



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 06:05 AM UTC

PDB ID : 6DLN / pdb_00006dlh
BMRB ID : 30472
Title : Oligomeric Structure of the HIV gp41 MPER-TMD in Phospholipid Bilayers
Authors : Kwon, B.; Lee, M.; Waring, A.J.; Hong, M.
Deposited on : 2018-06-01

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

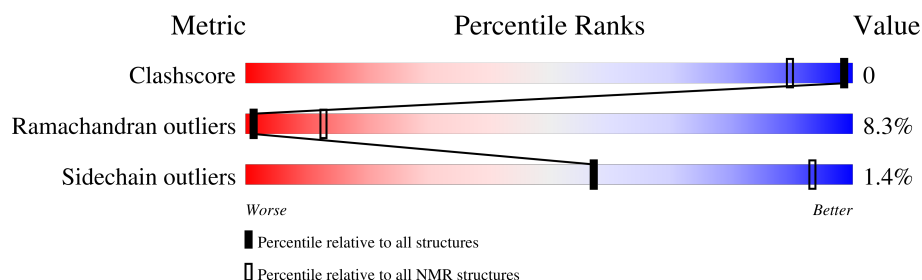
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 1%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	39	38% 56% 5%
1	B	39	44% 54% .
1	C	39	46% 49% 5%

2 Ensemble composition and analysis

This entry contains 10 models. Model 10 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:1-A:39, B:40-B:78, C:79-C:117 (117)	0.73	10

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

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

The models can be grouped into 2 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 7
2	8, 9, 10
Single-model clusters	2; 5; 6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2043 atoms, of which 1041 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transmembrane protein gp41.

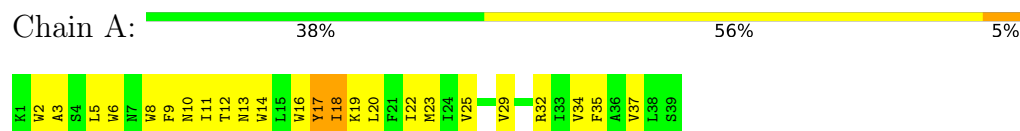
Mol	Chain	Residues	Atoms						Trace
1	A	39	Total	C	H	N	O	S	0
			681	234	347	52	47	1	
1	B	39	Total	C	H	N	O	S	0
			681	234	347	52	47	1	
1	C	39	Total	C	H	N	O	S	0
			681	234	347	52	47	1	

4 Residue-property plots

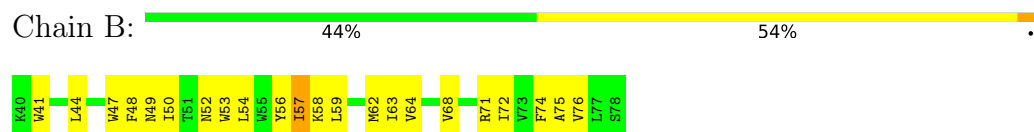
4.1 Average score per residue in the NMR ensemble

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

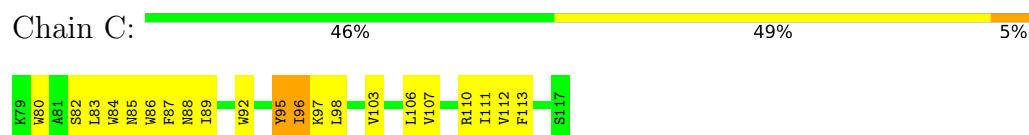
- Molecule 1: Transmembrane protein gp41



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- Molecule 1: Transmembrane protein gp41

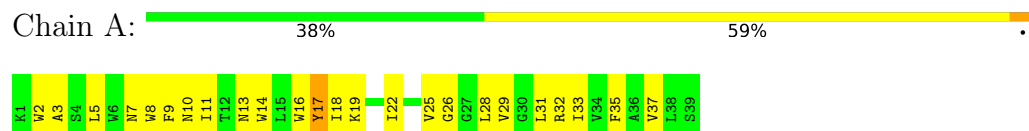


4.2 Scores per residue for each member of the ensemble

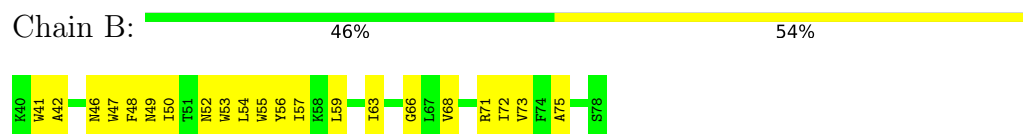
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

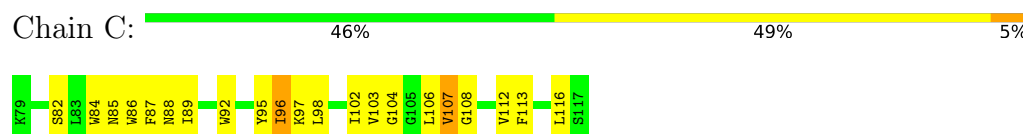
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

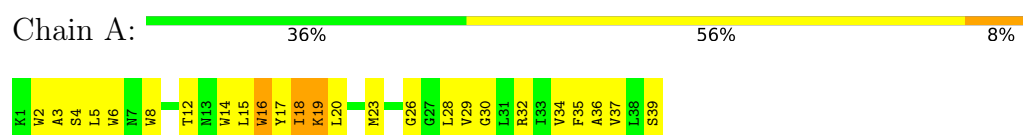


- Molecule 1: Transmembrane protein gp41

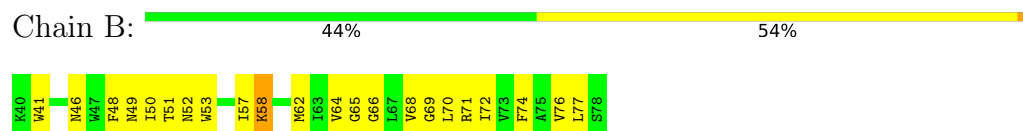


4.2.2 Score per residue for model 2

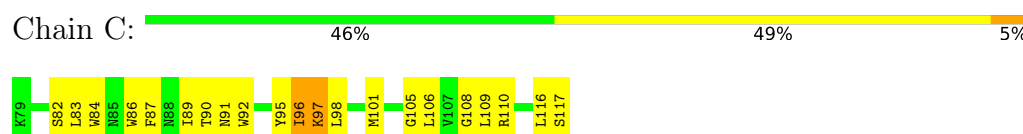
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

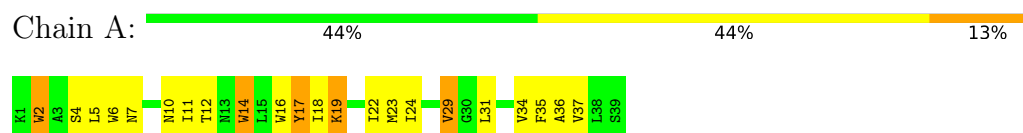


- Molecule 1: Transmembrane protein gp41

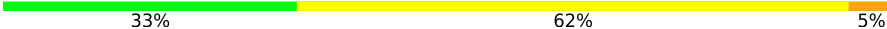


4.2.3 Score per residue for model 3

- Molecule 1: Transmembrane protein gp41

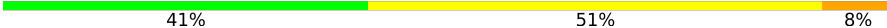


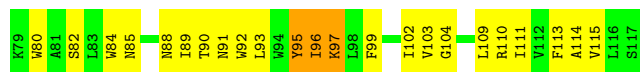
- Molecule 1: Transmembrane protein gp41

Chain B:  33% 62% 5%



- Molecule 1: Transmembrane protein gp41

Chain C:  41% 51% 8%



4.2.4 Score per residue for model 4

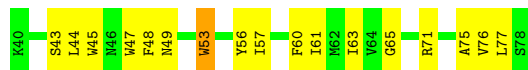
- Molecule 1: Transmembrane protein gp41

Chain A:  36% 59% 5%

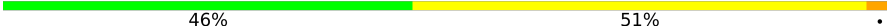


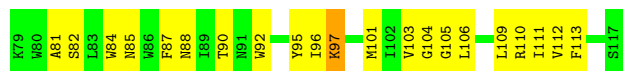
- Molecule 1: Transmembrane protein gp41

Chain B:  56% 41% 3%



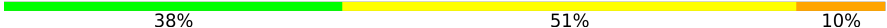
- Molecule 1: Transmembrane protein gp41

Chain C:  46% 51% 3%



4.2.5 Score per residue for model 5

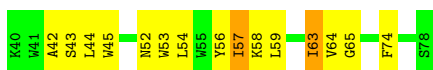
- Molecule 1: Transmembrane protein gp41

Chain A:  38% 51% 10%



- Molecule 1: Transmembrane protein gp41

Chain B:  62% 33% 5%



- Molecule 1: Transmembrane protein gp41

Chain C: 44% 51% 5%



4.2.6 Score per residue for model 6

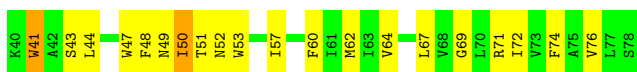
- Molecule 1: Transmembrane protein gp41

Chain A: 44% 46% 8% .



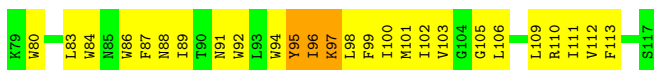
- Molecule 1: Transmembrane protein gp41

Chain B: 49% 46% 5%



- Molecule 1: Transmembrane protein gp41

Chain C: 33% 59% 8%



4.2.7 Score per residue for model 7

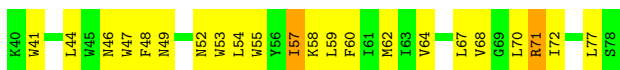
- Molecule 1: Transmembrane protein gp41

Chain A: 26% 62% 13%

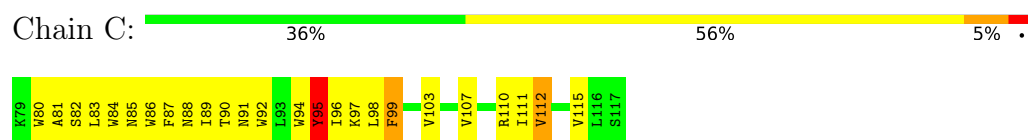


- Molecule 1: Transmembrane protein gp41

Chain B: 44% 51% 5%

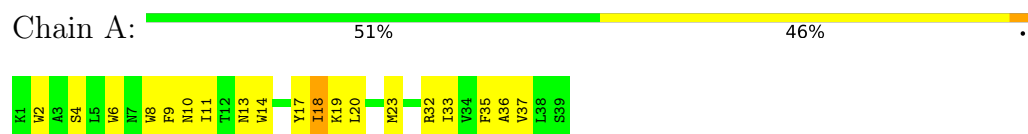


- Molecule 1: Transmembrane protein gp41

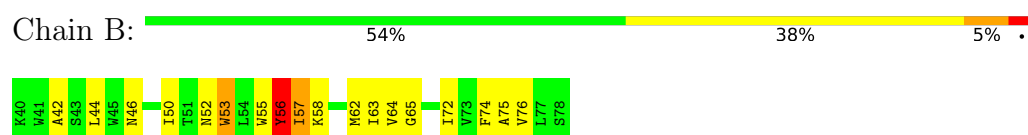


4.2.8 Score per residue for model 8

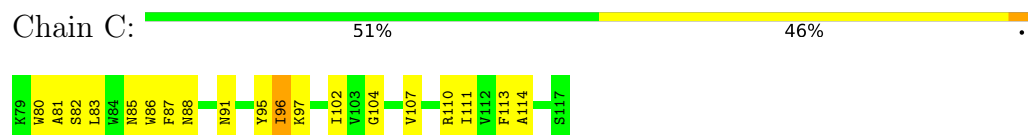
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

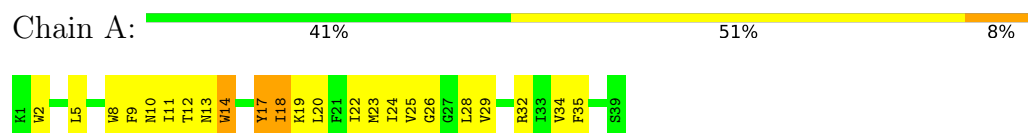


- Molecule 1: Transmembrane protein gp41

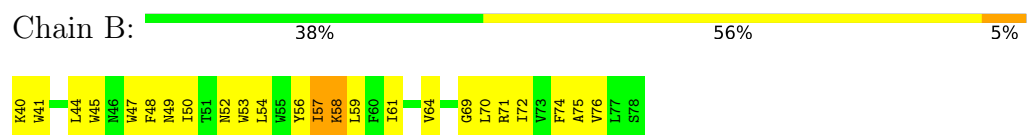


4.2.9 Score per residue for model 9

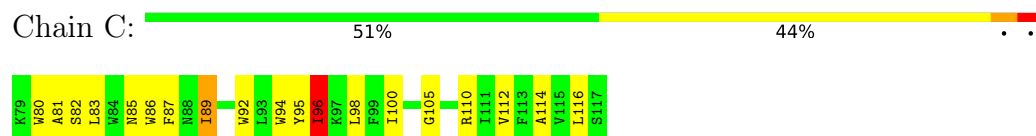
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41

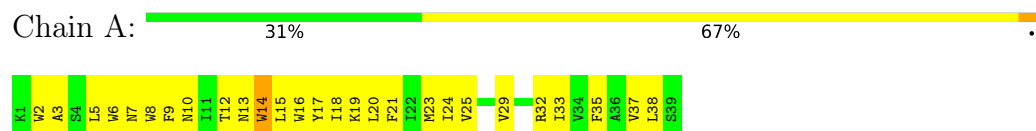


- Molecule 1: Transmembrane protein gp41

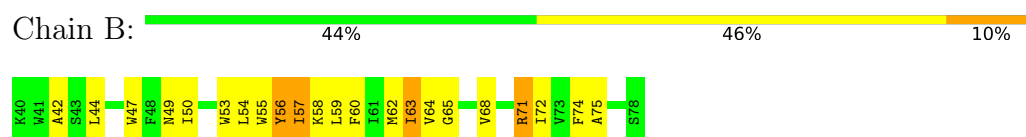


4.2.10 Score per residue for model 10 (medoid)

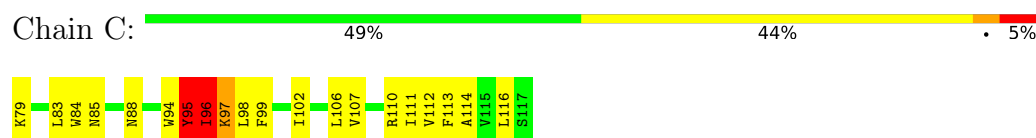
- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41



- Molecule 1: Transmembrane protein gp41



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
GROMACS	refinement	
CHARMM-GUI	refinement	
GROMACS	structure calculation	
CHARMM-GUI	structure calculation	

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	23
Number of shifts mapped to atoms	23
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.13±0.10	10±3/347 (2.9± 0.8%)	2.52±0.09	27±5/473 (5.7± 1.1%)
1	B	2.09±0.08	9±2/347 (2.6± 0.7%)	2.41±0.08	22±5/473 (4.8± 1.0%)
1	C	2.07±0.05	8±2/347 (2.2± 0.6%)	2.48±0.15	27±5/473 (5.8± 1.1%)
All	All	2.10	266/10410 (2.6%)	2.47	766/14190 (5.4%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.8±0.6
1	C	0.0±0.0	0.5±0.9
1	B	0.0±0.0	0.6±0.9
All	All	0	19

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	33	ILE	CA-C	10.16	1.65	1.52	1	1
1	A	16	TRP	NE1-CE2	-10.05	1.26	1.37	2	2
1	A	26	GLY	C-N	9.74	1.45	1.33	7	2
1	B	68	VAL	CA-C	-8.97	1.41	1.52	2	1
1	A	5	LEU	C-N	8.95	1.45	1.33	9	2
1	A	6	TRP	CA-CB	8.89	1.67	1.53	3	2
1	C	90	THR	CA-C	-8.83	1.41	1.52	4	1
1	A	26	GLY	CA-C	-8.76	1.42	1.52	2	1
1	A	29	VAL	CA-C	8.55	1.64	1.52	2	1
1	C	116	LEU	CA-CB	8.49	1.68	1.53	10	1
1	A	23	MET	C-N	8.44	1.44	1.33	5	3
1	A	4	SER	CA-C	8.43	1.63	1.52	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	109	LEU	CA-C	8.32	1.64	1.52	2	2
1	C	105	GLY	CA-C	-8.28	1.42	1.52	6	2
1	C	92	TRP	CA-CB	8.21	1.59	1.53	1	2
1	B	47	TRP	NE1-CE2	8.09	1.46	1.37	3	2
1	A	18	ILE	CA-C	8.07	1.62	1.52	4	2
1	A	16	TRP	CA-CB	7.94	1.64	1.53	5	2
1	A	11	ILE	CA-CB	7.67	1.63	1.54	1	1
1	B	72	ILE	CA-C	7.67	1.62	1.52	1	4
1	B	68	VAL	N-CA	7.65	1.55	1.46	3	1
1	C	84	TRP	N-CA	-7.63	1.37	1.46	7	1
1	A	20	LEU	N-CA	-7.57	1.35	1.46	9	2
1	C	89	ILE	CA-C	-7.50	1.43	1.52	6	2
1	A	10	ASN	N-CA	-7.37	1.37	1.46	9	1
1	C	85	ASN	N-CA	-7.35	1.36	1.46	8	1
1	C	100	ILE	CA-CB	-7.35	1.46	1.54	5	2
1	C	88	ASN	C-N	7.31	1.43	1.33	7	2
1	B	53	TRP	NE1-CE2	-7.30	1.29	1.37	4	1
1	C	90	THR	CA-CB	7.28	1.64	1.53	7	1
1	A	30	GLY	CA-C	-7.27	1.42	1.51	6	1
1	A	5	LEU	CA-CB	7.27	1.64	1.53	10	1
1	B	41	TRP	N-CA	-7.25	1.37	1.46	1	1
1	B	64	VAL	C-N	-7.20	1.24	1.33	2	2
1	A	21	PHE	CA-C	7.18	1.62	1.52	4	1
1	C	97	LYS	C-O	-7.13	1.16	1.24	3	1
1	A	3	ALA	C-N	7.12	1.43	1.33	7	1
1	C	97	LYS	CA-C	-7.10	1.43	1.52	8	1
1	B	61	ILE	CA-CB	-7.10	1.44	1.54	9	1
1	C	87	PHE	CA-CB	7.05	1.64	1.53	4	2
1	C	109	LEU	CA-CB	6.96	1.64	1.53	4	1
1	B	66	GLY	CA-C	-6.95	1.43	1.51	1	1
1	C	114	ALA	CA-C	6.93	1.61	1.52	9	1
1	A	23	MET	CA-C	6.92	1.62	1.52	4	1
1	B	71	ARG	CA-C	6.87	1.62	1.52	3	1
1	B	52	ASN	C-N	6.87	1.43	1.33	6	2
1	A	7	ASN	CA-C	-6.78	1.44	1.52	7	1
1	A	32	ARG	C-N	6.78	1.42	1.33	1	1
1	A	22	ILE	C-N	6.75	1.43	1.34	3	2
1	B	74	PHE	C-N	6.74	1.43	1.34	3	1
1	B	58	LYS	CA-CB	6.70	1.64	1.53	3	1
1	C	84	TRP	CA-C	6.69	1.61	1.52	3	2
1	B	62	MET	C-N	6.64	1.42	1.33	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	56	TYR	C-N	6.60	1.42	1.33	8	1
1	B	55	TRP	CA-C	6.60	1.60	1.52	8	3
1	B	50	ILE	N-CA	6.59	1.54	1.46	2	2
1	C	112	VAL	CA-CB	6.59	1.62	1.54	4	1
1	A	34	VAL	CA-C	-6.59	1.43	1.52	9	2
1	B	56	TYR	CA-C	-6.58	1.44	1.52	9	1
1	A	18	ILE	CA-CB	6.56	1.63	1.54	5	1
1	A	8	TRP	N-CA	-6.53	1.38	1.46	2	1
1	B	77	LEU	C-N	6.51	1.42	1.33	7	1
1	B	75	ALA	C-N	6.51	1.42	1.33	3	3
1	C	99	PHE	C-N	6.50	1.42	1.33	3	1
1	B	47	TRP	CA-C	6.46	1.61	1.52	1	2
1	A	25	VAL	CA-C	-6.44	1.45	1.52	10	1
1	B	48	PHE	CA-CB	6.40	1.63	1.53	1	2
1	A	32	ARG	CD-NE	6.39	1.55	1.46	4	2
1	A	15	LEU	CA-C	-6.38	1.44	1.52	10	1
1	A	16	TRP	CA-C	6.37	1.60	1.52	10	2
1	B	47	TRP	CA-CB	6.35	1.63	1.53	6	1
1	C	112	VAL	CA-C	-6.34	1.45	1.52	7	1
1	A	34	VAL	CA-CB	-6.33	1.46	1.54	2	1
1	B	71	ARG	N-CA	6.31	1.54	1.46	6	2
1	C	116	LEU	C-N	6.28	1.42	1.33	2	2
1	B	52	ASN	CA-CB	6.27	1.63	1.53	1	1
1	B	67	LEU	N-CA	6.27	1.53	1.46	3	2
1	C	96	ILE	N-CA	-6.27	1.38	1.46	9	1
1	C	88	ASN	CA-C	6.24	1.60	1.52	3	1
1	A	15	LEU	C-O	-6.23	1.15	1.24	6	1
1	A	31	LEU	CA-CB	6.20	1.62	1.53	4	1
1	A	11	ILE	CA-C	-6.18	1.45	1.52	9	1
1	B	50	ILE	CA-CB	6.18	1.62	1.54	10	1
1	B	57	ILE	N-CA	-6.17	1.38	1.46	7	1
1	A	31	LEU	C-N	6.13	1.42	1.33	1	1
1	B	61	ILE	C-N	6.12	1.42	1.33	4	1
1	A	13	ASN	CA-C	6.12	1.60	1.52	10	1
1	A	35	PHE	N-CA	-6.11	1.39	1.46	1	1
1	B	45	TRP	C-N	6.10	1.42	1.33	5	1
1	A	39	SER	CA-CB	6.08	1.65	1.53	2	3
1	B	40	LYS	C-N	6.07	1.42	1.33	9	1
1	A	2	TRP	CA-CB	6.06	1.63	1.53	5	2
1	A	17	TYR	CA-C	6.06	1.60	1.52	5	1
1	B	58	LYS	C-O	-6.05	1.16	1.24	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	C	83	LEU	CA-CB	6.05	1.62	1.53	10	1
1	A	9	PHE	CA-CB	6.04	1.62	1.53	7	1
1	A	36	ALA	N-CA	-6.03	1.39	1.46	3	2
1	A	10	ASN	CA-CB	6.02	1.62	1.53	1	1
1	B	71	ARG	C-N	-6.00	1.26	1.33	2	1
1	B	72	ILE	C-N	5.96	1.41	1.33	9	1
1	A	12	THR	CA-C	-5.95	1.45	1.52	10	2
1	B	57	ILE	CA-CB	5.92	1.62	1.54	5	1
1	B	70	LEU	CA-CB	5.91	1.62	1.53	7	1
1	C	89	ILE	N-CA	5.90	1.53	1.46	1	2
1	C	91	ASN	CA-C	5.87	1.60	1.53	2	1
1	C	101	MET	CA-C	5.87	1.60	1.52	2	1
1	A	38	LEU	N-CA	-5.86	1.39	1.46	6	1
1	B	48	PHE	CA-C	5.86	1.60	1.52	4	1
1	A	21	PHE	C-N	5.83	1.40	1.33	7	1
1	B	57	ILE	C-N	5.77	1.41	1.33	5	1
1	B	58	LYS	N-CA	5.76	1.53	1.46	7	1
1	B	70	LEU	CA-C	5.76	1.60	1.52	3	1
1	A	29	VAL	N-CA	-5.76	1.39	1.46	5	1
1	B	44	LEU	C-N	5.72	1.41	1.33	10	1
1	A	18	ILE	C-N	5.70	1.41	1.33	7	2
1	C	100	ILE	CA-C	-5.70	1.45	1.52	9	2
1	B	44	LEU	CA-C	5.69	1.60	1.52	6	2
1	B	63	ILE	CA-C	5.69	1.59	1.52	8	1
1	C	114	ALA	C-N	5.67	1.41	1.33	5	1
1	B	63	ILE	CA-CB	-5.67	1.47	1.54	3	1
1	C	96	ILE	C-N	5.67	1.39	1.32	3	1
1	A	35	PHE	CA-CB	5.64	1.62	1.53	2	1
1	A	37	VAL	CA-C	-5.64	1.46	1.52	3	2
1	B	44	LEU	CA-CB	5.64	1.62	1.53	7	2
1	B	49	ASN	CA-C	5.62	1.60	1.52	1	1
1	A	22	ILE	CA-CB	-5.61	1.47	1.54	9	2
1	B	72	ILE	CA-CB	-5.60	1.48	1.54	3	2
1	A	8	TRP	CA-CB	5.59	1.62	1.53	6	1
1	B	45	TRP	CZ2-CH2	5.58	1.47	1.37	5	1
1	C	84	TRP	CA-CB	5.58	1.62	1.53	2	1
1	B	42	ALA	C-N	5.56	1.41	1.33	1	1
1	A	19	LYS	CA-C	5.56	1.60	1.52	2	1
1	C	110	ARG	CA-C	5.56	1.60	1.52	8	1
1	C	113	PHE	N-CA	-5.55	1.39	1.46	3	2
1	B	45	TRP	CA-CB	5.55	1.61	1.53	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	9	PHE	C-O	-5.54	1.17	1.24	8	1
1	C	105	GLY	N-CA	5.54	1.52	1.45	4	1
1	C	91	ASN	N-CA	5.53	1.52	1.46	7	1
1	A	6	TRP	C-N	5.53	1.41	1.33	6	1
1	C	94	TRP	CA-CB	5.51	1.62	1.53	9	1
1	C	86	TRP	CA-CB	5.50	1.62	1.53	5	3
1	C	84	TRP	NE1-CE2	-5.49	1.31	1.37	3	1
1	C	112	VAL	N-CA	-5.48	1.40	1.46	7	2
1	A	3	ALA	C-O	5.48	1.30	1.24	2	1
1	B	51	THR	N-CA	5.46	1.52	1.46	6	1
1	A	31	LEU	N-CA	-5.45	1.39	1.46	6	1
1	B	41	TRP	CA-C	5.45	1.60	1.52	7	1
1	A	36	ALA	CA-C	-5.44	1.45	1.52	7	1
1	A	30	GLY	C-N	5.43	1.41	1.33	6	1
1	A	14	TRP	C-N	5.41	1.41	1.33	9	1
1	B	63	ILE	C-N	5.40	1.40	1.33	1	1
1	A	9	PHE	N-CA	5.39	1.52	1.46	1	1
1	A	29	VAL	CA-CB	-5.39	1.47	1.54	2	1
1	A	3	ALA	CA-C	5.38	1.59	1.52	5	1
1	A	28	LEU	C-O	-5.36	1.17	1.24	1	1
1	B	76	VAL	C-N	5.35	1.41	1.34	4	1
1	C	103	VAL	CA-CB	5.34	1.60	1.54	7	1
1	A	19	LYS	C-N	5.34	1.41	1.34	4	1
1	C	106	LEU	C-N	5.33	1.40	1.33	1	1
1	B	46	ASN	CA-CB	5.32	1.61	1.53	8	1
1	C	110	ARG	C-N	5.31	1.40	1.33	8	2
1	B	71	ARG	CA-CB	5.31	1.62	1.53	7	1
1	B	76	VAL	N-CA	5.31	1.52	1.46	2	1
1	A	21	PHE	CA-CB	5.31	1.61	1.53	6	1
1	A	20	LEU	CA-C	-5.30	1.45	1.52	8	2
1	A	14	TRP	CA-CB	5.27	1.62	1.53	10	1
1	A	2	TRP	N-CA	-5.27	1.42	1.47	1	1
1	B	63	ILE	N-CA	5.26	1.52	1.46	5	1
1	A	38	LEU	C-N	5.26	1.40	1.33	10	1
1	C	92	TRP	NE1-CE2	-5.25	1.31	1.37	2	1
1	B	60	PHE	N-CA	-5.24	1.40	1.46	6	1
1	B	47	TRP	CD2-CE2	5.23	1.50	1.41	6	1
1	B	64	VAL	CA-CB	-5.23	1.47	1.54	9	1
1	C	87	PHE	C-N	5.22	1.41	1.33	2	1
1	C	111	ILE	CA-C	5.21	1.58	1.52	3	1
1	B	65	GLY	C-N	5.21	1.40	1.33	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	52	ASN	CA-C	-5.20	1.46	1.52	5	1
1	A	12	THR	N-CA	-5.20	1.40	1.46	5	1
1	C	96	ILE	CA-C	-5.19	1.46	1.52	9	1
1	A	20	LEU	C-O	-5.19	1.17	1.24	7	1
1	C	110	ARG	CA-CB	5.19	1.61	1.53	4	1
1	B	71	ARG	CD-NE	5.18	1.53	1.46	2	1
1	B	45	TRP	CA-C	-5.17	1.46	1.52	5	1
1	B	49	ASN	CA-CB	5.16	1.61	1.53	7	1
1	A	17	TYR	C-N	5.15	1.40	1.33	5	1
1	C	104	GLY	C-N	5.15	1.40	1.34	1	1
1	B	65	GLY	CA-C	-5.14	1.45	1.52	8	1
1	A	28	LEU	N-CA	-5.14	1.40	1.46	4	1
1	A	6	TRP	C-O	-5.13	1.18	1.24	8	1
1	C	99	PHE	N-CA	5.13	1.52	1.46	6	1
1	A	38	LEU	CA-C	-5.12	1.45	1.52	7	1
1	C	94	TRP	CA-C	-5.12	1.46	1.52	9	1
1	C	104	GLY	CA-C	-5.09	1.46	1.52	4	1
1	B	65	GLY	C-O	-5.09	1.17	1.23	10	1
1	C	106	LEU	CB-CG	5.07	1.63	1.53	6	1
1	C	84	TRP	C-N	5.07	1.40	1.33	4	2
1	C	95	TYR	C-N	5.05	1.40	1.33	9	1
1	C	95	TYR	CA-CB	5.05	1.62	1.53	6	1
1	C	107	VAL	CA-CB	5.04	1.60	1.54	5	1
1	C	86	TRP	NE1-CE2	-5.04	1.31	1.37	2	1
1	C	95	TYR	N-CA	5.04	1.52	1.46	10	1
1	A	4	SER	C-O	-5.04	1.18	1.24	5	1
1	B	72	ILE	N-CA	5.03	1.52	1.46	6	1
1	A	37	VAL	CA-CB	5.02	1.60	1.54	1	1
1	A	25	VAL	CA-CB	5.01	1.60	1.54	1	1
1	C	107	VAL	CA-C	5.01	1.59	1.52	7	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	103	VAL	CA-C-N	13.20	134.63	119.98	6	3
1	C	103	VAL	C-N-CA	13.20	134.63	119.98	6	3
1	B	77	LEU	N-CA-C	10.50	124.00	111.82	4	1
1	C	90	THR	N-CA-C	10.40	122.20	111.07	4	1
1	C	80	TRP	N-CA-C	10.39	122.61	111.28	7	2
1	A	19	LYS	CA-C-N	10.30	135.11	120.28	10	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	19	LYS	C-N-CA	10.30	135.11	120.28	10	7
1	A	33	ILE	N-CA-C	10.08	120.95	110.36	10	1
1	B	71	ARG	NE-CZ-NH2	10.00	128.20	119.20	1	2
1	A	9	PHE	CA-CB-CG	9.79	123.59	113.80	4	3
1	C	110	ARG	NE-CZ-NH1	9.60	131.10	121.50	4	4
1	B	48	PHE	N-CA-C	9.52	121.65	111.28	6	2
1	A	11	ILE	N-CA-C	9.48	120.29	110.62	3	4
1	B	42	ALA	N-CA-C	9.45	121.18	111.07	10	3
1	A	7	ASN	CA-C-N	9.35	132.80	120.28	3	1
1	A	7	ASN	C-N-CA	9.35	132.80	120.28	3	1
1	A	7	ASN	N-CA-C	9.33	121.45	111.28	10	1
1	B	58	LYS	CA-C-N	9.33	137.46	121.14	9	4
1	B	58	LYS	C-N-CA	9.33	137.46	121.14	9	4
1	C	98	LEU	CA-C-O	9.31	130.76	119.49	1	1
1	B	64	VAL	N-CA-C	9.22	120.02	110.62	3	4
1	C	91	ASN	CA-CB-CG	9.21	121.81	112.60	6	1
1	A	13	ASN	N-CA-C	9.02	121.19	111.36	5	2
1	B	49	ASN	N-CA-C	8.95	120.65	111.07	4	2
1	C	88	ASN	CA-CB-CG	-8.94	103.66	112.60	6	5
1	A	3	ALA	N-CA-C	8.90	120.98	111.28	4	4
1	A	35	PHE	O-C-N	-8.87	112.86	122.09	10	4
1	B	68	VAL	N-CA-C	8.72	119.52	110.62	7	1
1	C	103	VAL	N-CA-CB	-8.62	99.53	110.57	1	1
1	C	97	LYS	CA-C-N	8.61	137.99	121.54	7	7
1	C	97	LYS	C-N-CA	8.61	137.99	121.54	7	7
1	C	85	ASN	CA-CB-CG	8.59	121.19	112.60	10	3
1	A	18	ILE	CA-C-N	8.54	137.86	121.54	9	2
1	A	18	ILE	C-N-CA	8.54	137.86	121.54	9	2
1	A	15	LEU	N-CA-C	-8.28	104.05	114.56	2	2
1	B	75	ALA	N-CA-C	8.22	120.32	111.36	8	3
1	B	65	GLY	CA-C-N	8.18	128.86	119.94	8	2
1	B	65	GLY	C-N-CA	8.18	128.86	119.94	8	2
1	C	88	ASN	N-CA-C	8.18	120.19	111.28	5	1
1	A	33	ILE	CA-C-N	8.11	133.28	120.47	5	2
1	A	33	ILE	C-N-CA	8.11	133.28	120.47	5	2
1	A	6	TRP	O-C-N	-8.10	112.91	122.15	10	2
1	A	37	VAL	N-CA-C	8.10	118.88	110.62	2	2
1	C	107	VAL	N-CA-C	8.09	118.87	110.62	8	2
1	A	10	ASN	N-CA-C	8.06	120.07	111.28	8	3
1	A	7	ASN	CA-CB-CG	-8.06	104.54	112.60	1	3
1	A	11	ILE	CA-C-N	8.00	130.84	120.44	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	11	ILE	C-N-CA	8.00	130.84	120.44	5	1
1	A	29	VAL	N-CA-C	7.99	118.77	110.62	5	5
1	B	72	ILE	N-CA-C	7.97	118.75	110.62	10	1
1	C	86	TRP	N-CA-C	7.96	120.96	111.33	6	1
1	C	99	PHE	CA-C-O	7.93	128.95	120.55	10	2
1	A	17	TYR	N-CA-C	7.89	127.61	110.80	5	5
1	B	63	ILE	N-CA-C	7.88	118.65	110.62	10	3
1	C	85	ASN	N-CA-C	7.84	119.82	111.28	9	1
1	A	24	ILE	N-CA-C	7.83	117.93	110.42	4	2
1	C	103	VAL	N-CA-C	7.74	117.85	110.42	7	4
1	C	110	ARG	CA-C-N	7.72	130.44	120.56	10	3
1	C	110	ARG	C-N-CA	7.72	130.44	120.56	10	3
1	B	55	TRP	CB-CG-CD2	-7.71	116.00	126.80	7	1
1	B	54	LEU	N-CA-C	-7.70	104.49	114.04	5	5
1	B	77	LEU	O-C-N	-7.67	111.52	122.41	3	1
1	C	110	ARG	N-CA-C	7.66	120.71	111.82	3	4
1	C	98	LEU	CA-C-N	7.64	132.29	120.82	2	5
1	C	98	LEU	C-N-CA	7.64	132.29	120.82	2	5
1	B	55	TRP	O-C-N	-7.62	114.79	123.48	7	1
1	B	59	LEU	CA-C-N	7.62	130.49	120.28	7	4
1	B	59	LEU	C-N-CA	7.62	130.49	120.28	7	4
1	C	107	VAL	N-CA-CB	7.60	120.88	110.54	10	1
1	B	63	ILE	O-C-N	-7.60	114.46	121.91	5	1
1	A	24	ILE	O-C-N	-7.55	114.05	121.83	9	1
1	C	101	MET	N-CA-C	7.52	119.48	111.28	5	1
1	A	5	LEU	N-CA-C	7.51	119.11	111.07	9	2
1	A	35	PHE	CA-CB-CG	-7.51	106.28	113.80	3	2
1	B	50	ILE	CA-C-N	7.51	130.20	120.44	10	4
1	B	50	ILE	C-N-CA	7.51	130.20	120.44	10	4
1	C	87	PHE	CA-CB-CG	-7.49	106.31	113.80	1	1
1	A	25	VAL	O-C-N	-7.47	114.13	121.90	7	2
1	C	106	LEU	N-CA-C	7.47	119.42	111.28	2	3
1	C	89	ILE	N-CA-CB	7.45	119.26	110.55	2	2
1	C	82	SER	CA-C-N	7.42	130.22	120.28	7	4
1	C	82	SER	C-N-CA	7.42	130.22	120.28	7	4
1	A	8	TRP	CA-C-O	7.42	128.41	120.55	4	1
1	A	2	TRP	CB-CG-CD2	-7.37	116.48	126.80	8	2
1	A	11	ILE	O-C-N	-7.36	114.73	121.87	7	3
1	B	44	LEU	N-CA-C	7.30	119.23	111.28	10	1
1	A	15	LEU	CA-C-N	7.28	133.24	123.05	6	1
1	A	15	LEU	C-N-CA	7.28	133.24	123.05	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	5	LEU	CA-C-N	7.24	130.58	120.29	7	2
1	A	5	LEU	C-N-CA	7.24	130.58	120.29	7	2
1	A	31	LEU	N-CA-C	7.22	119.16	111.28	4	1
1	A	34	VAL	CA-C-N	7.21	130.25	120.44	6	1
1	A	34	VAL	C-N-CA	7.21	130.25	120.44	6	1
1	B	49	ASN	CA-C-N	7.21	130.65	120.42	7	3
1	B	49	ASN	C-N-CA	7.21	130.65	120.42	7	3
1	A	8	TRP	CA-C-N	7.19	129.78	120.44	10	4
1	A	8	TRP	C-N-CA	7.19	129.78	120.44	10	4
1	B	72	ILE	CA-C-O	7.16	128.76	121.17	8	2
1	C	113	PHE	CA-C-N	7.16	129.88	120.28	6	2
1	C	113	PHE	C-N-CA	7.16	129.88	120.28	6	2
1	A	12	THR	N-CA-C	7.16	119.17	111.36	9	3
1	B	74	PHE	O-C-N	-7.15	114.54	122.12	2	3
1	C	102	ILE	N-CA-C	7.14	117.27	110.42	6	1
1	A	26	GLY	O-C-N	-7.12	115.29	122.19	9	2
1	A	25	VAL	CA-C-O	7.10	128.38	120.85	4	1
1	C	84	TRP	CA-C-N	7.09	130.10	120.38	10	2
1	C	84	TRP	C-N-CA	7.09	130.10	120.38	10	2
1	C	83	LEU	N-CA-C	7.09	118.66	111.07	2	3
1	A	32	ARG	NE-CZ-NH1	7.07	128.57	121.50	4	2
1	A	10	ASN	CA-CB-CG	-7.06	105.54	112.60	5	2
1	A	5	LEU	CA-C-O	7.05	128.25	120.63	4	1
1	A	6	TRP	CB-CG-CD1	7.04	137.46	126.90	5	1
1	C	82	SER	N-CA-CB	6.99	120.39	110.12	4	1
1	B	63	ILE	N-CA-CB	6.95	118.68	110.55	8	1
1	B	64	VAL	CA-C-N	6.95	129.04	120.22	2	3
1	B	64	VAL	C-N-CA	6.95	129.04	120.22	2	3
1	B	57	ILE	CA-C-N	6.95	134.80	121.54	10	7
1	B	57	ILE	C-N-CA	6.95	134.80	121.54	10	7
1	A	35	PHE	CA-C-N	6.92	129.55	120.28	3	1
1	A	35	PHE	C-N-CA	6.92	129.55	120.28	3	1
1	C	99	PHE	O-C-N	-6.92	114.79	122.12	10	1
1	B	48	PHE	CA-C-N	6.91	130.10	120.29	2	2
1	B	48	PHE	C-N-CA	6.91	130.10	120.29	2	2
1	C	81	ALA	CA-C-N	6.91	129.53	120.28	4	2
1	C	81	ALA	C-N-CA	6.91	129.53	120.28	4	2
1	C	90	THR	N-CA-CB	6.90	119.99	109.98	7	1
1	B	71	ARG	CA-C-N	6.84	129.18	120.56	4	3
1	B	71	ARG	C-N-CA	6.84	129.18	120.56	4	3
1	C	81	ALA	CA-C-O	6.83	127.67	120.42	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	56	TYR	N-CA-C	6.83	119.56	111.02	4	1
1	B	54	LEU	CA-C-O	6.81	128.22	119.98	1	2
1	C	98	LEU	O-C-N	-6.81	113.54	122.39	1	2
1	A	36	ALA	O-C-N	6.79	129.32	122.12	3	2
1	B	56	TYR	O-C-N	-6.78	115.06	123.33	10	1
1	C	103	VAL	CB-CA-C	-6.76	103.31	111.97	4	1
1	B	41	TRP	CB-CG-CD2	6.76	136.26	126.80	6	2
1	A	4	SER	N-CA-CB	6.75	119.80	110.01	5	2
1	C	112	VAL	CA-C-N	6.75	129.22	120.44	5	4
1	C	112	VAL	C-N-CA	6.75	129.22	120.44	5	4
1	B	67	LEU	CA-C-O	-6.75	113.73	120.82	3	1
1	C	89	ILE	CA-C-N	6.73	129.30	120.28	1	3
1	C	89	ILE	C-N-CA	6.73	129.30	120.28	1	3
1	A	32	ARG	NE-CZ-NH2	-6.73	113.14	119.20	5	2
1	A	2	TRP	O-C-N	-6.73	113.64	122.59	7	1
1	C	83	LEU	CA-C-N	6.72	129.18	120.44	7	2
1	C	83	LEU	C-N-CA	6.72	129.18	120.44	7	2
1	A	16	TRP	N-CA-CB	-6.71	99.47	110.42	10	1
1	B	44	LEU	CA-C-O	-6.71	112.25	119.97	9	1
1	C	87	PHE	CA-C-O	-6.70	113.78	120.82	6	1
1	C	83	LEU	O-C-N	-6.70	115.02	122.12	6	1
1	A	33	ILE	CA-C-O	6.69	128.45	121.29	4	1
1	A	16	TRP	CB-CG-CD2	6.68	136.16	126.80	3	1
1	C	92	TRP	CA-CB-CG	6.68	126.29	113.60	9	2
1	C	110	ARG	NH1-CZ-NH2	-6.68	110.62	119.30	7	3
1	A	23	MET	N-CA-C	6.67	119.56	111.82	3	4
1	B	47	TRP	CB-CG-CD1	-6.67	116.90	126.90	9	1
1	A	3	ALA	CA-C-N	6.66	129.10	120.44	2	1
1	A	3	ALA	C-N-CA	6.66	129.10	120.44	2	1
1	C	111	ILE	N-CA-C	-6.66	104.27	110.53	10	3
1	A	16	TRP	CA-C-N	6.65	134.24	121.54	4	2
1	A	16	TRP	C-N-CA	6.65	134.24	121.54	4	2
1	C	85	ASN	CA-C-O	6.64	127.61	119.97	8	1
1	B	65	GLY	CA-C-O	-6.64	113.62	120.66	4	2
1	C	96	ILE	CA-C-N	6.64	134.22	121.54	2	4
1	C	96	ILE	C-N-CA	6.64	134.22	121.54	2	4
1	C	106	LEU	CA-C-N	6.63	129.55	120.46	10	1
1	C	106	LEU	C-N-CA	6.63	129.55	120.46	10	1
1	C	104	GLY	CA-C-N	6.63	127.34	119.98	8	1
1	C	104	GLY	C-N-CA	6.63	127.34	119.98	8	1
1	C	86	TRP	CB-CG-CD2	6.62	136.07	126.80	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	VAL	O-C-N	6.62	128.64	121.83	6	1
1	A	23	MET	O-C-N	-6.62	114.13	122.27	10	2
1	B	67	LEU	N-CA-C	6.59	118.12	111.07	3	1
1	B	52	ASN	OD1-CG-ND2	6.59	129.19	122.60	5	1
1	C	111	ILE	N-CA-CB	6.58	118.25	110.55	6	2
1	A	2	TRP	CB-CG-CD1	6.58	136.76	126.90	8	2
1	C	84	TRP	N-CA-C	6.58	118.53	111.36	6	1
1	A	32	ARG	N-CA-CB	6.56	120.32	110.22	8	1
1	A	12	THR	CA-CB-OG1	6.55	119.43	109.60	9	2
1	C	95	TYR	N-CA-C	6.54	119.97	110.42	1	7
1	A	25	VAL	CA-C-N	6.54	127.20	120.00	6	3
1	A	25	VAL	C-N-CA	6.54	127.20	120.00	6	3
1	A	12	THR	N-CA-CB	6.54	119.55	110.07	2	1
1	C	81	ALA	N-CA-C	6.53	119.24	111.33	9	1
1	B	48	PHE	O-C-N	-6.52	115.35	122.07	4	1
1	C	91	ASN	OD1-CG-ND2	-6.52	116.08	122.60	8	1
1	C	84	TRP	CB-CG-CD2	6.51	135.91	126.80	1	3
1	A	29	VAL	CA-C-O	-6.49	113.97	120.85	6	1
1	C	111	ILE	O-C-N	-6.47	115.60	121.87	5	1
1	C	83	LEU	CA-C-O	-6.43	114.07	120.82	9	2
1	C	80	TRP	CB-CG-CD1	6.42	136.53	126.90	7	2
1	A	6	TRP	N-CA-CB	-6.40	100.68	110.16	10	1
1	C	88	ASN	CB-CG-ND2	6.40	126.00	116.40	4	1
1	A	2	TRP	CA-C-N	6.39	129.17	120.54	9	5
1	A	2	TRP	C-N-CA	6.39	129.17	120.54	9	5
1	A	27	GLY	N-CA-C	6.39	120.22	112.49	7	1
1	B	70	LEU	N-CA-C	6.38	119.91	111.75	2	1
1	C	86	TRP	CA-C-N	6.37	128.72	120.44	1	1
1	C	86	TRP	C-N-CA	6.37	128.72	120.44	1	1
1	B	50	ILE	N-CA-CB	6.36	119.19	110.54	6	1
1	C	114	ALA	N-CA-C	6.36	118.29	111.36	8	2
1	A	13	ASN	CA-CB-CG	-6.35	106.25	112.60	9	1
1	A	25	VAL	CB-CA-C	-6.35	103.84	111.97	1	1
1	B	55	TRP	CB-CG-CD1	6.33	136.40	126.90	7	1
1	A	29	VAL	CA-C-N	6.33	128.25	120.22	9	4
1	A	29	VAL	C-N-CA	6.33	128.25	120.22	9	4
1	C	79	LYS	CA-C-N	6.32	128.75	120.28	10	2
1	C	79	LYS	C-N-CA	6.32	128.75	120.28	10	2
1	C	95	TYR	CA-C-N	6.24	133.21	121.97	7	3
1	C	95	TYR	C-N-CA	6.24	133.21	121.97	7	3
1	A	8	TRP	N-CA-CB	-6.22	100.95	110.16	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	94	TRP	CA-C-O	-6.21	114.38	121.40	10	2
1	C	91	ASN	N-CA-C	6.21	117.72	111.07	7	1
1	B	66	GLY	CA-C-N	6.20	128.50	120.44	2	1
1	B	66	GLY	C-N-CA	6.20	128.50	120.44	2	1
1	C	104	GLY	CA-C-O	6.20	127.12	120.30	8	2
1	B	65	GLY	O-C-N	-6.18	116.19	122.19	5	2
1	A	32	ARG	N-CA-C	6.17	118.80	111.33	4	1
1	B	60	PHE	CA-CB-CG	6.17	119.97	113.80	7	1
1	B	71	ARG	NE-CZ-NH1	-6.16	115.34	121.50	1	1
1	A	35	PHE	N-CA-CB	6.15	118.99	110.07	6	1
1	C	104	GLY	O-C-N	-6.15	115.58	122.28	3	1
1	B	48	PHE	CA-CB-CG	6.14	119.94	113.80	2	1
1	C	91	ASN	O-C-N	-6.14	115.45	122.09	3	1
1	A	9	PHE	O-C-N	-6.12	115.77	122.07	10	1
1	C	113	PHE	CA-CB-CG	-6.12	107.69	113.80	6	2
1	B	62	MET	CA-C-O	-6.11	113.20	120.10	2	3
1	A	34	VAL	CA-C-O	6.11	127.06	120.47	4	1
1	A	20	LEU	CA-C-O	6.10	126.91	119.11	5	1
1	A	16	TRP	O-C-N	-6.09	116.10	123.29	7	1
1	C	94	TRP	CA-C-N	6.09	133.16	121.54	6	1
1	C	94	TRP	C-N-CA	6.09	133.16	121.54	6	1
1	B	56	TYR	CB-CG-CD2	-6.08	111.68	120.80	1	1
1	A	16	TRP	CA-C-O	-6.07	114.54	121.40	2	1
1	B	41	TRP	CB-CG-CD1	-6.07	117.79	126.90	6	1
1	C	82	SER	N-CA-C	6.07	117.89	111.28	1	2
1	C	107	VAL	CA-C-N	6.07	126.84	119.99	1	1
1	C	107	VAL	C-N-CA	6.07	126.84	119.99	1	1
1	B	69	GLY	O-C-N	-6.05	116.38	122.19	9	2
1	B	52	ASN	CA-CB-CG	-6.05	106.55	112.60	2	2
1	C	110	ARG	CB-CG-CD	6.03	125.17	111.30	7	2
1	B	74	PHE	CB-CA-C	6.03	120.80	110.79	10	2
1	C	111	ILE	CB-CA-C	-6.02	104.02	112.14	5	2
1	B	49	ASN	CA-CB-CG	6.01	118.61	112.60	2	1
1	A	6	TRP	CB-CG-CD2	-6.01	118.38	126.80	5	1
1	C	87	PHE	CA-C-N	6.01	128.66	120.54	9	1
1	C	87	PHE	C-N-CA	6.01	128.66	120.54	9	1
1	B	64	VAL	N-CA-CB	6.01	119.18	110.52	5	1
1	A	4	SER	CA-C-N	6.01	128.82	120.29	7	1
1	A	4	SER	C-N-CA	6.01	128.82	120.29	7	1
1	A	10	ASN	CB-CG-ND2	-5.99	107.41	116.40	9	1
1	C	111	ILE	CA-C-N	5.98	129.92	120.47	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	111	ILE	C-N-CA	5.98	129.92	120.47	8	2
1	A	6	TRP	CH2-CZ2-CE2	5.97	125.27	117.50	6	1
1	B	72	ILE	CA-C-N	5.97	130.08	120.82	3	2
1	B	72	ILE	C-N-CA	5.97	130.08	120.82	3	2
1	B	68	VAL	CB-CA-C	-5.95	104.10	112.14	7	1
1	B	76	VAL	CB-CA-C	-5.95	104.11	112.14	6	1
1	B	52	ASN	O-C-N	5.95	129.39	122.20	2	1
1	B	43	SER	N-CA-C	5.95	121.18	111.37	5	2
1	B	76	VAL	CA-CB-CG2	-5.94	100.30	110.40	8	1
1	A	11	ILE	CB-CA-C	5.93	120.15	112.14	9	2
1	B	63	ILE	CA-C-O	5.90	127.09	120.95	10	1
1	C	97	LYS	CB-CA-C	-5.89	108.78	115.79	3	1
1	A	4	SER	N-CA-C	5.89	117.37	111.07	2	1
1	B	77	LEU	CB-CA-C	5.89	121.30	110.11	2	1
1	C	101	MET	O-C-N	-5.88	114.55	122.43	4	1
1	A	25	VAL	N-CA-C	5.88	116.06	110.53	7	1
1	B	76	VAL	N-CA-CB	5.87	118.53	110.54	3	1
1	C	94	TRP	CA-CB-CG	5.85	124.72	113.60	6	1
1	B	56	TYR	CA-C-O	-5.84	114.85	122.45	4	1
1	C	85	ASN	OD1-CG-ND2	-5.83	116.77	122.60	1	3
1	C	81	ALA	O-C-N	-5.82	115.52	122.15	7	1
1	B	44	LEU	CA-C-N	5.82	128.39	120.54	8	2
1	B	44	LEU	C-N-CA	5.82	128.39	120.54	8	2
1	C	112	VAL	N-CA-C	-5.82	106.07	113.22	9	1
1	C	86	TRP	CB-CG-CD1	-5.80	118.20	126.90	7	1
1	A	32	ARG	CD-NE-CZ	-5.80	116.28	124.40	10	1
1	B	45	TRP	CB-CG-CD2	5.79	134.91	126.80	9	2
1	B	62	MET	N-CA-C	5.79	118.37	111.71	2	1
1	A	14	TRP	N-CA-CB	5.77	120.24	110.49	5	2
1	B	44	LEU	O-C-N	-5.77	115.17	122.27	3	3
1	A	10	ASN	CA-C-N	5.76	128.35	120.46	4	4
1	A	10	ASN	C-N-CA	5.76	128.35	120.46	4	4
1	A	12	THR	O-C-N	-5.76	115.59	122.15	9	2
1	A	24	ILE	CB-CA-C	-5.75	104.38	112.14	6	1
1	C	113	PHE	N-CA-C	-5.75	105.09	111.36	8	1
1	B	46	ASN	CA-C-N	5.74	127.97	120.28	7	1
1	B	46	ASN	C-N-CA	5.74	127.97	120.28	7	1
1	B	73	VAL	CA-CB-CG1	5.72	120.13	110.40	1	1
1	B	72	ILE	O-C-N	-5.72	116.30	121.91	6	2
1	B	52	ASN	CA-C-N	5.71	132.45	121.54	8	2
1	B	52	ASN	C-N-CA	5.71	132.45	121.54	8	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	LEU	N-CA-C	5.69	118.26	111.71	9	1
1	A	21	PHE	CA-C-N	-5.68	115.64	122.35	6	1
1	A	21	PHE	C-N-CA	-5.68	115.64	122.35	6	1
1	A	20	LEU	CA-C-N	5.68	128.16	120.38	4	1
1	A	20	LEU	C-N-CA	5.68	128.16	120.38	4	1
1	A	34	VAL	N-CA-C	5.68	116.45	110.72	3	1
1	B	64	VAL	CB-CA-C	5.68	119.81	112.14	8	1
1	A	31	LEU	N-CA-CB	5.67	119.08	110.28	3	1
1	B	49	ASN	OD1-CG-ND2	5.66	128.26	122.60	7	1
1	C	114	ALA	CA-C-N	5.66	128.22	120.46	3	1
1	C	114	ALA	C-N-CA	5.66	128.22	120.46	3	1
1	A	22	ILE	N-CA-C	-5.66	106.94	111.81	6	1
1	A	24	ILE	N-CA-CB	5.65	118.22	110.54	10	1
1	B	70	LEU	N-CA-CB	5.64	118.91	110.22	9	1
1	B	58	LYS	O-C-N	-5.64	115.08	122.59	3	1
1	A	23	MET	CG-SD-CE	-5.63	88.50	100.90	7	1
1	B	52	ASN	N-CA-C	5.63	117.11	110.97	1	1
1	B	46	ASN	CA-CB-CG	5.63	118.23	112.60	2	2
1	C	85	ASN	CA-C-N	5.62	127.82	120.28	4	1
1	C	85	ASN	C-N-CA	5.62	127.82	120.28	4	1
1	C	89	ILE	N-CA-C	5.62	116.08	110.23	9	1
1	C	116	LEU	N-CA-C	5.62	120.13	113.28	1	2
1	B	68	VAL	N-CA-CB	5.62	118.18	110.54	10	1
1	A	6	TRP	CA-CB-CG	5.61	124.26	113.60	6	1
1	C	84	TRP	CD2-CE2-CZ2	-5.61	116.80	122.40	6	1
1	C	88	ASN	CA-C-N	5.59	127.60	120.56	10	2
1	C	88	ASN	C-N-CA	5.59	127.60	120.56	10	2
1	A	29	VAL	CB-CA-C	-5.58	104.82	111.97	9	1
1	C	88	ASN	CB-CG-OD1	-5.58	109.65	120.80	4	1
1	A	30	GLY	CA-C-N	5.57	129.18	120.82	2	1
1	A	30	GLY	C-N-CA	5.57	129.18	120.82	2	1
1	C	90	THR	CA-CB-OG1	5.56	117.95	109.60	2	2
1	B	62	MET	N-CA-CB	5.55	119.61	110.39	6	3
1	A	11	ILE	CA-C-O	5.55	126.72	120.95	5	1
1	B	74	PHE	CA-C-O	5.55	126.43	120.55	9	2
1	A	9	PHE	CA-C-N	5.54	127.98	120.44	9	2
1	A	9	PHE	C-N-CA	5.54	127.98	120.44	9	2
1	B	57	ILE	CA-C-O	5.54	127.70	120.78	10	1
1	A	30	GLY	N-CA-C	5.54	119.34	112.64	2	1
1	C	94	TRP	CB-CG-CD1	-5.54	118.59	126.90	9	1
1	C	101	MET	N-CA-CB	5.53	118.85	110.28	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	84	TRP	CB-CG-CD1	5.52	135.18	126.90	10	2
1	B	52	ASN	CA-C-O	-5.52	114.56	121.02	2	1
1	C	98	LEU	N-CA-C	5.52	117.29	111.28	2	1
1	A	34	VAL	O-C-N	-5.52	115.57	121.80	4	1
1	A	16	TRP	CB-CG-CD1	5.52	135.17	126.90	4	1
1	C	105	GLY	CA-C-O	-5.51	115.07	120.75	9	1
1	C	80	TRP	CA-C-O	5.50	126.39	120.55	8	1
1	A	26	GLY	N-CA-C	5.49	119.14	112.49	2	1
1	B	72	ILE	N-CA-CB	-5.49	103.08	110.54	10	1
1	A	37	VAL	O-C-N	-5.48	116.56	121.87	2	1
1	A	2	TRP	N-CA-CB	5.47	119.73	110.49	10	1
1	C	117	SER	N-CA-CB	5.47	119.79	110.50	2	1
1	B	67	LEU	O-C-N	-5.47	116.33	122.12	6	2
1	A	5	LEU	O-C-N	-5.46	116.20	122.09	2	1
1	A	37	VAL	CA-C-O	-5.46	114.73	120.57	4	1
1	A	21	PHE	CB-CA-C	5.44	119.82	110.79	7	1
1	A	22	ILE	CA-C-O	5.44	126.50	120.46	7	1
1	B	47	TRP	O-C-N	-5.44	116.35	122.12	7	1
1	B	51	THR	CA-C-N	5.44	127.51	120.44	6	2
1	B	51	THR	C-N-CA	5.44	127.51	120.44	6	2
1	C	80	TRP	N-CA-CB	5.43	118.10	110.12	8	1
1	B	48	PHE	CA-C-O	-5.42	115.13	120.82	7	1
1	C	97	LYS	N-CA-C	5.41	119.27	109.32	3	1
1	B	61	ILE	O-C-N	-5.41	113.93	122.04	4	1
1	A	10	ASN	CB-CA-C	-5.41	101.49	110.68	3	1
1	C	112	VAL	CG1-CB-CG2	-5.41	98.91	110.80	10	1
1	C	101	MET	CG-SD-CE	-5.40	89.02	100.90	4	1
1	B	76	VAL	N-CA-C	5.39	117.79	111.05	9	1
1	C	93	LEU	CA-C-N	5.38	131.25	122.81	3	1
1	C	93	LEU	C-N-CA	5.38	131.25	122.81	3	1
1	A	13	ASN	CA-C-N	5.37	131.80	121.54	8	2
1	A	13	ASN	C-N-CA	5.37	131.80	121.54	8	2
1	C	108	GLY	O-C-N	5.37	127.34	122.19	2	1
1	B	42	ALA	N-CA-CB	-5.37	102.20	109.98	5	1
1	A	30	GLY	O-C-N	-5.35	116.84	122.13	2	1
1	C	96	ILE	CB-CA-C	5.35	120.06	111.29	8	1
1	C	115	VAL	CA-CB-CG1	5.32	119.44	110.40	3	1
1	B	50	ILE	N-CA-C	5.30	116.08	110.72	9	3
1	C	82	SER	O-C-N	-5.30	115.34	122.23	5	1
1	B	55	TRP	CA-C-N	5.30	131.66	121.54	7	1
1	B	55	TRP	C-N-CA	5.30	131.66	121.54	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	C	108	GLY	CA-C-N	5.30	127.91	120.28	1	1
1	C	108	GLY	C-N-CA	5.30	127.91	120.28	1	1
1	A	32	ARG	NH1-CZ-NH2	-5.30	112.42	119.30	6	1
1	B	46	ASN	CB-CG-ND2	5.30	124.35	116.40	7	1
1	A	10	ASN	N-CA-CB	5.29	117.83	109.94	5	1
1	B	61	ILE	CA-C-N	-5.29	111.27	121.58	4	1
1	B	61	ILE	C-N-CA	-5.29	111.27	121.58	4	1
1	A	16	TRP	CE2-CD2-CE3	5.29	124.08	118.80	1	1
1	B	53	TRP	N-CA-CB	5.28	119.41	110.49	8	1
1	C	91	ASN	CA-C-O	5.28	126.13	120.70	3	1
1	B	57	ILE	N-CA-CB	5.27	119.93	111.23	10	1
1	A	19	LYS	CA-C-O	-5.27	112.97	120.51	2	1
1	A	3	ALA	O-C-N	-5.27	116.64	122.07	7	1
1	B	69	GLY	CA-C-O	-5.26	115.34	120.75	2	1
1	A	6	TRP	CA-C-N	5.26	127.75	120.29	7	1
1	A	6	TRP	C-N-CA	5.26	127.75	120.29	7	1
1	B	75	ALA	O-C-N	-5.25	115.81	122.27	4	1
1	A	31	LEU	CA-C-O	5.25	126.12	120.55	4	2
1	A	36	ALA	N-CA-C	5.25	117.00	111.28	3	2
1	C	90	THR	O-C-N	-5.25	115.82	122.17	3	1
1	C	114	ALA	CA-C-O	5.25	125.98	120.42	10	1
1	A	28	LEU	N-CA-CB	5.24	117.61	110.01	2	1
1	B	45	TRP	CB-CG-CD1	-5.23	119.06	126.90	9	1
1	C	86	TRP	CA-CB-CG	5.22	123.52	113.60	6	3
1	C	102	ILE	CA-C-N	5.22	127.61	120.46	3	1
1	C	102	ILE	C-N-CA	5.22	127.61	120.46	3	1
1	B	55	TRP	CA-CB-CG	5.21	123.51	113.60	3	1
1	B	75	ALA	CA-C-N	-5.21	112.23	120.47	9	1
1	B	75	ALA	C-N-CA	-5.21	112.23	120.47	9	1
1	A	10	ASN	OD1-CG-ND2	-5.21	117.39	122.60	6	1
1	A	31	LEU	O-C-N	-5.21	116.60	122.12	7	1
1	A	12	THR	CA-C-O	5.19	126.05	120.55	3	1
1	A	17	TYR	CB-CG-CD1	-5.19	113.02	120.80	5	1
1	A	12	THR	CA-CB-CG2	5.18	119.31	110.50	2	1
1	A	18	ILE	N-CA-CB	5.17	119.77	111.23	6	1
1	C	87	PHE	CB-CG-CD1	-5.16	111.92	120.70	8	1
1	C	112	VAL	CB-CA-C	-5.16	105.18	112.14	4	1
1	A	7	ASN	CB-CG-ND2	5.15	124.13	116.40	5	1
1	A	26	GLY	CA-C-N	5.15	126.58	120.14	4	1
1	A	26	GLY	C-N-CA	5.15	126.58	120.14	4	1
1	A	29	VAL	CA-CB-CG1	5.15	119.15	110.40	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	VAL	CA-CB-CG2	-5.14	101.65	110.40	6	1
1	A	37	VAL	CA-CB-CG2	-5.14	101.66	110.40	10	1
1	A	9	PHE	CB-CA-C	5.14	118.95	110.88	9	1
1	B	67	LEU	CA-C-N	5.14	127.03	120.56	6	1
1	B	67	LEU	C-N-CA	5.14	127.03	120.56	6	1
1	B	46	ASN	CB-CA-C	-5.12	102.30	110.79	1	1
1	C	87	PHE	N-CA-C	5.11	116.85	111.28	7	1
1	B	52	ASN	CB-CG-ND2	5.11	124.07	116.40	7	1
1	C	102	ILE	O-C-N	-5.11	116.92	121.87	10	1
1	B	60	PHE	CA-C-O	-5.11	115.14	120.55	4	1
1	A	6	TRP	CA-C-O	5.09	125.82	120.42	10	1
1	A	21	PHE	CA-CB-CG	5.09	118.89	113.80	6	2
1	C	88	ASN	N-CA-CB	5.09	117.39	110.01	10	1
1	C	102	ILE	N-CA-CB	5.09	117.08	110.57	8	1
1	B	74	PHE	CA-CB-CG	-5.08	108.72	113.80	5	1
1	C	80	TRP	O-C-N	-5.08	116.74	122.12	3	2
1	A	2	TRP	CE3-CZ3-CH2	-5.07	114.51	121.10	1	1
1	A	8	TRP	CB-CG-CD2	-5.07	119.71	126.80	9	1
1	C	100	ILE	CA-CB-CG2	5.06	119.11	110.50	5	1
1	B	77	LEU	CA-C-O	5.06	125.20	119.18	3	1
1	B	43	SER	CA-C-O	5.06	126.31	120.90	4	1
1	A	35	PHE	N-CA-C	-5.05	105.86	111.36	5	1
1	A	6	TRP	N-CA-C	5.02	116.83	111.36	10	1
1	B	59	LEU	CA-C-O	5.00	125.14	119.18	10	1
1	B	71	ARG	N-CA-C	5.00	117.38	111.33	10	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	17	TYR	Sidechain	4
1	B	71	ARG	Sidechain	3
1	A	32	ARG	Sidechain	2
1	C	95	TYR	Sidechain	2
1	B	56	TYR	Sidechain	2
1	C	113	PHE	Sidechain	1
1	A	16	TRP	Peptide	1
1	A	9	PHE	Sidechain	1
1	C	99	PHE	Sidechain	1
1	C	115	VAL	Mainchain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	B	60	PHE	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	B	334	347	344	0±0
1	C	334	347	344	0±0
1	A	334	347	347	0±0
All	All	10020	10410	10350	4

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:68:VAL:HG21	1:C:103:VAL:HG13	0.46	1.87	3	1
1:B:68:VAL:HG22	1:C:107:VAL:CG2	0.43	2.43	1	1
1:A:35:PHE:CD2	1:A:35:PHE:C	0.42	2.97	5	1
1:B:59:LEU:O	1:B:63:ILE:HG22	0.41	2.16	5	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	37/39 (95%)	31±1 (84±3%)	2±1 (6±3%)	4±1 (10±3%)	1	9
1	B	37/39 (95%)	32±1 (85±2%)	2±1 (7±3%)	3±1 (8±3%)	1	14
1	C	37/39 (95%)	33±0 (88±1%)	2±1 (5±3%)	2±1 (7±3%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1110/1170 (95%)	953 (86%)	65 (6%)	92 (8%)	1 13

All 15 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	14	TRP	10
1	B	53	TRP	10
1	C	96	ILE	10
1	A	17	TYR	9
1	A	18	ILE	9
1	B	57	ILE	8
1	B	58	LYS	6
1	C	95	TYR	6
1	A	19	LYS	5
1	C	92	TRP	5
1	A	2	TRP	4
1	C	97	LYS	4
1	B	56	TYR	3
1	B	41	TRP	2
1	A	33	ILE	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	34/34 (100%)	34±0 (99±1%)	0±0 (1±1%)	76 96
1	B	34/34 (100%)	34±0 (99±1%)	0±0 (1±1%)	68 95
1	C	34/34 (100%)	33±1 (97±2%)	1±1 (3±2%)	41 88
All	All	1020/1020 (100%)	1006 (99%)	14 (1%)	57 93

All 13 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	C	96	ILE	2

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Mol	Chain	Res	Type	Models (Total)
1	C	102	ILE	1
1	A	29	VAL	1
1	B	40	LYS	1
1	C	109	LEU	1
1	C	97	LYS	1
1	C	103	VAL	1
1	A	34	VAL	1
1	B	50	ILE	1
1	C	111	ILE	1
1	C	112	VAL	1
1	C	89	ILE	1
1	B	63	ILE	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chemical_shift_mpertm.txt*

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	23
Number of shifts mapped to atoms	23
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

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

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 23 atoms were assigned a chemical shift out of a possible 1806. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	10/594 (2%)	0/243 (0%)	10/234 (4%)	0/117 (0%)
Sidechain	13/915 (1%)	0/615 (0%)	13/276 (5%)	0/24 (0%)
Aromatic	0/297 (0%)	0/147 (0%)	0/135 (0%)	0/15 (0%)
Overall	23/1806 (1%)	0/1005 (0%)	23/645 (4%)	0/156 (0%)

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

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 1%, i.e. 23 atoms were assigned a chemical shift out of a possible 1806. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	10/594 (2%)	0/243 (0%)	10/234 (4%)	0/117 (0%)
Sidechain	13/915 (1%)	0/615 (0%)	13/276 (5%)	0/24 (0%)
Aromatic	0/297 (0%)	0/147 (0%)	0/135 (0%)	0/15 (0%)
Overall	23/1806 (1%)	0/1005 (0%)	23/645 (4%)	0/156 (0%)

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

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

