	2:C:106:LEU:HG	0.65	1.91	13	14	
2:C:97:VAL:O	2:C:101:GLU:HG3	0.63	1.94	14	2	
1:A:14:LEU:HG	1:B:33:LEU:HD22	0.62	1.72	3	2	
1:A:36:PHE:O	1:A:40:TYR:HB2	0.61	1.95	12	2	
1:A:22:THR:HB	1:A:40:TYR:CE1	0.60	2.31	10	8	
1:A:18:LEU:HD21	1:A:44:LEU:HB2	0.60	1.74	1	11	
1:B:22:THR:O	1:B:25:VAL:HG22	0.59	1.97	18	17	
1:B:38:VAL:HA	1:B:41:PHE:CE2	0.59	2.33	13	3	
1:A:22:THR:O	1:A:26:LEU:HG	0.59	1.98	11	4	
1:A:18:LEU:HB3	1:A:40:TYR:CZ	0.58	2.32	13	11	
1:A:38:VAL:HA	1:B:41:PHE:CG	0.58	2.34	3	2	
2:C:94:ILE:O	2:C:98:VAL:HG23	0.58	1.99	12	4	
1:B:42:THR:O	1:B:46:GLU:HG2	0.57	1.98	18	2	
1:A:38:VAL:O	1:A:42:THR:HG23	0.55	2.00	8	2	
1:B:18:LEU:HA	1:B:21:TYR:CE2	0.55	2.37	2	2	
1:B:38:VAL:HA	1:B:41:PHE:CZ	0.54	2.37	13	3	
1:A:25:VAL:O	1:A:30:PRO:HD3	0.54	2.02	1	17	
1:A:21:TYR:CD2	1:A:43:ARG:HG3	0.54	2.38	13	1	
1:A:16:GLU:HA	1:A:19:GLN:NE2	0.54	2.17	8	1	
1:A:21:TYR:CD2	1:A:40:TYR:HA	0.54	2.38	17	2	
1:A:18:LEU:HB3	1:A:40:TYR:CE2	0.53	2.38	20	3	
1:B:28:GLN:HE21	1:B:28:GLN:HA	0.53	1.63	15	1	
1:A:39:GLU:O	1:A:43:ARG:HG2	0.53	2.04	8	6	
2:C:104:ALA:O	2:C:107:LYS:HG2	0.53	2.04	5	11	
1:A:19:GLN:O	1:A:22:THR:HG22	0.53	2.03	12	5	
2:C:86:THR:O	2:C:90:VAL:HG12	0.53	2.04	8	2	
1:B:39:GLU:O	1:B:43:ARG:HG2	0.53	2.04	12	1	
1:A:23:VAL:HG21	2:C:88:GLU:HA	0.52	1.81	1	3	
1:A:21:TYR:CD1	1:A:40:TYR:HA	0.52	2.40	13	2	
2:C:90:VAL:O	2:C:94:ILE:HG12	0.52	2.04	15	14	
1:A:18:LEU:CD2	1:A:44:LEU:HB2	0.52	2.35	15	11	
1:B:18:LEU:HA	1:B:21:TYR:CZ	0.52	2.40	2	1	
1:A:42:THR:O	1:A:46:GLU:HG2	0.52	2.05	8	2	
1:B:15:THR:O	1:B:19:GLN:HG3	0.51	2.06	4	4	
2:C:101:GLU:O	2:C:105:VAL:HG23	0.51	2.04	8	18	
1:A:44:LEU:O	1:A:48:ARG:HG2	0.51	2.05	13	2	
1:A:15:THR:O	1:A:19:GLN:HB2	0.51	2.06	19	1	
2:C:92:ALA:O	2:C:96:GLN:HB3	0.51	2.06	17	3	
1:A:21:TYR:O	1:A:25:VAL:HG23	0.50	2.07	11	12	
1:B:10:ILE:HD11	2:C:87:ALA:HA	0.50	1.83	6	2	
2:C:86:THR:O	2:C:90:VAL:HG23	0.50	2.06	6	2	

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



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	the officer of the second seco			Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:24:GLU:O	1:A:28:GLN:HG2	0.50	2.06	16	2
2:C:91:SER:O	2:C:95:VAL:HG23	0.50	2.07	8	1
1:A:38:VAL:HA	1:B:41:PHE:CD1	0.50	2.41	17	2
1:A:19:GLN:HA	1:A:22:THR:HG22	0.50	1.84	20	5
1:A:41:PHE:HB3	1:B:34:VAL:HG13	0.50	1.83	8	5
1:B:40:TYR:O	1:B:43:ARG:HG2	0.49	2.08	7	1
1:B:38:VAL:O	1:B:42:THR:HG22	0.49	2.07	11	1
1:A:18:LEU:HB3	1:A:40:TYR:CE1	0.49	2.42	12	5
1:A:19:GLN:O	1:A:23:VAL:HG23	0.49	2.08	3	6
1:A:44:LEU:HD12	1:B:34:VAL:HG21	0.49	1.84	16	3
1:A:16:GLU:O	1:A:19:GLN:HG2	0.48	2.08	18	1
1:B:12:PRO:HD2	1:B:15:THR:OG1	0.48	2.08	8	2
1:A:22:THR:HB	1:A:40:TYR:CE2	0.48	2.43	11	1
2:C:94:ILE:O	2:C:98:VAL:HG22	0.48	2.08	4	1
1:B:18:LEU:HA	1:B:21:TYR:CD2	0.48	2.43	19	1
1:B:34:VAL:O	1:B:38:VAL:HG23	0.48	2.09	3	3
1:A:41:PHE:HB2	1:B:41:PHE:CE2	0.47	2.44	17	3
1:A:11:PRO:N	1:A:12:PRO:HD3	0.47	2.23	6	2
1:A:45:ARG:O	1:A:48:ARG:HG2	0.47	2.09	1	1
1:A:34:VAL:HG12	1:B:44:LEU:HG	0.47	1.87	6	1
1:B:14:LEU:HD12	1:B:15:THR:N	0.47	2.25	6	6
1:B:29:GLN:HG3	1:B:36:PHE:HB2	0.47	1.86	13	1
1:A:22:THR:HB	1:A:40:TYR:CD1	0.46	2.44	18	2
1:A:15:THR:O	1:A:19:GLN:HB3	0.46	2.11	12	1
1:A:23:VAL:O	1:A:27:ARG:HG2	0.46	2.10	14	3
1:A:25:VAL:HG11	1:A:36:PHE:CD1	0.45	2.46	13	4
1:A:29:GLN:HA	1:A:29:GLN:OE1	0.45	2.11	13	1
1:B:30:PRO:HD2	1:B:33:LEU:HD23	0.45	1.89	18	4
1:A:16:GLU:O	1:A:19:GLN:HB3	0.45	2.12	14	1
1:A:18:LEU:HG	1:A:44:LEU:HD12	0.45	1.89	6	3
1:A:15:THR:O	1:A:19:GLN:HG2	0.44	2.12	7	1
1:B:29:GLN:O	1:B:33:LEU:HD23	0.44	2.12	11	2
1:B:10:ILE:O	1:B:12:PRO:HD3	0.44	2.13	5	2
1:B:24:GLU:O	1:B:28:GLN:HG2	0.44	2.12	9	1
1:A:27:ARG:NE	1:A:27:ARG:HA	0.44	2.28	1	1
1:A:8:ILE:HA	1:B:29:GLN:OE1	0.44	2.13	17	1
2:C:107:LYS:HE3	2:C:109:GLU:CG	0.43	2.43	19	1
1:B:20:GLY:O	1:B:24:GLU:HG2	0.43	2.14	13	3
1:A:14:LEU:CD2	1:B:34:VAL:HG23	0.43	2.44	8	1
1:A:23:VAL:HG23	2:C:87:ALA:HB3	0.43	1.91	15	1
1:A:25:VAL:O	1:A:28:GLN:HB3	0.43	2.13	14	1



Atom 1	Atom 2	$Cleah(\lambda)$	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:15:THR:O	1:A:19:GLN:HG3	0.42	2.15	4	1	
1:B:18:LEU:HD23	2:C:94:ILE:HG22	0.42	1.91	14	1	
1:B:19:GLN:O	1:B:23:VAL:HG23	0.42	2.14	18	1	
1:A:23:VAL:O	1:A:26:LEU:HD23	0.42	2.14	9	1	
2:C:104:ALA:HB1	2:C:109:GLU:HB3	0.42	1.90	14	1	
1:A:37:ALA:HA	1:A:40:TYR:CE1	0.42	2.49	7	1	
1:A:14:LEU:HA	1:A:44:LEU:HD11	0.42	1.89	7	1	
1:A:36:PHE:CZ	1:B:14:LEU:HG	0.42	2.49	9	1	
2:C:90:VAL:O	2:C:93:ARG:HG3	0.41	2.14	10	1	
2:C:94:ILE:O	2:C:98:VAL:HG13	0.41	2.16	16	1	
1:B:21:TYR:O	1:B:25:VAL:HG13	0.41	2.15	3	2	
1:A:8:ILE:HB	2:C:106:LEU:HD22	0.41	1.91	14	1	
1:B:20:GLY:O	1:B:24:GLU:HG3	0.41	2.16	19	1	
1:B:28:GLN:HG3	1:B:36:PHE:CZ	0.41	2.51	4	1	
1:B:29:GLN:N	1:B:30:PRO:HD3	0.41	2.31	9	1	
1:A:14:LEU:HG	1:B:33:LEU:HD12	0.41	1.93	12	2	
1:A:17:LEU:HB2	1:A:44:LEU:HD23	0.40	1.92	16	1	
1:A:27:ARG:HE	1:A:27:ARG:HA	0.40	1.77	11	1	
2:C:99:THR:O	2:C:103:VAL:HG23	0.40	2.17	20	2	
1:B:29:GLN:HA	1:B:29:GLN:HE21	0.40	1.76	20	1	
1:A:41:PHE:HZ	1:B:21:TYR:CD2	0.40	2.34	2	1	
1:B:16:GLU:O	1:B:19:GLN:HB3	0.40	2.17	3	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	А	42/52~(81%)	$40\pm1~(95\pm2\%)$	$2\pm1 (5\pm2\%)$	0±0 (0±1%)	32 76
1	В	37/52~(71%)	$34\pm1~(93\pm3\%)$	$2\pm1~(4\pm3\%)$	1±0 (3±1%)	6 42
2	С	24/28~(86%)	$24\pm0$ (99 $\pm2\%$ )	0±0 (1±2%)	0±0 (0±1%)	45 81
All	All	2060/2640~(78%)	1959~(95%)	78 (4%)	23 (1%)	15 64

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)
1	В	11	PRO	17
1	А	11	PRO	2
1	В	12	PRO	2
1	А	31	PRO	1
2	С	108	GLY	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	А	38/43~(88%)	$37 \pm 1 (97 \pm 2\%)$	$1\pm1~(2\pm2\%)$	43 90		
1	В	34/43~(79%)	$32\pm1$ (94 $\pm4\%$ )	$2\pm1~(6\pm4\%)$	17 68		
2	С	18/22~(82%)	$17 \pm 1 (97 \pm 4\%)$	$1\pm1 (3\pm4\%)$	37 86		
All	All	1800/2160~(83%)	1726 (96%)	74 (4%)	28 81		

All 27 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	В	10	ILE	15
1	А	19	GLN	10
1	В	14	LEU	8
1	В	21	TYR	3
1	В	28	GLN	3
1	В	41	PHE	3
2	С	96	GLN	3
1	В	15	THR	2
1	А	48	ARG	2
1	В	19	GLN	2
1	В	11	PRO	2
1	В	29	GLN	2
1	А	17	LEU	2
2	С	89	GLU	2
2	С	106	LEU	2
1	А	27	ARG	2
1	А	15	THR	1
2	С	88	GLU	1



	0	1	1 0	
Mol	Chain	Res	Type	Models (Total)
2	С	101	GLU	1
1	А	26	LEU	1
2	С	93	ARG	1
2	С	107	LYS	1
1	В	39	GLU	1
1	В	40	TYR	1
1	В	30	PRO	1
1	А	43	ARG	1
1	В	32	ASP	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 oligosaccharides 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 66% for the well-defined parts and 67% for the entire structure.

# 7.1 Chemical shift list 1

File name: working\_cs.cif

Chemical shift list name:  $starch\_output$ 

# 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	1760
Number of shifts mapped to atoms	1217
Number of unparsed shifts	0
Number of shifts with mapping errors	543
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

• No matching atom found in the structure. All 543 occurrences are reported below.

	Chain	Bos	Type	Type	Type Atom	Shift Data		
	Ullalli		туре	Atom	Value	Uncertainty	Ambiguity	
1	С	10	LYS	Н	7.932	0.003	1	
1	С	10	LYS	CA	55.766	0.078	1	
1	С	10	LYS	CB	33.233	0.005	1	
1	C	10	LYS	Ν	120.212	0.022	1	
1	С	11	ALA	Н	8.189	0.004	1	
1	С	11	ALA	HA	4.525	0.000	1	
1	С	11	ALA	HB1	1.33	0.000	1	
1	С	11	ALA	HB2	1.33	0.000	1	
1	С	11	ALA	HB3	1.33	0.000	1	
1	С	11	ALA	CA	50.598	0.000	1	
1	С	11	ALA	CB	18.158	0.000	1	
1	С	11	ALA	N	126.193	0.056	1	
1	С	13	HIS	CA	56.215	0.064	1	
1	С	13	HIS	CB	30.383	0.000	1	



		-		• •	Shift Data		
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	С	14	TRP	Н	7.832	0.004	1
1	С	14	TRP	HA	4.697	0.000	1
1	С	14	TRP	HB2	3.246	0.000	2
1	С	14	TRP	HB3	3.246	0.000	2
1	С	14	TRP	CA	57.565	0.013	1
1	С	14	TRP	CB	29.594	0.071	1
1	С	14	TRP	N	122.146	0.075	1
1	С	15	THR	Н	7.803	0.004	1
1	С	15	THR	HG21	1.024	0.000	1
1	С	15	THR	HG22	1.024	0.000	1
1	С	15	THR	HG23	1.024	0.000	1
1	C	15	THR	CA	61.501	0.121	1
1	С	15	THR	CB	70.172	0.045	1
1	C	15	THR	Ν	115.431	0.046	1
1	C	16	SER	Н	8.122	0.005	1
1	С	16	SER	CA	58.689	0.048	1
1	С	16	SER	CB	63.773	0.090	1
1	С	16	SER	Ν	117.493	0.034	1
1	С	17	ALA	Н	8.232	0.002	1
1	С	17	ALA	HB1	1.393	0.000	1
1	С	17	ALA	HB2	1.393	0.000	1
1	С	17	ALA	HB3	1.393	0.000	1
1	С	17	ALA	CA	52.931	0.032	1
1	C	17	ALA	CB	19.171	0.026	1
1	С	17	ALA	Ν	125.873	0.030	1
1	C	18	SER	Н	8.147	0.002	1
1	C	18	SER	CA	58.674	0.020	1
1	C	18	SER	CB	63.631	0.018	1
1	C	18	SER	Ν	114.521	0.018	1
1	С	19	LEU	Н	8.182	0.004	1
1	C	19	LEU	CA	55.689	0.058	1
1	C	19	LEU	CB	42.224	0.030	1
1	C	19	LEU	N	123.857	0.028	1
1	C	20	THR	Н	7.984	0.004	1
1	C	20	THR	HG21	1.19	0.000	1
1	С	20	THR	HG22	1.19	0.000	1
1	C	20	THR	HG23	1.19	0.000	1
1	C	20	THR	CA	62.24	0.094	1
1	C	20	THR	CB	69.746	0.026	1
1	C	20	THR	Ν	113.807	0.023	1
1	C	21	GLU	Н	8.243	0.003	1

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		-	-	• •	Shift Data			
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity	
1	С	21	GLU	CA	56.901	0.068	1	
1	С	21	GLU	CB	30.174	0.043	1	
1	С	21	GLU	N	122.99	0.045	1	
1	С	22	ALA	Н	8.185	0.002	1	
1	С	22	ALA	CA	52.878	0.011	1	
1	С	22	ALA	CB	19.099	0.060	1	
1	С	22	ALA	N	124.508	0.063	1	
1	С	23	ALA	Н	8.038	0.003	1	
1	С	23	ALA	CA	52.52	0.078	1	
1	С	23	ALA	CB	19.168	0.004	1	
1	С	23	ALA	Ν	122.333	0.029	1	
1	C	24	ALA	Н	7.999	0.004	1	
1	С	24	ALA	CA	52.319	0.063	1	
1	С	24	ALA	CB	19.25	0.009	1	
1	С	24	ALA	Ν	122.349	0.032	1	
1	С	25	HIS	Н	8.118	0.004	1	
1	C	25	HIS	CA	53.947	0.000	1	
1	C	25	HIS	CB	29.892	0.000	1	
1	C	25	HIS	Ν	118.968	0.017	1	
1	С	29	PRO	CB	31.999	0.029	1	
1	C	30	GLU	Н	8.494	0.002	1	
1	С	30	GLU	CA	56.889	0.000	1	
1	C	30	GLU	CB	30.02	0.000	1	
1	C	30	GLU	Ν	120.133	0.012	1	
1	С	35	GLY	CA	45.465	0.000	1	
1	C	36	GLY	Н	8.262	0.003	1	
1	C	36	GLY	CA	45.36	0.055	1	
1	C	36	GLY	N	108.858	0.030	1	
1	С	37	SER	Н	8.342	0.003	1	
1	С	37	SER	HA	4.491	0.000	1	
1	C	37	SER	HB2	3.919	0.000	2	
1	C	37	SER	HB3	3.919	0.000	2	
1	C	37	SER	CA	58.599	0.055	1	
1	C	37	SER	CB	63.938	0.026	1	
1	C	37	SER	N	115.567	0.102	1	
1	С	38	GLY	Н	8.498	0.004	1	
1	C	38	GLY	HA2	3.98	0.000	2	
1	C	38	GLY	HA3	3.98	0.000	2	
1	C	38	GLY	CA	45.545	0.000	1	
1	C	38	GLY	Ν	110.974	0.024	1	
1	C	39	GLU	CA	56.127	0.085	1	



			Shift Data				
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	С	39	GLU	CB	29.303	0.078	1
1	C	40	GLY	Н	8.468	0.003	1
1	С	40	GLY	CA	45.576	0.066	1
1	C	40	GLY	Ν	109.548	0.033	1
1	C	41	LEU	Н	8.032	0.004	1
1	C	41	LEU	HA	4.377	0.000	1
1	С	41	LEU	CA	55.319	0.023	1
1	C	41	LEU	CB	42.414	0.033	1
1	С	41	LEU	Ν	121.491	0.024	1
1	C	42	SER	Н	8.283	0.003	1
1	С	42	SER	HA	4.443	0.000	1
1	C	42	SER	CA	58.537	0.000	1
1	С	42	SER	CB	63.74	0.000	1
1	C	42	SER	Ν	116.324	0.033	1
1	С	43	ARG	CA	56.193	0.002	1
1	С	43	ARG	CB	30.834	0.055	1
1	С	44	SER	Н	8.264	0.003	1
1	С	44	SER	CA	58.394	0.067	1
1	С	44	SER	CB	63.908	0.032	1
1	С	44	SER	Ν	116.496	0.028	1
1	С	45	ALA	Н	8.357	0.004	1
1	С	45	ALA	HB1	1.399	0.000	1
1	С	45	ALA	HB2	1.399	0.000	1
1	С	45	ALA	HB3	1.399	0.000	1
1	С	45	ALA	CA	52.912	0.015	1
1	С	45	ALA	CB	19.166	0.048	1
1	С	45	ALA	Ν	125.9	0.034	1
1	С	46	ASN	Н	8.247	0.004	1
1	C	46	ASN	CA	53.228	0.052	1
1	С	46	ASN	CB	38.908	0.050	1
1	C	46	ASN	Ν	116.936	0.027	1
1	С	47	GLY	Н	8.127	0.006	1
1	C	47	GLY	HA2	3.846	0.000	2
1	С	47	GLY	HA3	3.846	0.000	2
1	С	47	GLY	CA	45.171	0.039	1
1	С	47	GLY	Ν	108.297	0.030	1
1	C	48	PHE	Н	7.995	0.005	1
1	С	48	PHE	HA	4.845	0.000	1
1	С	48	PHE	HB2	2.996	0.000	2
1	С	48	PHE	HB3	2.996	0.000	2
1	С	48	PHE	CA	55.795	0.000	1



		Б	<b>F</b>	• •	Shift Data			
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity	
1	С	48	PHE	CB	39.079	0.000	1	
1	С	48	PHE	N	120.855	0.027	1	
1	С	49	PRO	CA	63.177	0.019	1	
1	С	49	PRO	CB	31.672	0.030	1	
1	С	50	TYR	Н	8.043	0.004	1	
1	С	50	TYR	CA	57.953	0.052	1	
1	С	50	TYR	CB	38.848	0.041	1	
1	С	50	TYR	N	120.752	0.032	1	
1	С	51	ARG	Н	8.091	0.006	1	
1	С	51	ARG	HA	4.322	0.000	1	
1	С	51	ARG	HD2	3.163	0.000	2	
1	С	51	ARG	HD3	3.163	0.000	2	
1	С	51	ARG	CA	55.552	0.057	1	
1	С	51	ARG	CB	31.296	0.041	1	
1	С	51	ARG	N	123.699	0.048	1	
1	С	52	GLU	Н	8.472	0.006	1	
1	С	52	GLU	HA	4.177	0.000	1	
1	С	52	GLU	HB2	1.965	0.000	2	
1	С	52	GLU	HB3	1.965	0.000	2	
1	С	52	GLU	HG2	2.285	0.000	2	
1	С	52	GLU	HG3	2.285	0.000	2	
1	С	52	GLU	CA	57.055	0.101	1	
1	С	52	GLU	CB	30.162	0.050	1	
1	С	52	GLU	Ν	122.91	0.033	1	
1	С	53	GLU	Н	8.515	0.004	1	
1	С	53	GLU	HA	4.248	0.000	1	
1	С	53	GLU	HB2	1.956	0.000	2	
1	С	53	GLU	HB3	1.956	0.000	2	
1	C	53	GLU	HG2	2.252	0.000	2	
1	С	53	GLU	HG3	2.252	0.000	2	
1	C	53	GLU	CA	56.906	0.000	1	
1	С	53	GLU	Ν	121.243	0.030	1	
1	C	55	GLU	CA	57.073	0.087	1	
1	C	55	GLU	CB	30.217	0.039	1	
1	C	56	GLY	Н	8.372	0.003	1	
1	С	56	GLY	CA	45.382	0.045	1	
1	C	56	GLY	N	110.002	0.040	1	
1	С	57	ALA	Η	8.005	0.003	1	
1	С	57	ALA	CA	52.589	0.059	1	
1	С	57	ALA	CB	19.181	0.016	1	
1	С	57	ALA	N	123.533	0.043	1	



		Б		• •	Shift Data			
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity	
1	С	58	PHE	Н	8.199	0.003	1	
1	С	58	PHE	HA	4.588	0.000	1	
1	С	58	PHE	HB2	3.088	0.000	2	
1	С	58	PHE	HB3	3.088	0.000	2	
1	С	58	PHE	CA	57.772	0.013	1	
1	С	58	PHE	CB	39.336	0.045	1	
1	С	58	PHE	N	118.997	0.024	1	
1	С	59	GLY	Н	8.17	0.004	1	
1	С	59	GLY	HA2	3.886	0.000	2	
1	С	59	GLY	HA3	3.886	0.000	2	
1	С	59	GLY	CA	45.28	0.050	1	
1	С	59	GLY	N	110.023	0.033	1	
1	С	60	GLU	Н	8.253	0.004	1	
1	С	60	GLU	CA	56.667	0.032	1	
1	С	60	GLU	CB	30.168	0.078	1	
1	С	60	GLU	N	120.669	0.020	1	
1	С	61	HIS	Н	8.445	0.006	1	
1	С	61	HIS	HB2	3.17	0.000	2	
1	С	61	HIS	HB3	3.17	0.000	2	
1	С	61	HIS	CA	56.193	0.140	1	
1	С	61	HIS	CB	30.022	0.065	1	
1	С	61	HIS	N	119.659	0.033	1	
1	С	62	GLY	Н	8.313	0.003	1	
1	С	62	GLY	CA	45.461	0.055	1	
1	С	62	GLY	N	109.78	0.017	1	
1	С	63	SER	Н	8.283	0.003	1	
1	С	63	SER	CA	58.534	0.040	1	
1	С	63	SER	CB	63.82	0.011	1	
1	С	63	SER	Ν	115.699	0.032	1	
1	С	64	GLN	Н	8.475	0.007	1	
1	С	64	GLN	CA	56.239	0.028	1	
1	С	64	GLN	CB	29.396	0.021	1	
1	С	64	GLN	N	121.934	0.046	1	
1	С	65	GLY	Н	8.349	0.003	1	
1	С	65	GLY	CA	45.454	0.000	1	
1	С	65	GLY	N	109.669	0.027	1	
1	C	66	THR	Η	7.982	0.006	1	
1	С	66	THR	HG21	1.155	0.000	1	
1	C	66	THR	HG22	1.155	0.000	1	
1	С	66	THR	HG23	1.155	0.000	1	
1	С	66	THR	CA	61.895	0.108	1	

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		D		• •	Shift Data		
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	С	66	THR	CB	69.832	0.078	1
1	С	66	THR	N	113.791	0.048	1
1	С	67	TYR	Н	8.256	0.004	1
1	С	67	TYR	CA	58.011	0.109	1
1	С	67	TYR	CB	38.852	0.035	1
1	C	67	TYR	N	122.686	0.049	1
1	C	68	SER	Н	8.093	0.007	1
1	С	68	SER	HA	4.413	0.000	1
1	C	68	SER	HB2	3.806	0.000	2
1	С	68	SER	HB3	3.806	0.000	2
1	C	68	SER	CA	58.132	0.022	1
1	C	68	SER	CB	63.996	0.073	1
1	С	68	SER	N	117.468	0.032	1
1	C	69	ASP	Н	8.313	0.004	1
1	С	69	ASP	CA	54.326	0.046	1
1	C	69	ASP	CB	41.253	0.029	1
1	C	69	ASP	N	122.845	0.017	1
1	C	70	THR	Н	8.066	0.004	1
1	C	70	THR	CA	62.062	0.052	1
1	С	70	THR	CB	69.686	0.051	1
1	C	70	THR	N	114.328	0.030	1
1	С	71	LYS	Н	8.286	0.004	1
1	C	71	LYS	HA	4.33	0.000	1
1	C	71	LYS	CA	56.583	0.000	1
1	C	71	LYS	CB	32.82	0.000	1
1	С	71	LYS	N	123.394	0.041	1
1	C	72	GLU	CA	56.724	0.064	1
1	С	72	GLU	CB	30.11	0.110	1
1	С	73	ASN	H	8.388	0.003	1
1	С	73	ASN	CA	53.289	0.014	1
1	C	73	ASN	CB	39.059	0.031	1
1	C	73	ASN	N	119.385	0.026	1
1	С	74	GLY	Н	8.313	0.004	1
1	C	74	GLY	HA2	3.978	0.000	2
1	C	74	GLY	HA3	3.978	0.000	2
1	C	74	GLY	CA	45.533	0.066	1
1	C	74	GLY	N	109.119	0.025	1
1	C	75	ILE	H	8.022	0.003	1
1	C	75	ILE	HA	4.155	0.018	1
1	C	75	ILE	HB	1.813	0.010	1
1	C	75	ILE	HD11	0.811	0.006	1



		-			Shift Data			
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity	
1	С	75	ILE	HD12	0.811	0.006	1	
1	C	75	ILE	HD13	0.811	0.006	1	
1	С	75	ILE	HG12	1.426	0.029	1	
1	С	75	ILE	HG13	1.107	0.014	1	
1	C	75	ILE	HG21	0.885	0.013	1	
1	C	75	ILE	HG22	0.885	0.013	1	
1	C	75	ILE	HG23	0.885	0.013	1	
1	C	75	ILE	CA	61.345	0.056	1	
1	C	75	ILE	CB	38.686	0.071	1	
1	С	75	ILE	CD1	12.915	0.065	1	
1	С	75	ILE	CG1	27.143	0.193	1	
1	C	75	ILE	CG2	17.215	0.102	1	
1	С	75	ILE	Ν	119.822	0.024	1	
1	С	76	ASN	Н	8.528	0.004	1	
1	С	76	ASN	HA	4.724	0.000	1	
1	С	76	ASN	HB2	2.816	0.000	2	
1	С	76	ASN	HB3	2.816	0.000	2	
1	С	76	ASN	CA	53.424	0.083	1	
1	С	76	ASN	CB	38.9	0.030	1	
1	С	76	ASN	N	122.07	0.016	1	
1	С	77	GLY	Н	8.275	0.003	1	
1	С	77	GLY	CA	45.533	0.000	1	
1	С	77	GLY	N	109.431	0.028	1	
1	С	79	LEU	Н	8.269	0.003	1	
1	С	79	LEU	CA	55.288	0.005	1	
1	С	79	LEU	CB	42.301	0.036	1	
1	С	79	LEU	Ν	122.763	0.042	1	
1	С	80	THR	Н	8.168	0.016	1	
1	C	80	THR	HA	4.394	0.007	1	
1	С	80	THR	HB	4.247	0.005	1	
1	C	80	THR	HG21	1.177	0.010	1	
1	С	80	THR	HG22	1.177	0.010	1	
1	C	80	THR	HG23	1.177	0.010	1	
1	C	80	THR	CA	61.581	0.000	1	
1	С	80	THR	CB	70.027	0.023	1	
1	С	80	THR	CG2	21.608	0.015	1	
1	C	80	THR	N	114.341	0.010	1	
1	С	81	SER	Н	8.3	0.006	1	
1	C	81	SER	HA	4.399	0.001	1	
1	С	81	SER	HB2	3.824	0.012	2	
1	С	81	SER	HB3	3.824	0.012	2	



		Ъ		• •	Shift Data		
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	С	81	SER	CA	58.419	0.041	1
1	С	81	SER	CB	63.716	0.063	1
1	С	81	SER	N	117.698	0.049	1
1	С	82	ALA	Н	8.188	0.012	1
1	С	82	ALA	HA	4.27	0.024	1
1	С	82	ALA	HB1	1.34	0.011	1
1	С	82	ALA	HB2	1.34	0.011	1
1	С	82	ALA	HB3	1.34	0.011	1
1	С	82	ALA	CA	52.519	0.127	1
1	C	82	ALA	CB	19.207	0.046	1
1	C	82	ALA	Ν	124.612	0.012	1
1	С	83	ASP	Н	8.174	0.008	1
1	С	83	ASP	HA	4.52	0.005	1
1	C	83	ASP	HB2	2.644	0.020	2
1	С	83	ASP	HB3	2.644	0.020	2
1	С	83	ASP	CA	54.743	0.083	1
1	С	83	ASP	CB	41.166	0.039	1
1	С	83	ASP	N	118.873	0.016	1
1	С	84	ARG	Н	8.048	0.013	1
1	С	113	GLU	Н	8.066	0.003	1
1	C	113	GLU	HA	4.161	0.000	1
1	С	113	GLU	HB2	2.007	0.012	2
1	С	113	GLU	HB3	2.007	0.012	2
1	С	113	GLU	HG2	2.316	0.019	2
1	C	113	GLU	HG3	2.316	0.019	2
1	C	113	GLU	CB	29.876	0.000	1
1	C	113	GLU	Ν	120.143	0.011	1
1	C	114	ALA	Н	8.007	0.004	1
1	C	114	ALA	HA	4.201	0.008	1
1	C	114	ALA	HB1	1.381	0.009	1
1	C	114	ALA	HB2	1.381	0.009	1
1	С	114	ALA	HB3	1.381	0.009	1
1	C	114	ALA	CA	52.82	0.086	1
1	C	114	ALA	CB	18.935	0.004	1
1	C	114	ALA	Ν	123.121	0.028	1
1	С	115	GLN	Н	8.003	0.006	1
1	C	115	GLN	HA	4.194	0.018	1
1	C	115	GLN	HB2	1.977	0.003	2
1	C	115	GLN	HB3	1.977	0.003	2
1	C	115	GLN	HG2	2.322	0.016	2
1	C	115	GLN	HG3	2.322	0.016	2



		D		• •	Shift Data		
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	С	115	GLN	CA	56.569	0.017	1
1	С	115	GLN	CG	33.709	0.032	1
1	С	115	GLN	N	117.87	0.004	1
1	С	116	HIS	Н	8.131	0.013	1
1	С	116	HIS	HA	4.591	0.005	1
1	С	116	HIS	HB2	3.173	0.005	1
1	С	116	HIS	HB3	3.104	0.018	1
1	С	116	HIS	CA	56.381	0.121	1
1	С	116	HIS	CB	30.084	0.091	1
1	С	116	HIS	N	119.534	0.000	1
1	С	120	PRO	HA	4.38	0.016	1
1	С	120	PRO	HB2	1.876	0.003	1
1	С	120	PRO	HB3	2.258	0.010	1
1	С	120	PRO	HD2	3.646	0.013	1
1	С	120	PRO	HD3	3.817	0.022	1
1	С	120	PRO	HG2	1.907	0.002	1
1	С	120	PRO	HG3	1.999	0.005	1
1	С	120	PRO	CA	63.308	0.036	1
1	С	120	PRO	CB	31.543	0.339	1
1	С	120	PRO	CD	50.942	0.110	1
1	С	120	PRO	CG	27.315	0.024	1
1	С	121	ALA	Н	8.33	0.003	1
1	С	121	ALA	HA	4.365	0.000	1
1	С	121	ALA	HB1	1.351	0.000	1
1	С	121	ALA	HB2	1.351	0.000	1
1	С	121	ALA	HB3	1.351	0.000	1
1	С	121	ALA	CA	52.404	0.000	1
1	С	121	ALA	CB	19.219	0.000	1
1	С	121	ALA	N	124.37	0.047	1
1	С	122	ALA	Н	8.186	0.001	1
1	С	122	ALA	CA	51.921	0.101	1
1	С	122	ALA	CB	19.295	0.002	1
1	С	122	ALA	N	123.432	0.000	1
1	С	123	LEU	Н	8.15	0.004	1
1	С	123	LEU	CA	52.857	0.000	1
1	С	123	LEU	CB	41.72	0.000	1
1	С	124	PRO	CA	62.892	0.066	1
1	С	124	PRO	CB	31.915	0.031	1
1	С	125	LEU	Н	8.226	0.003	1
1	С	125	LEU	CA	55.116	0.025	1
1	С	125	LEU	CB	42.452	0.028	1

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		D	<b>D</b>	• •		Shift Data	1
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	C	125	LEU	Ν	122.551	0.037	1
1	С	126	ALA	Н	8.266	0.002	1
1	С	126	ALA	HA	4.317	0.000	1
1	С	126	ALA	HB1	1.399	0.000	1
1	С	126	ALA	HB2	1.399	0.000	1
1	С	126	ALA	HB3	1.399	0.000	1
1	C	126	ALA	CA	52.242	0.069	1
1	С	126	ALA	CB	19.271	0.020	1
1	C	126	ALA	Ν	125.189	0.041	1
1	C	127	ALA	Н	8.244	0.002	1
1	С	127	ALA	HA	4.279	0.000	1
1	C	127	ALA	HB1	1.4	0.000	1
1	С	127	ALA	HB2	1.4	0.000	1
1	С	127	ALA	HB3	1.4	0.000	1
1	С	127	ALA	CA	52.574	0.000	1
1	C	127	ALA	CB	19.296	0.000	1
1	C	127	ALA	Ν	123.661	0.030	1
1	C	128	GLU	Н	8.392	0.003	1
1	C	128	GLU	Ν	119.908	0.029	1
1	C	129	GLU	CA	56.608	0.026	1
1	С	129	GLU	CB	30.413	0.031	1
1	C	130	THR	Н	8.189	0.003	1
1	С	130	THR	HG21	1.19	0.000	1
1	С	130	THR	HG22	1.19	0.000	1
1	C	130	THR	HG23	1.19	0.000	1
1	C	130	THR	CA	62.066	0.027	1
1	C	130	THR	CB	69.823	0.002	1
1	C	130	THR	Ν	115.823	0.033	1
1	C	131	VAL	Н	8.089	0.003	1
1	С	131	VAL	HA	4.095	0.011	1
1	C	131	VAL	HB	2.041	0.010	1
1	С	131	VAL	HG11	0.896	0.011	2
1	C	131	VAL	HG12	0.896	0.011	2
1	C	131	VAL	HG13	0.896	0.011	2
1	C	131	VAL	HG21	0.896	0.011	2
1	C	131	VAL	HG22	0.896	0.011	2
1	C	131	VAL	HG23	0.896	0.011	2
1	C	131	VAL	CA	62.248	0.039	1
1	C	131	VAL	CB	32.822	0.101	1
1	C	131	VAL	CG1	20.866	0.082	1
1	C	131	VAL	N	122.399	0.037	1



		Ъ		• •	Shift Data		
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	С	132	ASN	Н	8.451	0.004	1
1	С	132	ASN	HA	4.751	0.000	1
1	С	132	ASN	CA	52.942	0.027	1
1	С	132	ASN	CB	39.07	0.030	1
1	С	132	ASN	N	122.555	0.030	1
1	С	133	LEU	Н	8.146	0.004	1
1	С	133	LEU	CA	52.957	0.000	1
1	С	133	LEU	CB	41.815	0.000	1
1	С	133	LEU	Ν	124.33	0.038	1
1	С	135	PRO	CA	62.747	0.000	1
1	С	135	PRO	CB	31.968	0.032	1
1	С	136	SER	Н	8.338	0.003	1
1	С	136	SER	HA	4.748	0.000	1
1	С	136	SER	HB2	3.851	0.000	2
1	С	136	SER	HB3	3.851	0.000	2
1	С	136	SER	CA	56.502	0.000	1
1	С	136	SER	CB	63.539	0.000	1
1	С	136	SER	N	117.564	0.057	1
1	С	139	PRO	CA	62.744	0.000	1
1	С	139	PRO	CB	31.963	0.032	1
1	С	140	SER	Н	8.378	0.003	1
1	С	140	SER	HA	4.763	0.000	1
1	С	140	SER	HB2	3.872	0.000	2
1	С	140	SER	HB3	3.872	0.000	2
1	С	140	SER	CA	56.408	0.000	1
1	С	140	SER	CB	63.5	0.000	1
1	С	140	SER	N	117.473	0.033	1
1	С	141	PRO	CA	63.283	0.005	1
1	С	141	PRO	CB	32.016	0.047	1
1	С	142	ALA	Н	8.357	0.003	1
1	С	142	ALA	HA	4.324	0.000	1
1	С	142	ALA	HB1	1.423	0.000	1
1	С	142	ALA	HB2	1.423	0.000	1
1	С	142	ALA	HB3	1.423	0.000	1
1	С	142	ALA	CA	52.773	0.035	1
1	C	142	ALA	CB	19.093	0.038	1
1	С	142	ALA	N	124.224	0.031	1
1	С	143	SER	Н	8.211	0.003	1
1	С	143	SER	HA	4.395	0.000	1
1	С	143	SER	HB2	3.894	0.000	2
1	C	143	SER	HB3	3.894	0.000	2

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		_			Shift Data		
List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	C	143	SER	CA	58.607	0.019	1
1	C	143	SER	CB	63.822	0.024	1
1	C	143	SER	Ν	114.828	0.033	1
1	C	144	GLU	Н	8.381	0.004	1
1	C	144	GLU	CA	56.963	0.000	1
1	C	144	GLU	CB	30.249	0.000	1
1	C	144	GLU	Ν	122.533	0.021	1
1	C	145	GLN	CA	56.112	0.052	1
1	C	145	GLN	CB	29.364	0.020	1
1	C	146	THR	Н	8.125	0.004	1
1	C	146	THR	HG21	1.217	0.000	1
1	С	146	THR	HG22	1.217	0.000	1
1	C	146	THR	HG23	1.217	0.000	1
1	C	146	THR	CA	62.179	0.004	1
1	C	146	THR	CB	69.734	0.032	1
1	C	146	THR	Ν	115.788	0.034	1
1	C	147	ALA	Н	8.259	0.002	1
1	С	147	ALA	HA	4.309	0.016	1
1	C	147	ALA	CA	52.58	0.125	1
1	С	147	ALA	CB	19.215	0.021	1
1	С	147	ALA	N	126.607	0.028	1
1	С	148	ALA	Н	8.192	0.003	1
1	C	148	ALA	CA	52.493	0.038	1
1	С	148	ALA	CB	19.127	0.073	1
1	С	148	ALA	N	123.37	0.036	1
1	C	149	LEU	Н	8.127	0.003	1
1	С	149	LEU	CA	55.331	0.000	1
1	C	149	LEU	CB	42.333	0.000	1
1	C	149	LEU	Ν	121.57	0.026	1
1	C	151	GLU	CA	56.593	0.052	1
1	C	151	GLU	CB	30.422	0.043	1
1	C	152	ALA	Н	8.326	0.003	1
1	C	152	ALA	HA	4.408	0.000	1
1	C	152	ALA	HB1	1.436	0.000	1
1	C	152	ALA	HB2	1.436	0.000	1
1	С	152	ALA	HB3	1.436	0.000	1
1	C	152	ALA	CA	52.749	0.042	1
1	С	152	ALA	CB	19.241	0.029	1
1	C	152	ALA	Ν	125.168	0.033	1
1	C	153	THR	Η	8.123	0.004	1
1	С	153	THR	HG21	1.233	0.000	1



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List ID	Chain	Res	Type	Atom	Value	Uncertainty	Ambiguity
1	С	153	THR	HG22	1.233	0.000	1
1	C	153	THR	HG23	1.233	0.000	1
1	С	153	THR	CA	61.726	0.055	1
1	С	153	THR	CB	69.905	0.045	1
1	С	153	THR	N	112.989	0.028	1
1	С	154	SER	Н	8.312	0.003	1
1	С	154	SER	CA	58.557	0.026	1
1	С	154	SER	CB	63.956	0.022	1
1	С	154	SER	N	117.896	0.043	1
1	С	155	GLY	Н	8.404	0.005	1
1	С	155	GLY	HA2	4.017	0.000	2
1	С	155	GLY	HA3	4.017	0.000	2
1	С	155	GLY	CA	45.346	0.027	1
1	С	155	GLY	N	110.902	0.032	1
1	С	156	GLU	Н	8.273	0.002	1
1	С	156	GLU	CA	56.6	0.032	1
1	С	156	GLU	CB	30.413	0.028	1
1	С	156	GLU	N	120.624	0.043	1
1	С	157	SER	Н	8.344	0.003	1
1	С	157	SER	HA	4.478	0.000	1
1	С	157	SER	HB2	3.89	0.000	2
1	С	157	SER	HB3	3.89	0.000	2
1	С	157	SER	CA	58.339	0.066	1
1	С	157	SER	CB	63.925	0.042	1
1	С	157	SER	N	116.872	0.036	1
1	С	158	ALA	Н	8.301	0.003	1
1	С	158	ALA	HA	4.383	0.000	1
1	С	158	ALA	HB1	1.404	0.000	1
1	C	158	ALA	HB2	1.404	0.000	1
1	С	158	ALA	HB3	1.404	0.000	1
1	C	158	ALA	CA	52.639	0.043	1
1	C	158	ALA	CB	19.316	0.026	1
1	С	158	ALA	N	126.702	0.038	1
1	С	159	GLN	H	8.288	0.006	1
1	С	159	GLN	CA	55.48	0.000	1
1	С	159	GLN	CB	32.897	0.000	1
1	C	159	GLN	N	119.165	0.018	1

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# 7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.



Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	212	$-0.44 \pm 0.18$	None needed ( $< 0.5$ ppm)
$^{13}C_{\beta}$	184	$0.17 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}C'$	0		None (insufficient data)
<sup>15</sup> N	205	$-0.11 \pm 0.14$	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 66%, i.e. 970 atoms were assigned a chemical shift out of a possible 1473. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}\mathbf{N}$
Backbone	364/504~(72%)	187/203~(92%)	84/206~(41%)	93/95~(98%)
Sidechain	606/886~(68%)	427/579~(74%)	179/274~(65%)	0/33~(0%)
Aromatic	0/83~(0%)	0/40~(0%)	0/42~(0%)	0/1~(0%)
Overall	970/1473~(66%)	614/822~(75%)	263/522~(50%)	93/129~(72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 1218 atoms were assigned a chemical shift out of a possible 1809. 0 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	$^{15}$ N
Backbone	474/649~(73%)	245/263~(93%)	111/264~(42%)	118/122 (97%)
Sidechain	744/1070~(70%)	523/701~(75%)	221/328~(67%)	0/41~(0%)
Aromatic	0/90~(0%)	0/44~(0%)	0/44~(0%)	0/2~(0%)
Overall	1218/1809~(67%)	768/1008~(76%)	332/636~(52%)	118/165~(72%)

## 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	В	8	ILE	CG2	28.02	10.93 - 24.12	8.0

# 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 welldefined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



Random coil index (RCI) for chain C:





# 8 NMR restraints analysis (i)

# 8.1 Conformationally restricting restraints (i)

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	0
Intra-residue ( i-j =0)	0
Sequential ( i-j =1)	0
Medium range ( $ i-j >1$ and $ i-j <5$ )	0
Long range $( i-j  \ge 5)$	0
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	174
Number of unmapped restraints	0
Number of restraints per residue	0
Number of long range restraints per residue <sup>1</sup>	0

<sup>1</sup>Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

# 8.2 Residual restraint violations (i)

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

# 8.2.1 Average number of distance violations per model (i)

Distance violations less than 0.1 Å are not included in the calculation. There are no distance restraints

# 8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than  $1^\circ$  are not included in the calculation.

Bins $(^{\circ})$	Average number of violations per model	Max $(^{\circ})$
1.0-10.0 (Small)	11.7	7.14



Bins $(^{\circ})$	Average number of violations per model	Max $(^{\circ})$
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None



# 9 Distance violation analysis (i)

No distance restraints data found



# 10 Dihedral-angle violation analysis (i)

# 10.1 Summary of dihedral-angle violations (i)

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than  $1^{\circ}$  are not included in the calculation.

Angle trine	Count 071		Vie	$Violated^3$			Consistently Violated <sup>4</sup>		
Angle type	Count	70	Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$	
PHI	87	50.0	23	26.4	13.2	0	0.0	0.0	
PSI	87	50.0	38	43.7	21.8	1	1.1	0.6	
Total	174	100.0	61	35.1	35.1	1	0.6	0.6	

 $^1$  percentage calculated with respect to total number of dihedral-angle restraints,  $^2$  percentage calculated with respect to number of restraints in a particular dihedral-angle type,  $^3$  violated in at least one model,  $^4$  violated in all the models

## 10.1.1 Bar chart : Distribution of dihedral-angles and violations (i)



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories



# 10.2 Dihedral-angle violation statistics for each model (i)

The following table provides the dihedral-angle violation statistics for each model in the ensemble. Violations less than  $1^{\circ}$  are not included in the statistics.

Model ID	Number of violations			Magn (°)	$M_{OV}$ (°)	SD (°)	Modian (°)	
Model ID	PHI	PSI	Total	Mean ()	max ()		Median ()	
1	3	10	13	2.12	5.34	1.19	1.72	
2	3	9	12	1.95	3.12	0.62	1.88	
3	3	7	10	1.82	4.05	0.85	1.52	
4	4	6	10	2.16	5.2	1.2	1.88	
5	5	6	11	2.62	7.14	1.85	1.78	
6	8	9	17	2.37	4.59	1.13	2.18	
7	3	11	14	2.16	5.3	1.28	1.84	
8	1	11	12	1.99	5.75	1.18	1.72	
9	6	8	14	2.03	4.63	1.09	1.56	
10	1	11	12	2.03	4.49	1.01	1.65	
11	2	11	13	2.37	6.34	1.74	1.63	
12	1	7	8	2.24	5.45	1.43	1.54	
13	5	8	13	2.19	5.4	1.14	1.73	
14	4	10	14	2.01	5.07	1.08	1.66	
15	2	8	10	2.03	4.79	1.03	1.72	
16	3	7	10	2.13	5.37	1.19	1.76	
17	3	6	9	2.4	6.44	1.52	2.13	
18	3	10	13	1.88	5.84	1.29	1.46	
19	1	7	8	2.39	6.11	1.58	1.84	
20	4	8	12	1.77	5.74	1.25	1.29	







The mean(dot), median(x) and the standard deviation are shown in blue with respect to the y axis on the right

# 10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Num	ber o	f violated restraints	Fraction of the ensemble			
PHI	PSI	Total	$\operatorname{Count}^1$	%		
9	8	17	1	5.0		
9	11	20	2	10.0		
1	6	7	3	15.0		
2	1	3	4	20.0		
0	4	4	5	25.0		
0	0	0	6	30.0		
0	2	2	7	35.0		
1	0	1	8	40.0		
0	0	0	9	45.0		
0	1	1	10	50.0		
0	0	0	11	55.0		



PHI

PSI

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Num	iber o	of violated restraints	Fraction of the ensemble						
PHI	PSI	Total	Count <sup>1</sup>	%					
0	1	1	12	60.0					
0	2	2	13	65.0					
0	0	0	14	70.0					
0	0	0	15	75.0					
0	1	1	16	80.0					
0	0	0	17	85.0					
0	0	0	18	90.0					
1	0	1	19	95.0					
0	1	1	20	100.0					

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 $^{1}$  Number of models with violations





# 10.4 Most violated dihedral-angle restraints in the ensemble (i)

# 10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models



in the ensemble



#### 10.4.2 Table: Most violated dihedral-angle restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	$Models^1$	Mean	$\mathbf{SD}^2$	Median
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	20	5.31	0.88	5.36
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	19	1.81	0.68	1.67
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	16	2.03	0.62	2.02
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	13	2.67	0.76	2.9
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	13	1.86	0.46	1.89
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	12	3.14	1.67	2.61
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	10	1.96	0.83	1.7
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	8	1.78	0.63	1.56
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	7	1.61	0.49	1.56
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	7	1.55	0.23	1.53
(1,78)	1:14:B:LEU:N	1:14:B:LEU:CA	1:14:B:LEU:C	1:15:B:THR:N	5	1.62	0.41	1.54
(1,104)	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	1:29:B:GLN:N	5	1.55	0.25	1.62
(1,90)	1:21:B:TYR:N	1:21:B:TYR:CA	1:21:B:TYR:C	1:22:B:THR:N	5	1.47	0.26	1.46
(1,52)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:GLU:N	5	1.29	0.22	1.17
(1,3)	1:8:A:ILE:C	1:9:A:GLN:N	1:9:A:GLN:CA	1:9:A:GLN:C	4	2.52	0.52	2.5
(1,36)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:GLN:N	4	1.84	0.29	1.9
(1,133)	2:86:C:THR:C	2:87:C:ALA:N	2:87:C:ALA:CA	2:87:C:ALA:C	4	1.74	0.48	1.7
(1,156)	2:98:C:VAL:N	2:98:C:VAL:CA	2:98:C:VAL:C	2:99:C:THR:N	3	1.9	0.42	1.66
(1,140)	2:90:C:VAL:N	2:90:C:VAL:CA	2:90:C:VAL:C	2:91:C:SER:N	3	1.71	0.15	1.64
(1,7)	1:12:A:PRO:C	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	3	1.59	0.42	1.33



Key	Atom-1	Atom-2	Atom-3	Atom-4	$\mathbf{Models}^1$	Mean	$\mathbf{SD}^2$	Median
(1,174)	2:109:C:GLU:N	2:109:C:GLU:CA	2:109:C:GLU:C	2:110:C:GLN:N	3	1.47	0.29	1.63
(1,94)	1:23:B:VAL:N	1:23:B:VAL:CA	1:23:B:VAL:C	1:24:B:GLU:N	3	1.44	0.28	1.49
(1,44)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLU:N	3	1.33	0.29	1.21
(1,130)	1:45:B:ARG:N	1:45:B:ARG:CA	1:45:B:ARG:C	1:46:B:GLU:N	3	1.31	0.21	1.45
(1,6)	1:10:A:ILE:N	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:PRO:N	2	3.6	0.74	3.6
(1,2)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:GLN:N	2	2.51	0.51	2.51
(1,70)	1:8:B:ILE:N	1:8:B:ILE:CA	1:8:B:ILE:C	1:9:B:GLN:N	2	2.18	0.28	2.18
(1,32)	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1:27:A:ARG:N	2	1.78	0.21	1.78
(1,167)	2:103:C:VAL:C	2:104:C:ALA:N	2:104:C:ALA:CA	2:104:C:ALA:C	2	1.78	0.68	1.78
(1,65)	1:45:A:ARG:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	2	1.67	0.46	1.67
(1,10)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	2	1.62	0.17	1.62
(1,12)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLU:N	2	1.58	0.42	1.58
(1,131)	2:85:C:GLU:C	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2	1.56	0.5	1.56
(1,103)	1:27:B:ARG:C	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	2	1.52	0.35	1.52
(1,137)	2:88:C:GLU:C	2:89:C:GLU:N	2:89:C:GLU:CA	2:89:C:GLU:C	2	1.38	0.07	1.38
(1,54)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:TYR:N	2	1.36	0.18	1.36
(1,64)	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	1:46:A:GLU:N	2	1.23	0.21	1.23
(1,150)	2:95:C:VAL:N	2:95:C:VAL:CA	2:95:C:VAL:C	2:96:C:GLN:N	2	1.22	0.15	1.22
(1,15)	1:16:A:GLU:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	2	1.18	0.07	1.18
(1,118)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:GLU:N	2	1.16	0.14	1.16
(1,47)	1:35:A:GLU:C	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	2	1.16	0.09	1.16
(1,136)	2:88:C:GLU:N	2:88:C:GLU:CA	2:88:C:GLU:C	2:89:C:GLU:N	2	1.15	0.12	1.15
(1,75)	1:12:B:PRO:C	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	2	1.14	0.09	1.14
(1,29)	1:24:A:GLU:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	2	1.02	0.03	1.02

<sup>1</sup> Number of violated models, <sup>2</sup>Standard deviation, All angle values are in degree (°)

# 10.5 All violated dihedral-angle restraints (i)

## 10.5.1 Histogram : Distribution of violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.





#### 10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation $(^{\circ})$
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	5	7.14
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	17	6.44
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	11	6.34
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	11	6.33
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	19	6.11
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	18	5.84
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	8	5.75
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	20	5.74
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	12	5.45
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	13	5.4
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	16	5.37
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	1	5.34
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	7	5.3
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	4	5.2
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	5	5.16
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	14	5.07
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	15	4.79
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	7	4.66
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	9	4.63
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	6	4.59
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	6	4.51



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Key	Atom-1	Atom-2	Atom-3	Atom-4	Atom-4 Model ID	
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	10	4.49
(1,6)	1:10:A:ILE:N	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:PRO:N	6	4.34
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	3	4.05
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	9	4.01
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	1	3.72
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	10	3.68
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	12	3.6
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	18	3.39
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	5	3.26
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	13	3.16
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	4	3.14
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	19	3.13
(1,38)	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1:30:A:PRO:N	2	3.12
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	5	3.12
(1,3)	1:8:A:ILE:C	1:9:A:GLN:N	1:9:A:GLN:CA	1:9:A:GLN:C	14	3.1
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	9	3.07
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	7	3.03
(1,2)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:GLN:N	6	3.02
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	13	3.0
(1,3)	1:8:A:ILE:C	1:9:A:GLN:N	1:9:A:GLN:CA	1:9:A:GLN:C	6	2.98
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	14	2.96
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	17	2.9
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	13	2.87
(1,6)	1:10:A:ILE:N	1:10:A:ILE:CA	1:10:A:ILE:C	1:11:A:PRO:N	16	2.85
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	15	2.76
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	19	2.71
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	1	2.69
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	4	2.67
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	2	2.63
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	1	2.63
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	2	2.49
(1,156)	2:98:C:VAL:N	2:98:C:VAL:CA	2:98:C:VAL:C	2:99:C:THR:N	10	2.49
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	14	2.46
(1,70)	1:8:B:ILE:N	1:8:B:ILE:CA	1:8:B:ILE:C	1:9:B:GLN:N	3	2.46
(1,167)	2:103:C:VAL:C	2:104:C:ALA:N	2:104:C:ALA:CA	2:104:C:ALA:C	6	2.45
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	16	2.4
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	2	2.4
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	6	2.39
(1,133)	2:86:C:THR:C	2:87:C:ALA:N	2:87:C:ALA:CA	2:87:C:ALA:C	11	2.36
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	7	2.32
(1,78)	1:14:B:LEU:N	1:14:B:LEU:CA	1:14:B:LEU:C	1:15:B:THR:N	9	2.3
$(1, \overline{48})$	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	2	2.28
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	8	2.26
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	6	2.24
$(1,5\overline{6})$	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	20	2.24
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	17	2.21
$(1, \overline{48})$	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	11	2.2
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	6	2.18
(1,7)	1:12:A:PRO:C	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	17	2.18
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	15	2.16
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	12	2.14



Continued from previous page							
Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation $(^{\circ})$	
(1, 36)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:GLN:N	19	2.14	
(1,65)	1:45:A:ARG:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	17	2.13	
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	11	2.09	
(1,131)	2:85:C:GLU:C	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	9	2.07	
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	8	2.05	
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	4	2.05	
(1,133)	2:86:C:THR:C	2:87:C:ALA:N	2:87:C:ALA:CA	2:87:C:ALA:C	7	2.04	
(1,114)	1:36:B:PHE:N	1:36:B:PHE:CA	1:36:B:PHE:C	1:37:B:ALA:N	3	2.03	
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	6	2.03	
(1, 36)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:GLN:N	7	2.03	
(1,3)	1:8:A:ILE:C	1:9:A:GLN:N	1:9:A:GLN:CA	1:9:A:GLN:C	13	2.02	
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	14	2.01	
(1,12)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLU:N	7	2.01	
(1,2)	1:8:A:ILE:N	1:8:A:ILE:CA	1:8:A:ILE:C	1:9:A:GLN:N	14	2.01	
(1, 32)	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1:27:A:ARG:N	9	2.0	
(1,3)	1:8:A:ILE:C	1:9:A:GLN:N	1:9:A:GLN:CA	1:9:A:GLN:C	10	1.97	
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	5	1.96	
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	10	1.94	
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	8	1.94	
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	16	1.93	
(1,140)	2:90:C:VAL:N	2:90:C:VAL:CA	2:90:C:VAL:C	2:91:C:SER:N	4	1.92	
(1,70)	1:8:B:ILE:N	1:8:B:ILE:CA	1:8:B:ILE:C	1:9:B:GLN:N	2	1.91	
(1,90)	1:21:B:TYR:N	1:21:B:TYR:CA	1:21:B:TYR:C	1:22:B:THR:N	1	1.9	
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	18	1.9	
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	20	1.89	
(1,103)	1:27:B:ARG:C	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	16	1.87	
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	8	1.87	
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	3	1.86	
(1,171)	2:105:C:VAL:C	2:106:C:LEU:N	2:106:C:LEU:CA	2:106:C:LEU:C	2	1.85	
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	13	1.85	
(1,104)	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	1:29:B:GLN:N	1	1.85	
(1,69)	1:7:B:HIS:C	1:8:B:ILE:N	1:8:B:ILE:CA	1:8:B:ILE:C	4	1.85	
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	15	1.85	
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	15	1.82	
(1,78)	1:14:B:LEU:N	1:14:B:LEU:CA	1:14:B:LEU:C	1:15:B:THR:N	11	1.79	
(1,10)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	8	1.79	
(1, 36)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:GLN:N	5	1.78	
(1,94)	1:23:B:VAL:N	1:23:B:VAL:CA	1:23:B:VAL:C	1:24:B:GLU:N	14	1.75	
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	2	1.74	
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	13	1.73	
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	10	1.72	
(1,44)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLU:N	1	1.72	
(1,174)	2:109:C:GLU:N	2:109:C:GLU:CA	2:109:C:GLU:C	2:110:C:GLN:N	18	1.71	
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	13	1.68	
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	13	1.68	
(1,45)	1:34:A:VAL:C	1:35:A:GLU:N	1:35:A:GLU:CA	1:35:A:GLU:C	1	1.67	
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	2	1.67	
(1,160)	2:100:C:ALA:N	2:100:C:ALA:CA	2:100:C:ALA:C	2:101:C:GLU:N	7	1.66	
(1,156)	2:98:C:VAL:N	2:98:C:VAL:CA	2:98:C:VAL:C	2:99:C:THR:N	8	1.66	
(1,89)	1:20:B:GLY:C	1:21:B:TYR:N	1:21:B:TYR:CA	1:21:B:TYR:C	6	1.66	
(1.74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	20	1.66	



Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation ( $^{\circ}$ )
(1,140)	2:90:C:VAL:N	2:90:C:VAL:CA	2:90:C:VAL:C	2:91:C:SER:N	16	1.64
(1,174)	2:109:C:GLU:N	2:109:C:GLU:CA	2:109:C:GLU:C	2:110:C:GLN:N	11	1.63
(1,104)	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	1:29:B:GLN:N	11	1.63
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	17	1.63
(1,104)	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	1:29:B:GLN:N	15	1.62
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	9	1.62
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	11	1.62
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	18	1.61
(1,104)	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	1:29:B:GLN:N	3	1.59
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	15	1.59
(1,140)	2:90:C:VAL:N	2:90:C:VAL:CA	2:90:C:VAL:C	2:91:C:SER:N	10	1.58
(1,52)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:GLU:N	17	1.58
(1,154)	2:97:C:VAL:N	2:97:C:VAL:CA	2:97:C:VAL:C	2:98:C:VAL:N	10	1.57
(1,32)	1:26:A:LEU:N	1:26:A:LEU:CA	1:26:A:LEU:C	1:27:A:ARG:N	14	1.57
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	14	1.56
(1,90)	1:21:B:TYR:N	1:21:B:TYR:CA	1:21:B:TYR:C	1:22:B:THR:N	6	1.56
(1,156)	2:98:C:VAL:N	2:98:C:VAL:CA	2:98:C:VAL:C	2:99:C:THR:N	12	1.55
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	1	1.55
(1,78)	1:14:B:LEU:N	1:14:B:LEU:CA	1:14:B:LEU:C	1:15:B:THR:N	19	1.54
(1,54)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:TYR:N	20	1.54
(1,52)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:GLU:N	8	1.53
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	6	1.53
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	4	1.53
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	12	1.53
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	18	1.52
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	13	1.52
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	9	1.5
(1,107)	1:32:B:ASP:C	1:33:B:LEU:N	1:33:B:LEU:CA	1:33:B:LEU:C	14	1.49
(1,94)	1:23:B:VAL:N	1:23:B:VAL:CA	1:23:B:VAL:C	1:24:B:GLU:N	11	1.49
(1,137)	2:88:C:GLU:C	2:89:C:GLU:N	2:89:C:GLU:CA	2:89:C:GLU:C	7	1.46
(1,130)	1:45:B:ARG:N	1:45:B:ARG:CA	1:45:B:ARG:C	1:46:B:GLU:N	18	1.46
(1,90)	1:21:B:TYR:N	1:21:B:TYR:CA	1:21:B:TYR:C	1:22:B:THR:N	7	1.46
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	3	1.46
(1,10)	1:14:A:LEU:N	1:14:A:LEU:CA	1:14:A:LEU:C	1:15:A:THR:N	15	1.46
(1,130)	1:45:B:ARG:N	1:45:B:ARG:CA	1:45:B:ARG:C	1:46:B:GLU:N	10	1.45
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	18	1.44
(1,64)	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	1:46:A:GLU:N	17	1.44
(1,71)	1:8:B:ILE:C	1:9:B:GLN:N	1:9:B:GLN:CA	1:9:B:GLN:C	6	1.41
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	16	1.41
(1,78)	1:14:B:LEU:N	1:14:B:LEU:CA	1:14:B:LEU:C	1:15:B:THR:N	8	1.39
(1,36)	1:28:A:GLN:N	1:28:A:GLN:CA	1:28:A:GLN:C	1:29:A:GLN:N	1	1.39
(1,150)	2:95:C:VAL:N	2:95:C:VAL:CA	2:95:C:VAL:C	2:96:C:GLN:N	19	1.37
(1,133)	2:86:C:THR:C	2:87:C:ALA:N	2:87:C:ALA:CA	2:87:C:ALA:C	5	1.37
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	16	1.37
(1,111)	1:34:B:VAL:C	1:35:B:GLU:N	1:35:B:GLU:CA	1:35:B:GLU:C	9	1.37
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	10	1.37
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	16	1.35
(1,28)	1:24:A:GLU:N	1:24:A:GLU:CA	1:24:A:GLU:C	1:25:A:VAL:N	12	1.34
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	18	1.34
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	20	1.33
(1,7)	1:12:A:PRO:C	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	3	1.33



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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation ( $^{\circ}$ )
(1,137)	2:88:C:GLU:C	2:89:C:GLU:N	2:89:C:GLU:CA	2:89:C:GLU:C	5	1.31
(1,118)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:GLU:N	8	1.3
(1,90)	1:21:B:TYR:N	1:21:B:TYR:CA	1:21:B:TYR:C	1:22:B:THR:N	9	1.28
(1,136)	2:88:C:GLU:N	2:88:C:GLU:CA	2:88:C:GLU:C	2:89:C:GLU:N	5	1.27
(1,7)	1:12:A:PRO:C	1:13:A:GLY:N	1:13:A:GLY:CA	1:13:A:GLY:C	5	1.27
(1,47)	1:35:A:GLU:C	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	3	1.25
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	20	1.25
(1,15)	1:16:A:GLU:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	13	1.25
(1,75)	1:12:B:PRO:C	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	6	1.23
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	8	1.22
(1,65)	1:45:A:ARG:C	1:46:A:GLU:N	1:46:A:GLU:CA	1:46:A:GLU:C	20	1.21
(1,44)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLU:N	13	1.21
(1,133)	2:86:C:THR:C	2:87:C:ALA:N	2:87:C:ALA:CA	2:87:C:ALA:C	9	1.2
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	3	1.2
(1,103)	1:27:B:ARG:C	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	15	1.18
(1,54)	1:39:A:GLU:N	1:39:A:GLU:CA	1:39:A:GLU:C	1:40:A:TYR:N	9	1.18
(1,5)	1:9:A:GLN:C	1:10:A:ILE:N	1:10:A:ILE:CA	1:10:A:ILE:C	6	1.18
(1,52)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:GLU:N	12	1.17
(1,14)	1:16:A:GLU:N	1:16:A:GLU:CA	1:16:A:GLU:C	1:17:A:LEU:N	8	1.16
(1,12)	1:15:A:THR:N	1:15:A:THR:CA	1:15:A:THR:C	1:16:A:GLU:N	2	1.16
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	7	1.15
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	5	1.15
(1,63)	1:44:A:LEU:C	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	20	1.15
(1,50)	1:37:A:ALA:N	1:37:A:ALA:CA	1:37:A:ALA:C	1:38:A:VAL:N	4	1.15
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	9	1.14
(1,90)	1:21:B:TYR:N	1:21:B:TYR:CA	1:21:B:TYR:C	1:22:B:THR:N	18	1.13
(1,123)	1:40:B:TYR:C	1:41:B:PHE:N	1:41:B:PHE:CA	1:41:B:PHE:C	4	1.11
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	11	1.11
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	12	1.11
(1,15)	1:16:A:GLU:C	1:17:A:LEU:N	1:17:A:LEU:CA	1:17:A:LEU:C	2	1.11
(1,167)	2:103:C:VAL:C	2:104:C:ALA:N	2:104:C:ALA:CA	2:104:C:ALA:C	20	1.1
(1,52)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:GLU:N	11	1.1
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	19	1.1
(1,78)	1:14:B:LEU:N	1:14:B:LEU:CA	1:14:B:LEU:C	1:15:B:THR:N	2	1.09
(1,104)	1:28:B:GLN:N	1:28:B:GLN:CA	1:28:B:GLN:C	1:29:B:GLN:N	16	1.08
(1,150)	2:95:C:VAL:N	2:95:C:VAL:CA	2:95:C:VAL:C	2:96:C:GLN:N	10	1.07
(1,126)	1:42:B:THR:N	1:42:B:THR:CA	1:42:B:THR:C	1:43:B:ARG:N	15	1.07
(1,94)	1:23:B:VAL:N	1:23:B:VAL:CA	1:23:B:VAL:C	1:24:B:GLU:N	18	1.07
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	11	1.07
(1,68)	1:47:A:ALA:N	1:47:A:ALA:CA	1:47:A:ALA:C	1:48:A:ARG:N	7	1.07
(1,47)	1:35:A:GLU:C	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	13	1.07
(1,174)	2:109:C:GLU:N	2:109:C:GLU:CA	2:109:C:GLU:C	2:110:C:GLN:N	20	1.06
(1,131)	2:85:C:GLU:C	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	1	1.06
(1,52)	1:38:A:VAL:N	1:38:A:VAL:CA	1:38:A:VAL:C	1:39:A:GLU:N	1	1.06
(1,44)	1:34:A:VAL:N	1:34:A:VAL:CA	1:34:A:VAL:C	1:35:A:GLU:N	17	1.05
(1,29)	1:24:A:GLU:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	14	1.05
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	7	1.04
(1,76)	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	1:14:B:LEU:N	6	1.04
(1,75)	1:12:B:PRO:C	1:13:B:GLY:N	1:13:B:GLY:CA	1:13:B:GLY:C	18	1.04
(1,148)	2:94:C:ILE:N	2:94:C:ILE:CA	2:94:C:1LE:C	2:95:C:VAL:N	10	1.03
(1,136)	2:88:C:GLU:N	2:88:C:GLU:CA	2:88:C:GLU:C	2:89:C:GLU:N	7	1.03



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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation ( $^{\circ}$ )
(1,118)	1:38:B:VAL:N	1:38:B:VAL:CA	1:38:B:VAL:C	1:39:B:GLU:N	14	1.03
(1,74)	1:10:B:ILE:N	1:10:B:ILE:CA	1:10:B:ILE:C	1:11:B:PRO:N	18	1.03
(1,37)	1:28:A:GLN:C	1:29:A:GLN:N	1:29:A:GLN:CA	1:29:A:GLN:C	14	1.03
(1,170)	2:105:C:VAL:N	2:105:C:VAL:CA	2:105:C:VAL:C	2:106:C:LEU:N	3	1.02
(1,130)	1:45:B:ARG:N	1:45:B:ARG:CA	1:45:B:ARG:C	1:46:B:GLU:N	14	1.02
(1,64)	1:45:A:ARG:N	1:45:A:ARG:CA	1:45:A:ARG:C	1:46:A:GLU:N	20	1.02
(1,56)	1:40:A:TYR:N	1:40:A:TYR:CA	1:40:A:TYR:C	1:41:A:PHE:N	19	1.01
(1,48)	1:36:A:PHE:N	1:36:A:PHE:CA	1:36:A:PHE:C	1:37:A:ALA:N	1	1.01
(1,132)	2:86:C:THR:N	2:86:C:THR:CA	2:86:C:THR:C	2:87:C:ALA:N	4	1.0
(1,29)	1:24:A:GLU:C	1:25:A:VAL:N	1:25:A:VAL:CA	1:25:A:VAL:C	9	1.0

