



# Full wwPDB NMR Structure Validation Report ⓘ

Mar 4, 2026 – 08:48 PM UTC

PDB ID : 2EVZ / pdb\_00002evz  
Title : Structure of RNA Binding Domains 3 and 4 of Polypyrimidine Tract Binding Protein  
Authors : Allain, F.H.; Auweter, S.D.  
Deposited on : 2005-11-01

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

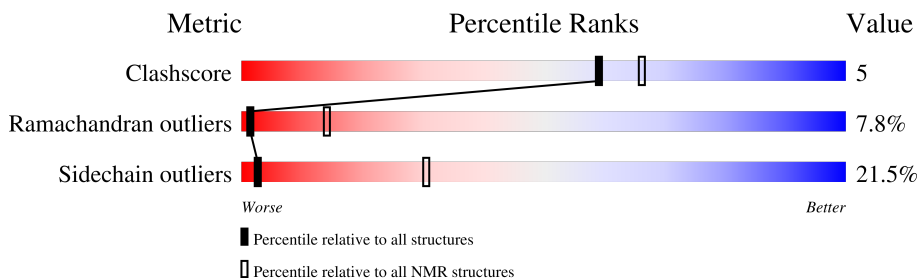
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	229	

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:13-A:47, A:52-A:91, A:104-A:108, A:126-A:208 (163)	0.68	18

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 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3259 atoms, of which 1641 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Polypyrimidine tract-binding protein 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	208	3259	1023	1641	296	295	4	0

There are 21 discrepancies between the modelled and reference sequences:

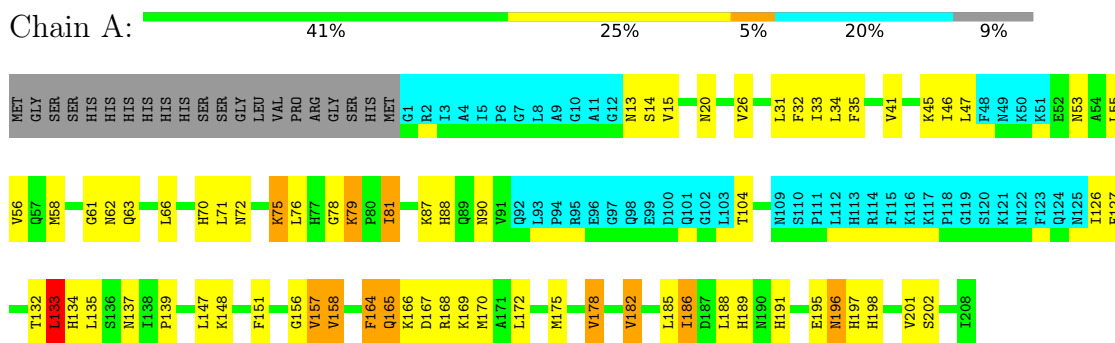
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	cloning artifact	UNP P26599
A	-19	GLY	-	cloning artifact	UNP P26599
A	-18	SER	-	cloning artifact	UNP P26599
A	-17	SER	-	cloning artifact	UNP P26599
A	-16	HIS	-	expression tag	UNP P26599
A	-15	HIS	-	expression tag	UNP P26599
A	-14	HIS	-	expression tag	UNP P26599
A	-13	HIS	-	expression tag	UNP P26599
A	-12	HIS	-	expression tag	UNP P26599
A	-11	HIS	-	expression tag	UNP P26599
A	-10	SER	-	cloning artifact	UNP P26599
A	-9	SER	-	cloning artifact	UNP P26599
A	-8	GLY	-	cloning artifact	UNP P26599
A	-7	LEU	-	cloning artifact	UNP P26599
A	-6	VAL	-	cloning artifact	UNP P26599
A	-5	PRO	-	cloning artifact	UNP P26599
A	-4	ARG	-	cloning artifact	UNP P26599
A	-3	GLY	-	cloning artifact	UNP P26599
A	-2	SER	-	cloning artifact	UNP P26599
A	-1	HIS	-	cloning artifact	UNP P26599
A	0	MET	-	cloning artifact	UNP P26599

## 4 Residue-property plots i

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

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

- Molecule 1: Polypyrimidine tract-binding protein 1

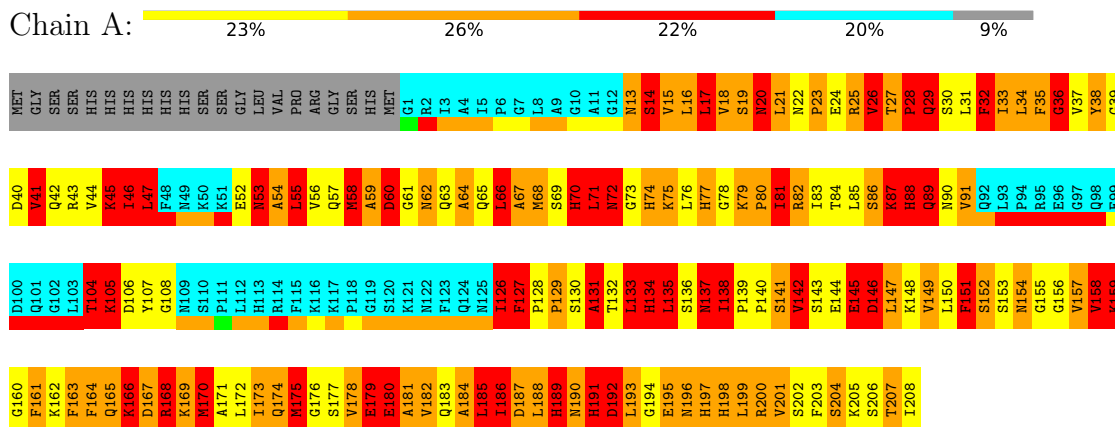


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

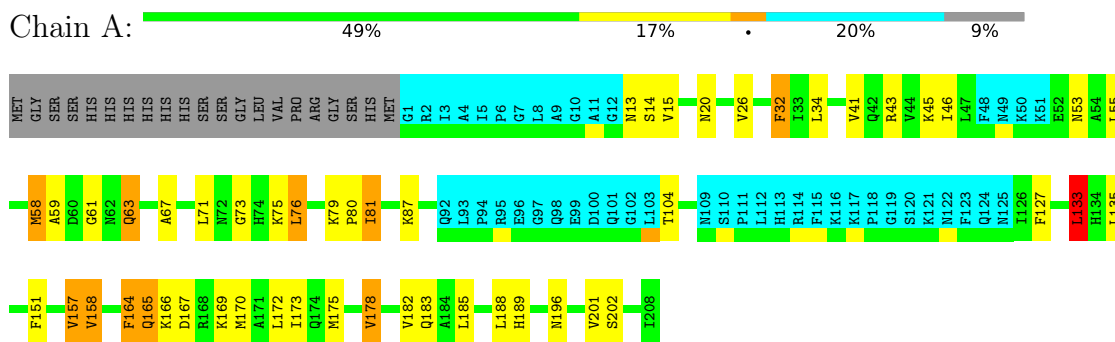
#### 4.2.1 Score per residue for model 1

- Molecule 1: Polypyrimidine tract-binding protein 1



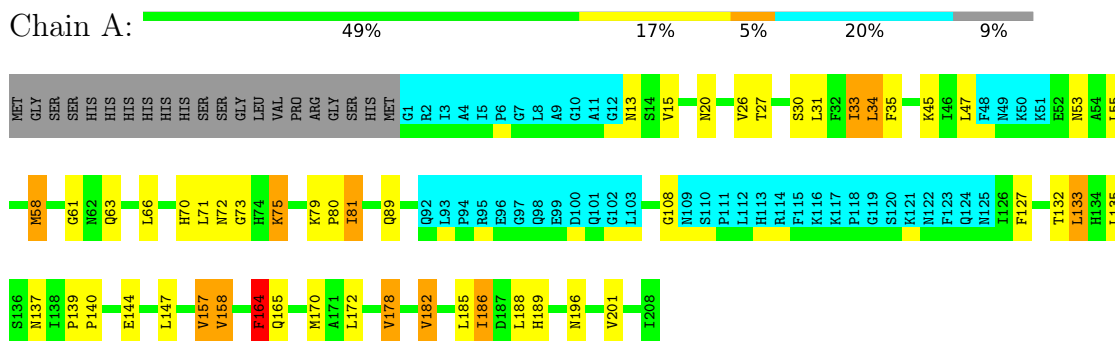
### 4.2.2 Score per residue for model 2

- Molecule 1: Polypyrimidine tract-binding protein 1



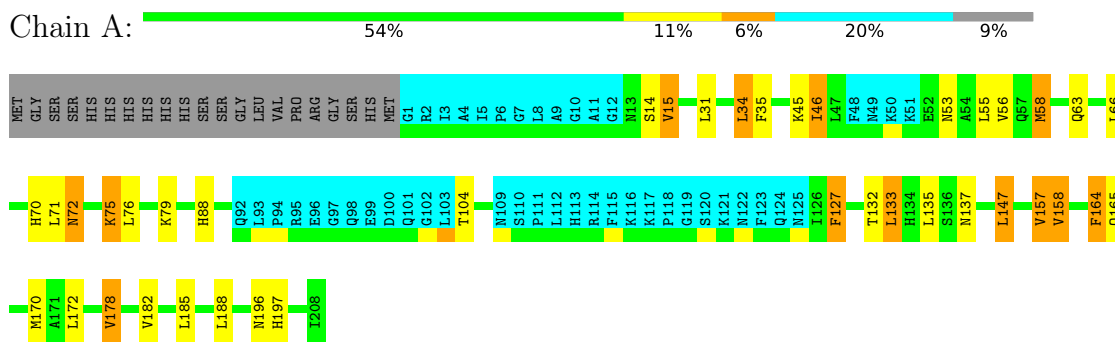
### 4.2.3 Score per residue for model 3

- Molecule 1: Polypyrimidine tract-binding protein 1



### 4.2.4 Score per residue for model 4

- Molecule 1: Polypyrimidine tract-binding protein 1



### 4.2.5 Score per residue for model 5

- Molecule 1: Polypyrimidine tract-binding protein 1

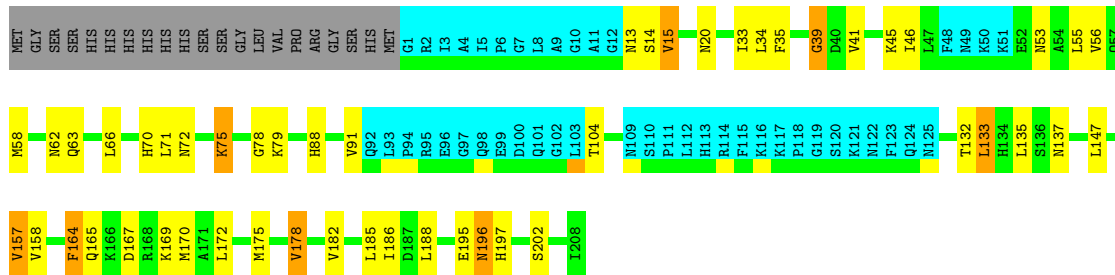
Chain A: 47% 20% 20% 9%



### 4.2.6 Score per residue for model 6

- Molecule 1: Polypyrimidine tract-binding protein 1

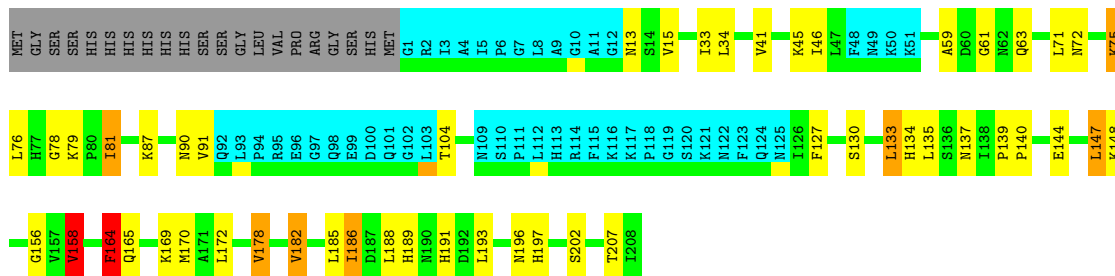
Chain A: 49% 18% 20% 9%



### 4.2.7 Score per residue for model 7

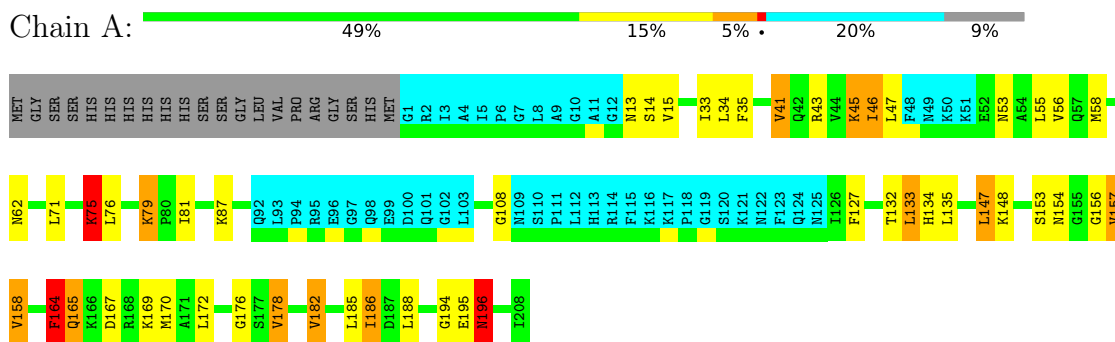
- Molecule 1: Polypyrimidine tract-binding protein 1

Chain A: 49% 18% 20% 9%



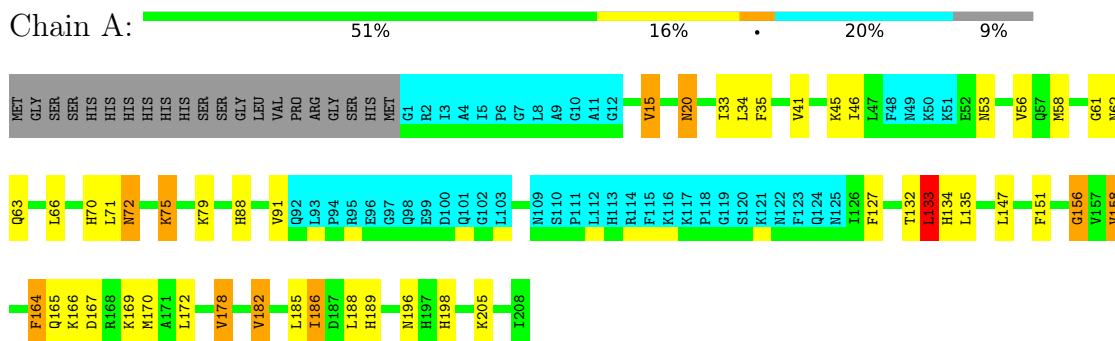
### 4.2.8 Score per residue for model 8

- Molecule 1: Polypyrimidine tract-binding protein 1



### 4.2.9 Score per residue for model 9

- Molecule 1: Polypyrimidine tract-binding protein 1



### 4.2.10 Score per residue for model 10

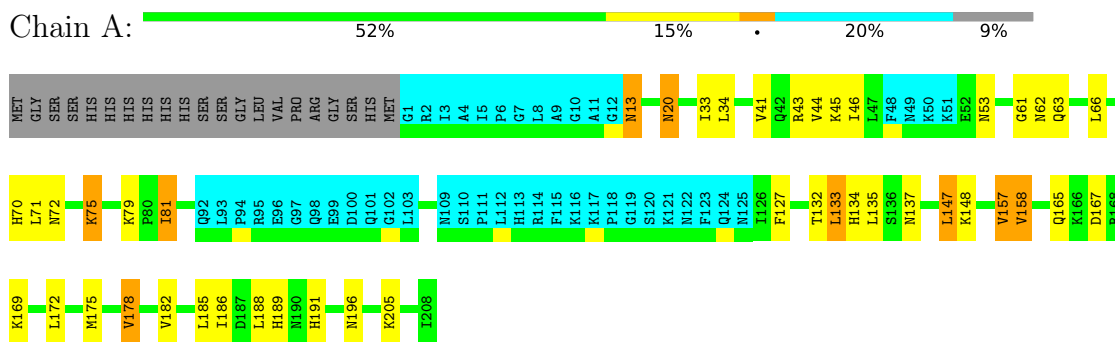
- Molecule 1: Polypyrimidine tract-binding protein 1





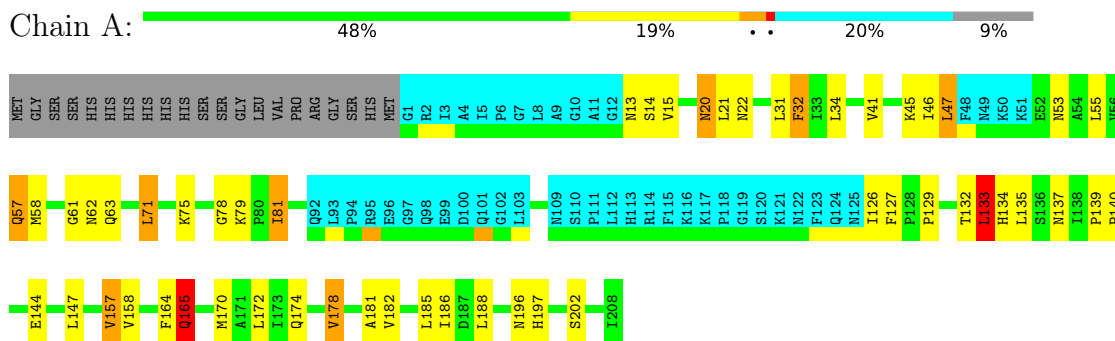
## 4.2.14 Score per residue for model 14

- Molecule 1: Polypyrimidine tract-binding protein 1



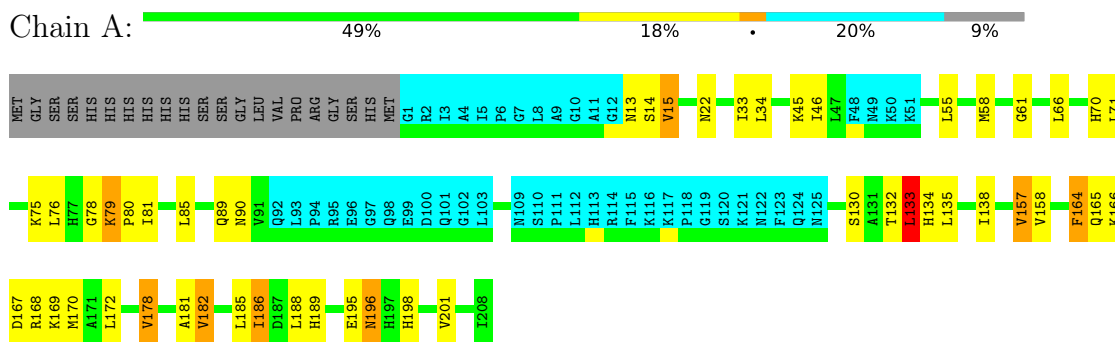
## 4.2.15 Score per residue for model 15

- Molecule 1: Polypyrimidine tract-binding protein 1



## 4.2.16 Score per residue for model 16

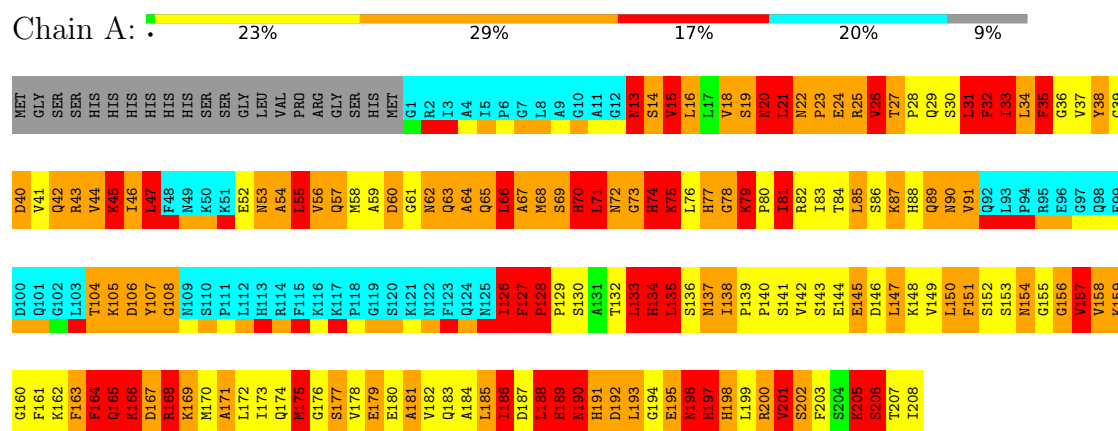
- Molecule 1: Polypyrimidine tract-binding protein 1





## 4.2.20 Score per residue for model 20

## • Molecule 1: Polypyrimidine tract-binding protein 1



## 5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 20 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
CYANA	structure solution	2.0
Amber	refinement	7.0

No chemical shift data was provided.

## 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	1.34±1.17	40±94/1297 ( 3.0± 7.3%)	2.24±1.02	88±156/1751 ( 5.1± 8.9%)
All	All	1.78	790/25940 ( 3.0%)	2.46	1770/35020 ( 5.1%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	6.8±16.1
All	All	0	137

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	70	HIS	CE1-NE2	18.56	1.51	1.32	19	1
1	A	44	VAL	CA-CB	-18.04	1.30	1.54	1	2
1	A	160	GLY	N-CA	-17.29	1.27	1.45	19	2
1	A	128	PRO	CA-C	16.53	1.67	1.52	20	2
1	A	140	PRO	N-CA	16.47	1.68	1.47	19	2
1	A	77	HIS	ND1-CE1	16.19	1.48	1.32	19	3
1	A	185	LEU	CA-C	-15.84	1.33	1.52	19	1
1	A	77	HIS	CA-C	15.55	1.73	1.52	19	2
1	A	162	LYS	CA-C	14.75	1.71	1.52	1	1
1	A	137	ASN	CA-C	14.61	1.72	1.52	1	1
1	A	132	THR	CA-CB	-14.30	1.35	1.52	1	2
1	A	131	ALA	CA-C	14.21	1.72	1.52	1	1
1	A	26	VAL	CA-C	13.93	1.68	1.52	1	1
1	A	135	LEU	CA-C	13.93	1.69	1.52	20	1
1	A	19	SER	CA-C	-13.37	1.36	1.52	19	1
1	A	62	ASN	CA-C	13.18	1.71	1.52	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	52	GLU	CA-C	13.11	1.69	1.52	20	2
1	A	169	LYS	C-N	-13.08	1.16	1.33	19	1
1	A	89	GLN	CA-C	13.04	1.70	1.53	20	1
1	A	60	ASP	N-CA	13.03	1.62	1.46	1	1
1	A	37	VAL	CA-C	12.90	1.67	1.52	19	3
1	A	154	ASN	CA-CB	12.90	1.73	1.53	20	1
1	A	139	PRO	CA-C	12.85	1.64	1.52	20	2
1	A	199	LEU	C-N	12.85	1.50	1.33	19	1
1	A	29	GLN	C-O	-12.84	1.07	1.24	19	2
1	A	23	PRO	CA-C	12.83	1.70	1.52	20	1
1	A	41	VAL	N-CA	12.72	1.62	1.46	19	1
1	A	25	ARG	C-O	12.71	1.40	1.24	1	1
1	A	24	GLU	N-CA	12.71	1.62	1.46	20	2
1	A	42	GLN	N-CA	-12.66	1.29	1.46	20	2
1	A	142	VAL	CA-C	12.58	1.66	1.53	19	1
1	A	26	VAL	N-CA	12.44	1.62	1.46	19	3
1	A	29	GLN	C-N	12.44	1.49	1.33	1	2
1	A	126	ILE	N-CA	12.34	1.61	1.46	1	2
1	A	156	GLY	N-CA	12.21	1.60	1.45	1	1
1	A	193	LEU	N-CA	12.20	1.61	1.46	19	1
1	A	130	SER	CA-C	12.03	1.67	1.52	20	2
1	A	88	HIS	N-CA	12.02	1.60	1.46	19	1
1	A	190	ASN	N-CA	-11.99	1.29	1.46	20	1
1	A	29	GLN	N-CA	11.97	1.60	1.46	20	2
1	A	134	HIS	CA-C	11.96	1.69	1.53	19	1
1	A	189	HIS	CG-ND1	11.89	1.51	1.38	1	2
1	A	15	VAL	N-CA	-11.87	1.31	1.46	1	2
1	A	24	GLU	CA-C	11.84	1.68	1.52	19	2
1	A	147	LEU	C-N	11.82	1.48	1.33	20	2
1	A	41	VAL	CA-C	11.68	1.67	1.52	1	2
1	A	186	ILE	CA-CB	11.64	1.68	1.54	20	1
1	A	24	GLU	C-O	-11.62	1.10	1.24	1	2
1	A	137	ASN	N-CA	11.59	1.61	1.46	19	2
1	A	23	PRO	CA-CB	11.56	1.70	1.53	19	2
1	A	134	HIS	N-CA	11.51	1.60	1.46	1	1
1	A	177	SER	N-CA	11.50	1.60	1.45	20	1
1	A	167	ASP	CA-C	11.47	1.68	1.52	20	1
1	A	88	HIS	CE1-NE2	11.46	1.44	1.32	20	1
1	A	34	LEU	C-N	-11.39	1.18	1.33	19	1
1	A	107	TYR	CA-CB	11.28	1.70	1.53	19	2
1	A	170	MET	SD-CE	11.27	2.07	1.79	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	36	GLY	C-N	11.21	1.44	1.33	20	2
1	A	55	LEU	CA-C	-11.15	1.39	1.52	19	1
1	A	134	HIS	CD2-NE2	11.10	1.50	1.37	20	2
1	A	198	HIS	CA-C	-11.08	1.38	1.52	20	2
1	A	145	GLU	CA-CB	-10.96	1.38	1.53	19	1
1	A	66	LEU	N-CA	-10.96	1.33	1.46	1	1
1	A	87	LYS	CA-C	10.94	1.67	1.52	1	3
1	A	40	ASP	CA-C	10.94	1.69	1.53	1	2
1	A	146	ASP	C-N	10.90	1.49	1.33	19	1
1	A	151	PHE	CA-C	10.89	1.68	1.52	20	1
1	A	108	GLY	C-N	10.85	1.47	1.33	1	1
1	A	200	ARG	NE-CZ	-10.78	1.21	1.33	20	1
1	A	148	LYS	C-N	10.78	1.47	1.33	20	1
1	A	199	LEU	CA-CB	10.68	1.71	1.53	19	1
1	A	56	VAL	CA-CB	-10.66	1.40	1.53	1	1
1	A	181	ALA	N-CA	10.60	1.59	1.46	1	2
1	A	196	ASN	N-CA	-10.58	1.34	1.46	1	1
1	A	74	HIS	CG-CD2	10.55	1.47	1.35	19	2
1	A	84	THR	CB-OG1	-10.55	1.26	1.43	20	1
1	A	90	ASN	CA-C	10.55	1.66	1.52	1	1
1	A	86	SER	C-O	-10.54	1.14	1.24	19	2
1	A	198	HIS	CB-CG	10.52	1.64	1.50	20	1
1	A	172	LEU	C-N	-10.52	1.22	1.33	19	2
1	A	134	HIS	ND1-CE1	10.51	1.43	1.32	19	2
1	A	74	HIS	CE1-NE2	-10.47	1.22	1.32	1	1
1	A	56	VAL	CA-C	10.46	1.66	1.52	1	2
1	A	82	ARG	CD-NE	10.46	1.60	1.46	20	2
1	A	134	HIS	C-O	-10.44	1.11	1.24	1	1
1	A	39	GLY	C-N	10.38	1.46	1.33	19	1
1	A	104	THR	CA-CB	10.34	1.70	1.53	20	2
1	A	53	ASN	CA-CB	10.33	1.73	1.53	20	2
1	A	129	PRO	CA-C	10.29	1.67	1.52	1	1
1	A	72	ASN	N-CA	10.28	1.59	1.46	19	2
1	A	47	LEU	CA-C	-10.27	1.39	1.52	20	3
1	A	147	LEU	CA-C	10.22	1.66	1.52	19	2
1	A	18	VAL	N-CA	10.21	1.59	1.46	1	2
1	A	13	ASN	CA-CB	10.20	1.70	1.53	1	1
1	A	83	ILE	C-N	-10.18	1.21	1.33	20	1
1	A	159	LYS	C-O	-10.16	1.09	1.23	19	2
1	A	60	ASP	CA-CB	10.16	1.70	1.53	1	2
1	A	85	LEU	CA-C	10.10	1.65	1.52	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	193	LEU	C-O	10.09	1.37	1.23	19	2
1	A	27	THR	CB-OG1	-10.03	1.27	1.43	20	2
1	A	185	LEU	CA-CB	-10.02	1.37	1.53	19	2
1	A	149	VAL	CA-CB	9.99	1.69	1.54	19	1
1	A	134	HIS	CB-CG	9.99	1.64	1.50	19	1
1	A	38	TYR	CA-C	9.92	1.65	1.52	19	1
1	A	139	PRO	C-O	9.91	1.35	1.24	19	1
1	A	200	ARG	CZ-NH1	-9.89	1.19	1.32	1	1
1	A	191	HIS	CB-CG	9.82	1.63	1.50	20	1
1	A	17	LEU	C-O	9.80	1.35	1.23	19	1
1	A	201	VAL	C-N	9.77	1.45	1.33	19	1
1	A	37	VAL	CA-CB	9.76	1.66	1.54	20	3
1	A	16	LEU	CA-CB	9.76	1.66	1.53	19	1
1	A	59	ALA	CA-CB	9.75	1.68	1.53	1	2
1	A	13	ASN	C-N	-9.75	1.20	1.33	20	2
1	A	133	LEU	N-CA	9.72	1.58	1.46	1	1
1	A	47	LEU	N-CA	9.70	1.60	1.46	1	1
1	A	65	GLN	CA-CB	9.67	1.68	1.53	1	1
1	A	187	ASP	N-CA	9.67	1.58	1.46	19	2
1	A	20	ASN	CA-C	9.64	1.65	1.52	1	2
1	A	203	PHE	C-O	9.61	1.35	1.24	19	1
1	A	106	ASP	N-CA	9.58	1.57	1.46	19	2
1	A	170	MET	CA-CB	-9.58	1.37	1.53	20	1
1	A	37	VAL	N-CA	9.57	1.56	1.46	1	1
1	A	128	PRO	CA-CB	-9.57	1.41	1.54	19	2
1	A	198	HIS	ND1-CE1	9.56	1.42	1.32	20	2
1	A	65	GLN	C-N	-9.55	1.22	1.33	20	3
1	A	21	LEU	CB-CG	9.52	1.72	1.53	19	2
1	A	166	LYS	CD-CE	9.52	1.81	1.52	1	1
1	A	179	GLU	C-N	9.46	1.46	1.33	20	1
1	A	138	ILE	N-CA	-9.44	1.37	1.47	20	1
1	A	81	ILE	N-CA	9.43	1.58	1.46	19	2
1	A	173	ILE	N-CA	9.43	1.56	1.46	1	1
1	A	165	GLN	N-CA	9.42	1.57	1.46	20	1
1	A	106	ASP	C-N	9.41	1.46	1.33	20	1
1	A	195	GLU	C-O	-9.40	1.12	1.24	19	1
1	A	45	LYS	C-N	-9.40	1.20	1.33	1	1
1	A	74	HIS	CD2-NE2	-9.40	1.27	1.37	20	1
1	A	137	ASN	C-N	-9.39	1.22	1.33	1	3
1	A	154	ASN	N-CA	-9.36	1.34	1.46	19	1
1	A	168	ARG	N-CA	9.32	1.58	1.46	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	191	HIS	CE1-NE2	9.31	1.41	1.32	1	2
1	A	188	LEU	CA-C	9.30	1.65	1.52	20	1
1	A	155	GLY	C-N	9.26	1.45	1.33	19	2
1	A	141	SER	N-CA	9.26	1.59	1.45	19	2
1	A	86	SER	CA-C	9.26	1.65	1.52	20	1
1	A	106	ASP	C-O	9.25	1.34	1.24	19	2
1	A	82	ARG	NE-CZ	-9.24	1.22	1.33	19	1
1	A	198	HIS	CG-ND1	9.24	1.48	1.38	19	1
1	A	196	ASN	CG-OD1	-9.24	1.05	1.23	20	1
1	A	89	GLN	CA-CB	9.23	1.66	1.53	20	1
1	A	39	GLY	N-CA	9.22	1.54	1.45	19	2
1	A	14	SER	N-CA	9.19	1.58	1.46	19	2
1	A	18	VAL	C-O	9.16	1.34	1.24	1	1
1	A	131	ALA	C-O	-9.12	1.11	1.24	19	1
1	A	30	SER	C-N	9.08	1.47	1.33	20	1
1	A	206	SER	CA-CB	9.07	1.66	1.53	1	1
1	A	203	PHE	CA-C	9.03	1.64	1.52	19	1
1	A	32	PHE	N-CA	8.94	1.56	1.46	19	1
1	A	152	SER	N-CA	-8.94	1.35	1.46	19	2
1	A	207	THR	CA-C	8.94	1.63	1.52	19	2
1	A	163	PHE	CA-CB	8.91	1.67	1.53	20	2
1	A	186	ILE	CA-C	8.91	1.64	1.52	1	1
1	A	74	HIS	ND1-CE1	-8.87	1.23	1.32	19	2
1	A	64	ALA	N-CA	-8.86	1.35	1.46	20	1
1	A	71	LEU	CA-C	8.85	1.64	1.52	19	1
1	A	84	THR	N-CA	8.85	1.57	1.46	19	2
1	A	45	LYS	CA-C	-8.83	1.42	1.52	1	1
1	A	157	VAL	CA-CB	-8.83	1.43	1.54	1	2
1	A	43	ARG	CA-CB	8.82	1.69	1.53	19	1
1	A	191	HIS	CA-C	-8.77	1.41	1.52	1	1
1	A	134	HIS	CA-CB	8.76	1.68	1.53	19	2
1	A	91	VAL	CA-C	-8.76	1.42	1.52	19	2
1	A	53	ASN	CA-C	8.73	1.63	1.52	19	3
1	A	183	GLN	CA-CB	8.71	1.67	1.53	20	1
1	A	22	ASN	CA-C	8.70	1.63	1.53	19	2
1	A	32	PHE	CA-CB	8.70	1.67	1.53	19	2
1	A	205	LYS	N-CA	-8.69	1.34	1.46	19	1
1	A	201	VAL	N-CA	8.67	1.57	1.46	1	3
1	A	202	SER	CA-C	8.66	1.63	1.53	1	2
1	A	82	ARG	CA-CB	8.66	1.68	1.53	20	1
1	A	104	THR	CA-C	8.63	1.65	1.53	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	147	LEU	CA-CB	8.61	1.67	1.53	1	2
1	A	74	HIS	CB-CG	8.56	1.62	1.50	19	2
1	A	184	ALA	CA-C	-8.48	1.40	1.52	1	1
1	A	27	THR	CA-CB	8.48	1.64	1.54	1	2
1	A	144	GLU	C-O	-8.48	1.14	1.24	1	1
1	A	135	LEU	C-O	8.45	1.34	1.23	20	1
1	A	140	PRO	CA-C	8.44	1.65	1.52	20	1
1	A	134	HIS	CG-ND1	8.44	1.47	1.38	1	1
1	A	83	ILE	C-O	-8.44	1.14	1.24	19	1
1	A	199	LEU	CA-C	8.42	1.65	1.53	19	2
1	A	73	GLY	CA-C	-8.41	1.40	1.51	20	1
1	A	59	ALA	C-O	8.40	1.34	1.24	20	1
1	A	58	MET	CG-SD	8.40	2.01	1.80	19	2
1	A	181	ALA	CA-C	8.39	1.64	1.52	19	1
1	A	183	GLN	N-CA	8.32	1.56	1.46	1	1
1	A	22	ASN	C-O	-8.32	1.15	1.24	20	2
1	A	38	TYR	N-CA	-8.32	1.36	1.46	1	1
1	A	76	LEU	N-CA	-8.31	1.36	1.46	1	3
1	A	91	VAL	N-CA	8.30	1.55	1.45	20	1
1	A	205	LYS	C-N	8.29	1.45	1.34	20	1
1	A	203	PHE	CA-CB	8.29	1.64	1.53	1	3
1	A	88	HIS	CG-ND1	8.28	1.47	1.38	19	2
1	A	91	VAL	CA-CB	8.25	1.64	1.54	1	1
1	A	19	SER	N-CA	-8.25	1.35	1.45	19	1
1	A	194	GLY	CA-C	-8.22	1.40	1.51	20	2
1	A	89	GLN	N-CA	8.18	1.56	1.46	1	2
1	A	18	VAL	CA-C	8.17	1.63	1.52	1	1
1	A	187	ASP	CB-CG	8.14	1.72	1.52	20	1
1	A	80	PRO	CA-C	8.11	1.64	1.52	20	2
1	A	126	ILE	CA-CB	8.11	1.68	1.55	19	2
1	A	77	HIS	N-CA	8.10	1.56	1.46	20	2
1	A	43	ARG	CD-NE	8.08	1.57	1.46	1	2
1	A	134	HIS	CE1-NE2	8.08	1.40	1.32	19	3
1	A	187	ASP	C-N	8.07	1.44	1.33	19	1
1	A	173	ILE	C-N	-8.05	1.22	1.33	20	1
1	A	129	PRO	CA-CB	-8.02	1.43	1.53	20	1
1	A	159	LYS	CA-C	8.01	1.63	1.52	19	1
1	A	70	HIS	CB-CG	8.01	1.61	1.50	1	1
1	A	74	HIS	CA-C	8.01	1.63	1.52	20	1
1	A	161	PHE	C-O	8.00	1.33	1.23	1	1
1	A	34	LEU	CA-C	8.00	1.63	1.52	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	182	VAL	CA-CB	-7.98	1.45	1.54	1	3
1	A	170	MET	C-O	7.96	1.33	1.23	19	2
1	A	104	THR	C-O	7.94	1.32	1.23	19	1
1	A	39	GLY	CA-C	7.93	1.60	1.51	20	1
1	A	81	ILE	C-N	-7.90	1.23	1.33	1	2
1	A	197	HIS	CB-CG	-7.87	1.39	1.50	1	1
1	A	164	PHE	C-O	7.85	1.33	1.24	19	1
1	A	53	ASN	C-O	7.85	1.33	1.23	20	1
1	A	188	LEU	CB-CG	7.84	1.69	1.53	1	1
1	A	28	PRO	N-CA	7.84	1.57	1.47	19	1
1	A	78	GLY	C-N	7.84	1.42	1.33	20	1
1	A	27	THR	CA-C	-7.83	1.42	1.52	20	2
1	A	55	LEU	CA-CB	-7.83	1.43	1.53	1	1
1	A	206	SER	N-CA	7.81	1.55	1.45	1	2
1	A	80	PRO	CA-CB	7.79	1.64	1.53	20	2
1	A	198	HIS	CG-CD2	7.79	1.44	1.35	1	1
1	A	169	LYS	CA-C	7.78	1.62	1.52	19	1
1	A	194	GLY	C-O	7.75	1.34	1.23	20	1
1	A	189	HIS	CB-CG	7.75	1.61	1.50	19	1
1	A	154	ASN	C-O	7.74	1.34	1.24	1	1
1	A	82	ARG	N-CA	7.74	1.56	1.46	20	1
1	A	162	LYS	N-CA	7.74	1.55	1.46	19	3
1	A	160	GLY	C-N	-7.74	1.24	1.33	20	1
1	A	34	LEU	N-CA	7.73	1.56	1.46	19	1
1	A	172	LEU	N-CA	-7.72	1.35	1.45	19	1
1	A	68	MET	CA-C	-7.72	1.43	1.52	20	2
1	A	175	MET	N-CA	7.71	1.56	1.46	19	2
1	A	151	PHE	C-N	7.68	1.44	1.33	1	1
1	A	57	GLN	C-O	-7.68	1.14	1.24	1	1
1	A	81	ILE	CA-C	7.67	1.62	1.52	1	2
1	A	177	SER	CA-CB	-7.67	1.40	1.53	20	1
1	A	87	LYS	N-CA	7.65	1.55	1.46	19	1
1	A	40	ASP	CG-OD1	7.64	1.39	1.25	19	1
1	A	163	PHE	C-O	7.63	1.32	1.23	20	1
1	A	178	VAL	CA-CB	-7.63	1.45	1.54	20	2
1	A	136	SER	CA-C	-7.62	1.43	1.52	1	1
1	A	173	ILE	C-O	-7.58	1.16	1.24	20	2
1	A	54	ALA	N-CA	-7.56	1.36	1.46	19	1
1	A	46	ILE	N-CA	7.54	1.54	1.46	1	1
1	A	180	GLU	C-N	7.52	1.43	1.33	1	2
1	A	62	ASN	N-CA	-7.51	1.36	1.46	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	63	GLN	C-O	-7.50	1.15	1.24	20	2
1	A	189	HIS	CD2-NE2	7.50	1.46	1.37	20	2
1	A	167	ASP	C-N	7.50	1.44	1.33	19	1
1	A	77	HIS	CE1-NE2	-7.49	1.25	1.32	1	1
1	A	159	LYS	CA-CB	7.47	1.65	1.53	19	1
1	A	203	PHE	C-N	-7.47	1.23	1.33	20	3
1	A	195	GLU	N-CA	7.47	1.55	1.46	19	3
1	A	141	SER	CA-C	-7.45	1.42	1.52	19	1
1	A	63	GLN	CD-OE1	7.45	1.37	1.23	1	1
1	A	74	HIS	CA-CB	-7.38	1.41	1.53	20	1
1	A	196	ASN	CA-C	7.38	1.63	1.52	1	2
1	A	67	ALA	C-O	-7.38	1.15	1.24	19	1
1	A	197	HIS	CD2-NE2	7.37	1.46	1.37	19	1
1	A	72	ASN	C-O	-7.36	1.14	1.24	19	2
1	A	148	LYS	N-CA	7.34	1.55	1.46	19	3
1	A	83	ILE	N-CA	7.31	1.55	1.46	1	3
1	A	165	GLN	CA-CB	7.31	1.65	1.53	1	1
1	A	16	LEU	N-CA	7.30	1.55	1.46	19	2
1	A	126	ILE	C-O	-7.29	1.15	1.24	1	1
1	A	153	SER	CA-CB	7.29	1.65	1.53	19	1
1	A	189	HIS	CA-CB	7.29	1.65	1.53	19	1
1	A	198	HIS	CA-CB	-7.29	1.42	1.53	19	1
1	A	168	ARG	C-N	7.27	1.43	1.33	1	1
1	A	47	LEU	C-N	-7.26	1.23	1.33	1	1
1	A	75	LYS	C-N	7.26	1.43	1.33	1	1
1	A	69	SER	C-O	7.26	1.33	1.24	20	1
1	A	56	VAL	N-CA	-7.26	1.37	1.46	19	1
1	A	174	GLN	CA-CB	7.26	1.66	1.53	20	1
1	A	138	ILE	CA-CB	-7.25	1.44	1.54	1	1
1	A	61	GLY	CA-C	-7.25	1.41	1.51	20	1
1	A	182	VAL	C-N	7.25	1.43	1.33	20	1
1	A	156	GLY	C-N	-7.24	1.23	1.33	20	1
1	A	75	LYS	CA-C	-7.22	1.43	1.52	20	1
1	A	191	HIS	C-N	-7.21	1.24	1.33	20	1
1	A	32	PHE	CA-C	7.21	1.62	1.52	1	1
1	A	189	HIS	CE1-NE2	7.21	1.39	1.32	19	2
1	A	21	LEU	C-O	7.21	1.32	1.23	1	1
1	A	187	ASP	C-O	7.21	1.33	1.24	1	2
1	A	41	VAL	C-N	7.19	1.43	1.33	20	2
1	A	139	PRO	CA-CB	-7.15	1.44	1.54	19	1
1	A	31	LEU	C-N	-7.14	1.25	1.33	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	180	GLU	CA-C	7.13	1.61	1.52	19	2
1	A	20	ASN	C-N	-7.11	1.23	1.33	19	2
1	A	138	ILE	CA-C	7.11	1.59	1.52	20	1
1	A	143	SER	CA-CB	7.06	1.63	1.53	1	1
1	A	30	SER	CA-C	-7.03	1.44	1.52	20	2
1	A	165	GLN	C-O	7.00	1.32	1.24	19	2
1	A	148	LYS	CA-C	6.98	1.62	1.52	19	2
1	A	163	PHE	CA-C	6.96	1.61	1.52	20	1
1	A	173	ILE	CA-C	-6.95	1.44	1.52	19	1
1	A	43	ARG	N-CA	6.94	1.54	1.45	1	2
1	A	56	VAL	C-O	-6.94	1.16	1.24	1	1
1	A	190	ASN	CA-CB	6.94	1.63	1.53	20	2
1	A	45	LYS	C-O	-6.93	1.15	1.23	20	1
1	A	150	LEU	CA-C	-6.93	1.43	1.52	20	2
1	A	169	LYS	N-CA	6.92	1.55	1.46	1	1
1	A	76	LEU	CA-CB	-6.92	1.42	1.53	20	2
1	A	127	PHE	C-O	-6.91	1.15	1.24	1	2
1	A	133	LEU	CA-C	6.90	1.61	1.52	20	3
1	A	35	PHE	N-CA	-6.89	1.36	1.46	20	2
1	A	178	VAL	CA-C	-6.89	1.44	1.52	19	1
1	A	206	SER	C-N	-6.88	1.24	1.33	1	1
1	A	59	ALA	N-CA	6.88	1.55	1.46	19	2
1	A	191	HIS	CG-CD2	-6.87	1.28	1.35	19	1
1	A	166	LYS	C-N	6.87	1.43	1.33	1	1
1	A	72	ASN	CA-CB	6.87	1.65	1.53	20	1
1	A	67	ALA	C-N	6.85	1.42	1.33	19	1
1	A	137	ASN	C-O	6.85	1.32	1.24	19	1
1	A	170	MET	N-CA	6.84	1.54	1.46	19	1
1	A	42	GLN	C-O	6.83	1.32	1.24	19	2
1	A	15	VAL	CA-CB	6.82	1.63	1.54	19	1
1	A	88	HIS	CB-CG	-6.81	1.40	1.50	19	1
1	A	154	ASN	CA-C	6.79	1.61	1.52	19	2
1	A	179	GLU	N-CA	-6.79	1.37	1.46	1	1
1	A	181	ALA	C-O	-6.78	1.16	1.24	1	1
1	A	163	PHE	C-N	6.78	1.43	1.33	19	1
1	A	105	LYS	C-N	-6.78	1.24	1.33	1	2
1	A	138	ILE	C-O	-6.73	1.16	1.24	1	1
1	A	28	PRO	CA-C	-6.72	1.42	1.52	19	1
1	A	32	PHE	CG-CD1	6.70	1.52	1.38	1	2
1	A	85	LEU	N-CA	6.70	1.54	1.45	1	1
1	A	168	ARG	CZ-NH2	-6.69	1.24	1.33	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	134	HIS	CG-CD2	-6.69	1.28	1.35	19	2
1	A	25	ARG	CA-CB	6.68	1.64	1.53	19	1
1	A	131	ALA	N-CA	6.65	1.54	1.46	19	1
1	A	188	LEU	CA-CB	6.65	1.65	1.53	1	1
1	A	157	VAL	N-CA	6.65	1.53	1.46	19	2
1	A	185	LEU	N-CA	6.64	1.54	1.46	19	1
1	A	65	GLN	CA-C	-6.64	1.43	1.52	19	1
1	A	192	ASP	N-CA	6.61	1.54	1.46	1	1
1	A	151	PHE	CG-CD2	6.60	1.52	1.38	1	2
1	A	137	ASN	CB-CG	-6.59	1.35	1.52	19	2
1	A	33	ILE	C-N	6.59	1.42	1.33	20	1
1	A	168	ARG	CZ-NH1	-6.58	1.23	1.32	20	1
1	A	30	SER	C-O	-6.57	1.16	1.24	20	2
1	A	189	HIS	C-O	6.57	1.32	1.24	19	1
1	A	77	HIS	CB-CG	6.56	1.59	1.50	20	1
1	A	64	ALA	CA-CB	6.56	1.63	1.53	1	1
1	A	168	ARG	NE-CZ	6.56	1.40	1.33	19	1
1	A	181	ALA	CA-CB	-6.56	1.43	1.53	20	1
1	A	166	LYS	N-CA	-6.56	1.37	1.46	1	1
1	A	196	ASN	CG-ND2	-6.53	1.19	1.33	19	1
1	A	152	SER	CB-OG	-6.53	1.29	1.42	20	1
1	A	20	ASN	N-CA	-6.52	1.37	1.46	19	1
1	A	55	LEU	CB-CG	6.52	1.66	1.53	20	1
1	A	16	LEU	C-O	-6.52	1.15	1.23	20	1
1	A	15	VAL	CB-CG2	6.50	1.74	1.52	1	1
1	A	76	LEU	CA-C	6.50	1.61	1.52	19	2
1	A	205	LYS	CA-C	6.46	1.61	1.52	1	1
1	A	177	SER	C-N	6.46	1.42	1.34	20	1
1	A	43	ARG	C-N	-6.46	1.25	1.33	19	1
1	A	136	SER	CA-CB	6.45	1.64	1.53	19	1
1	A	44	VAL	C-O	-6.42	1.17	1.24	19	1
1	A	144	GLU	CA-CB	6.41	1.63	1.53	1	2
1	A	204	SER	C-O	6.41	1.31	1.23	19	1
1	A	105	LYS	CA-C	6.40	1.61	1.52	1	1
1	A	90	ASN	N-CA	6.40	1.54	1.46	1	1
1	A	176	GLY	N-CA	6.39	1.54	1.45	19	1
1	A	105	LYS	C-O	-6.38	1.16	1.24	1	1
1	A	88	HIS	CD2-NE2	6.37	1.44	1.37	19	1
1	A	197	HIS	CA-C	-6.37	1.46	1.53	19	1
1	A	203	PHE	CE2-CZ	6.37	1.57	1.38	19	1
1	A	142	VAL	N-CA	-6.36	1.38	1.46	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	17	LEU	CB-CG	6.35	1.66	1.53	1	1
1	A	61	GLY	C-N	6.35	1.42	1.33	19	1
1	A	38	TYR	CE2-CZ	6.34	1.53	1.38	19	1
1	A	14	SER	C-N	-6.31	1.25	1.33	19	2
1	A	190	ASN	CA-C	6.30	1.61	1.52	19	1
1	A	108	GLY	N-CA	6.30	1.54	1.45	20	1
1	A	169	LYS	C-O	-6.28	1.16	1.24	1	1
1	A	84	THR	CA-C	6.28	1.61	1.52	19	1
1	A	168	ARG	CA-CB	6.28	1.63	1.53	19	1
1	A	70	HIS	CD2-NE2	6.28	1.44	1.37	1	1
1	A	198	HIS	CE1-NE2	6.28	1.38	1.32	20	2
1	A	149	VAL	CA-C	6.28	1.60	1.52	1	1
1	A	206	SER	C-O	6.28	1.31	1.23	19	2
1	A	159	LYS	N-CA	6.27	1.54	1.46	1	1
1	A	133	LEU	CB-CG	6.25	1.66	1.53	19	1
1	A	190	ASN	CG-OD1	-6.24	1.11	1.23	20	1
1	A	63	GLN	N-CA	6.21	1.53	1.46	20	1
1	A	62	ASN	CB-CG	6.19	1.67	1.52	1	1
1	A	67	ALA	N-CA	-6.17	1.38	1.46	1	2
1	A	52	GLU	CA-CB	-6.17	1.45	1.54	19	1
1	A	44	VAL	N-CA	-6.16	1.39	1.46	19	1
1	A	82	ARG	CZ-NH2	-6.16	1.25	1.33	1	2
1	A	207	THR	CB-OG1	-6.15	1.33	1.43	20	2
1	A	154	ASN	C-N	-6.14	1.24	1.33	1	1
1	A	188	LEU	N-CA	-6.14	1.37	1.46	1	1
1	A	154	ASN	CG-ND2	-6.12	1.20	1.33	19	1
1	A	135	LEU	N-CA	6.12	1.53	1.45	20	1
1	A	69	SER	CA-C	6.12	1.60	1.52	19	1
1	A	70	HIS	CG-ND1	6.12	1.45	1.38	19	1
1	A	69	SER	C-N	-6.11	1.26	1.33	1	1
1	A	202	SER	CB-OG	-6.11	1.29	1.42	19	1
1	A	67	ALA	CA-C	6.11	1.60	1.52	19	1
1	A	138	ILE	C-N	-6.11	1.26	1.33	19	1
1	A	37	VAL	C-N	6.10	1.42	1.33	1	1
1	A	108	GLY	C-O	6.10	1.32	1.23	1	1
1	A	42	GLN	CG-CD	6.09	1.67	1.52	1	1
1	A	161	PHE	CA-CB	6.09	1.64	1.53	19	1
1	A	77	HIS	CG-ND1	6.07	1.45	1.38	20	2
1	A	204	SER	CB-OG	6.04	1.54	1.42	19	2
1	A	68	MET	C-O	-6.04	1.16	1.24	1	1
1	A	66	LEU	C-N	-6.03	1.26	1.33	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	58	MET	CA-CB	-6.01	1.45	1.52	19	1
1	A	80	PRO	N-CA	6.01	1.55	1.47	19	1
1	A	70	HIS	C-O	6.01	1.31	1.24	20	1
1	A	20	ASN	CG-ND2	-6.01	1.20	1.33	20	1
1	A	140	PRO	C-N	-6.00	1.25	1.33	1	1
1	A	42	GLN	CA-C	6.00	1.60	1.52	1	1
1	A	164	PHE	N-CA	-5.96	1.38	1.46	19	2
1	A	166	LYS	CA-CB	5.96	1.63	1.53	1	1
1	A	60	ASP	C-N	-5.95	1.24	1.33	19	2
1	A	184	ALA	N-CA	-5.93	1.38	1.46	1	1
1	A	202	SER	CA-CB	5.93	1.62	1.54	1	1
1	A	157	VAL	C-N	5.92	1.41	1.33	19	1
1	A	16	LEU	CA-C	5.92	1.61	1.53	1	1
1	A	171	ALA	N-CA	-5.92	1.38	1.45	1	1
1	A	107	TYR	CE1-CZ	5.92	1.52	1.38	19	1
1	A	78	GLY	CA-C	5.91	1.60	1.51	19	2
1	A	80	PRO	C-N	5.90	1.41	1.33	20	1
1	A	198	HIS	C-N	5.90	1.41	1.33	19	1
1	A	63	GLN	C-N	-5.89	1.26	1.33	19	1
1	A	146	ASP	CA-C	-5.89	1.45	1.52	20	1
1	A	183	GLN	C-N	5.89	1.41	1.34	20	1
1	A	162	LYS	C-N	5.88	1.41	1.33	20	1
1	A	165	GLN	CA-C	-5.87	1.45	1.52	20	1
1	A	163	PHE	N-CA	5.87	1.53	1.46	1	1
1	A	155	GLY	C-O	5.87	1.32	1.24	19	2
1	A	188	LEU	C-O	-5.86	1.16	1.24	1	1
1	A	161	PHE	CA-C	5.86	1.59	1.52	1	1
1	A	75	LYS	CB-CG	5.85	1.70	1.52	20	1
1	A	158	VAL	CA-CB	5.84	1.62	1.54	20	1
1	A	81	ILE	CA-CB	-5.84	1.46	1.54	1	1
1	A	161	PHE	CB-CG	5.83	1.64	1.50	20	1
1	A	42	GLN	CD-OE1	-5.82	1.12	1.23	19	1
1	A	43	ARG	CZ-NH1	5.80	1.40	1.32	19	1
1	A	152	SER	C-N	5.79	1.42	1.33	20	1
1	A	153	SER	C-O	5.79	1.30	1.24	19	1
1	A	162	LYS	C-O	-5.79	1.18	1.24	19	1
1	A	166	LYS	CA-C	5.79	1.58	1.52	20	1
1	A	44	VAL	CA-C	5.79	1.59	1.52	20	1
1	A	107	TYR	CA-C	-5.77	1.45	1.52	1	1
1	A	62	ASN	CA-CB	5.76	1.63	1.53	19	2
1	A	195	GLU	CA-C	-5.76	1.45	1.52	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	126	ILE	CA-C	-5.75	1.45	1.52	1	2
1	A	182	VAL	N-CA	5.74	1.54	1.46	19	1
1	A	199	LEU	CG-CD1	-5.73	1.33	1.52	1	1
1	A	189	HIS	ND1-CE1	5.73	1.38	1.32	19	1
1	A	150	LEU	C-O	-5.72	1.17	1.24	20	1
1	A	167	ASP	C-O	-5.72	1.17	1.24	19	1
1	A	89	GLN	CD-NE2	-5.72	1.21	1.33	20	1
1	A	70	HIS	CA-CB	-5.72	1.44	1.53	19	1
1	A	129	PRO	N-CA	-5.71	1.40	1.47	20	1
1	A	175	MET	CA-C	5.71	1.60	1.52	1	1
1	A	65	GLN	N-CA	5.71	1.53	1.46	20	2
1	A	23	PRO	C-N	5.68	1.41	1.33	19	1
1	A	27	THR	N-CA	5.68	1.51	1.46	20	2
1	A	40	ASP	CA-CB	-5.68	1.45	1.53	1	1
1	A	41	VAL	CA-CB	5.67	1.62	1.54	19	1
1	A	169	LYS	CD-CE	5.67	1.69	1.52	19	1
1	A	82	ARG	CZ-NH1	5.65	1.40	1.32	19	1
1	A	161	PHE	N-CA	5.65	1.53	1.46	19	1
1	A	62	ASN	CG-OD1	-5.64	1.12	1.23	1	1
1	A	19	SER	CA-CB	5.64	1.63	1.54	1	1
1	A	174	GLN	C-N	-5.63	1.25	1.33	20	1
1	A	31	LEU	CA-C	-5.62	1.45	1.52	1	1
1	A	174	GLN	CA-C	-5.61	1.46	1.52	20	1
1	A	178	VAL	N-CA	5.61	1.53	1.46	20	1
1	A	187	ASP	CA-C	-5.61	1.45	1.52	1	1
1	A	64	ALA	CA-C	5.59	1.60	1.52	1	1
1	A	175	MET	SD-CE	-5.59	1.65	1.79	19	1
1	A	192	ASP	C-N	5.59	1.40	1.33	1	1
1	A	204	SER	C-N	5.58	1.42	1.33	19	1
1	A	202	SER	C-O	-5.58	1.19	1.24	20	1
1	A	186	ILE	CB-CG1	5.57	1.64	1.53	20	1
1	A	185	LEU	CG-CD2	5.56	1.71	1.52	19	1
1	A	40	ASP	CB-CG	5.56	1.66	1.52	19	2
1	A	156	GLY	C-O	5.56	1.31	1.23	20	1
1	A	17	LEU	C-N	-5.55	1.26	1.33	1	1
1	A	194	GLY	C-N	5.54	1.41	1.33	19	1
1	A	208	ILE	N-CA	5.53	1.56	1.46	20	1
1	A	157	VAL	C-O	-5.53	1.18	1.24	19	1
1	A	199	LEU	N-CA	5.52	1.53	1.45	20	1
1	A	72	ASN	C-N	-5.51	1.25	1.33	1	1
1	A	35	PHE	CD2-CE2	5.51	1.55	1.38	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	148	LYS	CA-CB	5.51	1.62	1.53	19	1
1	A	172	LEU	CA-CB	-5.51	1.43	1.54	19	1
1	A	186	ILE	C-N	5.50	1.41	1.33	19	1
1	A	82	ARG	C-N	-5.50	1.25	1.33	19	1
1	A	42	GLN	CA-CB	5.48	1.62	1.53	1	2
1	A	84	THR	CA-CB	5.48	1.62	1.53	1	1
1	A	105	LYS	N-CA	5.48	1.52	1.46	20	1
1	A	132	THR	C-N	-5.47	1.25	1.33	19	1
1	A	25	ARG	CZ-NH2	-5.47	1.26	1.33	20	1
1	A	106	ASP	CG-OD2	-5.46	1.15	1.25	20	1
1	A	198	HIS	C-O	5.46	1.30	1.24	20	1
1	A	191	HIS	C-O	-5.46	1.17	1.24	20	1
1	A	145	GLU	C-N	-5.45	1.26	1.34	1	1
1	A	19	SER	CB-OG	-5.44	1.31	1.42	1	1
1	A	137	ASN	CA-CB	5.44	1.62	1.53	1	2
1	A	31	LEU	C-O	-5.43	1.17	1.24	1	1
1	A	142	VAL	C-N	5.42	1.38	1.33	19	1
1	A	35	PHE	CA-CB	-5.41	1.44	1.53	20	1
1	A	81	ILE	CB-CG1	5.40	1.64	1.53	19	1
1	A	198	HIS	CD2-NE2	5.40	1.43	1.37	1	1
1	A	18	VAL	CA-CB	5.38	1.61	1.54	1	2
1	A	158	VAL	C-O	-5.37	1.17	1.24	20	1
1	A	153	SER	CA-C	5.36	1.59	1.52	19	1
1	A	170	MET	CG-SD	-5.36	1.67	1.80	20	1
1	A	36	GLY	N-CA	-5.35	1.36	1.45	1	1
1	A	70	HIS	N-CA	5.34	1.53	1.46	1	1
1	A	33	ILE	N-CA	-5.33	1.40	1.46	1	1
1	A	78	GLY	C-O	-5.32	1.16	1.23	1	1
1	A	16	LEU	CG-CD2	5.31	1.70	1.52	20	1
1	A	47	LEU	CA-CB	-5.29	1.46	1.52	19	2
1	A	75	LYS	N-CA	5.29	1.53	1.46	20	1
1	A	47	LEU	CB-CG	5.28	1.64	1.53	1	1
1	A	104	THR	N-CA	5.27	1.52	1.45	1	1
1	A	13	ASN	CA-C	5.27	1.59	1.52	20	1
1	A	65	GLN	C-O	-5.26	1.18	1.24	20	1
1	A	171	ALA	C-O	-5.25	1.17	1.23	1	1
1	A	66	LEU	CA-CB	5.24	1.61	1.53	19	1
1	A	44	VAL	C-N	-5.23	1.25	1.33	1	1
1	A	32	PHE	CB-CG	5.22	1.62	1.50	20	1
1	A	201	VAL	CA-C	5.21	1.59	1.52	19	1
1	A	43	ARG	CA-C	-5.21	1.46	1.52	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	70	HIS	CA-C	-5.21	1.46	1.52	19	1
1	A	142	VAL	CB-CG2	5.21	1.69	1.52	19	1
1	A	142	VAL	C-O	5.21	1.31	1.23	19	1
1	A	88	HIS	C-O	-5.20	1.17	1.24	1	1
1	A	191	HIS	CA-CB	5.19	1.62	1.53	1	1
1	A	151	PHE	C-O	5.19	1.30	1.24	20	1
1	A	189	HIS	C-N	-5.19	1.26	1.33	20	1
1	A	42	GLN	C-N	-5.19	1.26	1.33	20	1
1	A	31	LEU	N-CA	-5.18	1.39	1.46	19	1
1	A	187	ASP	CG-OD2	-5.18	1.15	1.25	19	1
1	A	166	LYS	C-O	5.17	1.30	1.24	1	1
1	A	46	ILE	CA-CB	5.17	1.62	1.54	19	2
1	A	160	GLY	CA-C	-5.16	1.47	1.52	20	1
1	A	185	LEU	CB-CG	5.16	1.63	1.53	19	1
1	A	165	GLN	C-N	-5.15	1.26	1.33	20	1
1	A	23	PRO	N-CA	-5.14	1.40	1.47	19	1
1	A	145	GLU	CD-OE2	5.14	1.35	1.25	20	1
1	A	69	SER	CA-CB	5.13	1.62	1.53	19	1
1	A	74	HIS	C-N	5.13	1.40	1.33	1	1
1	A	148	LYS	C-O	5.13	1.30	1.24	19	1
1	A	36	GLY	CA-C	5.12	1.58	1.51	1	1
1	A	52	GLU	C-O	-5.12	1.17	1.23	1	1
1	A	89	GLN	CG-CD	5.12	1.64	1.52	19	1
1	A	158	VAL	N-CA	-5.11	1.40	1.46	19	1
1	A	105	LYS	CA-CB	5.11	1.67	1.54	19	1
1	A	176	GLY	C-N	-5.11	1.27	1.33	20	1
1	A	35	PHE	C-O	-5.10	1.17	1.24	19	1
1	A	64	ALA	C-O	5.10	1.29	1.24	20	1
1	A	23	PRO	N-CD	5.10	1.54	1.47	20	1
1	A	74	HIS	C-O	-5.09	1.17	1.24	19	1
1	A	139	PRO	N-CA	5.09	1.57	1.46	19	1
1	A	159	LYS	CG-CD	5.08	1.67	1.52	20	1
1	A	192	ASP	CB-CG	5.07	1.64	1.52	20	1
1	A	200	ARG	N-CA	5.07	1.52	1.46	1	1
1	A	40	ASP	N-CA	5.06	1.52	1.46	19	1
1	A	13	ASN	C-O	5.06	1.30	1.24	19	1
1	A	53	ASN	C-N	-5.05	1.25	1.33	20	1
1	A	137	ASN	CG-OD1	5.04	1.33	1.23	19	1
1	A	86	SER	CA-CB	5.04	1.61	1.53	1	1
1	A	193	LEU	CB-CG	5.04	1.63	1.53	20	1
1	A	177	SER	CB-OG	5.04	1.52	1.42	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	66	LEU	C-O	5.04	1.30	1.23	19	1
1	A	132	THR	N-CA	5.04	1.52	1.46	20	1
1	A	149	VAL	C-N	5.03	1.40	1.33	19	1
1	A	203	PHE	CD2-CE2	5.02	1.53	1.38	1	1
1	A	33	ILE	C-O	-5.01	1.18	1.24	1	1
1	A	179	GLU	CA-CB	5.01	1.62	1.53	20	1
1	A	192	ASP	CA-C	5.00	1.59	1.52	19	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	A	156	GLY	N-CA-C	22.59	137.19	112.33	1	2
1	A	197	HIS	CB-CG-CD2	-22.23	102.30	131.20	1	2
1	A	22	ASN	OD1-CG-ND2	-22.08	100.52	122.60	20	2
1	A	72	ASN	OD1-CG-ND2	-20.21	102.39	122.60	1	1
1	A	174	GLN	OE1-CD-NE2	-19.14	103.46	122.60	1	3
1	A	57	GLN	OE1-CD-NE2	-18.88	103.72	122.60	20	2
1	A	53	ASN	OD1-CG-ND2	-18.51	104.09	122.60	19	2
1	A	14	SER	O-C-N	-17.56	99.24	122.59	1	2
1	A	139	PRO	N-CA-CB	17.30	119.86	103.08	20	1
1	A	169	LYS	CA-C-N	17.23	145.17	120.71	19	4
1	A	169	LYS	C-N-CA	17.23	145.17	120.71	19	4
1	A	43	ARG	NE-CZ-NH2	16.65	134.18	119.20	20	2
1	A	22	ASN	CA-C-O	-16.62	105.53	119.99	20	1
1	A	70	HIS	CE1-NE2-CD2	-16.61	92.39	109.00	19	1
1	A	65	GLN	O-C-N	16.50	139.19	122.03	1	2
1	A	58	MET	CA-C-O	-16.19	104.08	120.92	19	2
1	A	65	GLN	CA-C-O	-16.08	104.11	121.00	1	3
1	A	182	VAL	N-CA-CB	16.01	128.07	110.62	1	1
1	A	33	ILE	O-C-N	-15.97	106.26	121.91	19	2
1	A	62	ASN	CA-CB-CG	15.92	128.52	112.60	1	3
1	A	196	ASN	OD1-CG-ND2	-15.88	106.72	122.60	1	3
1	A	53	ASN	CA-CB-CG	15.87	128.47	112.60	1	3
1	A	74	HIS	O-C-N	-15.74	103.63	122.20	19	1
1	A	134	HIS	CA-CB-CG	15.66	129.46	113.80	1	10
1	A	88	HIS	CA-CB-CG	15.58	129.38	113.80	19	2
1	A	167	ASP	CA-CB-CG	15.21	127.81	112.60	1	2
1	A	197	HIS	CE1-NE2-CD2	-14.95	94.05	109.00	19	2
1	A	37	VAL	CA-CB-CG2	14.73	135.44	110.40	1	1
1	A	138	ILE	CA-C-N	14.70	135.52	120.38	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	138	ILE	C-N-CA	14.70	135.52	120.38	20	2
1	A	79	LYS	O-C-N	-14.67	109.07	121.54	20	1
1	A	22	ASN	CA-CB-CG	14.67	127.27	112.60	1	6
1	A	42	GLN	O-C-N	-14.27	105.56	122.11	1	1
1	A	85	LEU	N-CA-C	14.14	130.44	110.50	19	2
1	A	43	ARG	NH1-CZ-NH2	-14.11	100.95	119.30	20	2
1	A	144	GLU	CA-C-O	-14.02	105.65	121.07	1	2
1	A	24	GLU	CA-C-O	14.02	135.41	120.55	1	2
1	A	153	SER	N-CA-C	-14.01	96.23	113.18	20	3
1	A	165	GLN	N-CA-C	13.87	127.75	111.11	20	1
1	A	186	ILE	O-C-N	-13.85	105.26	122.57	1	1
1	A	42	GLN	CA-C-O	13.63	135.11	120.80	1	3
1	A	182	VAL	CA-CB-CG1	13.50	133.35	110.40	1	19
1	A	60	ASP	CA-CB-CG	13.43	126.03	112.60	1	1
1	A	29	GLN	OE1-CD-NE2	-13.41	109.19	122.60	19	2
1	A	63	GLN	O-C-N	13.36	136.46	122.03	1	1
1	A	132	THR	CA-CB-OG1	13.31	129.56	109.60	1	1
1	A	63	GLN	CA-C-N	13.11	139.01	120.79	19	16
1	A	63	GLN	C-N-CA	13.11	139.01	120.79	19	16
1	A	147	LEU	O-C-N	-13.11	105.16	122.59	19	1
1	A	47	LEU	CA-C-N	13.09	146.54	121.54	1	4
1	A	47	LEU	C-N-CA	13.09	146.54	121.54	1	4
1	A	21	LEU	O-C-N	-12.73	108.08	122.84	19	1
1	A	27	THR	CA-C-N	12.71	135.73	119.84	19	1
1	A	27	THR	C-N-CA	12.71	135.73	119.84	19	1
1	A	76	LEU	CA-C-O	12.67	135.00	121.07	20	2
1	A	127	PHE	CA-C-N	12.64	133.40	120.38	20	2
1	A	127	PHE	C-N-CA	12.64	133.40	120.38	20	2
1	A	46	ILE	CA-C-O	-12.63	106.97	120.36	20	2
1	A	183	GLN	CA-C-N	12.63	138.81	120.38	1	5
1	A	183	GLN	C-N-CA	12.63	138.81	120.38	1	5
1	A	188	LEU	CB-CG-CD1	12.63	148.58	110.70	19	1
1	A	150	LEU	CA-C-O	-12.60	107.72	120.70	1	2
1	A	62	ASN	OD1-CG-ND2	-12.45	110.15	122.60	1	2
1	A	35	PHE	CA-CB-CG	12.42	126.22	113.80	20	1
1	A	88	HIS	CB-CA-C	12.37	133.00	109.37	19	1
1	A	186	ILE	CB-CA-C	12.32	130.04	112.05	19	2
1	A	197	HIS	CA-C-N	12.31	139.34	120.75	1	2
1	A	197	HIS	C-N-CA	12.31	139.34	120.75	1	2
1	A	149	VAL	CA-CB-CG1	12.31	131.33	110.40	20	1
1	A	190	ASN	CA-CB-CG	12.27	124.87	112.60	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	158	VAL	CA-C-N	12.24	137.81	120.79	20	16
1	A	158	VAL	C-N-CA	12.24	137.81	120.79	20	16
1	A	128	PRO	CA-C-N	12.17	135.06	119.84	1	4
1	A	128	PRO	C-N-CA	12.17	135.06	119.84	1	4
1	A	207	THR	CA-CB-OG1	12.16	127.84	109.60	20	2
1	A	69	SER	CA-C-N	12.15	137.54	120.29	19	1
1	A	69	SER	C-N-CA	12.15	137.54	120.29	19	1
1	A	155	GLY	CA-C-N	-12.15	104.17	121.54	19	3
1	A	155	GLY	C-N-CA	-12.15	104.17	121.54	19	3
1	A	91	VAL	N-CA-C	12.12	121.72	111.90	20	1
1	A	151	PHE	CA-CB-CG	12.10	125.90	113.80	19	2
1	A	27	THR	CB-CA-C	12.04	127.51	109.08	1	2
1	A	38	TYR	CA-C-O	-12.04	107.65	120.42	1	1
1	A	170	MET	N-CA-C	12.00	127.63	110.23	19	2
1	A	177	SER	CA-C-N	-11.92	105.54	120.56	1	1
1	A	177	SER	C-N-CA	-11.92	105.54	120.56	1	1
1	A	54	ALA	O-C-N	-11.92	109.33	123.27	1	1
1	A	195	GLU	CA-C-N	11.89	144.25	121.54	19	9
1	A	195	GLU	C-N-CA	11.89	144.25	121.54	19	9
1	A	23	PRO	CA-C-N	11.84	144.15	121.54	19	2
1	A	23	PRO	C-N-CA	11.84	144.15	121.54	19	2
1	A	20	ASN	CA-CB-CG	11.84	124.44	112.60	19	1
1	A	34	LEU	O-C-N	11.63	134.13	122.03	20	2
1	A	67	ALA	CB-CA-C	11.62	130.07	110.79	1	3
1	A	79	LYS	CB-CG-CD	11.61	137.99	111.30	20	3
1	A	22	ASN	O-C-N	-11.58	108.46	121.43	1	3
1	A	45	LYS	CB-CA-C	11.48	132.08	109.35	19	1
1	A	197	HIS	CG-CD2-NE2	-11.48	95.72	107.20	20	2
1	A	89	GLN	OE1-CD-NE2	-11.40	111.20	122.60	19	1
1	A	183	GLN	OE1-CD-NE2	-11.39	111.20	122.60	20	2
1	A	185	LEU	CB-CA-C	11.39	133.10	110.42	1	1
1	A	43	ARG	O-C-N	-11.37	110.48	123.33	1	1
1	A	162	LYS	CA-C-O	11.36	134.23	121.51	1	1
1	A	75	LYS	CB-CG-CD	11.32	137.33	111.30	1	1
1	A	38	TYR	O-C-N	11.28	135.01	122.15	1	2
1	A	38	TYR	CB-CA-C	11.25	128.44	109.55	19	1
1	A	164	PHE	CA-CB-CG	11.22	125.02	113.80	20	3
1	A	130	SER	CA-C-N	11.20	138.52	120.60	1	3
1	A	130	SER	C-N-CA	11.20	138.52	120.60	1	3
1	A	75	LYS	CA-C-N	11.17	142.87	121.54	19	15
1	A	75	LYS	C-N-CA	11.17	142.87	121.54	19	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	GLN	CA-C-N	11.16	138.82	122.41	19	1
1	A	57	GLN	C-N-CA	11.16	138.82	122.41	19	1
1	A	202	SER	CA-CB-OG	-11.16	88.77	111.10	19	1
1	A	25	ARG	NH1-CZ-NH2	-11.16	104.80	119.30	1	2
1	A	134	HIS	CB-CG-CD2	-11.10	116.77	131.20	19	1
1	A	54	ALA	N-CA-CB	11.08	128.17	110.77	1	1
1	A	139	PRO	CA-N-CD	-11.07	96.50	112.00	20	1
1	A	74	HIS	CG-CD2-NE2	11.04	118.23	107.20	20	1
1	A	143	SER	CA-CB-OG	11.00	133.09	111.10	19	1
1	A	139	PRO	N-CD-CG	10.99	119.68	103.20	20	1
1	A	177	SER	CA-CB-OG	10.97	133.05	111.10	1	1
1	A	205	LYS	CA-C-N	10.96	140.82	122.07	19	1
1	A	205	LYS	C-N-CA	10.96	140.82	122.07	19	1
1	A	91	VAL	CA-C-N	10.95	138.44	123.00	1	3
1	A	91	VAL	C-N-CA	10.95	138.44	123.00	1	3
1	A	46	ILE	CA-C-N	-10.93	105.50	121.24	20	1
1	A	46	ILE	C-N-CA	-10.93	105.50	121.24	20	1
1	A	64	ALA	N-CA-C	-10.92	99.38	111.07	20	2
1	A	177	SER	CA-C-O	-10.85	109.61	121.33	20	2
1	A	189	HIS	CB-CG-CD2	-10.84	117.11	131.20	19	2
1	A	62	ASN	CA-C-N	10.84	135.68	120.29	20	14
1	A	62	ASN	C-N-CA	10.84	135.68	120.29	20	14
1	A	74	HIS	CB-CG-CD2	-10.82	117.14	131.20	20	2
1	A	133	LEU	CA-C-O	-10.82	108.79	120.80	19	2
1	A	199	LEU	CA-C-O	10.81	133.37	121.05	1	1
1	A	190	ASN	OD1-CG-ND2	-10.74	111.86	122.60	19	2
1	A	70	HIS	CB-CG-CD2	-10.67	117.33	131.20	20	1
1	A	55	LEU	O-C-N	10.65	135.72	123.05	1	1
1	A	135	LEU	O-C-N	-10.61	110.96	123.27	19	1
1	A	200	ARG	NE-CZ-NH1	-10.61	110.89	121.50	19	2
1	A	184	ALA	CB-CA-C	10.61	130.26	110.63	19	1
1	A	131	ALA	O-C-N	-10.61	107.82	122.46	19	1
1	A	208	ILE	CB-CG1-CD1	10.58	136.02	113.80	20	1
1	A	186	ILE	CA-C-O	10.55	133.97	120.78	1	2
1	A	80	PRO	CA-C-N	10.53	140.93	121.97	20	4
1	A	80	PRO	C-N-CA	10.53	140.93	121.97	20	4
1	A	88	HIS	CB-CG-CD2	-10.53	117.51	131.20	19	3
1	A	198	HIS	CA-CB-CG	10.49	124.29	113.80	19	3
1	A	24	GLU	N-CA-C	10.47	122.70	111.28	1	2
1	A	21	LEU	CD1-CG-CD2	-10.47	87.77	110.80	20	2
1	A	40	ASP	CA-C-O	10.47	132.98	121.05	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	175	MET	N-CA-CB	-10.45	92.82	110.49	1	2
1	A	157	VAL	CA-C-N	10.42	140.73	121.97	19	2
1	A	157	VAL	C-N-CA	10.42	140.73	121.97	19	2
1	A	129	PRO	O-C-N	10.42	136.71	122.64	1	2
1	A	198	HIS	CE1-NE2-CD2	-10.42	98.58	109.00	1	1
1	A	29	GLN	O-C-N	10.41	136.38	122.43	19	1
1	A	14	SER	CA-CB-OG	10.39	131.88	111.10	20	2
1	A	104	THR	CA-CB-OG1	10.38	125.16	109.60	20	3
1	A	156	GLY	CA-C-N	10.38	134.20	121.85	19	8
1	A	156	GLY	C-N-CA	10.38	134.20	121.85	19	8
1	A	196	ASN	CB-CG-OD1	10.37	141.54	120.80	1	3
1	A	39	GLY	CA-C-O	-10.32	110.51	121.35	19	1
1	A	16	LEU	N-CA-C	10.32	124.60	110.35	1	1
1	A	168	ARG	NE-CZ-NH2	10.28	128.45	119.20	1	2
1	A	82	ARG	NE-CZ-NH2	10.26	128.43	119.20	19	2
1	A	106	ASP	CB-CA-C	10.25	128.53	111.51	1	2
1	A	38	TYR	N-CA-C	-10.24	100.19	111.36	1	2
1	A	178	VAL	CA-CB-CG2	10.21	127.76	110.40	20	2
1	A	52	GLU	CA-C-N	10.21	139.00	121.64	20	1
1	A	52	GLU	C-N-CA	10.21	139.00	121.64	20	1
1	A	46	ILE	CA-CB-CG1	-10.20	93.07	110.40	1	1
1	A	72	ASN	O-C-N	10.18	136.12	122.59	19	2
1	A	187	ASP	CA-C-N	10.17	136.88	120.60	19	1
1	A	187	ASP	C-N-CA	10.17	136.88	120.60	19	1
1	A	202	SER	CA-C-O	10.17	131.52	120.94	20	1
1	A	196	ASN	CB-CA-C	10.17	127.81	111.23	1	1
1	A	74	HIS	CB-CG-ND1	10.17	137.96	122.70	20	2
1	A	128	PRO	O-C-N	-10.14	109.49	121.46	1	1
1	A	18	VAL	N-CA-CB	-10.13	99.18	112.34	19	1
1	A	142	VAL	CA-CB-CG1	10.10	127.58	110.40	19	2
1	A	197	HIS	ND1-CE1-NE2	10.10	118.50	108.40	19	2
1	A	29	GLN	CA-C-O	-10.10	106.96	119.38	19	3
1	A	87	LYS	CG-CD-CE	-10.09	88.09	111.30	1	2
1	A	138	ILE	N-CA-CB	10.05	125.29	111.21	1	2
1	A	68	MET	CA-CB-CG	10.04	134.19	114.10	1	1
1	A	59	ALA	N-CA-C	10.03	123.45	111.82	20	2
1	A	147	LEU	N-CA-C	10.00	122.13	111.03	20	1
1	A	157	VAL	CB-CA-C	-10.00	99.98	110.88	19	1
1	A	178	VAL	O-C-N	9.99	131.68	121.89	20	2
1	A	76	LEU	N-CA-C	9.99	123.21	111.02	20	1
1	A	35	PHE	CE1-CZ-CE2	9.98	137.96	120.00	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	158	VAL	CA-CB-CG2	9.96	127.33	110.40	1	2
1	A	17	LEU	CA-C-O	9.95	133.08	121.44	1	2
1	A	28	PRO	N-CD-CG	9.89	118.04	103.20	20	2
1	A	148	LYS	CB-CG-CD	9.89	134.05	111.30	20	2
1	A	206	SER	CA-C-N	9.89	140.43	121.54	20	2
1	A	206	SER	C-N-CA	9.89	140.43	121.54	20	2
1	A	28	PRO	CA-N-CD	-9.89	98.16	112.00	19	1
1	A	191	HIS	CE1-NE2-CD2	-9.87	99.13	109.00	1	1
1	A	152	SER	CA-CB-OG	-9.86	91.39	111.10	20	2
1	A	166	LYS	O-C-N	9.85	135.69	122.59	1	1
1	A	83	ILE	N-CA-C	-9.84	96.89	109.58	1	1
1	A	186	ILE	CA-CB-CG2	9.84	127.23	110.50	19	2
1	A	133	LEU	CA-C-N	9.81	134.73	120.90	20	19
1	A	133	LEU	C-N-CA	9.81	134.73	120.90	20	19
1	A	202	SER	O-C-N	-9.78	111.41	122.75	20	1
1	A	167	ASP	CA-C-O	9.76	130.89	120.55	19	1
1	A	89	GLN	CG-CD-NE2	9.76	131.03	116.40	19	2
1	A	37	VAL	N-CA-C	-9.75	99.81	113.07	19	1
1	A	55	LEU	CA-C-O	-9.75	110.40	120.54	1	1
1	A	139	PRO	CA-C-N	9.73	132.00	119.84	1	8
1	A	139	PRO	C-N-CA	9.73	132.00	119.84	1	8
1	A	147	LEU	CA-C-O	9.70	130.89	120.90	20	1
1	A	191	HIS	CG-CD2-NE2	9.68	116.88	107.20	1	2
1	A	20	ASN	CA-C-O	9.68	134.35	120.51	1	2
1	A	164	PHE	O-C-N	9.66	133.81	122.79	20	2
1	A	159	LYS	CA-C-N	9.65	129.93	121.82	20	2
1	A	159	LYS	C-N-CA	9.65	129.93	121.82	20	2
1	A	68	MET	CA-C-O	9.63	130.93	120.82	20	1
1	A	87	LYS	N-CA-CB	9.62	123.72	114.10	20	1
1	A	31	LEU	CD1-CG-CD2	9.59	131.90	110.80	19	1
1	A	43	ARG	CB-CA-C	-9.59	89.28	110.67	19	1
1	A	44	VAL	N-CA-CB	-9.59	96.05	111.58	19	2
1	A	77	HIS	CA-C-O	9.59	131.05	119.64	1	1
1	A	193	LEU	N-CA-C	-9.57	99.96	112.68	19	2
1	A	13	ASN	N-CA-CB	-9.56	94.33	110.49	1	2
1	A	137	ASN	OD1-CG-ND2	-9.56	113.04	122.60	20	3
1	A	40	ASP	N-CA-C	-9.54	95.12	110.20	20	1
1	A	178	VAL	N-CA-CB	9.53	122.39	110.47	20	20
1	A	77	HIS	N-CA-CB	9.52	126.69	110.51	1	1
1	A	128	PRO	N-CD-CG	9.49	117.43	103.20	20	2
1	A	147	LEU	N-CA-CB	-9.47	96.15	110.16	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	VAL	N-CA-C	9.45	121.97	108.17	19	3
1	A	198	HIS	ND1-CE1-NE2	9.45	117.84	108.40	1	2
1	A	88	HIS	CB-CG-ND1	9.44	136.86	122.70	19	1
1	A	13	ASN	OD1-CG-ND2	-9.43	113.17	122.60	1	2
1	A	189	HIS	ND1-CE1-NE2	9.42	117.82	108.40	1	3
1	A	194	GLY	O-C-N	9.42	131.88	122.65	1	2
1	A	144	GLU	CA-C-N	9.39	137.29	122.83	19	1
1	A	144	GLU	C-N-CA	9.39	137.29	122.83	19	1
1	A	184	ALA	N-CA-CB	-9.38	95.77	110.22	19	1
1	A	170	MET	O-C-N	-9.38	111.11	122.65	20	1
1	A	201	VAL	O-C-N	-9.36	114.20	123.19	1	1
1	A	86	SER	N-CA-CB	9.34	125.68	110.55	19	2
1	A	23	PRO	O-C-N	-9.33	110.04	122.64	19	1
1	A	161	PHE	CA-CB-CG	-9.32	104.48	113.80	20	2
1	A	22	ASN	CB-CG-ND2	-9.28	102.48	116.40	20	1
1	A	163	PHE	CA-CB-CG	9.28	123.08	113.80	19	2
1	A	105	LYS	CB-CG-CD	-9.26	90.00	111.30	19	1
1	A	70	HIS	CG-CD2-NE2	9.25	116.45	107.20	19	1
1	A	147	LEU	CA-C-N	9.25	133.01	120.44	1	14
1	A	147	LEU	C-N-CA	9.25	133.01	120.44	1	14
1	A	148	LYS	O-C-N	-9.24	112.11	122.09	1	1
1	A	187	ASP	CA-C-O	-9.23	109.87	120.20	20	1
1	A	137	ASN	CB-CG-OD1	9.21	139.21	120.80	19	1
1	A	81	ILE	O-C-N	9.20	134.07	122.57	1	1
1	A	17	LEU	O-C-N	-9.19	112.77	123.06	19	2
1	A	17	LEU	CA-C-N	9.18	138.50	121.97	1	1
1	A	17	LEU	C-N-CA	9.18	138.50	121.97	1	1
1	A	32	PHE	CB-CA-C	9.17	126.06	110.84	19	1
1	A	66	LEU	CB-CA-C	-9.16	96.15	110.81	1	2
1	A	91	VAL	CG1-CB-CG2	9.16	130.95	110.80	1	1
1	A	193	LEU	N-CA-CB	-9.15	96.57	110.20	20	1
1	A	191	HIS	ND1-CG-CD2	9.15	115.25	106.10	19	2
1	A	183	GLN	CA-C-O	-9.15	109.95	120.20	19	1
1	A	155	GLY	O-C-N	9.14	132.99	122.38	19	2
1	A	160	GLY	CA-C-O	-9.14	111.79	121.57	20	2
1	A	183	GLN	N-CA-C	9.13	123.43	111.75	19	3
1	A	86	SER	CA-C-N	9.11	135.24	121.40	19	1
1	A	86	SER	C-N-CA	9.11	135.24	121.40	19	1
1	A	180	GLU	O-C-N	-9.07	112.30	122.09	19	2
1	A	20	ASN	O-C-N	-9.06	110.54	122.59	1	1
1	A	18	VAL	CA-C-N	-9.05	107.62	122.82	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	VAL	C-N-CA	-9.05	107.62	122.82	1	2
1	A	75	LYS	CA-CB-CG	9.02	132.14	114.10	19	1
1	A	56	VAL	CA-CB-CG1	-9.01	95.08	110.40	1	1
1	A	58	MET	O-C-N	9.01	133.22	122.68	1	1
1	A	56	VAL	CB-CA-C	9.01	124.51	110.81	20	1
1	A	182	VAL	O-C-N	-9.00	111.32	122.57	20	2
1	A	160	GLY	O-C-N	-8.98	115.79	123.60	20	2
1	A	22	ASN	CA-C-N	8.98	131.06	119.84	1	2
1	A	22	ASN	C-N-CA	8.98	131.06	119.84	1	2
1	A	207	THR	N-CA-C	8.97	122.51	109.14	1	1
1	A	23	PRO	N-CA-C	8.96	130.93	112.47	20	1
1	A	74	HIS	CA-C-N	8.95	138.64	121.54	19	2
1	A	74	HIS	C-N-CA	8.95	138.64	121.54	19	2
1	A	193	LEU	CA-C-O	-8.95	110.30	120.24	20	1
1	A	67	ALA	N-CA-C	-8.95	101.22	110.97	19	1
1	A	107	TYR	CB-CG-CD2	8.94	134.21	120.80	20	2
1	A	189	HIS	CA-C-N	8.94	134.76	122.34	20	1
1	A	189	HIS	C-N-CA	8.94	134.76	122.34	20	1
1	A	74	HIS	CA-CB-CG	-8.93	104.87	113.80	1	3
1	A	106	ASP	CA-CB-CG	-8.93	103.67	112.60	19	1
1	A	128	PRO	CA-CB-CG	8.91	121.43	104.50	19	1
1	A	166	LYS	CB-CG-CD	8.90	131.77	111.30	20	2
1	A	162	LYS	N-CA-C	8.89	122.38	109.14	1	1
1	A	149	VAL	O-C-N	-8.88	113.19	121.89	1	1
1	A	129	PRO	CA-N-CD	-8.87	99.58	112.00	1	2
1	A	200	ARG	CA-CB-CG	8.87	131.84	114.10	1	1
1	A	192	ASP	CB-CA-C	8.87	125.06	112.11	20	2
1	A	41	VAL	CA-CB-CG1	8.87	125.47	110.40	20	3
1	A	82	ARG	CD-NE-CZ	8.87	136.81	124.40	19	1
1	A	31	LEU	O-C-N	-8.86	112.52	122.09	1	2
1	A	18	VAL	O-C-N	8.85	132.15	123.03	20	1
1	A	19	SER	N-CA-C	-8.84	94.04	109.06	20	2
1	A	141	SER	N-CA-CB	-8.83	97.09	110.16	20	2
1	A	167	ASP	CA-C-N	8.81	134.67	122.07	19	4
1	A	167	ASP	C-N-CA	8.81	134.67	122.07	19	4
1	A	65	GLN	OE1-CD-NE2	-8.79	113.81	122.60	19	1
1	A	61	GLY	O-C-N	-8.75	111.33	122.70	1	1
1	A	159	LYS	O-C-N	8.73	134.95	122.20	19	2
1	A	159	LYS	CB-CA-C	-8.72	95.17	109.56	19	1
1	A	14	SER	CA-C-N	8.72	137.66	121.97	1	2
1	A	14	SER	C-N-CA	8.72	137.66	121.97	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	LEU	CA-C-O	8.71	132.97	120.51	19	2
1	A	193	LEU	CA-C-N	8.71	136.29	122.01	1	1
1	A	193	LEU	C-N-CA	8.71	136.29	122.01	1	1
1	A	105	LYS	CB-CA-C	-8.70	93.11	110.42	1	1
1	A	104	THR	O-C-N	-8.70	112.51	122.68	20	3
1	A	130	SER	CA-C-O	8.70	131.23	121.40	1	2
1	A	157	VAL	CA-CB-CG2	8.69	125.17	110.40	1	1
1	A	154	ASN	OD1-CG-ND2	-8.68	113.92	122.60	1	3
1	A	164	PHE	N-CA-C	8.68	129.29	110.80	1	3
1	A	187	ASP	N-CA-C	8.67	122.85	111.75	20	2
1	A	197	HIS	ND1-CG-CD2	-8.67	97.43	106.10	19	1
1	A	149	VAL	N-CA-C	-8.66	100.74	110.62	1	1
1	A	168	ARG	NH1-CZ-NH2	-8.66	108.04	119.30	1	1
1	A	69	SER	CA-C-O	-8.66	110.31	120.10	20	1
1	A	140	PRO	CB-CA-C	8.65	125.84	111.56	19	1
1	A	126	ILE	CA-C-O	8.63	131.57	120.78	20	1
1	A	31	LEU	CA-C-N	8.61	132.16	120.54	1	1
1	A	31	LEU	C-N-CA	8.61	132.16	120.54	1	1
1	A	199	LEU	N-CA-CB	-8.60	97.96	110.26	20	1
1	A	157	VAL	N-CA-CB	8.59	124.20	112.35	19	1
1	A	196	ASN	N-CA-C	8.58	129.08	110.80	19	1
1	A	191	HIS	ND1-CE1-NE2	8.58	116.98	108.40	20	1
1	A	137	ASN	CB-CG-ND2	-8.56	103.56	116.40	19	1
1	A	196	ASN	O-C-N	-8.55	110.07	122.04	1	1
1	A	77	HIS	CB-CG-CD2	-8.54	120.11	131.20	20	2
1	A	196	ASN	N-CA-CB	-8.53	99.73	112.78	1	2
1	A	201	VAL	CA-C-O	8.53	128.97	120.96	1	2
1	A	37	VAL	CA-C-N	8.51	135.15	120.68	20	1
1	A	37	VAL	C-N-CA	8.51	135.15	120.68	20	1
1	A	132	THR	CA-C-N	-8.50	110.99	122.72	20	1
1	A	132	THR	C-N-CA	-8.50	110.99	122.72	20	1
1	A	168	ARG	CB-CA-C	8.50	124.21	111.80	19	1
1	A	104	THR	CA-C-N	8.49	136.08	121.64	20	9
1	A	104	THR	C-N-CA	8.49	136.08	121.64	20	9
1	A	150	LEU	O-C-N	8.48	131.25	122.09	1	1
1	A	149	VAL	CA-C-N	8.47	137.72	121.54	19	1
1	A	149	VAL	C-N-CA	8.47	137.72	121.54	19	1
1	A	43	ARG	N-CA-C	-8.46	96.53	109.14	20	1
1	A	18	VAL	CA-C-O	-8.46	112.69	120.22	19	2
1	A	129	PRO	N-CA-CB	8.46	110.70	103.17	20	1
1	A	70	HIS	ND1-CE1-NE2	8.44	116.84	108.40	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	82	ARG	NH1-CZ-NH2	-8.44	108.33	119.30	1	1
1	A	145	GLU	CB-CA-C	8.44	124.14	111.06	19	1
1	A	42	GLN	CA-C-N	8.43	135.85	122.36	19	1
1	A	42	GLN	C-N-CA	8.43	135.85	122.36	19	1
1	A	131	ALA	CA-C-N	8.43	134.80	122.41	1	2
1	A	131	ALA	C-N-CA	8.43	134.80	122.41	1	2
1	A	127	PHE	CA-CB-CG	8.42	122.22	113.80	20	1
1	A	55	LEU	N-CA-CB	-8.40	97.07	110.77	20	1
1	A	44	VAL	CA-C-N	8.39	135.99	122.81	1	2
1	A	44	VAL	C-N-CA	8.39	135.99	122.81	1	2
1	A	87	LYS	CB-CA-C	8.39	118.13	109.83	20	3
1	A	138	ILE	CA-CB-CG2	-8.38	96.25	110.50	19	2
1	A	163	PHE	CB-CG-CD1	-8.38	106.45	120.70	20	2
1	A	35	PHE	CA-C-O	8.38	129.43	120.55	1	1
1	A	141	SER	CA-CB-OG	8.35	127.80	111.10	20	1
1	A	190	ASN	CB-CG-OD1	8.35	137.49	120.80	19	2
1	A	195	GLU	O-C-N	-8.33	111.51	122.59	1	1
1	A	188	LEU	N-CA-CB	-8.32	99.40	110.88	20	1
1	A	66	LEU	O-C-N	-8.31	113.45	122.09	1	1
1	A	25	ARG	CA-C-O	-8.30	109.39	119.43	19	1
1	A	27	THR	O-C-N	8.30	128.40	121.35	1	1
1	A	42	GLN	CG-CD-NE2	8.29	128.84	116.40	19	2
1	A	139	PRO	N-CA-C	8.26	120.78	110.70	13	2
1	A	27	THR	CA-CB-CG2	8.26	124.54	110.50	1	2
1	A	206	SER	O-C-N	-8.26	112.78	122.20	20	2
1	A	43	ARG	CA-C-N	8.24	134.69	122.98	1	1
1	A	43	ARG	C-N-CA	8.24	134.69	122.98	1	1
1	A	172	LEU	N-CA-C	8.24	121.69	109.24	19	1
1	A	129	PRO	CA-C-N	-8.23	108.88	122.21	1	1
1	A	129	PRO	C-N-CA	-8.23	108.88	122.21	1	1
1	A	169	LYS	CA-CB-CG	8.23	130.56	114.10	1	1
1	A	135	LEU	CB-CG-CD1	8.23	135.39	110.70	19	1
1	A	43	ARG	N-CA-CB	-8.22	98.31	111.62	19	2
1	A	150	LEU	CD1-CG-CD2	-8.21	92.73	110.80	20	1
1	A	32	PHE	CA-CB-CG	8.21	122.01	113.80	20	5
1	A	130	SER	O-C-N	-8.20	113.24	123.17	1	1
1	A	85	LEU	CA-C-N	8.20	137.21	121.54	20	2
1	A	85	LEU	C-N-CA	8.20	137.21	121.54	20	2
1	A	82	ARG	CB-CG-CD	-8.19	92.47	111.30	1	1
1	A	19	SER	CA-C-O	8.18	132.25	121.78	19	2
1	A	208	ILE	CA-CB-CG2	-8.16	96.62	110.50	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	162	LYS	CA-CB-CG	8.16	130.41	114.10	19	1
1	A	148	LYS	CB-CA-C	8.13	124.34	110.84	20	1
1	A	138	ILE	CB-CA-C	8.12	118.96	111.00	20	2
1	A	68	MET	O-C-N	-8.12	112.29	122.27	1	2
1	A	66	LEU	CD1-CG-CD2	-8.09	93.01	110.80	19	1
1	A	190	ASN	N-CA-CB	8.08	124.58	112.30	1	2
1	A	44	VAL	CG1-CB-CG2	-8.08	93.03	110.80	1	2
1	A	83	ILE	CA-CB-CG2	8.08	124.23	110.50	1	1
1	A	138	ILE	O-C-N	-8.08	112.42	121.14	20	1
1	A	199	LEU	O-C-N	-8.06	113.50	123.01	1	1
1	A	197	HIS	CB-CA-C	-8.06	101.31	111.22	1	1
1	A	82	ARG	NE-CZ-NH1	-8.05	113.45	121.50	19	2
1	A	22	ASN	CB-CA-C	8.05	118.54	110.33	20	2
1	A	32	PHE	CB-CG-CD1	8.04	134.37	120.70	1	1
1	A	146	ASP	N-CA-C	-8.04	101.80	111.69	20	1
1	A	44	VAL	CA-CB-CG2	8.02	124.04	110.40	1	1
1	A	36	GLY	N-CA-C	-8.00	102.62	115.66	1	1
1	A	199	LEU	N-CA-C	8.00	120.91	110.43	20	1
1	A	179	GLU	CB-CG-CD	-7.99	99.02	112.60	1	1
1	A	140	PRO	CA-N-CD	-7.97	100.84	112.00	19	2
1	A	201	VAL	CA-CB-CG1	7.97	123.95	110.40	19	2
1	A	47	LEU	N-CA-C	7.96	121.29	109.59	20	4
1	A	19	SER	N-CA-CB	-7.95	98.79	111.43	1	1
1	A	89	GLN	CB-CA-C	-7.93	94.02	111.71	20	1
1	A	136	SER	CA-CB-OG	7.93	126.95	111.10	1	1
1	A	191	HIS	CB-CG-CD2	-7.93	120.90	131.20	20	2
1	A	174	GLN	CG-CD-NE2	-7.91	104.53	116.40	20	2
1	A	74	HIS	CB-CA-C	-7.91	96.23	109.99	19	2
1	A	33	ILE	N-CA-CB	7.90	118.91	110.62	1	1
1	A	151	PHE	CA-C-O	-7.89	109.73	119.28	20	2
1	A	145	GLU	CA-C-O	7.89	130.32	120.15	19	1
1	A	192	ASP	CA-C-O	7.88	131.88	122.03	20	1
1	A	185	LEU	N-CA-C	-7.87	94.04	110.80	1	2
1	A	81	ILE	CA-C-N	7.86	136.55	121.54	19	2
1	A	81	ILE	C-N-CA	7.86	136.55	121.54	19	2
1	A	156	GLY	CA-C-O	7.86	134.24	120.57	20	2
1	A	32	PHE	CB-CG-CD2	-7.86	107.35	120.70	1	1
1	A	108	GLY	O-C-N	7.83	132.88	122.70	20	1
1	A	56	VAL	CA-C-N	7.83	133.02	122.84	1	1
1	A	56	VAL	C-N-CA	7.83	133.02	122.84	1	1
1	A	140	PRO	O-C-N	7.82	133.19	122.64	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	GLN	N-CA-CB	7.80	121.59	110.12	20	1
1	A	56	VAL	O-C-N	-7.79	115.20	123.14	20	2
1	A	181	ALA	N-CA-C	7.79	120.75	111.33	19	1
1	A	33	ILE	CA-C-N	-7.78	109.24	120.29	1	1
1	A	33	ILE	C-N-CA	-7.78	109.24	120.29	1	1
1	A	56	VAL	N-CA-CB	-7.77	98.71	111.45	19	1
1	A	90	ASN	CA-CB-CG	7.76	120.36	112.60	20	2
1	A	174	GLN	CA-C-O	-7.76	112.47	120.54	19	1
1	A	179	GLU	CA-CB-CG	-7.75	98.60	114.10	20	1
1	A	153	SER	CB-CA-C	-7.73	96.09	110.01	1	1
1	A	105	LYS	CA-C-N	7.73	133.67	122.77	19	1
1	A	105	LYS	C-N-CA	7.73	133.67	122.77	19	1
1	A	162	LYS	CB-CA-C	-7.72	96.49	111.78	19	1
1	A	130	SER	CA-CB-OG	7.72	126.54	111.10	20	1
1	A	198	HIS	CA-C-N	7.72	132.46	121.42	1	1
1	A	198	HIS	C-N-CA	7.72	132.46	121.42	1	1
1	A	133	LEU	O-C-N	7.71	132.21	123.19	19	2
1	A	70	HIS	CA-C-O	-7.70	112.25	120.42	19	2
1	A	126	ILE	CB-CG1-CD1	-7.70	97.63	113.80	19	1
1	A	197	HIS	CA-CB-CG	-7.69	106.11	113.80	19	1
1	A	40	ASP	CA-CB-CG	7.69	120.29	112.60	20	2
1	A	188	LEU	N-CA-C	7.67	124.79	114.12	20	2
1	A	195	GLU	CB-CG-CD	-7.67	99.56	112.60	19	1
1	A	58	MET	N-CA-CB	-7.65	98.61	110.46	20	1
1	A	15	VAL	O-C-N	-7.64	113.01	122.57	19	1
1	A	71	LEU	N-CA-CB	-7.63	98.61	110.06	20	1
1	A	55	LEU	CB-CA-C	7.63	123.51	109.70	19	1
1	A	201	VAL	CB-CA-C	7.62	121.87	110.90	19	2
1	A	52	GLU	CG-CD-OE1	7.62	135.92	118.40	20	1
1	A	150	LEU	N-CA-C	7.62	119.36	111.14	1	1
1	A	157	VAL	CA-CB-CG1	-7.62	97.45	110.40	1	1
1	A	196	ASN	CA-C-O	7.61	127.93	119.78	1	1
1	A	183	GLN	O-C-N	-7.61	113.87	122.09	20	1
1	A	84	THR	O-C-N	7.61	132.71	122.59	19	1
1	A	86	SER	O-C-N	-7.59	112.50	122.59	1	2
1	A	151	PHE	CB-CG-CD1	-7.58	107.81	120.70	19	2
1	A	107	TYR	CB-CG-CD1	-7.58	109.43	120.80	20	1
1	A	58	MET	N-CA-C	7.58	121.58	110.59	1	1
1	A	108	GLY	CA-C-N	7.56	135.98	121.54	19	1
1	A	108	GLY	C-N-CA	7.56	135.98	121.54	19	1
1	A	157	VAL	CA-C-O	7.56	125.55	118.90	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	132	THR	OG1-CB-CG2	7.55	124.40	109.30	19	2
1	A	162	LYS	N-CA-CB	-7.54	98.22	111.49	19	1
1	A	89	GLN	CA-C-O	7.54	130.40	121.88	20	1
1	A	54	ALA	CA-C-O	7.53	129.34	121.36	19	2
1	A	64	ALA	CB-CA-C	7.53	122.70	110.88	20	1
1	A	83	ILE	CA-C-O	-7.53	112.16	121.11	20	2
1	A	195	GLU	CA-C-O	7.51	131.25	120.51	1	1
1	A	26	VAL	N-CA-CB	7.51	118.71	110.53	1	1
1	A	82	ARG	O-C-N	7.50	132.56	122.59	20	1
1	A	143	SER	N-CA-C	7.49	118.41	108.07	19	1
1	A	201	VAL	N-CA-C	7.49	118.24	108.35	20	1
1	A	130	SER	CB-CA-C	-7.49	93.59	110.07	1	2
1	A	104	THR	OG1-CB-CG2	-7.48	94.34	109.30	20	2
1	A	24	GLU	CA-C-N	7.47	137.55	121.64	20	1
1	A	24	GLU	C-N-CA	7.47	137.55	121.64	20	1
1	A	165	GLN	CB-CG-CD	-7.46	99.92	112.60	1	1
1	A	42	GLN	CB-CG-CD	7.46	125.28	112.60	19	1
1	A	41	VAL	N-CA-C	7.45	124.83	109.34	1	1
1	A	13	ASN	CA-C-N	7.43	135.73	121.54	19	1
1	A	13	ASN	C-N-CA	7.43	135.73	121.54	19	1
1	A	35	PHE	CZ-CE2-CD2	-7.43	106.63	120.00	1	1
1	A	177	SER	N-CA-CB	-7.43	97.72	111.53	1	1
1	A	151	PHE	CB-CA-C	7.42	125.19	110.42	19	1
1	A	30	SER	O-C-N	7.42	129.80	122.09	1	1
1	A	143	SER	N-CA-CB	7.41	122.54	110.97	1	2
1	A	150	LEU	CA-C-N	7.41	135.70	121.54	19	1
1	A	150	LEU	C-N-CA	7.41	135.70	121.54	19	1
1	A	21	LEU	CB-CG-CD2	7.40	132.90	110.70	20	1
1	A	34	LEU	N-CA-CB	-7.40	99.21	110.16	1	5
1	A	22	ASN	N-CA-CB	7.39	122.03	110.12	20	3
1	A	138	ILE	CA-C-O	7.38	129.83	119.95	1	2
1	A	153	SER	CA-C-N	7.37	130.16	120.28	20	3
1	A	153	SER	C-N-CA	7.37	130.16	120.28	20	3
1	A	199	LEU	CB-CA-C	7.36	122.72	109.83	19	1
1	A	154	ASN	CB-CG-ND2	7.36	127.44	116.40	20	1
1	A	29	GLN	CA-C-N	-7.36	108.43	120.72	19	1
1	A	29	GLN	C-N-CA	-7.36	108.43	120.72	19	1
1	A	144	GLU	O-C-N	7.35	129.74	122.09	20	2
1	A	83	ILE	CB-CA-C	-7.35	100.09	111.26	1	1
1	A	30	SER	N-CA-C	-7.34	102.30	111.11	1	1
1	A	133	LEU	CB-CA-C	7.34	121.84	109.80	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	39	GLY	O-C-N	-7.34	116.88	123.92	19	2
1	A	66	LEU	N-CA-C	7.34	119.91	111.11	1	2
1	A	61	GLY	CA-C-N	-7.33	110.46	120.28	20	2
1	A	61	GLY	C-N-CA	-7.33	110.46	120.28	20	2
1	A	69	SER	CB-CA-C	-7.33	97.07	110.63	20	1
1	A	77	HIS	CB-CA-C	-7.33	97.34	109.65	1	1
1	A	52	GLU	CA-C-O	-7.32	110.27	118.69	19	1
1	A	171	ALA	N-CA-C	7.31	119.17	108.86	19	1
1	A	78	GLY	CA-C-N	7.30	139.62	121.80	19	2
1	A	78	GLY	C-N-CA	7.30	139.62	121.80	19	2
1	A	146	ASP	CA-C-O	-7.30	111.57	119.97	1	1
1	A	163	PHE	N-CA-C	7.30	120.42	108.52	1	1
1	A	202	SER	N-CA-CB	-7.29	100.19	111.35	20	1
1	A	70	HIS	O-C-N	-7.29	113.58	122.19	1	1
1	A	163	PHE	O-C-N	-7.29	114.66	123.27	1	2
1	A	128	PRO	N-CA-CB	7.28	110.14	103.08	20	1
1	A	26	VAL	CG1-CB-CG2	-7.27	94.80	110.80	1	1
1	A	192	ASP	CA-C-N	-7.27	108.93	122.60	19	2
1	A	192	ASP	C-N-CA	-7.27	108.93	122.60	19	2
1	A	189	HIS	CG-CD2-NE2	-7.27	99.93	107.20	20	1
1	A	24	GLU	N-CA-CB	-7.26	99.45	110.12	1	1
1	A	140	PRO	N-CD-CG	7.26	114.09	103.20	1	1
1	A	142	VAL	N-CA-C	7.26	117.96	110.05	19	1
1	A	159	LYS	CA-C-O	-7.25	112.80	120.92	1	1
1	A	41	VAL	CA-C-N	7.22	135.33	121.54	19	1
1	A	41	VAL	C-N-CA	7.22	135.33	121.54	19	1
1	A	146	ASP	CA-CB-CG	-7.21	105.39	112.60	19	1
1	A	44	VAL	O-C-N	-7.21	115.68	123.18	1	2
1	A	106	ASP	N-CA-C	7.20	121.95	107.41	20	2
1	A	104	THR	CB-CA-C	-7.19	97.06	109.65	19	1
1	A	86	SER	CA-CB-OG	7.19	125.48	111.10	1	2
1	A	178	VAL	CA-C-O	-7.19	113.55	121.17	1	1
1	A	21	LEU	N-CA-CB	-7.19	98.34	110.49	20	2
1	A	43	ARG	CD-NE-CZ	-7.18	114.34	124.40	1	4
1	A	196	ASN	CA-CB-CG	7.18	119.78	112.60	20	1
1	A	181	ALA	CA-C-O	-7.18	112.88	120.63	19	1
1	A	170	MET	CG-SD-CE	-7.18	85.11	100.90	20	2
1	A	76	LEU	CB-CA-C	-7.17	98.84	110.74	1	1
1	A	31	LEU	CB-CA-C	7.17	122.23	110.90	1	1
1	A	178	VAL	CB-CA-C	-7.16	102.81	111.97	1	9
1	A	187	ASP	CA-CB-CG	7.16	119.76	112.60	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	21	LEU	CA-CB-CG	7.15	141.34	116.30	1	1
1	A	45	LYS	CA-CB-CG	7.12	128.34	114.10	20	1
1	A	142	VAL	O-C-N	7.12	131.51	122.61	20	1
1	A	19	SER	O-C-N	-7.12	113.08	122.97	19	1
1	A	162	LYS	CG-CD-CE	7.12	127.67	111.30	1	1
1	A	74	HIS	CA-C-O	-7.10	110.50	119.31	20	2
1	A	160	GLY	CA-C-N	7.08	137.11	121.81	20	1
1	A	160	GLY	C-N-CA	7.08	137.11	121.81	20	1
1	A	188	LEU	CA-C-N	-7.07	110.55	121.02	20	1
1	A	188	LEU	C-N-CA	-7.07	110.55	121.02	20	1
1	A	23	PRO	N-CA-CB	-7.07	95.83	103.25	20	1
1	A	181	ALA	O-C-N	-7.06	114.63	122.12	1	2
1	A	91	VAL	CA-C-O	7.05	126.92	120.30	20	2
1	A	152	SER	CA-C-O	-7.04	112.42	120.24	19	2
1	A	168	ARG	CD-NE-CZ	-7.04	114.55	124.40	1	1
1	A	74	HIS	ND1-CG-CD2	-7.03	99.07	106.10	20	2
1	A	79	LYS	CA-C-O	-7.02	113.33	119.72	1	1
1	A	38	TYR	CG-CD2-CE2	7.01	131.71	121.20	19	2
1	A	196	ASN	CA-C-N	7.00	132.18	122.79	19	1
1	A	196	ASN	C-N-CA	7.00	132.18	122.79	19	1
1	A	173	ILE	CA-CB-CG1	7.00	122.30	110.40	1	1
1	A	70	HIS	CA-CB-CG	-7.00	106.80	113.80	20	1
1	A	80	PRO	N-CD-CG	7.00	113.69	103.20	19	1
1	A	34	LEU	CA-C-O	-6.99	113.66	121.00	20	1
1	A	197	HIS	CA-C-O	-6.99	110.52	120.51	20	1
1	A	172	LEU	CA-C-O	-6.98	113.52	121.40	19	2
1	A	43	ARG	CA-C-O	6.97	128.80	120.99	1	1
1	A	45	LYS	CG-CD-CE	6.97	127.33	111.30	1	1
1	A	189	HIS	CA-CB-CG	-6.97	106.83	113.80	19	2
1	A	58	MET	CA-CB-CG	6.97	128.03	114.10	1	1
1	A	142	VAL	CA-C-O	-6.96	112.08	120.78	1	1
1	A	175	MET	CA-CB-CG	-6.96	100.18	114.10	1	2
1	A	204	SER	CA-C-O	6.96	129.47	121.47	1	1
1	A	70	HIS	N-CA-CB	-6.95	99.87	110.16	19	1
1	A	83	ILE	CB-CG1-CD1	6.95	128.39	113.80	19	1
1	A	75	LYS	CB-CA-C	6.92	124.20	110.42	20	3
1	A	46	ILE	CB-CA-C	6.92	122.09	110.95	19	1
1	A	183	GLN	CG-CD-NE2	6.91	126.77	116.40	20	2
1	A	57	GLN	CG-CD-NE2	6.91	126.77	116.40	20	1
1	A	41	VAL	O-C-N	-6.91	113.93	122.57	19	1
1	A	35	PHE	CD1-CE1-CZ	-6.90	107.58	120.00	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	THR	CA-CB-OG1	6.90	119.95	109.60	19	1
1	A	207	THR	N-CA-CB	-6.90	98.83	110.49	20	1
1	A	173	ILE	CB-CG1-CD1	6.90	128.29	113.80	19	1
1	A	157	VAL	N-CA-C	6.89	121.48	113.42	19	2
1	A	134	HIS	ND1-CE1-NE2	-6.89	101.51	108.40	19	1
1	A	21	LEU	CA-C-N	-6.89	110.71	120.49	1	1
1	A	21	LEU	C-N-CA	-6.89	110.71	120.49	1	1
1	A	76	LEU	O-C-N	6.89	130.03	122.11	1	1
1	A	13	ASN	N-CA-C	6.87	125.44	110.80	1	1
1	A	141	SER	O-C-N	-6.86	115.13	122.19	19	1
1	A	127	PHE	O-C-N	-6.86	113.43	121.32	20	1
1	A	71	LEU	CD1-CG-CD2	-6.85	95.74	110.80	1	1
1	A	145	GLU	CB-CG-CD	6.84	124.22	112.60	1	1
1	A	15	VAL	N-CA-C	6.82	123.53	109.34	20	1
1	A	33	ILE	CA-C-O	-6.82	114.32	121.41	1	1
1	A	153	SER	CA-CB-OG	6.81	124.73	111.10	19	1
1	A	54	ALA	CA-C-N	6.80	133.22	122.74	19	1
1	A	54	ALA	C-N-CA	6.80	133.22	122.74	19	1
1	A	33	ILE	N-CA-C	-6.79	103.17	110.23	1	1
1	A	188	LEU	O-C-N	-6.78	112.78	122.41	1	1
1	A	145	GLU	N-CA-CB	-6.76	100.22	110.91	19	1
1	A	151	PHE	CD1-CG-CD2	6.75	128.73	118.60	19	1
1	A	79	LYS	CA-C-N	6.75	128.28	119.84	19	1
1	A	79	LYS	C-N-CA	6.75	128.28	119.84	19	1
1	A	62	ASN	N-CA-C	6.74	121.10	112.34	1	2
1	A	139	PRO	CB-CA-C	-6.73	102.71	110.92	20	1
1	A	189	HIS	N-CA-CB	-6.72	98.89	109.51	20	1
1	A	37	VAL	CA-C-O	-6.72	111.10	119.43	19	1
1	A	39	GLY	CA-C-N	6.70	132.13	122.21	19	2
1	A	39	GLY	C-N-CA	6.70	132.13	122.21	19	2
1	A	203	PHE	CD1-CE1-CZ	-6.70	107.94	120.00	19	1
1	A	136	SER	CA-C-N	6.69	134.33	121.54	20	1
1	A	136	SER	C-N-CA	6.69	134.33	121.54	20	1
1	A	18	VAL	CA-CB-CG2	-6.69	99.02	110.40	1	2
1	A	35	PHE	CA-C-N	6.69	137.20	121.82	20	1
1	A	35	PHE	C-N-CA	6.69	137.20	121.82	20	1
1	A	21	LEU	CB-CG-CD1	6.68	130.75	110.70	1	1
1	A	76	LEU	N-CA-CB	-6.68	99.66	109.82	20	2
1	A	66	LEU	CB-CG-CD2	-6.67	90.68	110.70	1	1
1	A	15	VAL	CA-CB-CG2	6.66	121.73	110.40	20	1
1	A	169	LYS	CA-C-O	6.66	126.14	118.55	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	VAL	O-C-N	6.65	131.10	122.26	19	2
1	A	86	SER	CB-CA-C	-6.65	100.08	114.10	19	2
1	A	55	LEU	CA-C-N	6.64	132.15	123.11	1	2
1	A	55	LEU	C-N-CA	6.64	132.15	123.11	1	2
1	A	64	ALA	N-CA-CB	-6.64	99.72	109.82	19	1
1	A	89	GLN	CA-C-N	6.63	134.21	121.54	19	2
1	A	89	GLN	C-N-CA	6.63	134.21	121.54	19	2
1	A	162	LYS	O-C-N	-6.63	114.61	122.96	1	1
1	A	60	ASP	N-CA-CB	6.63	121.69	110.49	20	1
1	A	29	GLN	CG-CD-NE2	6.62	126.33	116.40	19	1
1	A	161	PHE	N-CA-CB	6.62	121.76	110.57	1	1
1	A	127	PHE	CB-CA-C	6.61	123.19	110.17	1	1
1	A	105	LYS	O-C-N	6.60	131.37	122.59	1	1
1	A	203	PHE	CA-CB-CG	6.60	120.40	113.80	1	1
1	A	90	ASN	OD1-CG-ND2	6.59	129.19	122.60	19	2
1	A	52	GLU	CB-CA-C	6.59	120.69	111.86	1	2
1	A	158	VAL	N-CA-C	6.58	123.04	109.34	1	2
1	A	137	ASN	O-C-N	-6.58	113.84	122.59	1	2
1	A	176	GLY	O-C-N	-6.58	115.86	122.18	20	1
1	A	202	SER	CB-CA-C	-6.58	100.22	114.10	1	1
1	A	204	SER	N-CA-C	6.57	120.20	110.48	1	1
1	A	170	MET	N-CA-CB	6.56	119.74	109.83	19	1
1	A	176	GLY	N-CA-C	-6.56	104.89	112.50	20	1
1	A	73	GLY	CA-C-N	6.55	132.60	121.14	20	1
1	A	73	GLY	C-N-CA	6.55	132.60	121.14	20	1
1	A	183	GLN	CB-CA-C	-6.54	97.78	110.46	19	2
1	A	104	THR	CA-C-O	6.53	129.53	121.89	20	1
1	A	15	VAL	CA-CB-CG1	-6.53	99.30	110.40	19	1
1	A	53	ASN	N-CA-C	6.53	119.03	108.32	20	1
1	A	81	ILE	N-CA-C	6.52	117.58	110.21	15	4
1	A	140	PRO	CA-C-O	-6.52	108.73	120.60	1	1
1	A	150	LEU	N-CA-CB	6.52	119.52	110.07	1	1
1	A	52	GLU	O-C-N	6.52	128.91	122.19	19	2
1	A	46	ILE	CG1-CB-CG2	6.50	130.19	110.70	19	1
1	A	133	LEU	CA-CB-CG	6.50	139.03	116.30	19	1
1	A	137	ASN	CA-C-N	6.50	134.15	122.13	19	1
1	A	137	ASN	C-N-CA	6.50	134.15	122.13	19	1
1	A	176	GLY	CA-C-N	6.49	133.00	122.29	1	1
1	A	176	GLY	C-N-CA	6.49	133.00	122.29	1	1
1	A	198	HIS	N-CA-CB	-6.49	100.50	110.04	1	1
1	A	140	PRO	CA-C-N	6.49	129.50	120.29	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	140	PRO	C-N-CA	6.49	129.50	120.29	20	1
1	A	141	SER	N-CA-C	6.49	118.43	111.36	20	1
1	A	60	ASP	CB-CA-C	-6.49	97.51	110.42	20	1
1	A	107	TYR	CB-CA-C	6.47	123.30	110.42	20	2
1	A	148	LYS	N-CA-CB	6.47	119.45	110.07	1	1
1	A	191	HIS	N-CA-CB	6.45	121.39	110.49	1	1
1	A	203	PHE	CB-CA-C	-6.45	100.28	110.79	1	1
1	A	166	LYS	N-CA-C	6.45	124.53	110.80	19	1
1	A	69	SER	N-CA-C	6.44	119.29	111.82	1	1
1	A	170	MET	CA-C-N	6.44	133.41	121.62	20	1
1	A	170	MET	C-N-CA	6.44	133.41	121.62	20	1
1	A	161	PHE	CA-C-N	6.44	132.66	122.36	1	1
1	A	161	PHE	C-N-CA	6.44	132.66	122.36	1	1
1	A	25	ARG	O-C-N	6.42	130.68	122.39	19	1
1	A	129	PRO	N-CD-CG	6.42	112.83	103.20	19	1
1	A	83	ILE	N-CA-CB	6.41	117.52	110.53	19	1
1	A	54	ALA	N-CA-C	6.41	118.85	108.34	1	1
1	A	53	ASN	CA-C-N	6.41	131.81	122.77	1	1
1	A	53	ASN	C-N-CA	6.41	131.81	122.77	1	1
1	A	80	PRO	O-C-N	-6.41	113.99	122.64	1	1
1	A	55	LEU	CD1-CG-CD2	6.41	124.90	110.80	19	1
1	A	34	LEU	N-CA-C	-6.41	104.38	111.36	1	1
1	A	187	ASP	CB-CG-OD1	-6.40	103.68	118.40	1	1
1	A	40	ASP	CA-C-N	-6.40	110.45	121.97	1	1
1	A	40	ASP	C-N-CA	-6.40	110.45	121.97	1	1
1	A	91	VAL	CA-CB-CG1	6.39	121.26	110.40	20	2
1	A	186	ILE	CB-CG1-CD1	-6.39	100.39	113.80	1	2
1	A	205	LYS	CB-CG-CD	6.38	125.98	111.30	19	1
1	A	57	GLN	CA-CB-CG	-6.38	101.34	114.10	1	1
1	A	187	ASP	O-C-N	-6.38	114.10	122.59	19	1
1	A	45	LYS	CA-C-O	-6.38	113.33	120.66	19	1
1	A	106	ASP	O-C-N	6.38	130.73	123.27	19	1
1	A	77	HIS	ND1-CG-CD2	6.36	112.46	106.10	19	2
1	A	164	PHE	CG-CD1-CE1	-6.35	109.91	120.70	19	1
1	A	35	PHE	O-C-N	-6.34	115.40	122.12	1	1
1	A	193	LEU	O-C-N	-6.34	115.44	122.03	1	1
1	A	150	LEU	CB-CG-CD2	-6.33	91.71	110.70	1	1
1	A	69	SER	N-CA-CB	6.33	119.97	110.22	20	1
1	A	170	MET	CA-C-O	-6.32	114.24	121.19	19	2
1	A	45	LYS	CA-C-N	6.32	132.15	122.68	19	5
1	A	45	LYS	C-N-CA	6.32	132.15	122.68	19	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	180	GLU	CB-CG-CD	6.31	123.33	112.60	1	1
1	A	70	HIS	ND1-CG-CD2	-6.30	99.80	106.10	1	1
1	A	80	PRO	CB-CA-C	6.30	121.96	111.56	19	1
1	A	152	SER	N-CA-CB	-6.30	101.49	110.81	20	1
1	A	204	SER	O-C-N	-6.30	115.84	122.96	1	1
1	A	13	ASN	CA-CB-CG	-6.29	106.31	112.60	19	2
1	A	25	ARG	NE-CZ-NH2	6.29	124.86	119.20	1	1
1	A	157	VAL	O-C-N	-6.29	114.71	122.57	20	1
1	A	148	LYS	CA-C-O	-6.28	111.53	120.51	19	2
1	A	161	PHE	O-C-N	6.28	130.42	123.52	20	1
1	A	52	GLU	N-CA-C	-6.27	104.26	112.41	20	1
1	A	190	ASN	CA-C-N	6.26	133.50	121.54	1	2
1	A	190	ASN	C-N-CA	6.26	133.50	121.54	1	2
1	A	88	HIS	N-CA-CB	-6.26	99.94	110.83	19	1
1	A	173	ILE	O-C-N	-6.26	116.46	123.03	20	1
1	A	198	HIS	CB-CA-C	6.25	120.81	109.62	1	1
1	A	53	ASN	CB-CG-OD1	-6.25	108.30	120.80	20	2
1	A	171	ALA	CA-C-O	-6.24	114.55	121.23	20	1
1	A	189	HIS	ND1-CG-CD2	6.23	112.33	106.10	19	2
1	A	141	SER	CA-C-N	6.22	133.17	121.97	1	2
1	A	141	SER	C-N-CA	6.22	133.17	121.97	1	2
1	A	204	SER	CA-C-N	6.22	131.26	120.68	1	1
1	A	204	SER	C-N-CA	6.22	131.26	120.68	1	1
1	A	58	MET	CB-CA-C	6.20	121.85	111.30	19	2
1	A	189	HIS	CG-ND1-CE1	-6.20	98.76	109.30	1	2
1	A	184	ALA	N-CA-C	6.19	119.67	111.75	1	1
1	A	182	VAL	CA-C-O	-6.17	113.61	120.46	19	1
1	A	159	LYS	CA-CB-CG	-6.17	101.77	114.10	19	1
1	A	69	SER	CA-CB-OG	6.16	123.41	111.10	1	1
1	A	27	THR	CA-C-O	-6.15	113.79	119.76	20	2
1	A	68	MET	CG-SD-CE	-6.15	87.37	100.90	1	1
1	A	126	ILE	CA-CB-CG1	-6.15	99.95	110.40	20	3
1	A	89	GLN	CA-CB-CG	6.15	126.39	114.10	19	1
1	A	67	ALA	N-CA-CB	6.14	118.88	109.91	19	1
1	A	136	SER	CA-C-O	6.14	128.22	121.40	20	1
1	A	126	ILE	N-CA-CB	-6.13	101.02	112.36	19	1
1	A	179	GLU	CG-CD-OE1	6.12	132.49	118.40	1	1
1	A	134	HIS	CB-CG-ND1	6.12	131.88	122.70	19	1
1	A	25	ARG	CA-C-N	-6.12	113.22	121.66	1	1
1	A	25	ARG	C-N-CA	-6.12	113.22	121.66	1	1
1	A	70	HIS	CB-CA-C	-6.10	98.78	109.02	20	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	88	HIS	ND1-CE1-NE2	-6.09	102.31	108.40	20	2
1	A	137	ASN	CA-C-O	6.09	129.22	120.51	19	1
1	A	63	GLN	OE1-CD-NE2	-6.09	116.51	122.60	1	1
1	A	82	ARG	CA-CB-CG	6.09	126.27	114.10	1	1
1	A	45	LYS	N-CA-CB	-6.09	100.96	111.55	10	4
1	A	13	ASN	O-C-N	-6.08	113.55	122.43	19	2
1	A	59	ALA	N-CA-CB	-6.08	100.21	110.49	19	1
1	A	46	ILE	N-CA-C	6.08	117.23	108.48	1	1
1	A	89	GLN	CB-CG-CD	6.08	122.93	112.60	1	1
1	A	46	ILE	O-C-N	-6.08	116.66	122.98	19	1
1	A	28	PRO	CA-C-N	-6.07	112.14	120.28	20	1
1	A	28	PRO	C-N-CA	-6.07	112.14	120.28	20	1
1	A	142	VAL	CG1-CB-CG2	6.07	124.16	110.80	20	1
1	A	90	ASN	N-CA-C	6.07	123.73	110.80	20	2
1	A	191	HIS	O-C-N	6.07	130.66	122.59	1	1
1	A	34	LEU	CA-C-N	6.06	128.40	120.28	1	1
1	A	34	LEU	C-N-CA	6.06	128.40	120.28	1	1
1	A	160	GLY	N-CA-C	-6.06	100.23	111.14	19	1
1	A	46	ILE	N-CA-CB	-6.06	104.46	112.34	4	3
1	A	129	PRO	CA-C-O	-6.05	114.91	121.27	20	1
1	A	175	MET	CA-C-O	6.05	129.17	120.51	1	1
1	A	179	GLU	N-CA-C	6.04	117.95	111.36	19	1
1	A	151	PHE	CG-CD1-CE1	-6.04	110.43	120.70	19	1
1	A	154	ASN	CA-CB-CG	6.04	118.64	112.60	19	1
1	A	28	PRO	CB-CA-C	-6.04	102.80	112.21	1	1
1	A	172	LEU	O-C-N	-6.02	115.89	123.17	19	2
1	A	151	PHE	CD1-CE1-CZ	-6.02	109.17	120.00	20	1
1	A	15	VAL	CA-C-O	-6.01	113.27	120.78	1	1
1	A	21	LEU	CA-C-O	5.99	129.50	121.89	19	2
1	A	47	LEU	CB-CG-CD2	5.97	128.61	110.70	19	2
1	A	72	ASN	CA-C-N	5.96	130.86	122.63	3	4
1	A	72	ASN	C-N-CA	5.96	130.86	122.63	3	4
1	A	137	ASN	CA-CB-CG	-5.96	106.64	112.60	19	1
1	A	90	ASN	N-CA-CB	-5.95	101.37	111.31	1	1
1	A	146	ASP	CA-C-N	5.95	132.91	121.54	19	1
1	A	146	ASP	C-N-CA	5.95	132.91	121.54	19	1
1	A	38	TYR	CD1-CG-CD2	-5.95	109.17	118.10	1	1
1	A	187	ASP	OD1-CG-OD2	-5.95	108.62	122.90	19	1
1	A	63	GLN	CA-C-O	-5.95	114.78	120.90	1	1
1	A	131	ALA	CA-C-O	5.94	126.68	119.31	19	1
1	A	139	PRO	CA-C-O	-5.94	111.95	120.56	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	126	ILE	CA-C-N	5.93	136.28	121.80	1	1
1	A	126	ILE	C-N-CA	5.93	136.28	121.80	1	1
1	A	174	GLN	N-CA-CB	5.93	120.15	110.37	19	1
1	A	81	ILE	CB-CG1-CD1	5.92	126.23	113.80	1	1
1	A	180	GLU	N-CA-CB	5.91	119.50	110.39	1	1
1	A	66	LEU	N-CA-CB	5.91	118.55	109.91	20	1
1	A	174	GLN	CA-CB-CG	-5.91	102.28	114.10	20	1
1	A	167	ASP	O-C-N	-5.91	114.73	122.59	1	2
1	A	72	ASN	CA-CB-CG	5.91	118.51	112.60	19	1
1	A	191	HIS	CB-CG-ND1	-5.90	113.85	122.70	19	1
1	A	77	HIS	O-C-N	5.89	130.25	122.36	20	1
1	A	26	VAL	CA-CB-CG2	5.87	120.39	110.40	1	1
1	A	165	GLN	CB-CA-C	5.87	119.46	109.72	1	1
1	A	81	ILE	CA-C-O	-5.87	113.45	120.78	19	1
1	A	81	ILE	CA-CB-CG2	5.85	120.45	110.50	1	1
1	A	179	GLU	CA-C-N	5.85	129.84	121.71	1	1
1	A	179	GLU	C-N-CA	5.85	129.84	121.71	1	1
1	A	77	HIS	CB-CG-ND1	5.84	131.47	122.70	1	1
1	A	33	ILE	CB-CA-C	5.84	119.45	111.97	19	1
1	A	52	GLU	OE1-CD-OE2	-5.84	108.89	122.90	1	1
1	A	105	LYS	CA-CB-CG	5.84	125.78	114.10	20	1
1	A	198	HIS	CB-CG-CD2	-5.84	123.61	131.20	19	1
1	A	62	ASN	CB-CG-OD1	-5.83	109.14	120.80	20	2
1	A	126	ILE	CA-CB-CG2	-5.83	100.59	110.50	19	1
1	A	18	VAL	CB-CA-C	-5.83	101.74	111.29	1	2
1	A	131	ALA	N-CA-C	-5.82	105.67	112.89	19	1
1	A	148	LYS	CA-C-N	5.82	127.89	120.56	8	6
1	A	148	LYS	C-N-CA	5.82	127.89	120.56	8	6
1	A	134	HIS	CG-CD2-NE2	5.81	113.01	107.20	1	1
1	A	182	VAL	N-CA-C	-5.80	105.43	111.58	19	1
1	A	90	ASN	CB-CG-OD1	5.80	132.40	120.80	1	1
1	A	191	HIS	CA-C-O	-5.80	112.22	120.51	1	1
1	A	90	ASN	O-C-N	-5.79	114.89	122.59	19	1
1	A	135	LEU	N-CA-C	5.78	118.19	109.23	19	1
1	A	34	LEU	CB-CG-CD2	5.77	128.01	110.70	1	1
1	A	77	HIS	CG-ND1-CE1	-5.76	99.50	109.30	20	2
1	A	13	ASN	CA-C-O	-5.76	111.73	119.11	19	1
1	A	203	PHE	CA-C-N	5.76	133.06	122.92	20	1
1	A	203	PHE	C-N-CA	5.76	133.06	122.92	20	1
1	A	152	SER	N-CA-C	5.76	118.77	111.69	19	1
1	A	127	PHE	CA-C-O	-5.73	112.30	120.16	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	169	LYS	N-CA-C	-5.73	98.59	110.80	1	1
1	A	172	LEU	N-CA-CB	-5.73	101.72	111.69	19	1
1	A	27	THR	CA-CB-OG1	-5.71	101.03	109.60	1	1
1	A	88	HIS	CA-C-O	5.71	126.87	120.70	19	2
1	A	177	SER	O-C-N	-5.71	117.31	123.42	19	1
1	A	188	LEU	CB-CA-C	5.71	122.37	110.32	19	1
1	A	175	MET	O-C-N	-5.71	115.63	122.65	20	1
1	A	198	HIS	ND1-CG-CD2	5.67	111.77	106.10	20	1
1	A	87	LYS	O-C-N	-5.67	116.33	121.89	20	1
1	A	153	SER	N-CA-CB	5.67	119.93	110.41	20	1
1	A	145	GLU	CA-CB-CG	-5.67	102.77	114.10	19	1
1	A	90	ASN	CA-C-O	5.65	128.59	120.51	19	1
1	A	136	SER	N-CA-C	5.65	116.85	108.60	19	1
1	A	203	PHE	CD1-CG-CD2	5.64	127.06	118.60	20	1
1	A	106	ASP	N-CA-CB	-5.63	101.93	110.77	19	1
1	A	151	PHE	CG-CD2-CE2	-5.63	111.13	120.70	19	1
1	A	70	HIS	CA-C-N	5.62	128.86	120.31	19	1
1	A	70	HIS	C-N-CA	5.62	128.86	120.31	19	1
1	A	145	GLU	O-C-N	-5.62	115.41	122.20	1	1
1	A	84	THR	CA-C-N	5.61	133.09	123.05	1	1
1	A	84	THR	C-N-CA	5.61	133.09	123.05	1	1
1	A	194	GLY	N-CA-C	5.61	122.82	115.47	13	1
1	A	141	SER	CA-C-O	-5.61	111.81	120.16	1	1
1	A	38	TYR	N-CA-CB	-5.61	102.41	110.65	19	1
1	A	64	ALA	CA-C-O	5.60	126.67	120.63	1	1
1	A	168	ARG	N-CA-CB	-5.60	103.50	111.84	19	1
1	A	142	VAL	CB-CA-C	-5.59	105.44	111.59	19	2
1	A	19	SER	CA-C-N	5.58	132.21	121.54	20	1
1	A	19	SER	C-N-CA	5.58	132.21	121.54	20	1
1	A	28	PRO	N-CA-CB	5.58	109.11	103.25	19	1
1	A	184	ALA	CA-C-O	5.58	126.40	120.10	19	2
1	A	151	PHE	N-CA-CB	-5.58	101.07	110.49	1	1
1	A	200	ARG	CA-C-N	5.57	131.76	122.57	19	1
1	A	200	ARG	C-N-CA	5.57	131.76	122.57	19	1
1	A	76	LEU	CA-C-N	-5.57	112.79	122.36	20	1
1	A	76	LEU	C-N-CA	-5.57	112.79	122.36	20	1
1	A	74	HIS	ND1-CE1-NE2	5.55	113.95	108.40	1	1
1	A	200	ARG	NE-CZ-NH2	-5.55	114.21	119.20	20	1
1	A	38	TYR	CA-CB-CG	-5.55	103.92	113.90	1	1
1	A	44	VAL	CA-CB-CG1	5.54	119.82	110.40	1	1
1	A	191	HIS	CA-C-N	5.54	132.12	121.54	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	191	HIS	C-N-CA	5.54	132.12	121.54	1	3
1	A	198	HIS	N-CA-C	-5.53	102.82	110.35	1	1
1	A	87	LYS	CA-C-O	5.53	126.45	119.98	19	1
1	A	62	ASN	CA-C-O	5.53	126.14	119.61	1	1
1	A	57	GLN	CB-CA-C	5.52	118.95	110.62	19	1
1	A	206	SER	N-CA-C	5.52	119.09	110.32	19	2
1	A	202	SER	N-CA-C	5.52	115.31	108.19	1	1
1	A	165	GLN	CA-C-N	5.52	132.08	121.54	2	4
1	A	165	GLN	C-N-CA	5.52	132.08	121.54	2	4
1	A	77	HIS	ND1-CE1-NE2	5.51	113.91	108.40	20	1
1	A	130	SER	N-CA-C	5.49	117.53	109.24	19	1
1	A	71	LEU	O-C-N	5.49	127.94	122.12	20	1
1	A	27	THR	OG1-CB-CG2	-5.48	98.34	109.30	20	1
1	A	82	ARG	CG-CD-NE	-5.47	99.97	112.00	1	1
1	A	55	LEU	N-CA-C	5.47	117.55	108.20	1	1
1	A	164	PHE	CA-C-N	5.47	131.98	121.54	10	2
1	A	164	PHE	C-N-CA	5.47	131.98	121.54	10	2
1	A	72	ASN	CB-CG-OD1	5.46	131.72	120.80	1	2
1	A	166	LYS	CA-C-O	-5.46	112.71	120.51	1	1
1	A	134	HIS	O-C-N	5.45	129.06	122.85	19	1
1	A	150	LEU	CB-CA-C	-5.45	102.30	110.90	1	2
1	A	44	VAL	CA-C-O	5.45	125.77	120.27	1	1
1	A	72	ASN	CB-CA-C	5.44	121.25	110.42	20	1
1	A	79	LYS	CB-CA-C	5.44	116.21	108.76	11	2
1	A	74	HIS	CE1-NE2-CD2	-5.44	103.56	109.00	20	2
1	A	174	GLN	CA-C-N	5.43	131.91	121.54	19	1
1	A	174	GLN	C-N-CA	5.43	131.91	121.54	19	1
1	A	179	GLU	O-C-N	5.42	128.33	122.15	19	1
1	A	91	VAL	N-CA-CB	-5.42	103.88	111.25	1	1
1	A	199	LEU	CA-C-N	5.42	130.63	122.99	1	1
1	A	199	LEU	C-N-CA	5.42	130.63	122.99	1	1
1	A	172	LEU	CB-CG-CD2	5.41	126.94	110.70	20	1
1	A	203	PHE	CG-CD1-CE1	-5.41	111.51	120.70	20	1
1	A	161	PHE	N-CA-C	-5.41	100.30	108.52	19	1
1	A	179	GLU	CA-C-O	5.40	128.23	120.51	1	1
1	A	207	THR	CA-C-N	5.40	131.42	121.70	20	1
1	A	207	THR	C-N-CA	5.40	131.42	121.70	20	1
1	A	200	ARG	CB-CA-C	5.39	119.66	109.37	20	1
1	A	23	PRO	CB-CA-C	-5.38	102.68	111.56	1	1
1	A	82	ARG	CA-C-N	5.38	129.31	122.37	17	1
1	A	82	ARG	C-N-CA	5.38	129.31	122.37	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	173	ILE	CG1-CB-CG2	-5.38	94.57	110.70	19	1
1	A	149	VAL	CG1-CB-CG2	-5.38	98.97	110.80	20	1
1	A	64	ALA	CA-C-N	5.37	131.80	121.54	19	1
1	A	64	ALA	C-N-CA	5.37	131.80	121.54	19	1
1	A	164	PHE	CD1-CG-CD2	5.37	126.66	118.60	1	1
1	A	58	MET	CA-C-N	5.37	131.80	121.54	19	2
1	A	58	MET	C-N-CA	5.37	131.80	121.54	19	2
1	A	173	ILE	CA-CB-CG2	5.37	119.63	110.50	19	1
1	A	70	HIS	CG-ND1-CE1	-5.37	100.17	109.30	19	1
1	A	89	GLN	N-CA-C	5.36	122.22	110.80	1	1
1	A	143	SER	CA-C-N	5.36	127.78	120.54	20	1
1	A	143	SER	C-N-CA	5.36	127.78	120.54	20	1
1	A	182	VAL	CB-CA-C	-5.36	102.51	111.29	20	1
1	A	26	VAL	CB-CA-C	-5.35	104.19	111.15	1	1
1	A	40	ASP	CB-CA-C	-5.35	103.78	111.91	19	1
1	A	128	PRO	CB-CA-C	5.35	117.44	110.92	20	1
1	A	195	GLU	CG-CD-OE1	-5.35	106.10	118.40	1	1
1	A	208	ILE	CA-CB-CG1	5.35	119.49	110.40	1	1
1	A	189	HIS	CB-CA-C	5.34	119.06	110.29	1	1
1	A	20	ASN	CB-CA-C	5.34	115.12	109.83	15	2
1	A	36	GLY	O-C-N	-5.34	114.66	122.19	1	1
1	A	21	LEU	CB-CA-C	5.34	121.05	110.42	20	1
1	A	194	GLY	CA-C-N	5.33	127.96	120.28	20	2
1	A	194	GLY	C-N-CA	5.33	127.96	120.28	20	2
1	A	17	LEU	CD1-CG-CD2	5.32	122.51	110.80	1	1
1	A	33	ILE	CA-CB-CG1	-5.32	101.36	110.40	1	1
1	A	142	VAL	N-CA-CB	-5.31	102.46	111.23	1	1
1	A	35	PHE	CB-CG-CD2	-5.31	111.67	120.70	20	1
1	A	91	VAL	O-C-N	5.31	128.75	123.18	1	1
1	A	23	PRO	CB-CG-CD	-5.30	89.14	106.10	20	1
1	A	185	LEU	CD1-CG-CD2	-5.30	99.14	110.80	19	1
1	A	158	VAL	CB-CA-C	-5.29	102.61	111.29	1	2
1	A	72	ASN	CB-CG-ND2	5.29	124.34	116.40	19	1
1	A	85	LEU	N-CA-CB	-5.28	102.57	110.17	19	1
1	A	107	TYR	CD1-CG-CD2	5.28	126.02	118.10	19	1
1	A	200	ARG	NH1-CZ-NH2	-5.27	112.45	119.30	20	1
1	A	68	MET	CB-CG-SD	5.26	128.48	112.70	1	1
1	A	198	HIS	CG-ND1-CE1	-5.26	100.36	109.30	19	1
1	A	192	ASP	OD1-CG-OD2	-5.25	110.29	122.90	1	1
1	A	67	ALA	O-C-N	5.25	128.15	122.11	20	1
1	A	203	PHE	O-C-N	5.25	129.21	123.22	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	135	LEU	CB-CA-C	-5.25	97.91	109.56	19	1
1	A	145	GLU	CG-CD-OE1	5.24	130.46	118.40	19	1
1	A	190	ASN	CB-CA-C	5.24	120.86	110.42	19	1
1	A	180	GLU	CA-C-N	5.24	127.56	120.38	20	1
1	A	180	GLU	C-N-CA	5.24	127.56	120.38	20	1
1	A	75	LYS	O-C-N	5.24	129.56	122.59	19	1
1	A	182	VAL	CA-C-N	5.24	127.56	120.44	20	1
1	A	182	VAL	C-N-CA	5.24	127.56	120.44	20	1
1	A	55	LEU	CA-CB-CG	5.23	134.59	116.30	1	1
1	A	26	VAL	CA-C-N	5.22	133.90	123.56	1	1
1	A	26	VAL	C-N-CA	5.22	133.90	123.56	1	1
1	A	40	ASP	CB-CG-OD1	5.22	130.41	118.40	1	1
1	A	197	HIS	CB-CG-ND1	-5.22	114.88	122.70	19	1
1	A	18	VAL	CA-CB-CG1	5.21	119.26	110.40	1	1
1	A	208	ILE	N-CA-CB	-5.21	102.64	111.50	20	1
1	A	53	ASN	CA-C-O	5.21	127.62	121.58	19	1
1	A	32	PHE	CA-C-N	5.21	131.35	121.97	20	1
1	A	32	PHE	C-N-CA	5.21	131.35	121.97	20	1
1	A	29	GLN	CB-CA-C	5.20	119.42	110.79	20	1
1	A	153	SER	O-C-N	-5.20	114.84	122.43	20	1
1	A	145	GLU	N-CA-C	5.19	119.24	113.01	20	1
1	A	29	GLN	CA-CB-CG	5.19	124.48	114.10	19	1
1	A	47	LEU	O-C-N	-5.19	116.42	122.96	20	1
1	A	203	PHE	N-CA-C	-5.18	100.86	109.46	19	1
1	A	164	PHE	N-CA-CB	-5.17	101.75	110.49	1	1
1	A	80	PRO	CA-C-O	5.17	130.01	120.60	19	1
1	A	89	GLN	O-C-N	-5.17	115.36	122.23	20	1
1	A	198	HIS	CA-C-O	5.17	126.58	120.69	20	1
1	A	26	VAL	CA-CB-CG1	5.16	119.18	110.40	1	1
1	A	149	VAL	CA-CB-CG2	-5.15	101.65	110.40	20	1
1	A	57	GLN	N-CA-C	-5.14	99.41	108.20	1	1
1	A	30	SER	CA-C-N	5.13	127.43	120.65	3	1
1	A	30	SER	C-N-CA	5.13	127.43	120.65	3	1
1	A	41	VAL	CB-CA-C	5.13	117.77	111.25	10	3
1	A	25	ARG	N-CA-C	-5.13	105.32	112.45	1	1
1	A	172	LEU	CA-C-N	5.13	129.79	121.95	19	1
1	A	172	LEU	C-N-CA	5.13	129.79	121.95	19	1
1	A	159	LYS	N-CA-C	5.12	119.53	113.12	19	1
1	A	13	ASN	CB-CG-OD1	5.12	131.03	120.80	1	1
1	A	184	ALA	CA-C-N	5.12	131.31	121.54	1	1
1	A	184	ALA	C-N-CA	5.12	131.31	121.54	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	27	THR	N-CA-C	5.11	112.82	108.22	19	1
1	A	79	LYS	CG-CD-CE	-5.11	99.55	111.30	1	1
1	A	88	HIS	N-CA-C	5.11	117.44	110.55	20	1
1	A	163	PHE	CA-C-O	-5.10	115.14	120.80	20	1
1	A	132	THR	CA-C-O	5.09	125.75	120.40	20	2
1	A	165	GLN	CA-C-O	5.09	127.79	120.51	19	1
1	A	134	HIS	ND1-CG-CD2	5.09	111.19	106.10	19	1
1	A	22	ASN	N-CA-C	-5.09	98.48	109.01	20	1
1	A	135	LEU	CD1-CG-CD2	-5.08	99.62	110.80	19	1
1	A	40	ASP	O-C-N	-5.08	117.01	123.01	20	1
1	A	129	PRO	CB-CA-C	5.08	118.32	111.71	20	1
1	A	75	LYS	N-CA-C	5.07	121.61	110.80	19	1
1	A	59	ALA	CB-CA-C	5.06	119.19	110.79	1	1
1	A	165	GLN	CG-CD-OE1	-5.05	110.70	120.80	1	1
1	A	165	GLN	O-C-N	5.05	129.08	122.87	1	1
1	A	179	GLU	CG-CD-OE2	-5.05	106.79	118.40	1	1
1	A	168	ARG	NE-CZ-NH1	5.04	126.54	121.50	19	1
1	A	46	ILE	CB-CG1-CD1	-5.04	103.22	113.80	1	1
1	A	207	THR	CA-CB-CG2	5.03	119.05	110.50	19	1
1	A	158	VAL	CA-CB-CG1	5.03	118.95	110.40	19	1
1	A	178	VAL	N-CA-C	5.02	115.24	110.42	1	1
1	A	71	LEU	CB-CA-C	-5.02	102.40	110.74	1	1
1	A	26	VAL	O-C-N	5.02	128.77	122.59	20	1
1	A	68	MET	CA-C-N	5.02	127.26	120.38	17	1
1	A	68	MET	C-N-CA	5.02	127.26	120.38	17	1
1	A	196	ASN	CB-CG-ND2	-5.02	108.87	116.40	19	1
1	A	104	THR	N-CA-C	5.01	117.17	110.35	7	1
1	A	174	GLN	CG-CD-OE1	5.01	130.82	120.80	1	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	38	TYR	Sidechain	3
1	A	70	HIS	Mainchain,Sidechain	3
1	A	74	HIS	Sidechain,Mainchain	3
1	A	77	HIS	Sidechain	3
1	A	163	PHE	Sidechain,Mainchain	3
1	A	200	ARG	Sidechain	3
1	A	25	ARG	Mainchain,Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	32	PHE	Mainchain,Sidechain	2
1	A	53	ASN	Sidechain	2
1	A	60	ASP	Mainchain	2
1	A	82	ARG	Sidechain	2
1	A	86	SER	Mainchain	2
1	A	104	THR	Mainchain	2
1	A	127	PHE	Sidechain	2
1	A	134	HIS	Sidechain	2
1	A	137	ASN	Mainchain	2
1	A	159	LYS	Mainchain	2
1	A	161	PHE	Sidechain	2
1	A	179	GLU	Sidechain,Mainchain	2
1	A	181	ALA	Mainchain	2
1	A	185	LEU	Mainchain	2
1	A	189	HIS	Sidechain,Mainchain	2
1	A	191	HIS	Sidechain	2
1	A	197	HIS	Sidechain	2
1	A	43	ARG	Sidechain	2
1	A	79	LYS	Mainchain	2
1	A	107	TYR	Sidechain	2
1	A	128	PRO	Peptide,Mainchain	2
1	A	133	LEU	Mainchain	2
1	A	151	PHE	Mainchain,Sidechain	2
1	A	168	ARG	Sidechain,Mainchain	2
1	A	206	SER	Mainchain	2
1	A	13	ASN	Mainchain	1
1	A	14	SER	Mainchain	1
1	A	36	GLY	Mainchain	1
1	A	47	LEU	Mainchain	1
1	A	54	ALA	Mainchain	1
1	A	55	LEU	Mainchain	1
1	A	68	MET	Mainchain	1
1	A	72	ASN	Sidechain	1
1	A	88	HIS	Sidechain	1
1	A	131	ALA	Mainchain	1
1	A	135	LEU	Mainchain	1
1	A	145	GLU	Sidechain	1
1	A	146	ASP	Sidechain	1
1	A	152	SER	Mainchain	1
1	A	158	VAL	Mainchain	1
1	A	170	MET	Mainchain	1
1	A	180	GLU	Mainchain,Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	182	VAL	Mainchain	1
1	A	186	ILE	Mainchain	1
1	A	198	HIS	Mainchain	1
1	A	18	VAL	Mainchain	1
1	A	19	SER	Mainchain	1
1	A	20	ASN	Mainchain,Sidechain	1
1	A	33	ILE	Mainchain	1
1	A	39	GLY	Mainchain	1
1	A	45	LYS	Mainchain	1
1	A	58	MET	Mainchain	1
1	A	62	ASN	Mainchain	1
1	A	78	GLY	Mainchain	1
1	A	130	SER	Mainchain	1
1	A	143	SER	Mainchain	1
1	A	149	VAL	Mainchain	1
1	A	153	SER	Mainchain	1
1	A	183	GLN	Sidechain	1
1	A	187	ASP	Sidechain	1
1	A	192	ASP	Mainchain,Sidechain	1
1	A	203	PHE	Sidechain	1
1	A	22	ASN	Sidechain	1
1	A	24	GLU	Mainchain,Sidechain	1
1	A	31	LEU	Mainchain	1
1	A	46	ILE	Mainchain	1
1	A	57	GLN	Sidechain	1
1	A	65	GLN	Mainchain	1
1	A	66	LEU	Mainchain	1
1	A	69	SER	Mainchain	1
1	A	71	LEU	Mainchain	1
1	A	87	LYS	Mainchain	1
1	A	105	LYS	Mainchain	1
1	A	157	VAL	Mainchain	1
1	A	164	PHE	Sidechain	1
1	A	165	GLN	Mainchain	1
1	A	171	ALA	Mainchain	1
1	A	188	LEU	Mainchain	1
1	A	193	LEU	Mainchain	1
1	A	195	GLU	Mainchain	1

## 6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1272	1291	1291	12±16
All	All	25440	25820	25819	237

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:A:166:LYS:CD	1:A:166:LYS:CE	1.55	1.81	1	1
1:A:58:MET:SD	1:A:58:MET:CG	1.47	2.01	19	1
1:A:170:MET:CE	1:A:170:MET:SD	1.43	2.07	1	1
1:A:140:PRO:N	1:A:140:PRO:CA	1.42	1.68	19	1
1:A:73:GLY:HA2	1:A:81:ILE:HD11	0.93	1.37	1	4
1:A:73:GLY:CA	1:A:81:ILE:HD11	0.89	1.96	1	1
1:A:34:LEU:HD12	1:A:38:TYR:CE2	0.83	2.07	19	1
1:A:81:ILE:H	1:A:81:ILE:HD13	0.79	1.38	3	4
1:A:35:PHE:O	1:A:58:MET:HE1	0.78	1.78	1	3
1:A:66:LEU:HD21	1:A:70:HIS:CD2	0.76	2.16	1	9
1:A:35:PHE:CD2	1:A:56:VAL:HG11	0.74	2.18	20	10
1:A:170:MET:CE	1:A:170:MET:CG	0.74	2.65	1	1
1:A:66:LEU:C	1:A:66:LEU:HD23	0.73	2.08	1	2
1:A:21:LEU:HD13	1:A:52:GLU:O	0.69	1.87	19	1
1:A:133:LEU:H	1:A:133:LEU:HD23	0.69	1.47	20	2
1:A:34:LEU:HD12	1:A:38:TYR:HE2	0.68	1.47	19	1
1:A:164:PHE:CE1	1:A:172:LEU:HD13	0.67	2.25	11	14
1:A:189:HIS:HB2	1:A:201:VAL:CG1	0.67	2.20	1	5
1:A:81:ILE:H	1:A:81:ILE:CD1	0.66	2.02	3	4
1:A:17:LEU:HD21	1:A:53:ASN:CG	0.65	2.16	1	1
1:A:166:LYS:CE	1:A:166:LYS:CG	0.65	2.73	1	1
1:A:45:LYS:HD3	1:A:104:THR:HG23	0.63	1.70	19	1
1:A:70:HIS:CD2	1:A:128:PRO:HA	0.63	2.29	20	1
1:A:140:PRO:N	1:A:140:PRO:C	0.62	2.52	19	1
1:A:58:MET:SD	1:A:58:MET:CB	0.62	2.86	19	1
1:A:139:PRO:C	1:A:140:PRO:CA	0.62	2.66	19	1
1:A:21:LEU:HD13	1:A:26:VAL:HG21	0.62	1.70	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:LEU:HD12	1:A:53:ASN:HB2	0.62	1.71	1	1
1:A:73:GLY:H	1:A:81:ILE:CG1	0.61	2.07	1	1
1:A:135:LEU:HD21	1:A:173:ILE:HG22	0.60	1.74	1	1
1:A:66:LEU:O	1:A:70:HIS:HB2	0.59	1.97	19	1
1:A:133:LEU:HD23	1:A:133:LEU:N	0.58	2.13	20	2
1:A:57:GLN:HE22	1:A:90:ASN:ND2	0.57	1.96	19	1
1:A:17:LEU:HD23	1:A:18:VAL:N	0.55	2.16	1	1
1:A:185:LEU:O	1:A:186:ILE:C	0.55	2.47	1	1
1:A:150:LEU:HB3	1:A:188:LEU:HD21	0.55	1.78	19	1
1:A:33:ILE:O	1:A:37:VAL:HG22	0.55	2.02	19	1
1:A:29:GLN:HA	1:A:32:PHE:HB3	0.54	1.78	19	1
1:A:36:GLY:HA2	1:A:41:VAL:H	0.54	1.62	1	1
1:A:73:GLY:HA2	1:A:81:ILE:CD1	0.54	2.22	1	1
1:A:81:ILE:HD13	1:A:81:ILE:N	0.54	2.17	20	4
1:A:159:LYS:HB2	1:A:175:MET:O	0.54	2.03	1	1
1:A:13:ASN:HD21	1:A:85:LEU:CD2	0.53	2.16	17	2
1:A:14:SER:HB3	1:A:60:ASP:HA	0.53	1.80	1	1
1:A:138:ILE:CG1	1:A:138:ILE:O	0.52	2.57	19	1
1:A:73:GLY:H	1:A:81:ILE:HG12	0.52	1.64	1	1
1:A:134:HIS:CD2	1:A:134:HIS:C	0.52	2.87	1	1
1:A:73:GLY:N	1:A:81:ILE:HD11	0.52	2.20	1	1
1:A:33:ILE:HG21	1:A:186:ILE:HG22	0.52	1.82	20	2
1:A:66:LEU:C	1:A:66:LEU:CD2	0.51	2.79	1	1
1:A:151:PHE:CE2	1:A:188:LEU:HD23	0.51	2.40	19	1
1:A:138:ILE:HD11	1:A:169:LYS:O	0.51	2.06	1	1
1:A:166:LYS:CD	1:A:166:LYS:NZ	0.50	2.65	1	1
1:A:21:LEU:HD13	1:A:26:VAL:CG2	0.50	2.36	1	1
1:A:40:ASP:N	1:A:63:GLN:OE1	0.50	2.44	19	1
1:A:57:GLN:HE22	1:A:90:ASN:HD21	0.50	1.50	19	1
1:A:59:ALA:HB3	1:A:63:GLN:HG3	0.50	1.81	2	2
1:A:170:MET:CE	1:A:170:MET:CB	0.50	2.90	1	1
1:A:58:MET:CG	1:A:58:MET:CE	0.50	2.84	19	1
1:A:165:GLN:HG2	1:A:166:LYS:H	0.49	1.66	20	1
1:A:145:GLU:HG2	1:A:145:GLU:O	0.49	2.07	19	1
1:A:189:HIS:N	1:A:201:VAL:CG1	0.49	2.76	19	1
1:A:134:HIS:O	1:A:135:LEU:HD13	0.49	2.07	20	1
1:A:55:LEU:C	1:A:55:LEU:CD1	0.48	2.86	20	1
1:A:165:GLN:HG2	1:A:166:LYS:N	0.48	2.22	20	1
1:A:182:VAL:O	1:A:186:ILE:HG23	0.48	2.07	16	10
1:A:31:LEU:HD12	1:A:31:LEU:C	0.48	2.33	15	2
1:A:45:LYS:C	1:A:46:ILE:HD12	0.48	2.34	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:GLY:C	1:A:58:MET:HE2	0.48	2.34	6	1
1:A:66:LEU:O	1:A:67:ALA:C	0.48	2.54	1	1
1:A:45:LYS:O	1:A:54:ALA:HB1	0.48	2.09	20	1
1:A:31:LEU:HD11	1:A:44:VAL:HG13	0.47	1.86	13	1
1:A:29:GLN:HE21	1:A:29:GLN:C	0.47	2.16	1	1
1:A:31:LEU:HD11	1:A:44:VAL:CG1	0.47	2.39	13	2
1:A:81:ILE:N	1:A:81:ILE:CD1	0.47	2.78	20	1
1:A:45:LYS:CE	1:A:91:VAL:HG11	0.47	2.40	1	1
1:A:17:LEU:C	1:A:18:VAL:HG23	0.47	2.35	19	1
1:A:43:ARG:HG3	1:A:43:ARG:HH11	0.47	1.69	20	1
1:A:19:SER:O	1:A:20:ASN:HB3	0.47	2.10	20	2
1:A:33:ILE:CG2	1:A:185:LEU:HD11	0.46	2.40	1	1
1:A:45:LYS:HE3	1:A:91:VAL:HG11	0.46	1.87	1	1
1:A:44:VAL:HG22	1:A:56:VAL:HG13	0.46	1.87	20	1
1:A:17:LEU:HD23	1:A:18:VAL:H	0.46	1.71	1	1
1:A:131:ALA:O	1:A:174:GLN:HG2	0.46	2.10	1	1
1:A:66:LEU:HD23	1:A:66:LEU:O	0.46	2.09	1	1
1:A:22:ASN:O	1:A:26:VAL:HG22	0.46	2.11	5	1
1:A:58:MET:HA	1:A:58:MET:HE3	0.46	1.87	2	1
1:A:20:ASN:CG	1:A:20:ASN:O	0.45	2.58	20	1
1:A:158:VAL:CG1	1:A:175:MET:HE1	0.45	2.42	20	1
1:A:28:PRO:HG3	1:A:46:ILE:HD12	0.45	1.87	1	1
1:A:178:VAL:C	1:A:180:GLU:N	0.45	2.75	1	1
1:A:157:VAL:HG23	1:A:176:GLY:H	0.45	1.72	18	4
1:A:31:LEU:HD13	1:A:56:VAL:CG2	0.45	2.42	17	1
1:A:133:LEU:HD21	1:A:151:PHE:CE1	0.45	2.46	2	4
1:A:35:PHE:CD2	1:A:56:VAL:CG1	0.45	2.95	20	1
1:A:37:VAL:HG21	1:A:203:PHE:CE2	0.45	2.46	19	1
1:A:16:LEU:HD21	1:A:64:ALA:HB1	0.45	1.88	20	1
1:A:133:LEU:N	1:A:133:LEU:CD2	0.45	2.79	20	1
1:A:151:PHE:CD1	1:A:184:ALA:HB1	0.45	2.47	1	1
1:A:21:LEU:HG	1:A:26:VAL:HG21	0.45	1.89	19	2
1:A:15:VAL:HG11	1:A:88:HIS:HB3	0.45	1.88	19	1
1:A:42:GLN:HB2	1:A:57:GLN:HB3	0.45	1.88	19	1
1:A:169:LYS:HB3	1:A:170:MET:SD	0.44	2.52	19	1
1:A:55:LEU:C	1:A:55:LEU:HD13	0.44	2.37	20	1
1:A:79:LYS:HE3	1:A:81:ILE:HG22	0.44	1.88	8	1
1:A:31:LEU:O	1:A:32:PHE:C	0.44	2.56	19	2
1:A:71:LEU:O	1:A:81:ILE:HG13	0.44	2.12	19	1
1:A:145:GLU:O	1:A:149:VAL:HG23	0.44	2.13	1	1
1:A:81:ILE:C	1:A:81:ILE:HD13	0.44	2.38	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:MET:HG3	1:A:59:ALA:N	0.44	2.27	1	1
1:A:168:ARG:HE	1:A:168:ARG:C	0.44	2.21	1	1
1:A:138:ILE:O	1:A:138:ILE:HG13	0.43	2.12	19	1
1:A:18:VAL:HB	1:A:54:ALA:HB3	0.43	1.90	20	1
1:A:175:MET:SD	1:A:175:MET:N	0.43	2.91	1	1
1:A:133:LEU:HD22	1:A:173:ILE:HG22	0.43	1.90	10	2
1:A:58:MET:CE	1:A:58:MET:HA	0.43	2.43	19	1
1:A:67:ALA:O	1:A:71:LEU:HB2	0.43	2.14	1	2
1:A:71:LEU:O	1:A:81:ILE:HD11	0.43	2.13	15	1
1:A:73:GLY:H	1:A:81:ILE:HG13	0.42	1.73	20	1
1:A:104:THR:HG22	1:A:105:LYS:N	0.42	2.29	1	1
1:A:21:LEU:CD1	1:A:26:VAL:HG21	0.42	2.42	1	1
1:A:151:PHE:HA	1:A:154:ASN:HD21	0.42	1.75	1	1
1:A:45:LYS:HE3	1:A:91:VAL:HG22	0.42	1.90	6	1
1:A:161:PHE:CD1	1:A:162:LYS:N	0.42	2.87	19	1
1:A:71:LEU:O	1:A:73:GLY:N	0.42	2.52	20	1
1:A:190:ASN:HA	1:A:199:LEU:O	0.42	2.15	1	1
1:A:133:LEU:HD12	1:A:151:PHE:HE1	0.42	1.75	19	1
1:A:76:LEU:O	1:A:79:LYS:HE2	0.42	2.14	16	1
1:A:132:THR:HG21	1:A:206:SER:O	0.42	2.15	19	1
1:A:19:SER:O	1:A:20:ASN:CB	0.42	2.68	20	1
1:A:142:VAL:HG13	1:A:146:ASP:HB3	0.42	1.91	1	1
1:A:58:MET:HG2	1:A:64:ALA:CA	0.42	2.45	1	1
1:A:15:VAL:HG13	1:A:55:LEU:HD11	0.42	1.90	20	1
1:A:40:ASP:HB2	1:A:59:ALA:HB2	0.41	1.92	19	1
1:A:136:SER:N	1:A:200:ARG:O	0.41	2.53	19	1
1:A:148:LYS:HB2	1:A:161:PHE:CD2	0.41	2.49	19	1
1:A:133:LEU:H	1:A:133:LEU:CD2	0.41	2.27	1	1
1:A:57:GLN:HE22	1:A:91:VAL:HG12	0.41	1.75	17	1
1:A:33:ILE:HD12	1:A:186:ILE:HA	0.41	1.91	1	1
1:A:165:GLN:C	1:A:165:GLN:HE21	0.41	2.23	19	1
1:A:74:HIS:O	1:A:75:LYS:C	0.41	2.62	20	1
1:A:45:LYS:HD3	1:A:104:THR:CG2	0.41	2.45	19	1
1:A:186:ILE:HD13	1:A:186:ILE:HG21	0.41	1.72	1	1
1:A:31:LEU:C	1:A:31:LEU:HD12	0.41	2.41	17	1
1:A:145:GLU:O	1:A:145:GLU:CG	0.41	2.69	20	1
1:A:81:ILE:CD1	1:A:81:ILE:N	0.41	2.83	1	2
1:A:81:ILE:HD13	1:A:81:ILE:H	0.41	1.76	1	1
1:A:66:LEU:CD2	1:A:70:HIS:CG	0.41	3.04	19	1
1:A:79:LYS:HA	1:A:80:PRO:HD2	0.41	1.60	19	1
1:A:127:PHE:CE2	1:A:205:LYS:HB3	0.41	2.51	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD11	1:A:64:ALA:O	0.41	2.16	1	1
1:A:21:LEU:HD22	1:A:53:ASN:C	0.40	2.41	20	1
1:A:133:LEU:HD21	1:A:181:ALA:HB1	0.40	1.93	15	2
1:A:170:MET:CE	1:A:170:MET:HB2	0.40	2.46	1	1
1:A:151:PHE:HA	1:A:154:ASN:ND2	0.40	2.31	1	1
1:A:106:ASP:C	1:A:108:GLY:H	0.40	2.22	20	1
1:A:194:GLY:C	1:A:196:ASN:H	0.40	2.25	8	1
1:A:68:MET:HG3	1:A:69:SER:N	0.40	2.32	19	1
1:A:189:HIS:C	1:A:190:ASN:HD22	0.40	2.24	20	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	162/229 (71%)	125±7 (77±4%)	24±4 (15±2%)	13±5 (8±3%)	1	14
All	All	3240/4580 (71%)	2502 (77%)	484 (15%)	254 (8%)	1	14

All 59 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	158	VAL	19
1	A	127	PHE	15
1	A	15	VAL	14
1	A	165	GLN	14
1	A	61	GLY	13
1	A	14	SER	12
1	A	20	ASN	10
1	A	197	HIS	10
1	A	196	ASN	10
1	A	157	VAL	9
1	A	78	GLY	9
1	A	72	ASN	6
1	A	87	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	166	LYS	6
1	A	140	PRO	6
1	A	126	ILE	5
1	A	81	ILE	5
1	A	156	GLY	5
1	A	129	PRO	4
1	A	164	PHE	4
1	A	191	HIS	4
1	A	195	GLU	4
1	A	108	GLY	4
1	A	90	ASN	4
1	A	75	LYS	4
1	A	80	PRO	3
1	A	88	HIS	3
1	A	76	LEU	3
1	A	59	ALA	3
1	A	198	HIS	3
1	A	41	VAL	2
1	A	60	ASP	2
1	A	137	ASN	2
1	A	192	ASP	2
1	A	77	HIS	2
1	A	207	THR	2
1	A	47	LEU	2
1	A	168	ARG	2
1	A	23	PRO	1
1	A	89	GLN	1
1	A	142	VAL	1
1	A	151	PHE	1
1	A	167	ASP	1
1	A	170	MET	1
1	A	175	MET	1
1	A	179	GLU	1
1	A	39	GLY	1
1	A	131	ALA	1
1	A	13	ASN	1
1	A	28	PRO	1
1	A	63	GLN	1
1	A	82	ARG	1
1	A	147	LEU	1
1	A	150	LEU	1
1	A	154	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	187	ASP	1
1	A	21	LEU	1
1	A	32	PHE	1
1	A	128	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	144/197 (73%)	113±9 (79±6%)	31±9 (21±6%)	3	30
All	All	2880/3940 (73%)	2261 (79%)	619 (21%)	3	30

All 99 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	34	LEU	20
1	A	79	LYS	20
1	A	133	LEU	20
1	A	135	LEU	20
1	A	185	LEU	20
1	A	188	LEU	20
1	A	71	LEU	19
1	A	75	LYS	18
1	A	196	ASN	18
1	A	157	VAL	16
1	A	186	ILE	16
1	A	178	VAL	16
1	A	58	MET	15
1	A	170	MET	15
1	A	13	ASN	15
1	A	132	THR	15
1	A	41	VAL	14
1	A	46	ILE	14
1	A	164	PHE	14
1	A	33	ILE	14
1	A	45	LYS	13

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Mol	Chain	Res	Type	Models (Total)
1	A	55	LEU	13
1	A	53	ASN	12
1	A	169	LYS	12
1	A	81	ILE	11
1	A	147	LEU	11
1	A	137	ASN	11
1	A	20	ASN	9
1	A	76	LEU	9
1	A	167	ASP	9
1	A	15	VAL	9
1	A	175	MET	8
1	A	202	SER	8
1	A	165	GLN	7
1	A	87	LYS	5
1	A	154	ASN	5
1	A	205	LYS	5
1	A	26	VAL	4
1	A	89	GLN	4
1	A	126	ILE	4
1	A	138	ILE	4
1	A	193	LEU	4
1	A	31	LEU	4
1	A	144	GLU	4
1	A	90	ASN	4
1	A	85	LEU	4
1	A	27	THR	3
1	A	32	PHE	3
1	A	127	PHE	3
1	A	158	VAL	3
1	A	168	ARG	3
1	A	192	ASP	3
1	A	91	VAL	3
1	A	21	LEU	3
1	A	172	LEU	3
1	A	189	HIS	3
1	A	62	ASN	2
1	A	66	LEU	2
1	A	134	HIS	2
1	A	191	HIS	2
1	A	72	ASN	2
1	A	130	SER	2
1	A	88	HIS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	47	LEU	2
1	A	198	HIS	2
1	A	23	PRO	2
1	A	40	ASP	2
1	A	166	LYS	2
1	A	201	VAL	2
1	A	206	SER	2
1	A	17	LEU	1
1	A	28	PRO	1
1	A	29	GLN	1
1	A	105	LYS	1
1	A	141	SER	1
1	A	142	VAL	1
1	A	187	ASP	1
1	A	204	SER	1
1	A	207	THR	1
1	A	148	LYS	1
1	A	57	GLN	1
1	A	174	GLN	1
1	A	183	GLN	1
1	A	19	SER	1
1	A	65	GLN	1
1	A	74	HIS	1
1	A	146	ASP	1
1	A	149	VAL	1
1	A	162	LYS	1
1	A	195	GLU	1
1	A	14	SER	1
1	A	25	ARG	1
1	A	35	PHE	1
1	A	42	GLN	1
1	A	63	GLN	1
1	A	68	MET	1
1	A	150	LEU	1
1	A	177	SER	1
1	A	190	ASN	1

### 6.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	19-A	2
1	1-A	1
1	20-A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	45:LYS	C	46:ILE	N	1.20
20	A	13:ASN	C	14:SER	N	1.20
19	A	34:LEU	C	35:PHE	N	1.18
19	A	169:LYS	C	170:MET	N	1.16

## 7 Chemical shift validation

No chemical shift data were provided