



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:33 AM UTC

PDB ID : 9NM2 / pdb_00009nm2
BMRB ID : 31232
Title : Dimeric Structure of full-length CrgA, a Cell Division Protein from Mycobacterium tuberculosis, in Lipid Bilayers
Authors : Shin, Y.; Prasad, R.; Das, N.; Taylor, J.A.; Qin, H.; Hu, W.; Hu, Y.-Y.; Fu, R.; Zhang, R.; Zhou, H.-X.; Cross, T.A.
Deposited on : 2025-03-03

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
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

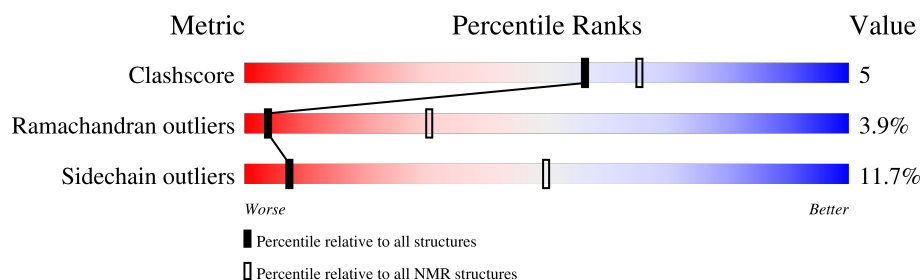
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 3%.

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	102	
1	B	102	

2 Ensemble composition and analysis

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:17-A:93, B:17-B:93 (154)	0.25	3

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2478 atoms, of which 1266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cell division protein CrgA.

Mol	Chain	Residues	Atoms						Trace
1	A	77	Total	C	H	N	O	S	0
			1239	411	633	97	92	6	
1	B	77	Total	C	H	N	O	S	0
			1239	411	633	97	92	6	

There are 18 discrepancies between the modelled and reference sequences:

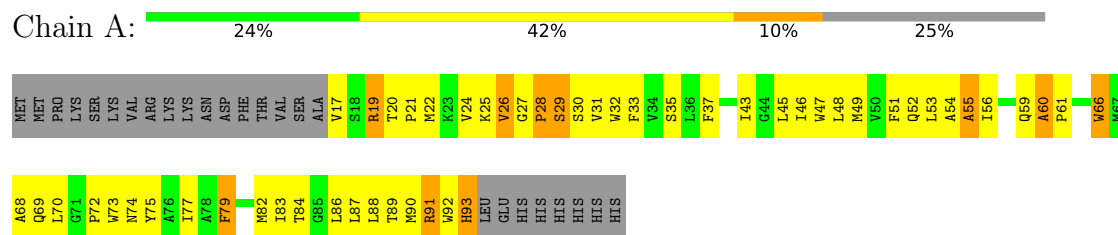
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P9WP57
A	94	LEU	-	expression tag	UNP P9WP57
A	95	GLU	-	expression tag	UNP P9WP57
A	96	HIS	-	expression tag	UNP P9WP57
A	97	HIS	-	expression tag	UNP P9WP57
A	98	HIS	-	expression tag	UNP P9WP57
A	99	HIS	-	expression tag	UNP P9WP57
A	100	HIS	-	expression tag	UNP P9WP57
A	101	HIS	-	expression tag	UNP P9WP57
B	0	MET	-	initiating methionine	UNP P9WP57
B	94	LEU	-	expression tag	UNP P9WP57
B	95	GLU	-	expression tag	UNP P9WP57
B	96	HIS	-	expression tag	UNP P9WP57
B	97	HIS	-	expression tag	UNP P9WP57
B	98	HIS	-	expression tag	UNP P9WP57
B	99	HIS	-	expression tag	UNP P9WP57
B	100	HIS	-	expression tag	UNP P9WP57
B	101	HIS	-	expression tag	UNP P9WP57

4 Residue-property plots

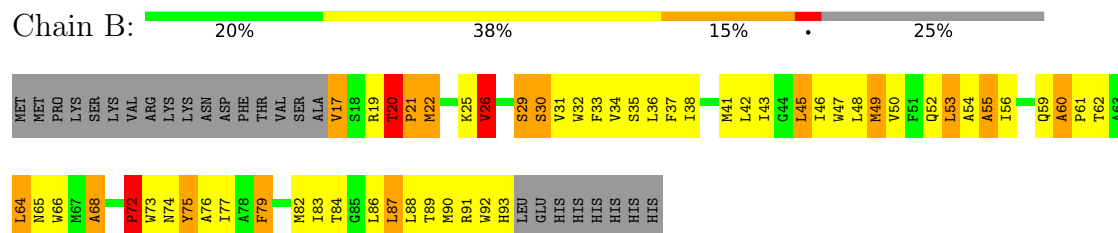
4.1 Average score per residue in the NMR ensemble

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: Cell division protein CrgA



- Molecule 1: Cell division protein CrgA

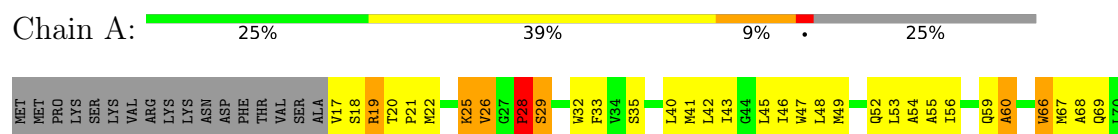


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

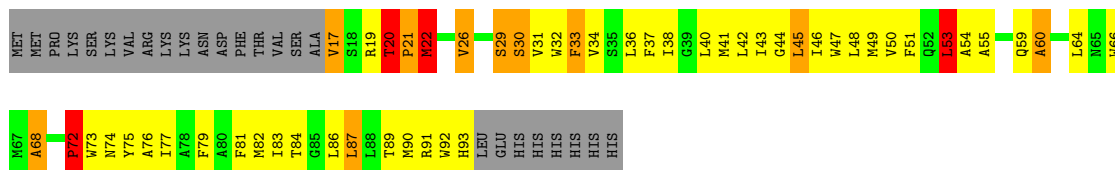
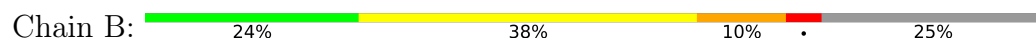
4.2.1 Score per residue for model 1

- Molecule 1: Cell division protein CrgA



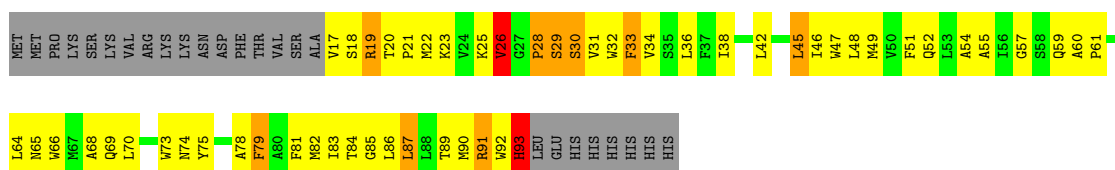
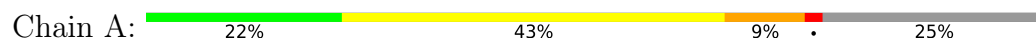


- Molecule 1: Cell division protein CrgA

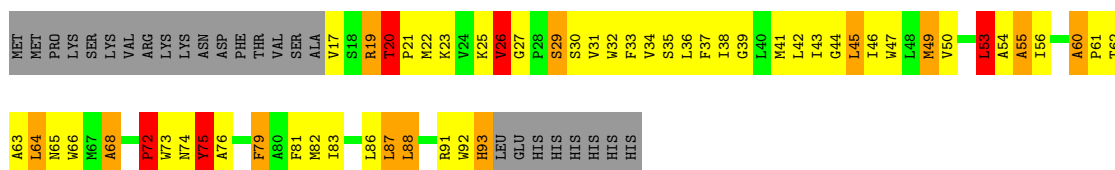
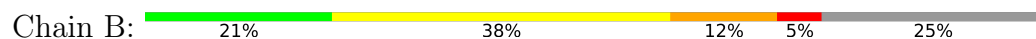


4.2.2 Score per residue for model 2

- Molecule 1: Cell division protein CrgA

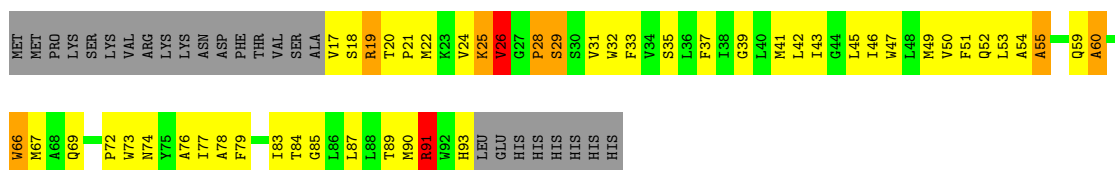


- Molecule 1: Cell division protein CrgA

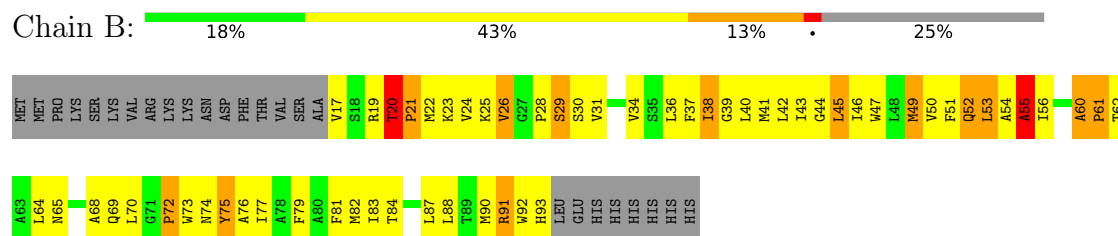


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Cell division protein CrgA

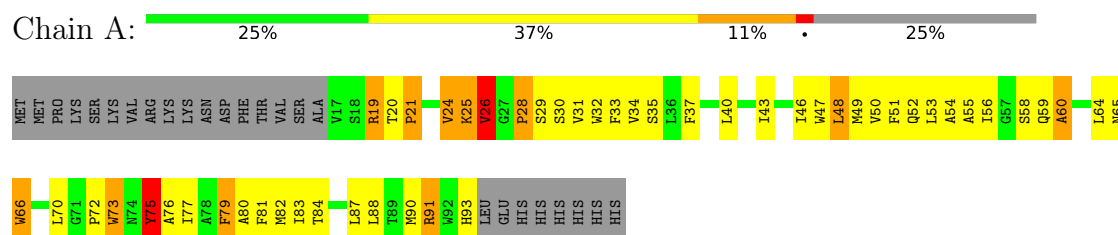


- Molecule 1: Cell division protein CrgA

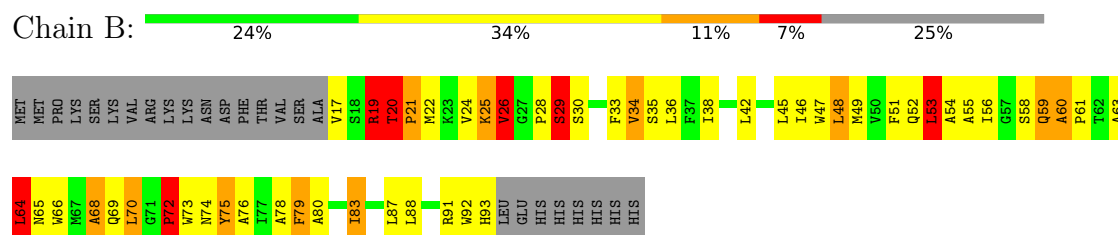


4.2.4 Score per residue for model 4

- Molecule 1: Cell division protein CrgA

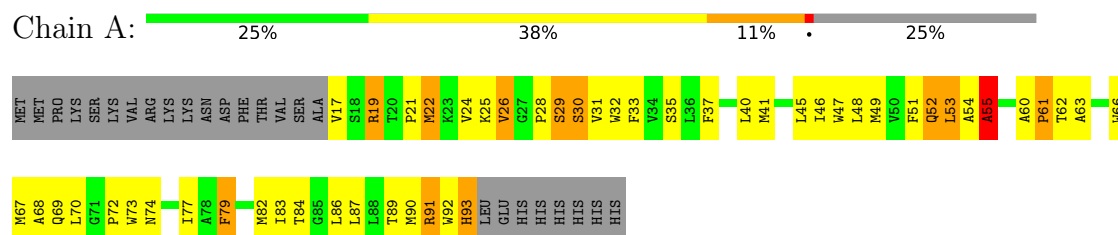


- Molecule 1: Cell division protein CrgA

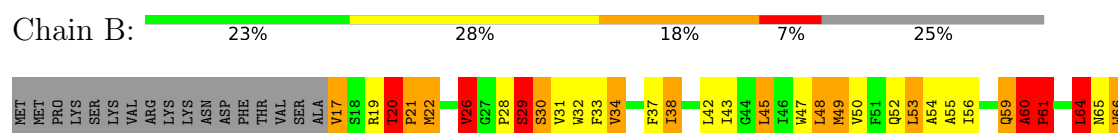


4.2.5 Score per residue for model 5

- Molecule 1: Cell division protein CrgA



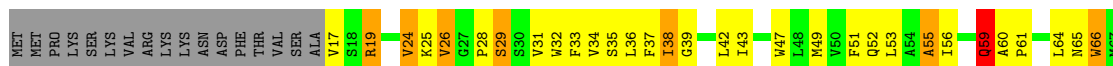
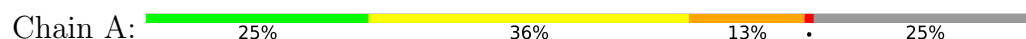
- Molecule 1: Cell division protein CrgA



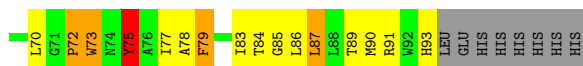
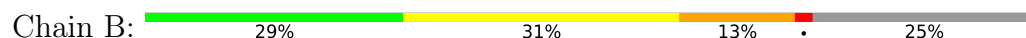


4.2.6 Score per residue for model 6

- Molecule 1: Cell division protein CrgA

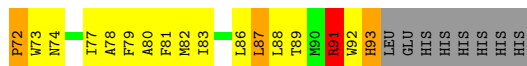
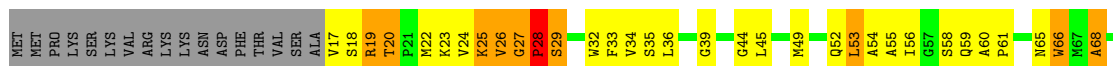
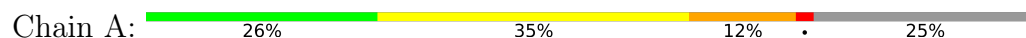


- Molecule 1: Cell division protein CrgA

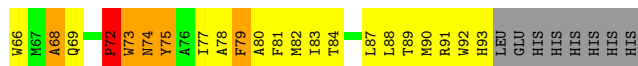
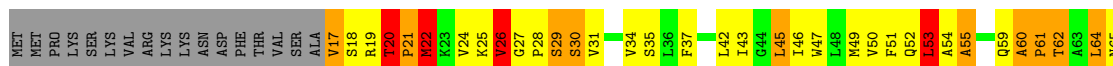
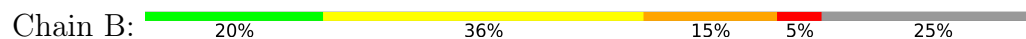


4.2.7 Score per residue for model 7

- Molecule 1: Cell division protein CrgA

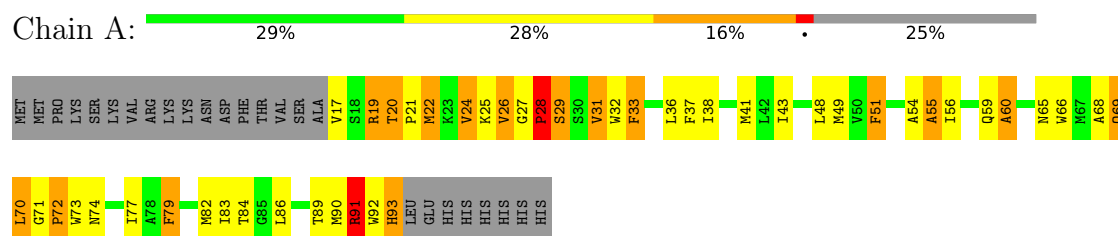


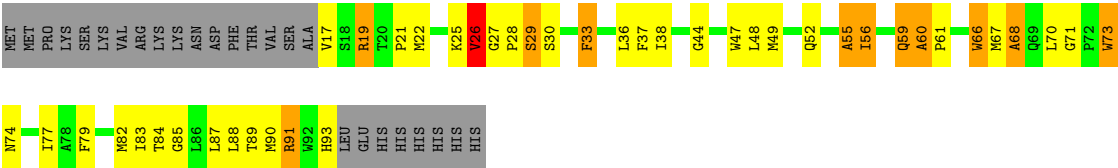
- Molecule 1: Cell division protein CrgA



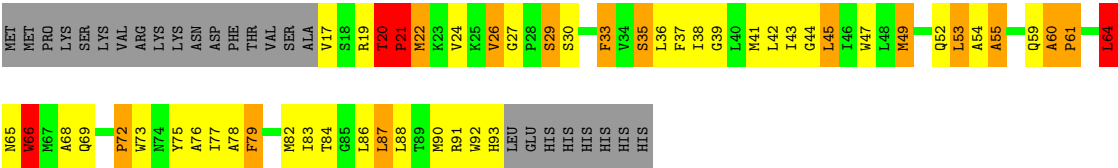
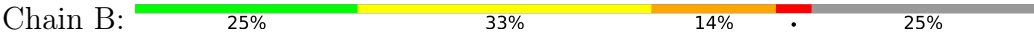
4.2.8 Score per residue for model 8

- Molecule 1: Cell division protein CrgA





● Molecule 1: Cell division protein CrgA



5 Refinement protocol and experimental data overview

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

Of the 13 calculated structures, 10 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
NAMD	refinement	2.13
X-PLOR NIH	structure calculation	3.4

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	69
Number of shifts mapped to atoms	69
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

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 i

6.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.15±0.07	17±4/626 (2.7± 0.7%)	2.71±0.07	60±4/854 (7.0± 0.5%)
1	B	2.26±0.07	24±5/626 (3.8± 0.8%)	2.99±0.06	69±7/854 (8.0± 0.8%)
All	All	2.21	407/12520 (3.3%)	2.85	1281/17080 (7.5%)

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	6.9±1.4
1	B	1.0±0.0	6.6±1.0
All	All	10	135

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	B	20	THR	CA-CB	14.05	1.74	1.53	10	10
1	B	61	PRO	CA-CB	10.25	1.60	1.53	4	3
1	B	61	PRO	N-CA	9.70	1.54	1.47	2	1
1	A	20	THR	CA-C	-9.46	1.45	1.52	4	2
1	A	25	LYS	CA-C	-9.09	1.41	1.52	3	1
1	B	21	PRO	CA-CB	8.92	1.63	1.53	4	2
1	A	32	TRP	N-CA	-8.52	1.36	1.46	1	1
1	A	30	SER	CA-C	-8.48	1.42	1.52	5	3
1	B	91	ARG	CD-NE	8.47	1.58	1.46	3	2
1	B	33	PHE	CA-CB	8.41	1.66	1.53	1	1
1	B	54	ALA	CA-C	8.29	1.63	1.52	8	4
1	A	26	VAL	CA-C	-8.26	1.42	1.52	6	3
1	A	61	PRO	CA-CB	8.13	1.65	1.53	2	2
1	B	74	ASN	CA-CB	7.97	1.66	1.53	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	26	VAL	C-N	7.95	1.45	1.33	8	1
1	A	92	TRP	NE1-CE2	-7.91	1.28	1.37	5	1
1	A	72	PRO	N-CA	7.88	1.53	1.47	6	2
1	A	72	PRO	CA-CB	7.80	1.58	1.53	6	2
1	A	64	LEU	CA-C	7.78	1.61	1.52	4	2
1	B	19	ARG	C-O	-7.76	1.15	1.23	1	1
1	A	19	ARG	CA-C	7.66	1.61	1.52	6	1
1	A	86	LEU	CA-C	7.54	1.62	1.52	8	1
1	B	88	LEU	N-CA	-7.53	1.37	1.46	4	1
1	A	93	HIS	ND1-CE1	7.51	1.40	1.32	4	2
1	B	65	ASN	N-CA	-7.49	1.36	1.46	4	2
1	B	83	ILE	CA-C	-7.48	1.43	1.52	2	2
1	A	77	ILE	CA-CB	-7.45	1.45	1.54	3	4
1	B	31	VAL	N-CA	-7.41	1.37	1.46	7	2
1	A	32	TRP	C-N	7.40	1.43	1.33	7	2
1	A	93	HIS	CB-CG	7.38	1.60	1.50	7	2
1	B	23	LYS	CA-CB	7.37	1.66	1.53	2	1
1	A	84	THR	C-N	7.33	1.43	1.33	6	2
1	B	91	ARG	CA-CB	7.32	1.64	1.53	4	1
1	A	55	ALA	C-N	7.25	1.42	1.33	4	1
1	B	54	ALA	N-CA	7.24	1.54	1.46	6	4
1	A	67	MET	CA-C	-7.22	1.43	1.52	10	2
1	A	69	GLN	CA-CB	7.21	1.65	1.53	2	1
1	A	64	LEU	N-CA	-7.19	1.37	1.46	2	1
1	B	66	TRP	NE1-CE2	-7.19	1.29	1.37	10	1
1	A	77	ILE	CA-C	7.18	1.61	1.52	3	1
1	B	73	TRP	CA-CB	7.17	1.64	1.53	4	1
1	B	77	ILE	C-N	7.13	1.43	1.33	5	1
1	B	27	GLY	CA-C	-7.12	1.41	1.51	7	1
1	B	65	ASN	CA-C	-7.09	1.44	1.52	5	2
1	A	40	LEU	N-CA	-7.08	1.37	1.46	4	1
1	A	18	SER	CA-C	-7.05	1.44	1.52	2	1
1	A	30	SER	C-N	7.03	1.42	1.33	2	1
1	A	29	SER	C-N	7.00	1.42	1.33	2	1
1	B	32	TRP	CA-CB	6.97	1.64	1.53	6	2
1	B	32	TRP	NE1-CE2	-6.97	1.29	1.37	5	2
1	B	49	MET	CA-CB	6.96	1.64	1.53	7	1
1	A	36	LEU	N-CA	-6.94	1.38	1.46	7	1
1	B	31	VAL	C-N	6.92	1.42	1.33	7	1
1	B	89	THR	CA-C	6.91	1.61	1.52	7	1
1	B	52	GLN	C-O	-6.90	1.16	1.24	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	25	LYS	C-N	6.86	1.42	1.33	7	1
1	A	44	GLY	CA-C	6.86	1.59	1.52	7	1
1	B	76	ALA	C-N	6.84	1.42	1.33	10	1
1	B	93	HIS	ND1-CE1	6.84	1.39	1.32	5	4
1	A	23	LYS	N-CA	-6.79	1.37	1.46	2	1
1	B	50	VAL	CA-CB	6.75	1.62	1.54	1	2
1	A	82	MET	CA-C	-6.75	1.44	1.52	5	2
1	B	47	TRP	C-N	6.73	1.42	1.33	3	1
1	A	89	THR	N-CA	6.70	1.54	1.46	6	2
1	B	49	MET	C-N	6.70	1.42	1.33	8	1
1	B	66	TRP	CA-C	6.69	1.60	1.52	8	2
1	A	85	GLY	CA-C	-6.69	1.44	1.52	6	1
1	B	27	GLY	N-CA	6.65	1.53	1.44	2	3
1	A	92	TRP	CA-C	6.63	1.61	1.52	9	2
1	B	60	ALA	CA-C	6.61	1.61	1.52	1	1
1	B	45	LEU	CA-CB	6.61	1.63	1.53	3	1
1	B	26	VAL	C-N	6.61	1.43	1.33	6	1
1	B	22	MET	CA-C	-6.58	1.44	1.52	1	2
1	A	89	THR	CA-CB	6.58	1.63	1.53	5	1
1	B	40	LEU	CA-CB	6.57	1.63	1.53	1	1
1	B	61	PRO	C-N	6.55	1.42	1.33	5	4
1	B	82	MET	CA-CB	6.55	1.63	1.53	8	1
1	B	46	ILE	CA-C	6.53	1.61	1.52	2	1
1	B	18	SER	CA-CB	6.51	1.65	1.53	7	1
1	A	54	ALA	CA-C	6.46	1.61	1.52	5	2
1	A	35	SER	CA-C	6.46	1.61	1.52	9	1
1	B	36	LEU	CA-CB	6.46	1.63	1.53	2	2
1	A	67	MET	C-N	6.43	1.42	1.33	9	1
1	B	45	LEU	N-CA	-6.42	1.38	1.46	1	1
1	B	65	ASN	CA-CB	6.41	1.64	1.53	10	1
1	B	45	LEU	C-N	6.39	1.42	1.33	7	1
1	A	77	ILE	C-O	-6.38	1.17	1.24	3	1
1	A	46	ILE	CA-C	-6.38	1.45	1.52	9	2
1	A	72	PRO	C-N	-6.38	1.25	1.33	4	1
1	A	83	ILE	CA-CB	6.36	1.62	1.54	3	3
1	A	47	TRP	CA-C	6.34	1.60	1.52	9	2
1	A	91	ARG	CA-C	6.34	1.61	1.52	8	1
1	B	29	SER	N-CA	6.30	1.53	1.46	6	1
1	B	35	SER	C-N	6.29	1.42	1.33	8	1
1	B	75	TYR	N-CA	-6.26	1.39	1.46	2	3
1	B	50	VAL	C-O	6.26	1.31	1.24	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	31	VAL	CA-C	-6.24	1.44	1.52	1	2
1	B	44	GLY	CA-C	-6.23	1.45	1.52	2	2
1	B	69	GLN	N-CA	-6.23	1.39	1.46	7	1
1	B	91	ARG	NE-CZ	-6.22	1.26	1.33	3	1
1	B	92	TRP	CA-C	6.20	1.60	1.52	2	2
1	B	24	VAL	N-CA	6.18	1.53	1.46	3	1
1	B	81	PHE	CA-CB	6.18	1.62	1.53	1	2
1	A	45	LEU	C-N	6.17	1.41	1.33	5	2
1	B	20	THR	CA-C	6.17	1.59	1.52	8	1
1	B	50	VAL	N-CA	6.16	1.53	1.46	7	1
1	B	68	ALA	N-CA	-6.12	1.38	1.46	5	2
1	B	63	ALA	C-O	-6.12	1.17	1.23	4	1
1	B	85	GLY	CA-C	6.12	1.58	1.52	6	1
1	B	19	ARG	CD-NE	6.11	1.54	1.46	8	2
1	B	70	LEU	C-N	6.10	1.42	1.33	4	1
1	B	69	GLN	CA-CB	6.09	1.64	1.54	4	1
1	A	72	PRO	CA-C	6.09	1.61	1.52	8	2
1	B	53	LEU	C-N	6.09	1.41	1.33	5	1
1	A	78	ALA	N-CA	-6.09	1.39	1.46	3	1
1	B	90	MET	CA-CB	6.08	1.62	1.53	8	1
1	A	93	HIS	CG-CD2	6.07	1.42	1.35	2	1
1	B	43	ILE	C-N	6.07	1.41	1.33	1	2
1	B	55	ALA	CA-C	6.06	1.60	1.52	5	3
1	A	67	MET	N-CA	6.06	1.53	1.46	5	2
1	B	56	ILE	N-CA	6.06	1.53	1.46	6	1
1	B	42	LEU	N-CA	6.05	1.53	1.46	10	3
1	B	93	HIS	CB-CG	6.03	1.58	1.50	6	2
1	B	64	LEU	N-CA	-6.03	1.38	1.46	4	1
1	A	45	LEU	CA-C	-6.02	1.44	1.52	2	1
1	B	33	PHE	CA-C	6.02	1.60	1.52	10	3
1	A	60	ALA	CA-C	6.02	1.60	1.52	1	1
1	A	53	LEU	N-CA	6.02	1.53	1.46	4	1
1	A	83	ILE	CA-C	6.02	1.60	1.52	10	1
1	A	68	ALA	CA-CB	-6.02	1.44	1.53	10	2
1	A	90	MET	CA-C	6.00	1.60	1.52	4	1
1	A	36	LEU	C-N	5.99	1.41	1.33	6	2
1	B	79	PHE	CA-CB	5.99	1.62	1.53	8	1
1	B	50	VAL	C-N	5.98	1.41	1.33	5	1
1	A	33	PHE	CA-CB	5.98	1.62	1.53	9	1
1	B	43	ILE	CA-CB	-5.98	1.47	1.54	9	1
1	B	74	ASN	N-CA	5.97	1.53	1.46	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	91	ARG	CA-C	-5.97	1.45	1.52	9	1
1	B	70	LEU	CA-C	-5.95	1.45	1.52	8	1
1	A	37	PHE	C-O	5.94	1.30	1.24	4	1
1	B	78	ALA	CA-C	5.94	1.60	1.52	10	1
1	B	80	ALA	CA-C	-5.94	1.45	1.52	8	1
1	A	91	ARG	CD-NE	5.93	1.54	1.46	4	1
1	A	33	PHE	N-CA	5.93	1.53	1.46	6	1
1	B	88	LEU	CA-C	-5.92	1.45	1.52	3	1
1	A	92	TRP	N-CA	-5.92	1.39	1.46	5	1
1	A	75	TYR	CA-CB	5.92	1.62	1.53	2	1
1	A	67	MET	CA-CB	5.92	1.65	1.53	1	1
1	A	24	VAL	N-CA	5.90	1.53	1.46	3	1
1	A	22	MET	CA-C	5.89	1.59	1.52	3	1
1	A	51	PHE	CA-CB	5.89	1.62	1.53	6	1
1	B	36	LEU	CA-C	-5.89	1.45	1.52	3	1
1	B	93	HIS	CG-ND1	5.86	1.44	1.38	2	1
1	B	59	GLN	C-O	5.86	1.30	1.23	4	1
1	A	59	GLN	CA-C	-5.85	1.45	1.52	10	2
1	A	93	HIS	CE1-NE2	-5.85	1.26	1.32	4	1
1	B	87	LEU	CA-CB	5.83	1.62	1.53	2	1
1	B	19	ARG	CA-C	-5.83	1.45	1.52	7	1
1	B	25	LYS	N-CA	-5.82	1.38	1.46	7	1
1	B	62	THR	CA-C	-5.80	1.45	1.52	7	3
1	B	19	ARG	C-N	5.79	1.41	1.33	1	2
1	B	36	LEU	C-N	-5.79	1.26	1.33	1	3
1	B	51	PHE	C-N	5.78	1.41	1.33	4	1
1	B	20	THR	N-CA	5.78	1.54	1.46	10	1
1	A	38	ILE	CA-C	-5.77	1.45	1.52	2	1
1	B	75	TYR	C-O	-5.76	1.17	1.24	8	1
1	A	92	TRP	C-O	-5.75	1.17	1.24	1	1
1	A	61	PRO	C-N	5.75	1.41	1.33	7	1
1	B	48	LEU	N-CA	-5.75	1.39	1.46	5	1
1	A	60	ALA	CA-CB	5.73	1.62	1.53	8	1
1	A	48	LEU	C-N	5.73	1.41	1.33	8	2
1	B	42	LEU	CA-CB	5.72	1.62	1.53	8	2
1	B	26	VAL	CA-C	-5.70	1.45	1.52	3	2
1	B	35	SER	CA-CB	5.69	1.62	1.53	9	3
1	A	32	TRP	NE1-CE2	5.68	1.43	1.37	8	1
1	A	40	LEU	CA-C	5.67	1.60	1.52	9	2
1	A	56	ILE	CB-CG1	5.67	1.64	1.53	7	1
1	B	49	MET	N-CA	-5.66	1.39	1.46	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	84	THR	N-CA	5.66	1.53	1.46	9	2
1	B	42	LEU	C-N	5.65	1.41	1.33	3	1
1	A	92	TRP	CD2-CE3	-5.64	1.31	1.40	1	1
1	B	93	HIS	CD2-NE2	5.64	1.44	1.37	3	1
1	A	68	ALA	C-O	-5.64	1.16	1.23	2	1
1	A	47	TRP	NE1-CE2	5.63	1.43	1.37	10	2
1	B	58	SER	N-CA	5.63	1.53	1.46	4	1
1	B	55	ALA	CA-CB	5.62	1.62	1.53	3	1
1	A	91	ARG	CA-CB	5.62	1.62	1.53	7	1
1	B	43	ILE	N-CA	-5.61	1.40	1.46	3	1
1	B	93	HIS	CE1-NE2	-5.59	1.26	1.32	2	1
1	A	79	PHE	CA-C	-5.59	1.45	1.52	7	1
1	A	42	LEU	N-CA	5.59	1.53	1.46	2	1
1	B	86	LEU	CA-CB	5.58	1.61	1.53	2	2
1	B	51	PHE	CA-C	-5.56	1.45	1.52	7	1
1	B	37	PHE	C-N	5.54	1.41	1.34	3	4
1	B	24	VAL	C-O	-5.53	1.18	1.24	8	1
1	A	45	LEU	CA-CB	5.52	1.61	1.53	3	1
1	B	73	TRP	NE1-CE2	-5.52	1.31	1.37	6	1
1	B	49	MET	CA-C	-5.51	1.45	1.52	9	1
1	A	58	SER	CA-C	-5.51	1.45	1.52	4	1
1	B	92	TRP	N-CA	-5.50	1.39	1.46	2	2
1	B	24	VAL	C-N	-5.50	1.26	1.33	3	1
1	B	30	SER	N-CA	5.46	1.52	1.46	8	1
1	A	83	ILE	C-N	5.46	1.41	1.33	9	1
1	A	74	ASN	CA-C	5.46	1.59	1.52	1	1
1	B	47	TRP	CA-C	-5.46	1.45	1.52	5	1
1	A	33	PHE	C-O	-5.45	1.17	1.24	4	1
1	A	86	LEU	CA-CB	5.45	1.61	1.53	8	2
1	A	88	LEU	N-CA	-5.44	1.39	1.46	6	1
1	A	75	TYR	N-CA	-5.44	1.40	1.46	6	1
1	A	53	LEU	C-N	-5.43	1.26	1.33	6	2
1	A	46	ILE	N-CA	-5.42	1.40	1.46	5	1
1	A	75	TYR	CA-C	5.42	1.59	1.52	9	1
1	A	73	TRP	NE1-CE2	5.41	1.43	1.37	5	1
1	A	47	TRP	C-N	5.39	1.40	1.33	2	2
1	B	56	ILE	CA-C	5.39	1.59	1.52	3	1
1	B	53	LEU	CA-CB	5.39	1.61	1.53	4	1
1	B	63	ALA	CA-C	5.39	1.58	1.52	2	1
1	A	48	LEU	N-CA	-5.39	1.39	1.46	5	1
1	B	59	GLN	C-N	5.38	1.44	1.33	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	49	MET	N-CA	-5.37	1.39	1.46	10	1
1	B	25	LYS	CA-C	5.37	1.58	1.52	2	1
1	B	86	LEU	CB-CG	5.35	1.64	1.53	5	1
1	A	42	LEU	C-N	5.35	1.40	1.33	3	1
1	B	34	VAL	CA-C	5.34	1.59	1.52	3	1
1	B	52	GLN	N-CA	-5.32	1.40	1.46	10	1
1	B	90	MET	CA-C	-5.31	1.45	1.52	9	2
1	B	22	MET	CA-CB	5.30	1.62	1.53	5	1
1	A	76	ALA	N-CA	-5.30	1.40	1.46	6	1
1	A	42	LEU	CA-C	5.29	1.59	1.52	1	1
1	B	48	LEU	CA-C	-5.29	1.46	1.52	4	1
1	A	51	PHE	CG-CD2	5.29	1.50	1.38	4	1
1	B	58	SER	C-O	5.29	1.29	1.23	6	1
1	A	76	ALA	C-O	-5.28	1.18	1.24	9	1
1	B	87	LEU	C-O	-5.28	1.18	1.24	5	2
1	B	89	THR	C-N	-5.28	1.27	1.33	8	1
1	A	88	LEU	C-O	-5.28	1.18	1.24	10	1
1	B	71	GLY	N-CA	5.27	1.51	1.44	5	1
1	B	87	LEU	CA-C	-5.26	1.46	1.52	6	1
1	A	29	SER	CA-C	5.26	1.59	1.52	9	1
1	B	47	TRP	NE1-CE2	5.25	1.43	1.37	8	1
1	A	31	VAL	CA-CB	5.25	1.61	1.54	3	1
1	A	91	ARG	N-CA	5.25	1.52	1.46	8	1
1	A	73	TRP	CA-C	5.23	1.59	1.52	3	1
1	B	41	MET	C-O	-5.23	1.18	1.24	1	1
1	B	45	LEU	CB-CG	5.23	1.64	1.53	8	1
1	B	39	GLY	CA-C	-5.22	1.46	1.52	10	1
1	B	52	GLN	CA-CB	5.22	1.61	1.53	10	1
1	A	43	ILE	CB-CG1	5.21	1.63	1.53	8	1
1	A	22	MET	N-CA	-5.21	1.39	1.46	3	1
1	B	82	MET	C-N	5.21	1.40	1.33	3	2
1	B	24	VAL	CA-C	-5.19	1.46	1.52	7	1
1	A	39	GLY	N-CA	5.19	1.52	1.45	3	1
1	A	82	MET	CA-CB	5.18	1.61	1.53	9	1
1	A	48	LEU	CA-CB	5.18	1.61	1.53	4	1
1	B	85	GLY	N-CA	5.18	1.52	1.45	9	1
1	B	38	ILE	N-CA	5.17	1.52	1.46	5	1
1	B	72	PRO	N-CA	-5.17	1.40	1.47	2	1
1	A	63	ALA	CA-C	5.16	1.58	1.52	9	1
1	B	83	ILE	C-N	5.16	1.40	1.33	10	1
1	B	26	VAL	C-O	-5.16	1.18	1.24	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	92	TRP	CA-CB	5.15	1.61	1.53	5	1
1	A	25	LYS	C-O	5.15	1.29	1.23	7	1
1	B	73	TRP	CZ2-CH2	5.15	1.47	1.37	7	1
1	A	53	LEU	CB-CG	5.15	1.63	1.53	5	1
1	B	56	ILE	C-N	5.15	1.41	1.33	5	1
1	B	41	MET	CA-CB	-5.14	1.45	1.53	6	1
1	A	66	TRP	NE1-CE2	5.14	1.43	1.37	10	1
1	A	77	ILE	CB-CG1	5.13	1.63	1.53	6	1
1	B	92	TRP	NE1-CE2	-5.13	1.31	1.37	2	1
1	B	41	MET	CA-C	5.13	1.59	1.52	9	1
1	A	40	LEU	C-O	5.11	1.29	1.24	1	1
1	B	17	VAL	C-N	5.11	1.40	1.33	8	1
1	B	33	PHE	C-N	5.11	1.40	1.33	2	1
1	A	66	TRP	C-O	-5.11	1.18	1.23	10	1
1	A	29	SER	N-CA	5.10	1.52	1.46	10	1
1	B	45	LEU	CA-C	5.09	1.59	1.52	6	1
1	A	22	MET	CG-SD	5.08	1.93	1.80	5	1
1	A	66	TRP	N-CA	5.07	1.52	1.46	3	1
1	A	66	TRP	CD2-CE3	-5.07	1.32	1.40	7	1
1	A	43	ILE	CA-C	5.07	1.59	1.52	3	1
1	A	68	ALA	N-CA	-5.07	1.39	1.45	7	1
1	A	44	GLY	C-N	5.06	1.40	1.33	9	1
1	A	89	THR	CA-C	-5.06	1.46	1.52	8	1
1	B	45	LEU	C-O	-5.05	1.18	1.24	10	1
1	B	73	TRP	C-N	5.05	1.40	1.33	4	1
1	B	92	TRP	CZ2-CH2	5.05	1.46	1.37	7	1
1	B	76	ALA	CA-C	-5.05	1.46	1.52	8	1
1	A	79	PHE	C-O	-5.04	1.18	1.24	1	1
1	B	73	TRP	CA-C	-5.04	1.46	1.52	10	1
1	B	93	HIS	CG-CD2	5.04	1.41	1.35	4	1
1	A	24	VAL	C-O	-5.04	1.19	1.24	6	1
1	B	42	LEU	CA-C	-5.04	1.46	1.52	7	1
1	A	88	LEU	CA-C	5.03	1.59	1.52	1	1
1	A	41	MET	C-N	5.03	1.40	1.33	3	1
1	B	41	MET	N-CA	-5.02	1.40	1.46	8	1
1	A	89	THR	C-N	5.01	1.40	1.33	6	1
1	A	43	ILE	C-N	5.00	1.40	1.33	4	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	B	20	THR	N-CA-C	20.27	159.48	108.40	6	10
1	B	29	SER	N-CA-C	20.11	133.35	111.03	6	10
1	B	20	THR	CB-CA-C	-19.76	80.80	109.45	5	10
1	B	54	ALA	N-CA-C	16.59	128.82	111.07	6	8
1	B	30	SER	N-CA-C	13.62	125.82	110.97	6	8
1	B	53	LEU	CA-C-N	-13.17	103.32	120.44	7	8
1	B	53	LEU	C-N-CA	-13.17	103.32	120.44	7	8
1	A	73	TRP	N-CA-C	13.14	127.05	111.02	9	8
1	B	20	THR	N-CA-CB	-12.82	82.11	110.95	2	10
1	B	53	LEU	N-CA-C	12.56	124.97	111.28	2	3
1	A	19	ARG	O-C-N	-12.29	108.46	123.33	1	10
1	A	79	PHE	CA-CB-CG	-12.19	101.61	113.80	3	8
1	A	29	SER	N-CA-C	12.06	136.50	110.80	1	10
1	B	93	HIS	CA-CB-CG	11.50	125.30	113.80	8	1
1	B	20	THR	CA-CB-CG2	11.49	130.03	110.50	4	10
1	B	73	TRP	N-CA-C	11.48	123.77	111.03	5	8
1	B	26	VAL	N-CA-C	-11.43	91.53	108.45	1	5
1	B	79	PHE	CA-CB-CG	-11.35	102.45	113.80	6	7
1	A	26	VAL	N-CA-C	-11.32	91.82	108.12	5	6
1	A	69	GLN	OE1-CD-NE2	-11.08	111.52	122.60	5	2
1	B	91	ARG	NE-CZ-NH1	11.02	132.52	121.50	9	5
1	A	55	ALA	N-CA-C	10.90	126.41	110.28	4	10
1	A	49	MET	N-CA-C	10.53	122.34	111.07	7	5
1	B	54	ALA	N-CA-CB	-10.48	94.81	110.01	5	1
1	A	91	ARG	NE-CZ-NH2	-10.39	109.85	119.20	6	3
1	B	55	ALA	N-CA-C	10.32	132.78	110.80	9	10
1	B	20	THR	CA-CB-OG1	10.12	124.77	109.60	7	6
1	A	67	MET	O-C-N	-9.98	111.26	123.33	1	1
1	A	51	PHE	CA-CB-CG	-9.94	103.86	113.80	9	5
1	A	86	LEU	N-CA-C	9.92	122.09	111.28	5	1
1	A	91	ARG	NE-CZ-NH1	9.88	131.38	121.50	2	4
1	A	90	MET	CA-C-N	9.86	135.29	120.31	5	6
1	A	90	MET	C-N-CA	9.86	135.29	120.31	5	6
1	B	68	ALA	N-CA-C	9.80	124.03	109.24	8	3
1	A	52	GLN	N-CA-CB	9.62	124.28	109.94	3	1
1	A	91	ARG	N-CA-C	9.58	122.73	111.71	6	6
1	B	38	ILE	CA-C-N	9.56	130.55	119.94	5	4
1	B	38	ILE	C-N-CA	9.56	130.55	119.94	5	4
1	B	50	VAL	N-CA-C	9.55	119.51	110.53	1	4
1	B	91	ARG	CA-C-N	9.47	132.97	120.28	4	4
1	B	91	ARG	C-N-CA	9.47	132.97	120.28	4	4
1	B	26	VAL	O-C-N	-9.46	112.98	123.20	4	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	81	PHE	N-CA-C	9.34	121.07	111.07	6	2
1	A	54	ALA	N-CA-C	9.34	121.46	111.28	8	7
1	B	61	PRO	CA-C-O	-9.22	114.49	121.31	4	2
1	B	89	THR	CA-C-N	9.21	132.62	120.28	8	5
1	B	89	THR	C-N-CA	9.21	132.62	120.28	8	5
1	A	75	TYR	CB-CA-C	9.09	125.15	110.88	9	2
1	B	74	ASN	OD1-CG-ND2	-9.03	113.57	122.60	9	2
1	A	47	TRP	N-CA-C	8.99	120.69	111.07	5	2
1	B	76	ALA	N-CA-C	8.96	121.05	111.28	4	3
1	A	58	SER	O-C-N	-8.87	112.54	123.36	9	2
1	A	74	ASN	N-CA-C	8.83	120.83	111.03	2	6
1	B	27	GLY	O-C-N	-8.77	113.00	121.77	7	2
1	B	78	ALA	CA-C-N	8.77	131.84	120.44	5	1
1	B	78	ALA	C-N-CA	8.77	131.84	120.44	5	1
1	A	26	VAL	CA-C-N	-8.74	108.14	121.87	8	7
1	A	26	VAL	C-N-CA	-8.74	108.14	121.87	8	7
1	B	91	ARG	NH1-CZ-NH2	-8.70	107.99	119.30	6	6
1	B	38	ILE	CB-CA-C	-8.65	100.46	112.14	6	4
1	A	60	ALA	O-C-N	-8.61	111.42	121.32	4	2
1	B	90	MET	N-CA-C	8.59	120.64	111.28	6	3
1	A	20	THR	O-C-N	-8.56	113.16	121.38	7	1
1	B	91	ARG	CA-C-O	8.54	129.48	120.42	9	3
1	B	78	ALA	CA-C-O	8.47	129.72	120.82	6	2
1	B	74	ASN	N-CA-C	8.46	120.27	111.14	3	3
1	A	26	VAL	O-C-N	-8.44	113.95	123.07	6	2
1	B	40	LEU	N-CA-C	8.40	120.06	111.07	9	3
1	A	52	GLN	O-C-N	-8.40	113.21	122.12	6	3
1	A	41	MET	N-CA-C	8.37	120.03	111.07	5	3
1	A	86	LEU	CA-C-N	8.37	131.49	120.28	7	2
1	A	86	LEU	C-N-CA	8.37	131.49	120.28	7	2
1	A	37	PHE	CA-CB-CG	-8.35	105.45	113.80	6	1
1	A	52	GLN	N-CA-C	8.35	120.38	111.28	2	3
1	A	21	PRO	N-CA-CB	-8.33	93.44	102.60	8	2
1	A	26	VAL	N-CA-CB	8.32	123.67	111.52	5	4
1	A	77	ILE	N-CA-C	8.31	118.40	110.42	5	5
1	B	20	THR	O-C-N	-8.31	113.22	121.94	2	3
1	B	83	ILE	CB-CA-C	-8.31	101.33	111.97	6	6
1	B	72	PRO	N-CA-CB	-8.30	94.54	103.25	9	4
1	A	79	PHE	N-CA-C	8.28	120.30	111.28	4	6
1	B	84	THR	CA-C-N	8.26	129.10	119.94	1	4
1	B	84	THR	C-N-CA	8.26	129.10	119.94	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	85	GLY	CA-C-N	-8.20	109.30	120.28	8	1
1	B	85	GLY	C-N-CA	-8.20	109.30	120.28	8	1
1	A	90	MET	N-CA-C	8.19	120.21	111.28	10	1
1	B	26	VAL	CA-C-N	-8.19	109.02	121.87	10	10
1	B	26	VAL	C-N-CA	-8.19	109.02	121.87	10	10
1	B	19	ARG	O-C-N	-8.14	113.48	123.33	3	2
1	A	40	LEU	CA-C-N	8.09	131.33	120.65	4	1
1	A	40	LEU	C-N-CA	8.09	131.33	120.65	4	1
1	B	83	ILE	CA-C-N	8.09	130.96	120.44	7	2
1	B	83	ILE	C-N-CA	8.09	130.96	120.44	7	2
1	B	80	ALA	N-CA-C	8.09	120.10	111.28	9	3
1	A	32	TRP	N-CA-C	8.06	120.07	111.28	5	1
1	A	81	PHE	CA-C-N	8.06	130.91	120.44	2	1
1	A	81	PHE	C-N-CA	8.06	130.91	120.44	2	1
1	A	40	LEU	N-CA-C	8.05	120.05	111.28	5	1
1	B	79	PHE	N-CA-C	8.04	119.67	111.07	4	4
1	A	54	ALA	CA-C-N	8.03	132.91	121.42	7	4
1	A	54	ALA	C-N-CA	8.03	132.91	121.42	7	4
1	B	91	ARG	N-CA-C	7.98	119.61	111.07	7	2
1	B	49	MET	N-CA-C	7.97	119.60	111.07	9	3
1	A	39	GLY	O-C-N	-7.95	114.56	122.19	6	1
1	B	56	ILE	CA-C-O	7.94	128.78	120.36	8	3
1	A	72	PRO	N-CA-CB	-7.94	97.49	102.81	1	4
1	B	35	SER	N-CA-C	7.87	119.86	111.28	6	3
1	A	43	ILE	CB-CA-C	7.85	122.74	112.14	9	2
1	A	32	TRP	O-C-N	-7.84	114.00	122.07	3	2
1	A	43	ILE	N-CA-CB	-7.82	99.90	110.54	4	1
1	B	26	VAL	CA-C-O	-7.79	112.19	120.76	1	1
1	B	52	GLN	N-CA-CB	7.78	121.36	110.07	5	2
1	B	29	SER	CB-CA-C	-7.78	98.02	110.86	9	6
1	B	87	LEU	CA-C-N	7.77	130.69	120.28	4	4
1	B	87	LEU	C-N-CA	7.77	130.69	120.28	4	4
1	A	29	SER	N-CA-CB	-7.76	97.37	110.49	4	5
1	B	21	PRO	N-CA-C	7.76	125.92	113.12	5	6
1	B	53	LEU	O-C-N	-7.75	112.74	122.27	3	3
1	B	75	TYR	CB-CA-C	7.73	123.01	110.88	10	2
1	A	55	ALA	O-C-N	-7.72	113.43	122.93	3	2
1	A	88	LEU	CA-C-N	7.71	130.46	120.44	9	2
1	A	88	LEU	C-N-CA	7.71	130.46	120.44	9	2
1	B	54	ALA	CA-C-N	7.70	136.25	121.54	9	3
1	B	54	ALA	C-N-CA	7.70	136.25	121.54	9	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	74	ASN	OD1-CG-ND2	-7.70	114.90	122.60	7	2
1	A	93	HIS	N-CA-CB	-7.70	97.41	110.50	9	3
1	B	60	ALA	CA-C-O	-7.70	109.62	120.16	2	1
1	A	89	THR	N-CA-C	7.69	119.30	111.07	1	1
1	A	79	PHE	N-CA-CB	7.69	121.43	110.12	4	2
1	B	76	ALA	CA-C-N	7.67	130.23	120.56	5	2
1	B	76	ALA	C-N-CA	7.67	130.23	120.56	5	2
1	B	91	ARG	NE-CZ-NH2	7.63	126.06	119.20	3	4
1	B	54	ALA	CA-C-O	7.62	128.70	120.55	10	3
1	B	19	ARG	NH1-CZ-NH2	-7.61	109.41	119.30	2	2
1	A	48	LEU	N-CA-CB	7.60	121.03	110.01	10	2
1	A	83	ILE	CB-CA-C	7.59	122.70	112.22	4	5
1	B	46	ILE	N-CA-C	7.59	118.36	110.62	3	4
1	A	84	THR	N-CA-CB	7.57	121.24	110.12	1	6
1	B	45	LEU	O-C-N	-7.56	114.28	122.07	1	1
1	A	19	ARG	NE-CZ-NH1	7.56	129.06	121.50	6	1
1	A	27	GLY	O-C-N	-7.56	114.21	121.77	8	3
1	A	67	MET	CA-C-O	7.55	129.66	120.60	1	1
1	A	24	VAL	CA-C-O	7.55	127.73	120.25	8	1
1	A	37	PHE	CB-CA-C	7.52	123.28	110.79	5	2
1	B	60	ALA	CA-C-N	-7.49	114.08	121.65	9	1
1	B	60	ALA	C-N-CA	-7.49	114.08	121.65	9	1
1	B	87	LEU	N-CA-C	7.48	119.44	111.28	9	2
1	B	74	ASN	CA-C-O	7.47	128.67	120.82	4	1
1	B	19	ARG	NE-CZ-NH2	-7.47	112.48	119.20	1	2
1	B	53	LEU	CB-CA-C	7.46	123.18	110.79	8	3
1	B	93	HIS	CG-CD2-NE2	7.42	114.62	107.20	2	1
1	A	85	GLY	N-CA-C	7.41	121.63	112.73	10	1
1	B	76	ALA	CA-C-O	7.41	128.60	120.82	1	1
1	A	82	MET	CG-SD-CE	-7.40	84.61	100.90	8	1
1	A	66	TRP	O-C-N	-7.40	114.34	123.36	7	4
1	A	25	LYS	O-C-N	-7.39	114.34	123.36	2	2
1	B	83	ILE	O-C-N	7.39	129.59	121.90	9	2
1	B	25	LYS	O-C-N	-7.38	114.35	123.36	4	4
1	B	19	ARG	NE-CZ-NH1	7.37	128.87	121.50	2	1
1	B	82	MET	O-C-N	-7.35	114.50	122.07	2	1
1	A	24	VAL	N-CA-C	7.35	118.90	108.17	5	1
1	B	53	LEU	N-CA-CB	7.34	120.90	110.12	8	4
1	B	68	ALA	CA-C-O	7.33	128.96	120.89	3	2
1	B	90	MET	O-C-N	-7.33	114.35	122.12	3	4
1	A	65	ASN	OD1-CG-ND2	-7.33	115.27	122.60	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	76	ALA	CA-C-N	7.32	129.78	120.56	4	1
1	A	76	ALA	C-N-CA	7.32	129.78	120.56	4	1
1	B	65	ASN	O-C-N	-7.32	114.43	123.36	7	1
1	B	88	LEU	CB-CA-C	7.29	122.90	110.79	9	1
1	A	51	PHE	N-CA-C	7.29	118.87	111.07	2	3
1	A	52	GLN	OE1-CD-NE2	-7.28	115.32	122.60	9	4
1	B	32	TRP	O-C-N	-7.27	114.58	122.07	1	1
1	A	89	THR	CA-C-N	7.24	129.99	120.28	7	2
1	A	89	THR	C-N-CA	7.24	129.99	120.28	7	2
1	B	41	MET	N-CA-C	7.22	118.80	111.07	2	3
1	B	31	VAL	CA-C-N	7.22	129.82	120.44	1	2
1	B	31	VAL	C-N-CA	7.22	129.82	120.44	1	2
1	A	31	VAL	CA-C-N	7.21	129.81	120.44	8	3
1	A	31	VAL	C-N-CA	7.21	129.81	120.44	8	3
1	A	48	LEU	CA-C-O	-7.19	112.92	120.55	9	1
1	A	87	LEU	CA-C-N	7.19	129.92	120.28	2	3
1	A	87	LEU	C-N-CA	7.19	129.92	120.28	2	3
1	A	35	SER	N-CA-C	7.19	118.76	111.07	9	3
1	A	52	GLN	CA-C-N	7.17	129.89	120.28	10	5
1	A	52	GLN	C-N-CA	7.17	129.89	120.28	10	5
1	A	93	HIS	CE1-NE2-CD2	-7.16	101.84	109.00	5	6
1	A	43	ILE	CA-C-N	7.15	127.92	119.98	8	1
1	A	43	ILE	C-N-CA	7.15	127.92	119.98	8	1
1	A	46	ILE	N-CA-C	7.14	117.28	110.42	5	2
1	B	88	LEU	O-C-N	-7.14	114.55	122.12	2	2
1	A	77	ILE	N-CA-CB	7.14	119.71	110.57	9	2
1	A	34	VAL	N-CA-C	7.13	117.26	110.42	9	3
1	B	60	ALA	O-C-N	-7.12	113.13	121.32	5	4
1	B	30	SER	CA-C-N	7.11	130.20	120.46	9	3
1	B	30	SER	C-N-CA	7.11	130.20	120.46	9	3
1	A	82	MET	N-CA-C	7.10	118.67	111.07	5	2
1	B	30	SER	CA-C-O	7.09	128.21	120.90	2	3
1	A	19	ARG	NE-CZ-NH2	-7.08	112.83	119.20	3	2
1	A	91	ARG	N-CA-CB	7.07	120.52	110.12	4	3
1	A	42	LEU	N-CA-C	7.04	118.60	111.07	6	1
1	A	30	SER	CA-C-N	7.04	130.10	120.46	2	2
1	A	30	SER	C-N-CA	7.04	130.10	120.46	2	2
1	A	66	TRP	CA-CB-CG	7.03	126.95	113.60	7	1
1	B	46	ILE	CA-C-O	7.02	128.30	120.85	7	2
1	B	46	ILE	O-C-N	7.02	129.06	121.83	4	4
1	B	73	TRP	CA-C-O	-7.01	113.64	121.00	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	83	ILE	N-CA-C	7.00	117.14	110.42	10	2
1	B	80	ALA	CA-C-O	6.99	128.16	120.82	7	2
1	A	92	TRP	N-CA-C	-6.98	103.69	111.71	7	2
1	B	21	PRO	N-CA-CB	-6.98	98.14	102.81	5	1
1	B	61	PRO	N-CA-CB	-6.97	98.14	102.81	2	3
1	B	49	MET	CB-CA-C	6.97	121.82	110.88	1	1
1	A	22	MET	CA-C-N	6.96	132.69	122.39	5	1
1	A	22	MET	C-N-CA	6.96	132.69	122.39	5	1
1	A	33	PHE	O-C-N	6.95	129.22	122.07	2	1
1	A	37	PHE	N-CA-C	6.94	118.84	111.28	5	1
1	A	70	LEU	CA-C-N	6.93	132.75	121.87	10	2
1	A	70	LEU	C-N-CA	6.93	132.75	121.87	10	2
1	A	38	ILE	N-CA-C	6.92	117.07	110.42	6	2
1	B	52	GLN	N-CA-C	6.89	118.44	111.07	8	1
1	B	92	TRP	N-CA-C	6.88	118.78	111.28	9	2
1	A	35	SER	N-CA-CB	6.88	120.23	110.12	5	2
1	A	93	HIS	CA-CB-CG	6.87	120.67	113.80	9	1
1	A	55	ALA	CA-C-O	6.86	128.87	121.05	7	2
1	A	84	THR	O-C-N	-6.84	114.87	122.12	1	3
1	A	23	LYS	O-C-N	-6.83	115.03	123.36	7	1
1	A	89	THR	CA-C-O	6.82	127.98	120.82	8	2
1	A	39	GLY	N-CA-C	6.81	120.90	112.73	6	1
1	B	31	VAL	CA-C-O	6.80	128.06	120.85	7	1
1	B	74	ASN	CA-C-N	6.79	129.27	120.44	5	4
1	B	74	ASN	C-N-CA	6.79	129.27	120.44	5	4
1	B	52	GLN	CA-C-N	6.79	129.38	120.28	5	2
1	B	52	GLN	C-N-CA	6.79	129.38	120.28	5	2
1	B	67	MET	N-CA-CB	6.79	122.22	110.81	5	1
1	A	93	HIS	ND1-CE1-NE2	6.77	115.17	108.40	2	3
1	A	68	ALA	N-CA-C	6.77	119.46	109.24	2	1
1	B	44	GLY	N-CA-C	6.75	120.33	112.50	10	2
1	B	28	PRO	CA-C-N	6.74	131.79	120.88	3	2
1	B	28	PRO	C-N-CA	6.74	131.79	120.88	3	2
1	B	48	LEU	CA-C-N	6.74	129.20	120.44	6	2
1	B	48	LEU	C-N-CA	6.74	129.20	120.44	6	2
1	A	83	ILE	N-CA-C	6.70	117.46	110.62	6	6
1	A	19	ARG	N-CA-C	-6.70	97.67	109.06	1	1
1	B	55	ALA	CA-C-O	6.67	130.05	120.51	3	2
1	A	71	GLY	CA-C-O	-6.67	111.98	121.52	1	2
1	A	84	THR	CA-C-N	6.65	127.36	119.98	8	5
1	A	84	THR	C-N-CA	6.65	127.36	119.98	8	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	34	VAL	N-CA-CB	-6.64	102.78	110.55	2	1
1	A	91	ARG	CB-CA-C	6.63	122.89	110.63	8	1
1	A	74	ASN	CA-C-N	6.63	129.06	120.44	10	3
1	A	74	ASN	C-N-CA	6.63	129.06	120.44	10	3
1	A	79	PHE	CA-C-O	-6.62	113.53	120.55	10	5
1	A	78	ALA	N-CA-C	6.62	118.15	111.07	3	5
1	A	24	VAL	CB-CA-C	6.61	119.11	110.12	7	2
1	B	82	MET	N-CA-C	6.60	119.31	111.33	10	3
1	B	42	LEU	CA-C-N	6.59	128.87	120.56	6	3
1	B	42	LEU	C-N-CA	6.59	128.87	120.56	6	3
1	A	80	ALA	O-C-N	-6.59	115.23	122.09	4	1
1	A	49	MET	CA-C-O	-6.59	113.90	120.82	4	1
1	B	88	LEU	CA-C-O	-6.59	113.57	120.55	10	1
1	A	69	GLN	O-C-N	-6.59	113.83	122.59	3	2
1	B	43	ILE	N-CA-C	6.57	116.73	110.42	8	2
1	A	82	MET	CA-C-O	-6.57	113.92	120.82	2	2
1	A	74	ASN	CA-C-O	6.56	127.66	120.90	7	2
1	A	65	ASN	CA-CB-CG	6.55	119.15	112.60	6	4
1	B	93	HIS	ND1-CE1-NE2	6.55	114.95	108.40	9	3
1	B	20	THR	CA-C-O	-6.54	112.58	119.13	10	2
1	B	31	VAL	N-CA-C	6.54	117.32	110.72	7	2
1	B	29	SER	CA-C-N	-6.53	111.75	120.63	10	2
1	B	29	SER	C-N-CA	-6.53	111.75	120.63	10	2
1	B	47	TRP	O-C-N	-6.53	115.20	122.12	1	3
1	B	21	PRO	CA-C-O	-6.51	114.35	121.77	4	2
1	B	31	VAL	O-C-N	6.50	128.17	121.87	2	1
1	B	39	GLY	O-C-N	-6.49	115.95	122.19	2	1
1	B	59	GLN	CB-CG-CD	6.49	123.64	112.60	5	2
1	A	84	THR	N-CA-C	6.49	118.36	111.28	8	1
1	A	35	SER	CA-C-O	-6.49	113.54	120.42	7	1
1	A	53	LEU	N-CA-C	6.49	118.35	111.28	7	1
1	A	37	PHE	CA-C-N	6.47	128.71	120.56	10	2
1	A	37	PHE	C-N-CA	6.47	128.71	120.56	10	2
1	A	19	ARG	N-CA-CB	6.46	121.67	110.81	2	5
1	B	38	ILE	N-CA-CB	6.46	119.32	110.54	6	2
1	A	32	TRP	CD2-CE2-CZ2	-6.45	115.95	122.40	4	2
1	B	65	ASN	CA-CB-CG	6.43	119.03	112.60	2	2
1	B	43	ILE	CA-C-N	6.42	127.07	119.94	3	3
1	B	43	ILE	C-N-CA	6.42	127.07	119.94	3	3
1	B	77	ILE	N-CA-C	6.42	117.17	110.62	8	4
1	A	30	SER	N-CA-C	6.42	119.59	111.69	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	33	PHE	CA-C-O	6.41	127.55	120.82	2	1
1	B	33	PHE	CA-CB-CG	-6.40	107.40	113.80	8	3
1	A	92	TRP	CA-C-O	6.39	127.33	120.55	9	1
1	B	28	PRO	N-CA-CB	6.38	109.62	102.60	5	2
1	A	32	TRP	CA-C-O	-6.38	114.12	120.82	6	2
1	B	86	LEU	CA-C-N	6.38	128.73	120.44	6	4
1	B	86	LEU	C-N-CA	6.38	128.73	120.44	6	4
1	B	19	ARG	N-CA-CB	6.37	122.53	111.13	5	2
1	B	49	MET	CA-C-N	-6.35	111.77	120.46	5	2
1	B	49	MET	C-N-CA	-6.35	111.77	120.46	5	2
1	A	24	VAL	O-C-N	-6.34	116.22	123.07	4	2
1	A	20	THR	CB-CA-C	-6.33	100.52	110.02	3	1
1	B	78	ALA	N-CA-C	6.33	118.17	111.28	5	3
1	A	33	PHE	N-CA-CB	6.32	119.18	110.01	10	1
1	B	47	TRP	N-CA-C	6.32	117.83	111.07	2	1
1	A	82	MET	CA-C-N	6.32	129.39	120.42	4	2
1	A	82	MET	C-N-CA	6.32	129.39	120.42	4	2
1	A	63	ALA	N-CA-C	6.32	119.87	108.69	5	2
1	A	72	PRO	CB-CA-C	6.31	122.14	112.10	1	1
1	A	87	LEU	N-CA-C	6.31	117.82	111.07	2	2
1	A	74	ASN	O-C-N	-6.30	115.23	122.03	7	1
1	B	44	GLY	CA-C-O	6.29	127.79	121.00	6	1
1	A	70	LEU	N-CA-C	6.28	119.81	108.69	9	1
1	B	39	GLY	CA-C-O	6.27	127.93	120.90	3	2
1	B	79	PHE	N-CA-CB	6.26	119.08	110.01	1	1
1	B	34	VAL	CA-C-N	6.25	128.56	120.44	1	4
1	B	34	VAL	C-N-CA	6.25	128.56	120.44	1	4
1	A	58	SER	CA-C-O	6.23	127.94	120.28	7	1
1	B	23	LYS	O-C-N	-6.22	115.77	123.36	2	1
1	B	81	PHE	N-CA-C	6.21	118.05	111.28	7	2
1	B	57	GLY	O-C-N	-6.21	114.62	122.70	9	1
1	B	64	LEU	N-CA-CB	6.21	121.24	110.81	5	2
1	B	42	LEU	CA-C-O	6.19	127.32	120.82	4	2
1	A	64	LEU	O-C-N	-6.19	115.81	123.36	6	1
1	A	42	LEU	CA-C-N	6.18	128.57	120.60	1	2
1	A	42	LEU	C-N-CA	6.18	128.57	120.60	1	2
1	A	33	PHE	CA-CB-CG	-6.17	107.63	113.80	8	2
1	A	18	SER	N-CA-C	6.17	119.18	108.76	9	1
1	B	35	SER	CB-CA-C	-6.16	100.57	110.79	4	2
1	A	43	ILE	O-C-N	-6.15	115.90	121.87	6	2
1	B	19	ARG	CG-CD-NE	-6.15	98.47	112.00	9	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	47	TRP	CE3-CZ3-CH2	6.15	129.09	121.10	10	1
1	A	47	TRP	CB-CG-CD1	-6.13	117.71	126.90	6	2
1	A	79	PHE	CB-CA-C	6.12	121.25	110.85	1	1
1	A	45	LEU	O-C-N	-6.10	115.78	122.07	7	2
1	B	72	PRO	CA-C-N	6.09	128.69	120.65	1	1
1	B	72	PRO	C-N-CA	6.09	128.69	120.65	1	1
1	A	89	THR	O-C-N	-6.09	115.80	122.07	2	3
1	B	56	ILE	O-C-N	-6.08	116.50	123.07	2	2
1	B	92	TRP	CA-C-N	6.08	132.64	121.70	10	2
1	B	92	TRP	C-N-CA	6.08	132.64	121.70	10	2
1	A	44	GLY	O-C-N	-6.07	116.28	122.17	10	1
1	A	91	ARG	CA-C-N	6.07	128.41	120.28	3	4
1	A	91	ARG	C-N-CA	6.07	128.41	120.28	3	4
1	A	86	LEU	O-C-N	-6.07	115.82	122.07	1	1
1	A	77	ILE	O-C-N	-6.06	115.60	121.90	10	1
1	A	69	GLN	CB-CG-CD	-6.05	102.31	112.60	3	1
1	B	42	LEU	O-C-N	-6.04	115.71	122.12	2	3
1	A	25	LYS	CA-C-O	-6.04	112.05	120.21	8	1
1	A	65	ASN	O-C-N	-6.04	115.99	123.36	7	1
1	A	83	ILE	CA-CB-CG2	-6.03	100.24	110.50	4	1
1	B	59	GLN	OE1-CD-NE2	-6.03	116.57	122.60	8	2
1	A	18	SER	CA-C-O	6.03	127.70	120.28	3	1
1	A	84	THR	CA-CB-OG1	6.03	118.64	109.60	2	2
1	B	81	PHE	O-C-N	-6.03	115.73	122.12	7	1
1	B	68	ALA	O-C-N	-6.02	116.74	123.48	3	1
1	A	56	ILE	N-CA-CB	6.01	120.30	111.52	8	2
1	B	84	THR	O-C-N	6.01	128.26	122.07	6	1
1	A	31	VAL	N-CA-CB	6.00	118.24	110.57	4	1
1	A	19	ARG	CG-CD-NE	-5.99	98.83	112.00	8	1
1	A	31	VAL	CB-CA-C	5.99	119.63	111.97	8	1
1	A	70	LEU	CA-C-O	-5.98	114.31	120.89	2	4
1	B	69	GLN	N-CA-C	-5.97	104.12	112.12	10	1
1	B	77	ILE	CB-CA-C	-5.95	104.22	112.02	1	1
1	B	37	PHE	CA-CB-CG	-5.95	107.85	113.80	9	1
1	A	52	GLN	CA-C-O	5.95	126.86	120.55	4	1
1	B	52	GLN	OE1-CD-NE2	-5.93	116.67	122.60	3	3
1	B	32	TRP	N-CA-C	5.91	117.40	111.07	9	1
1	B	70	LEU	CA-C-N	5.91	131.15	121.87	3	1
1	B	70	LEU	C-N-CA	5.91	131.15	121.87	3	1
1	A	56	ILE	O-C-N	-5.90	116.83	123.20	1	2
1	B	43	ILE	O-C-N	-5.88	116.14	121.91	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	22	MET	N-CA-C	5.87	119.08	108.69	5	1
1	A	45	LEU	CA-C-N	5.87	128.17	120.60	7	1
1	A	45	LEU	C-N-CA	5.87	128.17	120.60	7	1
1	B	83	ILE	N-CA-CB	5.87	117.42	110.55	1	4
1	A	67	MET	CA-C-N	-5.87	112.97	122.36	3	1
1	A	67	MET	C-N-CA	-5.87	112.97	122.36	3	1
1	A	31	VAL	CA-CB-CG2	5.86	120.37	110.40	2	1
1	A	83	ILE	O-C-N	-5.86	115.80	121.83	4	2
1	A	62	THR	N-CA-C	5.86	119.06	108.69	5	1
1	B	25	LYS	CA-C-O	5.85	127.34	120.20	6	1
1	A	40	LEU	O-C-N	-5.84	115.93	122.12	5	1
1	A	34	VAL	CA-CB-CG2	-5.83	100.48	110.40	7	1
1	A	34	VAL	N-CA-CB	-5.83	103.73	110.55	6	1
1	B	73	TRP	O-C-N	-5.83	116.06	122.07	10	1
1	B	66	TRP	O-C-N	-5.83	116.28	123.33	6	2
1	A	35	SER	O-C-N	-5.82	116.07	122.07	1	2
1	A	32	TRP	CB-CG-CD1	-5.82	118.17	126.90	8	1
1	A	22	MET	O-C-N	-5.82	116.29	123.33	5	2
1	A	77	ILE	CA-CB-CG1	5.80	120.26	110.40	5	1
1	B	45	LEU	CA-C-O	-5.80	114.40	120.55	10	1
1	B	47	TRP	CA-C-O	-5.80	114.69	120.90	4	1
1	B	75	TYR	CA-C-N	5.80	127.98	120.44	7	3
1	B	75	TYR	C-N-CA	5.80	127.98	120.44	7	3
1	A	36	LEU	CA-C-N	5.80	127.98	120.44	8	2
1	A	36	LEU	C-N-CA	5.80	127.98	120.44	8	2
1	A	66	TRP	CB-CG-CD1	-5.79	118.21	126.90	10	3
1	B	93	HIS	CE1-NE2-CD2	-5.79	103.21	109.00	9	2
1	A	91	ARG	CB-CG-CD	5.79	124.62	111.30	5	2
1	B	23	LYS	CA-C-N	5.79	131.04	122.99	2	1
1	B	23	LYS	C-N-CA	5.79	131.04	122.99	2	1
1	A	53	LEU	CB-CA-C	5.78	120.39	110.79	6	2
1	B	90	MET	CA-C-O	5.78	126.62	119.97	10	1
1	B	69	GLN	O-C-N	-5.78	115.19	121.95	10	1
1	A	69	GLN	CB-CA-C	5.77	121.91	110.42	5	1
1	B	70	LEU	CA-C-O	5.77	128.00	120.21	6	2
1	B	84	THR	N-CA-CB	5.77	118.37	110.01	7	2
1	B	56	ILE	N-CA-CB	5.75	119.92	111.52	5	1
1	A	49	MET	O-C-N	-5.74	116.04	122.12	1	3
1	B	87	LEU	CA-C-O	-5.73	114.80	120.82	4	2
1	A	55	ALA	N-CA-CB	5.73	118.39	109.97	10	1
1	A	30	SER	N-CA-CB	5.72	118.37	110.07	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	78	ALA	CA-C-O	5.72	126.83	120.82	3	1
1	B	48	LEU	N-CA-C	-5.71	104.97	111.14	1	1
1	B	73	TRP	CA-C-N	5.71	127.87	120.44	10	1
1	B	73	TRP	C-N-CA	5.71	127.87	120.44	10	1
1	A	60	ALA	CA-C-N	5.71	126.98	119.84	9	1
1	A	60	ALA	C-N-CA	5.71	126.98	119.84	9	1
1	B	45	LEU	N-CA-C	-5.70	104.97	111.07	6	2
1	A	37	PHE	O-C-N	-5.70	116.20	122.07	8	3
1	B	84	THR	CA-C-O	-5.70	114.84	120.82	8	1
1	A	25	LYS	CA-C-N	-5.69	114.50	122.75	7	2
1	A	25	LYS	C-N-CA	-5.69	114.50	122.75	7	2
1	A	27	GLY	CA-C-O	-5.68	113.39	121.52	9	1
1	B	79	PHE	CB-CA-C	5.68	119.80	110.88	5	1
1	A	48	LEU	CD1-CG-CD2	-5.67	98.32	110.80	1	1
1	A	88	LEU	O-C-N	-5.67	116.11	122.12	9	1
1	A	46	ILE	N-CA-CB	5.67	117.18	110.55	1	2
1	A	25	LYS	N-CA-C	5.67	118.72	108.69	2	2
1	A	76	ALA	O-C-N	-5.66	116.24	122.07	4	2
1	A	75	TYR	O-C-N	5.66	127.90	122.07	9	2
1	A	17	VAL	CA-CB-CG2	5.66	120.02	110.40	9	1
1	B	93	HIS	CB-CG-ND1	5.66	131.18	122.70	8	1
1	B	81	PHE	CA-CB-CG	-5.65	108.15	113.80	1	1
1	B	79	PHE	CA-C-N	5.65	127.85	120.28	6	3
1	B	79	PHE	C-N-CA	5.65	127.85	120.28	6	3
1	B	30	SER	N-CA-CB	-5.65	101.79	109.98	9	1
1	B	41	MET	O-C-N	-5.64	116.14	122.12	10	3
1	B	79	PHE	CA-C-O	-5.64	114.90	120.82	5	1
1	B	35	SER	CA-C-N	5.64	127.77	120.44	7	1
1	B	35	SER	C-N-CA	5.64	127.77	120.44	7	1
1	B	20	THR	CA-C-N	-5.63	112.80	119.84	6	1
1	B	20	THR	C-N-CA	-5.63	112.80	119.84	6	1
1	A	34	VAL	CA-CB-CG1	5.63	119.97	110.40	7	1
1	B	80	ALA	N-CA-CB	-5.63	101.85	110.01	7	2
1	A	82	MET	O-C-N	-5.62	116.28	122.07	6	1
1	B	47	TRP	CD2-CE2-CZ2	5.61	128.01	122.40	10	2
1	A	85	GLY	O-C-N	-5.61	116.80	122.19	2	2
1	B	22	MET	CB-CA-C	-5.61	99.83	109.65	8	1
1	A	57	GLY	O-C-N	-5.60	115.42	122.70	2	1
1	A	75	TYR	CA-C-O	5.60	126.49	120.55	4	2
1	B	64	LEU	O-C-N	-5.60	116.52	123.36	10	2
1	B	48	LEU	O-C-N	-5.58	116.20	122.12	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	86	LEU	N-CA-CB	5.58	118.31	110.12	1	2
1	B	43	ILE	CA-C-O	5.57	126.75	120.95	10	3
1	A	19	ARG	NH1-CZ-NH2	5.57	126.55	119.30	3	1
1	B	76	ALA	O-C-N	-5.57	116.33	122.07	10	1
1	A	85	GLY	CA-C-N	5.57	127.74	120.28	3	1
1	A	85	GLY	C-N-CA	5.57	127.74	120.28	3	1
1	A	44	GLY	CA-C-N	5.56	127.67	120.44	10	1
1	A	44	GLY	C-N-CA	5.56	127.67	120.44	10	1
1	B	75	TYR	N-CA-CB	-5.56	101.95	110.12	3	1
1	A	50	VAL	CA-C-N	5.55	127.72	120.28	3	1
1	A	50	VAL	C-N-CA	5.55	127.72	120.28	3	1
1	B	42	LEU	N-CA-C	5.54	117.00	111.07	9	2
1	A	60	ALA	CB-CA-C	5.54	121.09	110.17	8	1
1	B	88	LEU	N-CA-CB	5.54	118.04	110.01	5	1
1	B	25	LYS	CG-CD-CE	5.53	124.03	111.30	2	1
1	B	91	ARG	O-C-N	-5.53	115.85	122.15	9	2
1	B	54	ALA	O-C-N	-5.53	116.38	122.07	5	1
1	B	93	HIS	N-CA-CB	5.52	119.89	110.50	1	1
1	B	82	MET	CA-C-N	5.52	127.51	120.56	1	2
1	B	82	MET	C-N-CA	5.52	127.51	120.56	1	2
1	A	39	GLY	CA-C-N	5.50	127.97	120.54	7	1
1	A	39	GLY	C-N-CA	5.50	127.97	120.54	7	1
1	A	65	ASN	CB-CA-C	-5.50	100.03	109.65	7	1
1	B	37	PHE	O-C-N	-5.50	116.29	122.12	10	1
1	A	51	PHE	O-C-N	5.49	127.73	122.07	2	1
1	A	45	LEU	CB-CA-C	-5.49	101.51	110.85	5	1
1	B	42	LEU	CB-CA-C	-5.48	101.69	110.79	2	1
1	B	91	ARG	CB-CA-C	-5.48	102.27	110.88	4	1
1	B	62	THR	O-C-N	-5.48	116.67	123.36	8	1
1	A	20	THR	CA-C-O	-5.47	114.11	119.69	8	2
1	B	68	ALA	N-CA-CB	5.47	120.43	111.08	9	1
1	A	92	TRP	CD2-CE2-CZ2	-5.47	116.93	122.40	5	1
1	A	34	VAL	CA-C-N	5.46	127.59	120.28	2	1
1	A	34	VAL	C-N-CA	5.46	127.59	120.28	2	1
1	B	51	PHE	CA-C-N	5.45	127.52	120.44	1	1
1	B	51	PHE	C-N-CA	5.45	127.52	120.44	1	1
1	A	48	LEU	O-C-N	-5.44	116.47	122.07	10	1
1	B	66	TRP	CD2-CE2-CZ2	-5.42	116.98	122.40	1	1
1	A	73	TRP	O-C-N	-5.42	116.39	122.03	10	1
1	B	59	GLN	N-CA-CB	5.42	119.92	110.81	5	1
1	A	69	GLN	CG-CD-NE2	5.42	124.53	116.40	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	22	MET	O-C-N	-5.41	116.76	123.36	10	1
1	B	23	LYS	CB-CA-C	5.40	119.09	109.65	3	1
1	B	47	TRP	CB-CA-C	-5.39	102.42	110.88	3	1
1	A	79	PHE	CB-CG-CD2	5.38	129.84	120.70	6	1
1	B	73	TRP	CB-CA-C	-5.37	102.69	110.96	7	3
1	A	73	TRP	CG-CD2-CE3	5.36	139.26	133.90	9	1
1	A	55	ALA	CA-C-N	-5.36	115.54	122.99	10	1
1	A	55	ALA	C-N-CA	-5.36	115.54	122.99	10	1
1	A	54	ALA	CA-C-O	5.35	126.22	120.55	2	1
1	B	50	VAL	CG1-CB-CG2	-5.34	99.06	110.80	8	1
1	B	75	TYR	N-CA-C	5.33	117.09	111.28	6	1
1	A	72	PRO	CA-C-O	-5.33	117.28	121.38	1	1
1	A	88	LEU	N-CA-C	5.33	117.09	111.28	4	1
1	B	52	GLN	O-C-N	-5.32	116.08	122.15	4	1
1	B	74	ASN	N-CA-CB	-5.32	102.30	110.01	4	1
1	B	36	LEU	CA-C-O	-5.31	114.92	120.55	8	1
1	A	85	GLY	CA-C-O	5.31	126.22	120.75	10	1
1	B	50	VAL	CA-C-O	5.31	126.80	121.17	8	1
1	B	70	LEU	CB-CA-C	5.30	118.81	109.80	3	1
1	A	41	MET	CA-C-N	5.29	127.37	120.28	8	1
1	A	41	MET	C-N-CA	5.29	127.37	120.28	8	1
1	A	76	ALA	N-CA-C	5.29	116.85	111.14	1	1
1	B	23	LYS	CG-CD-CE	5.29	123.45	111.30	8	1
1	A	32	TRP	CH2-CZ2-CE2	5.28	124.36	117.50	2	1
1	A	71	GLY	O-C-N	-5.28	116.49	121.77	6	1
1	A	93	HIS	CG-CD2-NE2	5.28	112.48	107.20	5	1
1	B	34	VAL	N-CA-C	5.27	116.00	110.62	1	1
1	B	84	THR	CB-CA-C	-5.27	102.05	110.79	5	1
1	A	46	ILE	CA-CB-CG2	5.27	119.45	110.50	9	1
1	B	32	TRP	CH2-CZ2-CE2	5.26	124.34	117.50	2	1
1	A	70	LEU	CB-CA-C	5.26	121.64	110.07	4	1
1	B	68	ALA	CA-C-N	5.25	131.57	121.54	1	1
1	B	68	ALA	C-N-CA	5.25	131.57	121.54	1	1
1	A	83	ILE	CB-CG1-CD1	5.24	124.80	113.80	9	1
1	B	50	VAL	CA-C-N	5.23	127.55	120.44	6	1
1	B	50	VAL	C-N-CA	5.23	127.55	120.44	6	1
1	A	56	ILE	N-CA-C	-5.23	99.99	107.78	4	1
1	B	34	VAL	CB-CA-C	5.23	118.66	111.97	4	1
1	B	50	VAL	N-CA-CB	5.22	118.42	110.58	9	1
1	B	47	TRP	NE1-CE2-CD2	5.22	114.18	107.40	3	1
1	A	33	PHE	N-CA-C	5.21	116.64	111.07	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	37	PHE	N-CA-CB	5.20	117.55	110.01	7	1
1	B	68	ALA	CB-CA-C	-5.20	99.13	109.79	1	1
1	B	73	TRP	CB-CG-CD2	5.20	134.08	126.80	4	1
1	B	41	MET	CG-SD-CE	-5.19	89.48	100.90	3	1
1	B	59	GLN	CG-CD-NE2	5.19	124.19	116.40	7	1
1	B	60	ALA	CB-CA-C	5.19	120.39	110.17	6	1
1	B	77	ILE	N-CA-CB	5.19	116.62	110.55	6	1
1	B	28	PRO	N-CD-CG	5.18	110.02	103.80	7	1
1	A	26	VAL	CA-CB-CG1	5.18	119.20	110.40	1	1
1	B	62	THR	N-CA-C	5.18	117.86	108.69	3	1
1	A	81	PHE	CD1-CG-CD2	-5.17	110.84	118.60	6	1
1	A	18	SER	N-CA-CB	5.17	119.74	110.80	1	1
1	B	93	HIS	ND1-CG-CD2	-5.17	100.94	106.10	2	1
1	B	86	LEU	N-CA-C	5.17	116.91	111.28	8	1
1	A	83	ILE	N-CA-CB	5.16	117.56	110.54	3	2
1	A	30	SER	CB-CA-C	-5.16	102.74	110.90	10	1
1	A	80	ALA	CA-C-N	5.15	127.19	120.28	7	1
1	A	80	ALA	C-N-CA	5.15	127.19	120.28	7	1
1	B	93	HIS	CB-CG-CD2	-5.15	124.51	131.20	8	1
1	A	75	TYR	N-CA-C	5.15	116.89	111.28	1	1
1	A	40	LEU	N-CA-CB	-5.14	102.56	110.12	5	1
1	A	71	GLY	CA-C-N	5.14	126.84	121.65	1	1
1	A	71	GLY	C-N-CA	5.14	126.84	121.65	1	1
1	A	67	MET	CG-SD-CE	-5.13	89.60	100.90	1	1
1	B	61	PRO	O-C-N	-5.13	115.72	122.64	3	1
1	B	45	LEU	CD1-CG-CD2	-5.13	99.52	110.80	9	1
1	A	59	GLN	OE1-CD-NE2	-5.12	117.48	122.60	6	1
1	A	84	THR	CA-C-O	-5.11	115.13	120.55	5	1
1	B	43	ILE	CA-CB-CG1	-5.11	101.71	110.40	5	1
1	A	19	ARG	CD-NE-CZ	-5.11	117.25	124.40	5	1
1	A	18	SER	CA-C-N	5.10	131.14	122.37	7	1
1	A	18	SER	C-N-CA	5.10	131.14	122.37	7	1
1	A	56	ILE	CA-C-O	5.06	125.73	120.36	6	1
1	A	77	ILE	CA-C-O	-5.06	115.43	121.05	9	1
1	B	32	TRP	CD2-CE2-CZ2	-5.06	117.34	122.40	2	1
1	B	80	ALA	CA-C-N	5.06	127.06	120.28	5	1
1	B	80	ALA	C-N-CA	5.06	127.06	120.28	5	1
1	A	48	LEU	N-CA-C	5.04	117.16	111.11	2	1
1	A	51	PHE	CB-CG-CD1	-5.04	112.12	120.70	2	1
1	B	51	PHE	CB-CG-CD1	5.04	129.28	120.70	8	1
1	A	22	MET	CG-SD-CE	-5.04	89.80	100.90	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	69	GLN	CA-C-O	5.04	125.46	119.67	3	1
1	B	65	ASN	CA-C-O	5.03	126.47	120.28	7	1
1	A	61	PRO	N-CA-C	5.03	122.83	112.47	5	1
1	B	26	VAL	N-CA-CB	5.02	119.69	111.45	1	1
1	B	77	ILE	O-C-N	5.02	126.83	121.91	3	1
1	A	37	PHE	CA-C-O	-5.02	115.55	120.82	9	1
1	A	40	LEU	CA-C-O	5.01	125.86	120.55	5	1
1	B	83	ILE	CA-C-O	-5.00	115.50	121.05	9	1
1	B	51	PHE	N-CA-C	-5.00	105.74	111.14	1	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	20	THR	CA	10

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	19	ARG	Mainchain,Sidechain,Peptide	10
1	A	26	VAL	Peptide	10
1	B	20	THR	Peptide	10
1	B	29	SER	Peptide	10
1	B	72	PRO	Peptide	10
1	A	28	PRO	Peptide	9
1	B	26	VAL	Peptide	9
1	A	25	LYS	Peptide	8
1	B	75	TYR	Sidechain	8
1	B	53	LEU	Peptide	7
1	A	68	ALA	Peptide	6
1	A	55	ALA	Peptide	6
1	A	79	PHE	Sidechain	5
1	A	75	TYR	Sidechain	3
1	B	79	PHE	Sidechain	3
1	A	91	ARG	Sidechain	2
1	A	93	HIS	Sidechain	2
1	B	55	ALA	Peptide	2
1	B	68	ALA	Peptide	2
1	B	33	PHE	Sidechain	2
1	B	51	PHE	Sidechain	1
1	B	91	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	81	PHE	Sidechain	1
1	B	19	ARG	Sidechain	1
1	A	73	TRP	Peptide	1
1	A	51	PHE	Sidechain	1
1	A	92	TRP	Peptide	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	A	606	633	632	5±1
1	B	606	633	632	9±4
All	All	12120	12660	12640	121

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:20:THR:CB	1:B:20:THR:CA	1.59	1.74	2	3
1:B:20:THR:CB	1:B:20:THR:C	1.21	2.13	10	3
1:B:20:THR:CB	1:B:20:THR:N	1.09	2.15	2	3
1:B:20:THR:N	1:B:20:THR:HB	0.96	1.74	9	3
1:B:20:THR:CA	1:B:20:THR:HB	0.89	1.97	9	3
1:B:19:ARG:C	1:B:20:THR:HB	0.76	2.05	9	3
1:B:20:THR:CB	1:B:21:PRO:N	0.65	2.59	10	1
1:A:17:VAL:N	1:A:29:SER:HG	0.65	1.89	3	9
1:B:22:MET:SD	1:B:93:HIS:HB3	0.62	2.35	5	1
1:B:17:VAL:N	1:B:30:SER:HG	0.60	1.95	6	5
1:B:45:LEU:HD13	1:B:76:ALA:HA	0.59	1.75	5	2
1:A:33:PHE:CD1	1:B:22:MET:HE1	0.58	2.33	8	4
1:A:22:MET:HE1	1:B:33:PHE:CD1	0.57	2.34	1	1
1:A:17:VAL:N	1:A:30:SER:HG	0.57	1.98	2	3
1:A:26:VAL:HG12	1:A:33:PHE:HB2	0.55	1.77	3	3
1:B:64:LEU:HD23	1:B:66:TRP:CH2	0.55	2.37	6	5
1:B:60:ALA:HB1	1:B:61:PRO:CD	0.54	2.32	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:38:ILE:HD11	1:B:87:LEU:CD1	0.54	2.32	3	1
1:A:22:MET:CG	1:A:93:HIS:HB3	0.53	2.33	8	2
1:A:68:ALA:HB2	1:B:62:THR:HG23	0.52	1.80	7	1
1:B:20:THR:HG23	1:B:21:PRO:N	0.52	2.20	5	10
1:A:26:VAL:O	1:A:29:SER:HA	0.51	2.05	9	1
1:A:91:ARG:HA	1:A:91:ARG:HE	0.50	1.66	8	3
1:B:52:GLN:HA	1:B:55:ALA:HB3	0.50	1.83	3	1
1:A:33:PHE:CE1	1:B:22:MET:HE1	0.49	2.42	8	1
1:B:79:PHE:O	1:B:83:ILE:HG13	0.48	2.09	4	1
1:A:33:PHE:CG	1:B:22:MET:HE1	0.48	2.44	1	1
1:B:26:VAL:H	1:B:29:SER:HB3	0.47	1.70	5	1
1:B:73:TRP:CG	1:B:74:ASN:N	0.47	2.81	7	1
1:A:49:MET:HE2	1:A:49:MET:HA	0.47	1.87	2	1
1:A:73:TRP:CE2	1:B:59:GLN:HB3	0.46	2.45	1	4
1:B:49:MET:O	1:B:53:LEU:HB2	0.46	2.11	10	2
1:B:73:TRP:H	1:B:73:TRP:CD1	0.46	2.28	5	1
1:A:27:GLY:HA2	1:A:28:PRO:C	0.46	2.35	7	2
1:B:53:LEU:HD23	1:B:68:ALA:HB2	0.46	1.86	10	2
1:B:53:LEU:HB3	1:B:68:ALA:HB2	0.46	1.85	1	2
1:A:48:LEU:HD23	1:A:75:TYR:CZ	0.46	2.45	4	1
1:B:20:THR:CG2	1:B:21:PRO:N	0.45	2.79	3	3
1:A:22:MET:SD	1:B:26:VAL:HB	0.45	2.51	2	1
1:A:60:ALA:HB1	1:A:61:PRO:CD	0.45	2.42	9	2
1:B:45:LEU:CD1	1:B:76:ALA:HA	0.45	2.41	5	1
1:B:48:LEU:HD23	1:B:75:TYR:CE2	0.45	2.47	4	1
1:B:22:MET:HB3	1:B:93:HIS:HB3	0.44	1.90	2	1
1:A:22:MET:SD	1:A:93:HIS:HB3	0.44	2.52	7	2
1:B:20:THR:C	1:B:20:THR:OG1	0.43	2.59	10	1
1:B:53:LEU:HD23	1:B:68:ALA:CB	0.43	2.44	4	1
1:B:75:TYR:CE1	1:B:79:PHE:CD1	0.42	3.07	2	2
1:A:24:VAL:HG23	1:B:24:VAL:HG22	0.42	1.91	4	1
1:B:20:THR:C	1:B:20:THR:CG2	0.42	2.90	2	1
1:A:60:ALA:HB1	1:A:61:PRO:HD2	0.41	1.90	9	1
1:A:22:MET:HB3	1:A:93:HIS:HB3	0.41	1.92	5	1
1:B:19:ARG:O	1:B:20:THR:HB	0.41	2.04	4	1
1:A:59:GLN:HB3	1:B:73:TRP:CE2	0.41	2.51	6	1
1:A:20:THR:HA	1:A:22:MET:H	0.41	1.76	8	1
1:A:52:GLN:HA	1:A:55:ALA:HB3	0.40	1.94	5	1
1:A:38:ILE:HD13	1:A:83:ILE:HG22	0.40	1.94	6	1
1:B:22:MET:HE2	1:B:24:VAL:CG2	0.40	2.46	10	1
1:B:25:LYS:HA	1:B:29:SER:HB3	0.40	1.93	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:48:LEU:HD23	1:B:75:TYR:CZ	0.40	2.52	5	1
1:B:35:SER:HA	1:B:38:ILE:HD12	0.40	1.92	10	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	75/102 (74%)	68±1 (90±1%)	5±1 (6±1%)	3±1 (4±1%)	4	30
1	B	75/102 (74%)	68±1 (91±1%)	4±1 (5±2%)	3±1 (4±1%)	4	30
All	All	1500/2040 (74%)	1360 (91%)	81 (5%)	59 (4%)	4	30

All 11 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	60	ALA	10
1	B	60	ALA	10
1	B	72	PRO	10
1	A	28	PRO	8
1	A	21	PRO	7
1	B	21	PRO	5
1	B	55	ALA	4
1	A	71	GLY	2
1	A	61	PRO	1
1	B	61	PRO	1
1	A	72	PRO	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	63/87 (72%)	57±2 (90±3%)	6±2 (10±3%)	10	55
1	B	63/87 (72%)	54±2 (86±4%)	9±2 (14±4%)	6	45
All	All	1260/1740 (72%)	1112 (88%)	148 (12%)	7	50

All 44 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	66	TRP	10
1	B	17	VAL	10
1	B	20	THR	10
1	B	64	LEU	10
1	A	59	GLN	9
1	A	87	LEU	9
1	A	91	ARG	9
1	B	45	LEU	9
1	B	87	LEU	7
1	B	72	PRO	6
1	B	26	VAL	5
1	B	49	MET	5
1	A	53	LEU	4
1	B	34	VAL	4
1	B	66	TRP	4
1	A	28	PRO	3
1	B	22	MET	3
1	A	72	PRO	2
1	B	88	LEU	2
1	A	24	VAL	2
1	B	61	PRO	2
1	A	45	LEU	1
1	A	26	VAL	1
1	A	50	VAL	1
1	A	75	TYR	1
1	B	56	ILE	1
1	B	70	LEU	1
1	B	38	ILE	1
1	B	59	GLN	1
1	B	82	MET	1
1	B	86	LEU	1
1	A	20	THR	1
1	A	22	MET	1
1	A	31	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	38	ILE	1
1	A	69	GLN	1
1	A	70	LEU	1
1	B	23	LYS	1
1	B	67	MET	1
1	B	83	ILE	1
1	A	46	ILE	1
1	A	83	ILE	1
1	B	79	PHE	1
1	A	56	ILE	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 3% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping [i](#)

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

Total number of shifts	69
Number of shifts mapped to atoms	69
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	65

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	69	-7.01 ± 8.19	None needed (imprecise)

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 3%, i.e. 69 atoms were assigned a chemical shift out of a possible 2198. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	69/766 (9%)	0/312 (0%)	0/308 (0%)	69/146 (47%)
Sidechain	0/1180 (0%)	0/798 (0%)	0/356 (0%)	0/26 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/252 (0%)	0/126 (0%)	0/114 (0%)	0/12 (0%)
Overall	69/2198 (3%)	0/1236 (0%)	0/778 (0%)	69/184 (38%)

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 3%, i.e. 69 atoms were assigned a chemical shift out of a possible 2198. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	69/766 (9%)	0/312 (0%)	0/308 (0%)	69/146 (47%)
Sidechain	0/1180 (0%)	0/798 (0%)	0/356 (0%)	0/26 (0%)
Aromatic	0/252 (0%)	0/126 (0%)	0/114 (0%)	0/12 (0%)
Overall	69/2198 (3%)	0/1236 (0%)	0/778 (0%)	69/184 (38%)

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 ⓘ

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

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	35	SER	N	228.00	99.14 – 133.45	32.6
1	A	30	SER	N	225.00	99.14 – 133.45	31.7
1	A	39	GLY	N	220.00	91.59 – 127.52	30.7
1	A	80	ALA	N	229.00	106.13 – 140.55	30.7
1	A	49	MET	N	222.00	102.99 – 137.21	29.8
1	A	87	LEU	N	230.00	102.77 – 140.89	28.4
1	A	76	ALA	N	221.00	106.13 – 140.55	28.4
1	A	42	LEU	N	226.00	102.77 – 140.89	27.3
1	A	45	LEU	N	225.00	102.77 – 140.89	27.1
1	A	73	TRP	N	225.00	101.51 – 141.60	25.8
1	A	51	PHE	N	225.00	99.93 – 140.82	25.6
1	A	88	LEU	N	219.00	102.77 – 140.89	25.5
1	A	85	GLY	N	201.00	91.59 – 127.52	25.4
1	A	90	MET	N	207.00	102.99 – 137.21	25.4
1	A	46	ILE	N	227.00	100.55 – 142.30	25.3
1	A	48	LEU	N	216.00	102.77 – 140.89	24.7

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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	41	MET	N	203.00	102.99 – 137.21	24.2
1	A	79	PHE	N	219.00	99.93 – 140.82	24.1
1	A	38	ILE	N	222.00	100.55 – 142.30	24.1
1	A	84	THR	N	227.00	91.89 – 138.78	23.8
1	A	77	ILE	N	220.00	100.55 – 142.30	23.6
1	A	83	ILE	N	219.00	100.55 – 142.30	23.4
1	A	74	ASN	N	209.00	99.66 – 138.23	23.4
1	A	44	GLY	N	193.00	91.59 – 127.52	23.2
1	A	31	VAL	N	221.00	99.23 – 142.92	22.9
1	A	32	TRP	N	213.00	101.51 – 141.60	22.8
1	A	92	TRP	N	213.00	101.51 – 141.60	22.8
1	A	78	ALA	N	201.00	106.13 – 140.55	22.6
1	A	36	LEU	N	207.00	102.77 – 140.89	22.3
1	A	37	PHE	N	209.00	99.93 – 140.82	21.7
1	A	81	PHE	N	209.00	99.93 – 140.82	21.7
1	A	82	MET	N	194.00	102.99 – 137.21	21.6
1	A	86	LEU	N	204.00	102.77 – 140.89	21.6
1	A	89	THR	N	216.00	91.89 – 138.78	21.5
1	A	43	ILE	N	209.00	100.55 – 142.30	21.0
1	A	34	VAL	N	211.00	99.23 – 142.92	20.6
1	A	33	PHE	N	204.00	99.93 – 140.82	20.4
1	A	40	LEU	N	198.00	102.77 – 140.89	20.0
1	A	29	SER	N	179.00	99.14 – 133.45	18.3
1	A	75	TYR	N	190.00	100.12 – 140.79	17.1
1	A	47	TRP	N	188.00	101.51 – 141.60	16.6
1	A	91	ARG	N	177.00	102.91 – 138.82	15.6
1	A	54	ALA	N	173.00	106.13 – 140.55	14.4
1	A	53	LEU	N	175.00	102.77 – 140.89	13.9
1	A	19	ARG	N	73.00	102.91 – 138.82	-13.3
1	A	63	ALA	N	78.00	106.13 – 140.55	-13.2
1	A	64	LEU	N	74.00	102.77 – 140.89	-12.6
1	A	55	ALA	N	166.00	106.13 – 140.55	12.4
1	A	17	VAL	N	175.00	99.23 – 142.92	12.3
1	A	23	LYS	N	77.00	102.74 – 139.42	-12.0
1	A	25	LYS	N	77.00	102.74 – 139.42	-12.0
1	A	18	SER	N	77.00	99.14 – 133.45	-11.4
1	A	58	SER	N	77.00	99.14 – 133.45	-11.4
1	A	50	VAL	N	171.00	99.23 – 142.92	11.4
1	A	62	THR	N	62.00	91.89 – 138.78	-11.4
1	A	24	VAL	N	72.00	99.23 – 142.92	-11.2
1	A	65	ASN	N	77.00	99.66 – 138.23	-10.9
1	A	26	VAL	N	74.00	99.23 – 142.92	-10.8

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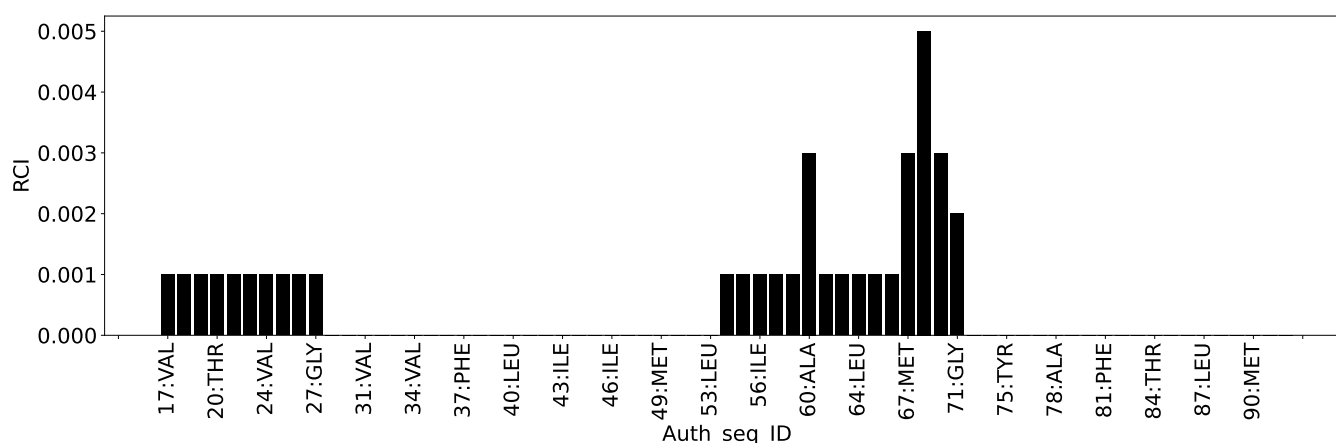
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List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	56	ILE	N	78.00	100.55 – 142.30	-10.4
1	A	57	GLY	N	74.00	91.59 – 127.52	-9.9
1	A	66	TRP	N	85.00	101.51 – 141.60	-9.1
1	A	22	MET	N	89.00	102.99 – 137.21	-9.1
1	A	20	THR	N	74.00	91.89 – 138.78	-8.8
1	A	27	GLY	N	78.00	91.59 – 127.52	-8.8
1	A	70	LEU	N	97.00	102.77 – 140.89	-6.5

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:



8 NMR restraints analysis

No restraints data found

9 Distance violation analysis ⓘ

No distance restraints data found

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found