



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 08:21 PM BST

PDB ID : 2EVZ
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
A user guide is available at
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

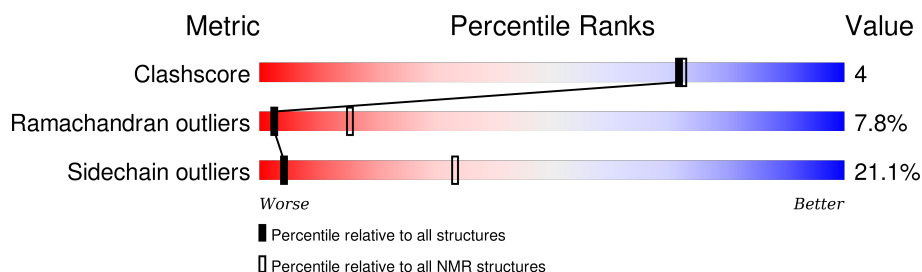
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>41%</div> <div>27%</div> <div>•</div> <div>20%</div> <div>9%</div> </div>

2 Ensemble composition and analysis ⓘ

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)	0.39	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
1	A	208	Total	C	H	N	O	S	0
			3259	1023	1641	296	295	4	

There are 21 discrepancies between the modelled and reference sequences:

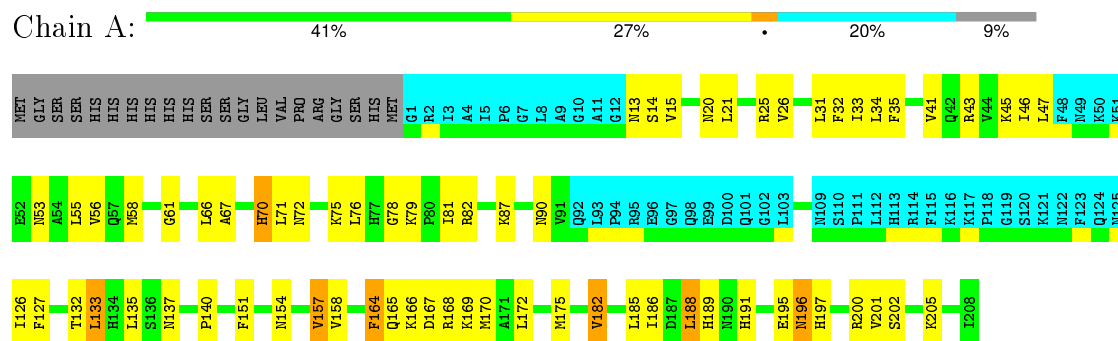
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	CLONING ARTIFACT	UNP P26599
A	-19	GLY	-	CLONING ARTIFACT	UNP P26599
A	-18	SER	-	CLONING ARTIFACT	UNP P26599
A	-17	SER	-	CLONING ARTIFACT	UNP P26599
A	-16	HIS	-	EXPRESSION TAG	UNP P26599
A	-15	HIS	-	EXPRESSION TAG	UNP P26599
A	-14	HIS	-	EXPRESSION 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 and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Polypyrimidine tract-binding protein 1

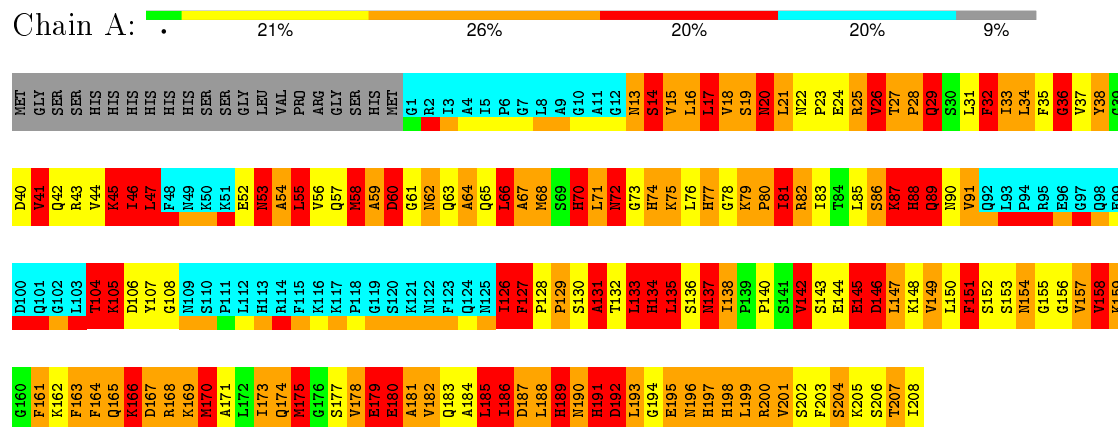


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

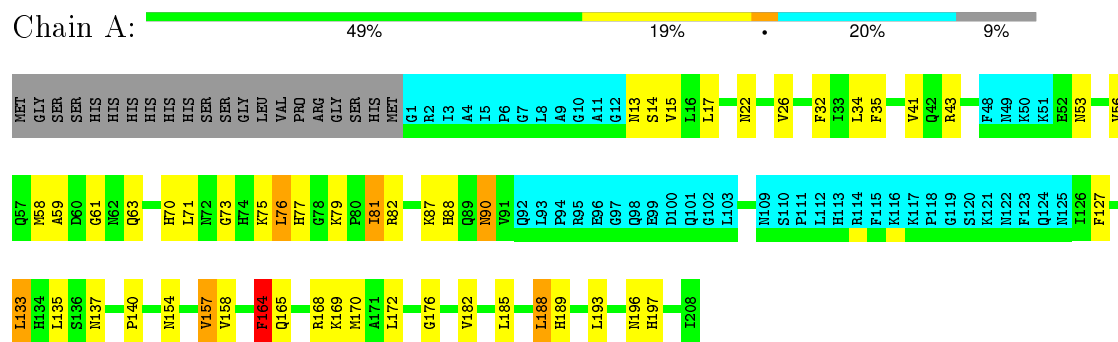
4.2.1 Score per residue for model 1

- Molecule 1: Polypyrimidine tract-binding protein 1



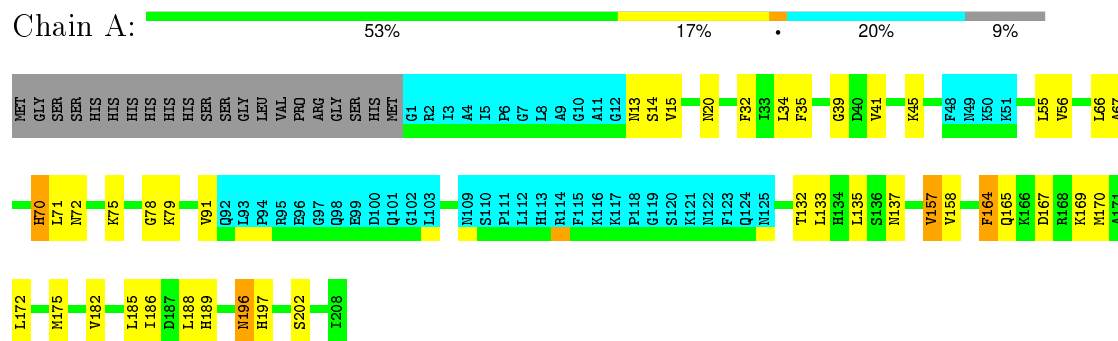
4.2.5 Score per residue for model 5

- Molecule 1: Polypyrimidine tract-binding protein 1



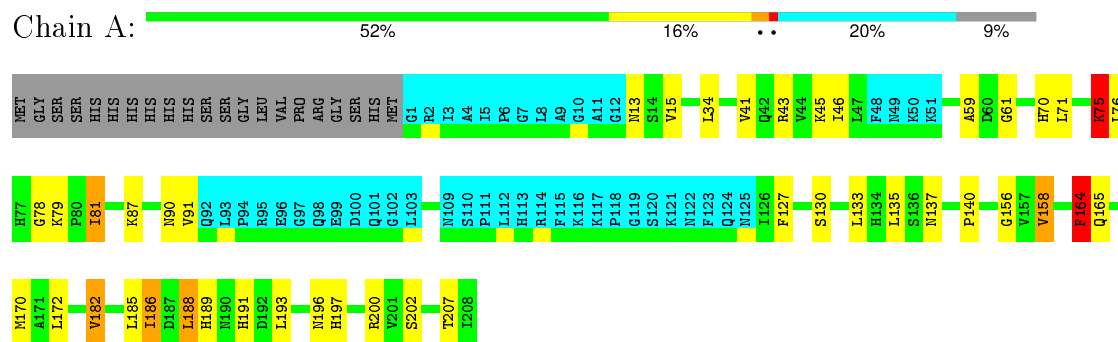
4.2.6 Score per residue for model 6

- Molecule 1: Polypyrimidine tract-binding protein 1



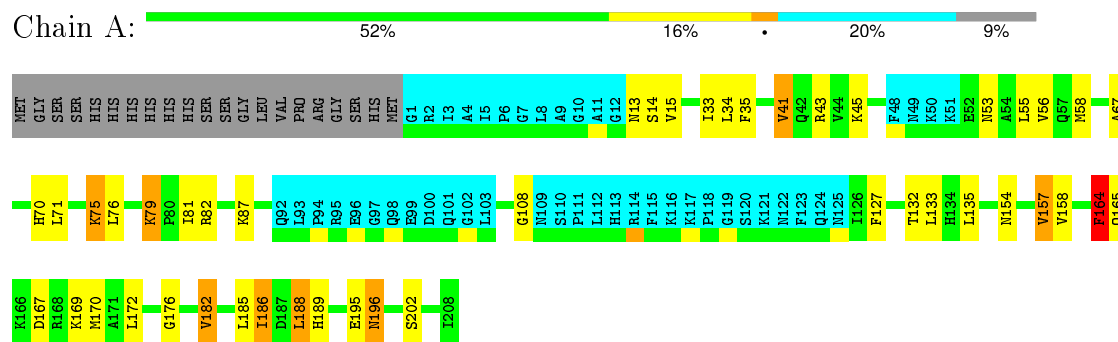
4.2.7 Score per residue for model 7

- Molecule 1: Polypyrimidine tract-binding protein 1



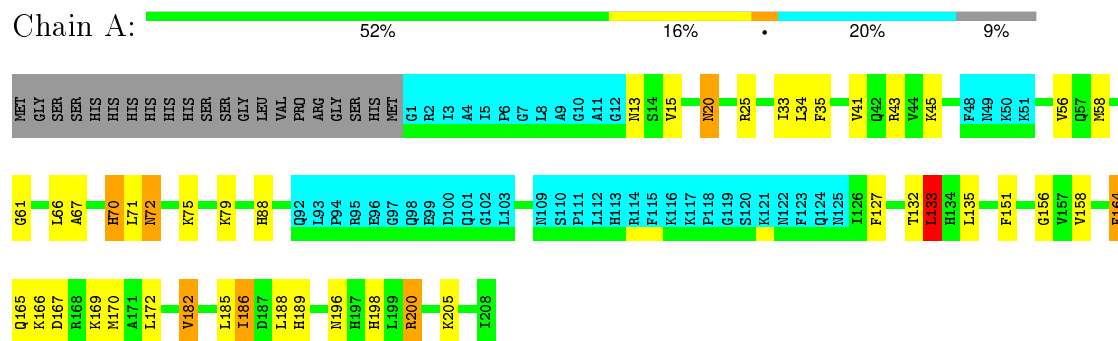
4.2.8 Score per residue for model 8

- Molecule 1: Polypyrimidine tract-binding protein 1



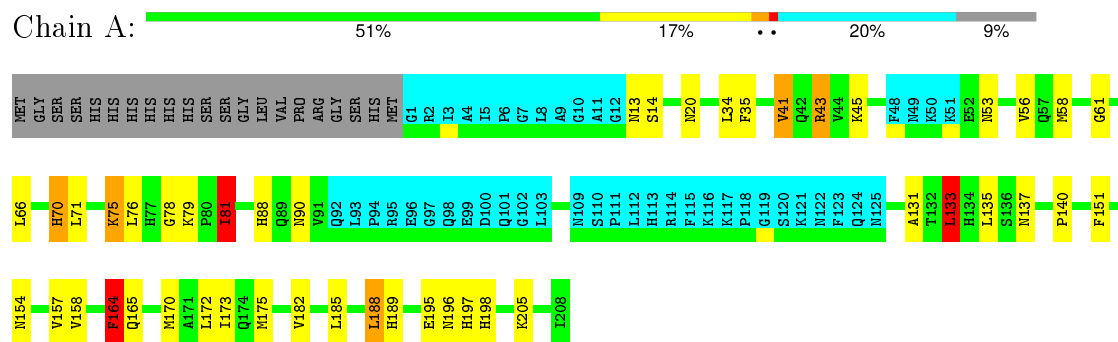
4.2.9 Score per residue for model 9

- Molecule 1: Polypyrimidine tract-binding protein 1



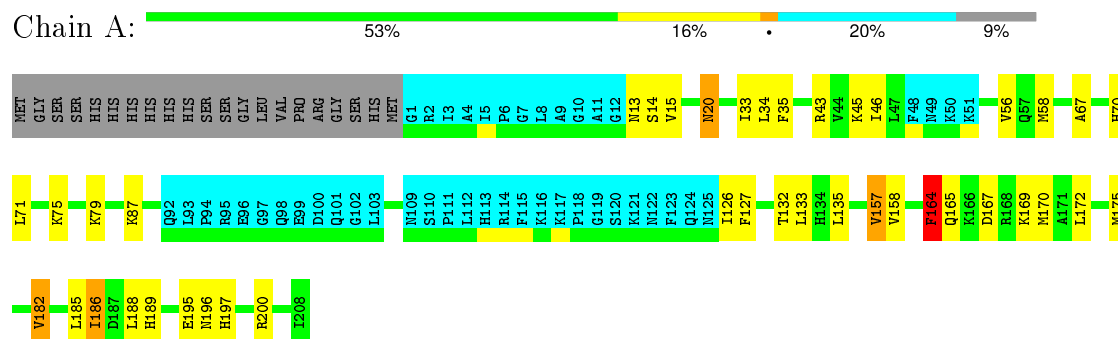
4.2.10 Score per residue for model 10

- Molecule 1: Polypyrimidine tract-binding protein 1



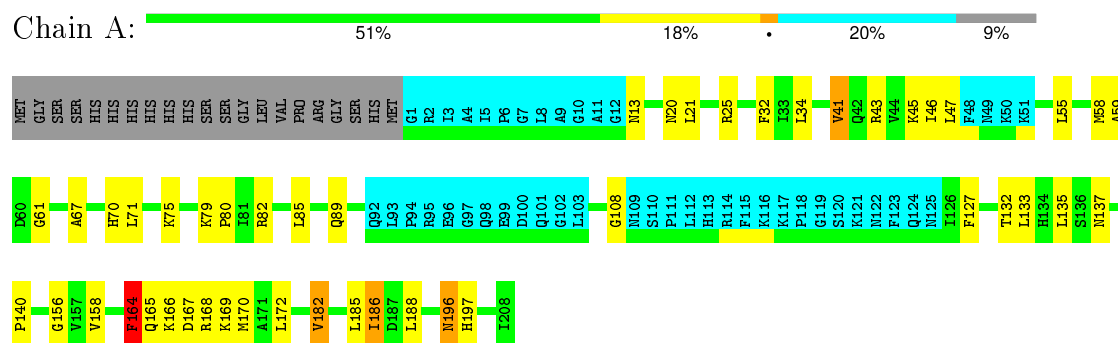
4.2.11 Score per residue for model 11

- Molecule 1: Polypyrimidine tract-binding protein 1



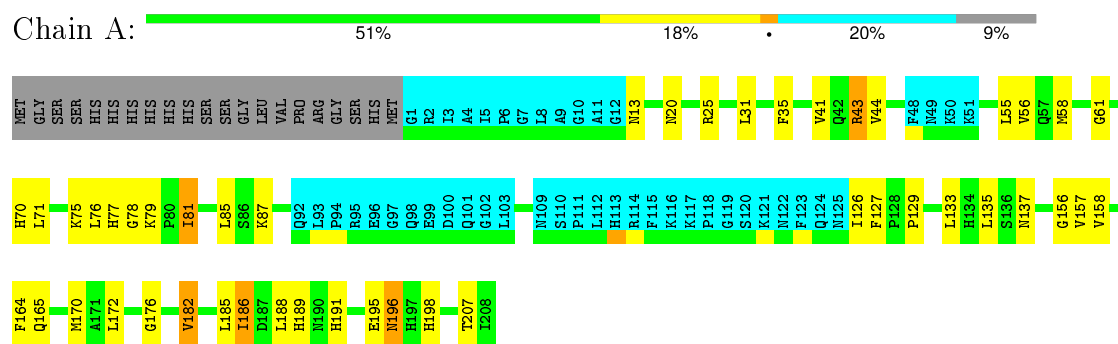
4.2.12 Score per residue for model 12

- Molecule 1: Polypyrimidine tract-binding protein 1



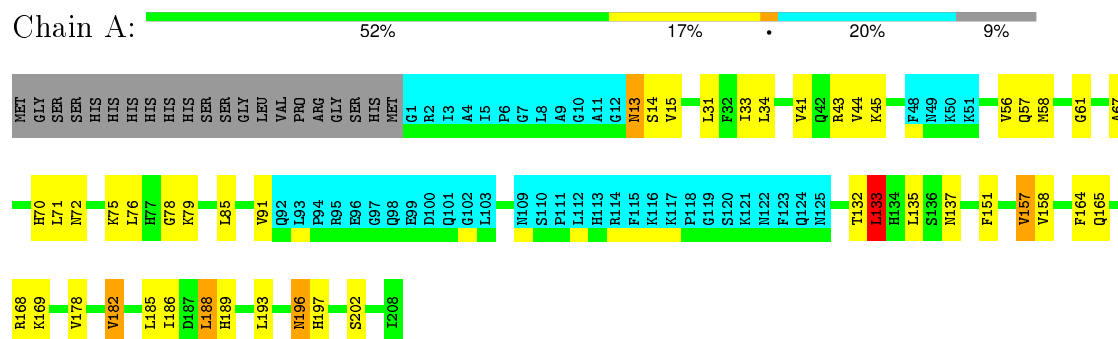
4.2.13 Score per residue for model 13

- Molecule 1: Polypyrimidine tract-binding protein 1



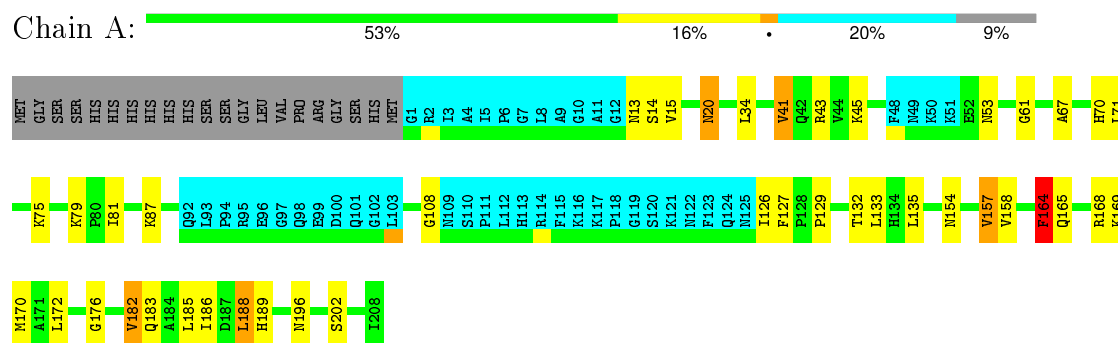
4.2.17 Score per residue for model 17

- Molecule 1: Polypyrimidine tract-binding protein 1



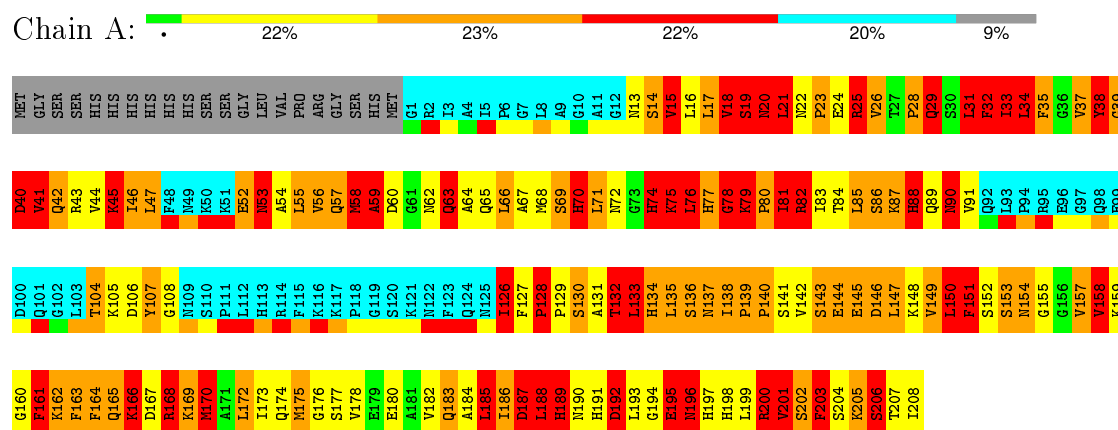
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Polypyrimidine tract-binding protein 1



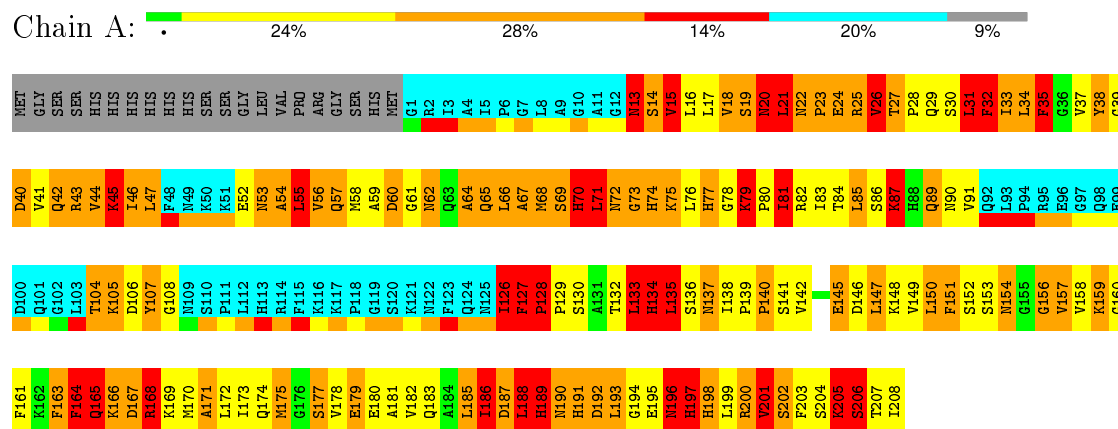
4.2.19 Score per residue for model 19

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

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.99±0.83	18±44/1297 (1.4±3.4%)	1.64±0.89	46±95/1751 (2.6±5.4%)
All	All	1.29	365/25940 (1.4%)	1.86	918/35020 (2.6%)

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	160	GLY	N-CA	-12.51	1.27	1.46	19	1
1	A	140	PRO	N-CA	12.44	1.68	1.47	19	2
1	A	166	LYS	CD-CE	11.90	1.81	1.51	1	1
1	A	38	TYR	CE2-CZ	11.48	1.53	1.38	19	1
1	A	44	VAL	CA-CB	-11.38	1.30	1.54	1	1
1	A	200	ARG	CZ-NH1	-10.88	1.19	1.33	1	1
1	A	203	PHE	CE2-CZ	10.74	1.57	1.37	19	1
1	A	107	TYR	CE1-CZ	10.69	1.52	1.38	19	1
1	A	152	SER	CB-OG	-10.12	1.29	1.42	20	1
1	A	15	VAL	CB-CG2	10.07	1.74	1.52	1	1
1	A	187	ASP	CB-CG	9.84	1.72	1.51	20	2
1	A	156	GLY	N-CA	9.53	1.60	1.46	1	1
1	A	202	SER	CB-OG	-9.48	1.29	1.42	19	2
1	A	32	PHE	CG-CD1	9.45	1.52	1.38	1	2
1	A	151	PHE	CG-CD2	9.30	1.52	1.38	1	2
1	A	204	SER	CB-OG	9.22	1.54	1.42	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	200	ARG	NE-CZ	-9.12	1.21	1.33	20	1
1	A	25	ARG	C-O	8.92	1.40	1.23	1	1
1	A	23	PRO	CA-C	8.89	1.70	1.52	20	1
1	A	206	SER	CA-CB	8.84	1.66	1.52	1	1
1	A	190	ASN	N-CA	-8.62	1.29	1.46	20	1
1	A	145	GLU	CD-OE2	8.60	1.35	1.25	20	2
1	A	180	GLU	CD-OE2	-8.51	1.16	1.25	20	1
1	A	82	ARG	CD-NE	8.49	1.60	1.46	20	2
1	A	19	SER	CB-OG	-8.45	1.31	1.42	1	1
1	A	177	SER	CA-CB	-8.41	1.40	1.52	20	3
1	A	29	GLN	C-O	-8.37	1.07	1.23	19	1
1	A	60	ASP	N-CA	8.32	1.62	1.46	1	1
1	A	23	PRO	CA-CB	8.32	1.70	1.53	19	1
1	A	42	GLN	N-CA	-8.25	1.29	1.46	20	1
1	A	198	HIS	CB-CG	8.24	1.64	1.50	20	1
1	A	84	THR	CB-OG1	-8.19	1.26	1.43	20	1
1	A	107	TYR	CE2-CZ	8.17	1.49	1.38	19	1
1	A	196	ASN	CG-OD1	-8.16	1.05	1.24	20	1
1	A	24	GLU	N-CA	8.12	1.62	1.46	20	1
1	A	107	TYR	CG-CD2	8.05	1.49	1.39	19	1
1	A	142	VAL	CB-CG2	8.04	1.69	1.52	19	2
1	A	153	SER	CA-CB	8.03	1.65	1.52	19	1
1	A	26	VAL	N-CA	8.03	1.62	1.46	19	1
1	A	70	HIS	CE1-NE2	8.03	1.51	1.32	19	1
1	A	35	PHE	CD2-CE2	7.97	1.55	1.39	1	1
1	A	41	VAL	N-CA	7.95	1.62	1.46	19	1
1	A	58	MET	CG-SD	7.92	2.01	1.81	19	1
1	A	134	HIS	CB-CG	7.83	1.64	1.50	19	1
1	A	82	ARG	NE-CZ	-7.82	1.22	1.33	19	1
1	A	154	ASN	CA-CB	7.79	1.73	1.53	20	1
1	A	169	LYS	C-N	-7.79	1.16	1.34	19	1
1	A	27	THR	CB-OG1	-7.78	1.27	1.43	20	2
1	A	130	SER	CB-OG	-7.76	1.32	1.42	20	2
1	A	53	ASN	CA-CB	7.75	1.73	1.53	20	2
1	A	136	SER	CA-CB	7.71	1.64	1.52	19	1
1	A	126	ILE	N-CA	7.71	1.61	1.46	1	1
1	A	191	HIS	CB-CG	7.69	1.63	1.50	20	1
1	A	193	LEU	N-CA	7.68	1.61	1.46	19	1
1	A	177	SER	CB-OG	7.68	1.52	1.42	1	2
1	A	77	HIS	CA-C	7.68	1.73	1.52	19	1
1	A	59	ALA	CA-CB	7.65	1.68	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	185	LEU	CA-C	-7.62	1.33	1.52	19	1
1	A	131	ALA	CA-C	7.59	1.72	1.52	1	1
1	A	60	ASP	CA-CB	7.58	1.70	1.53	1	1
1	A	179	GLU	CD-OE2	7.51	1.33	1.25	20	1
1	A	161	PHE	CB-CG	7.47	1.64	1.51	20	2
1	A	137	ASN	CA-C	7.46	1.72	1.52	1	1
1	A	199	LEU	CA-CB	7.46	1.71	1.53	19	1
1	A	193	LEU	C-O	7.45	1.37	1.23	19	1
1	A	15	VAL	N-CA	-7.42	1.31	1.46	1	1
1	A	73	GLY	CA-C	-7.40	1.40	1.51	20	1
1	A	137	ASN	N-CA	7.39	1.61	1.46	19	2
1	A	107	TYR	CA-CB	7.38	1.70	1.53	19	2
1	A	128	PRO	CA-C	7.34	1.67	1.52	20	1
1	A	170	MET	CA-CB	-7.33	1.37	1.53	20	1
1	A	168	ARG	CZ-NH1	-7.31	1.23	1.33	20	1
1	A	169	LYS	CD-CE	7.28	1.69	1.51	19	1
1	A	29	GLN	N-CA	7.25	1.60	1.46	20	1
1	A	199	LEU	C-N	7.24	1.50	1.34	19	1
1	A	203	PHE	CD2-CE2	7.23	1.53	1.39	1	1
1	A	194	GLY	CA-C	-7.23	1.40	1.51	20	1
1	A	62	ASN	CA-C	7.22	1.71	1.52	1	1
1	A	88	HIS	N-CA	7.21	1.60	1.46	19	1
1	A	159	LYS	C-O	-7.19	1.09	1.23	19	1
1	A	62	ASN	CB-CG	7.16	1.67	1.51	1	1
1	A	145	GLU	CA-CB	-7.13	1.38	1.53	19	1
1	A	52	GLU	CD-OE2	-7.13	1.17	1.25	1	1
1	A	136	SER	CB-OG	7.12	1.51	1.42	1	2
1	A	19	SER	CA-CB	7.12	1.63	1.52	1	1
1	A	195	GLU	CD-OE2	7.12	1.33	1.25	1	1
1	A	153	SER	CB-OG	7.10	1.51	1.42	20	1
1	A	177	SER	N-CA	7.09	1.60	1.46	20	1
1	A	162	LYS	CA-C	7.09	1.71	1.52	1	1
1	A	129	PRO	CA-C	7.08	1.67	1.52	1	1
1	A	43	ARG	CA-CB	7.06	1.69	1.53	19	1
1	A	134	HIS	N-CA	7.06	1.60	1.46	1	1
1	A	42	GLN	CG-CD	7.06	1.67	1.51	1	1
1	A	132	THR	CA-CB	-7.04	1.35	1.53	1	1
1	A	155	GLY	C-N	7.03	1.45	1.33	19	1
1	A	47	LEU	N-CA	6.94	1.60	1.46	1	1
1	A	185	LEU	CA-CB	-6.92	1.37	1.53	19	2
1	A	74	HIS	CG-CD2	6.89	1.47	1.35	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	21	LEU	CB-CG	6.88	1.72	1.52	19	1
1	A	179	GLU	CG-CD	6.87	1.62	1.51	1	1
1	A	143	SER	CA-CB	6.86	1.63	1.52	1	1
1	A	137	ASN	CB-CG	6.86	1.66	1.51	20	2
1	A	24	GLU	CD-OE1	-6.84	1.18	1.25	19	2
1	A	89	GLN	CA-C	6.78	1.70	1.52	20	1
1	A	38	TYR	CE1-CZ	6.78	1.47	1.38	1	1
1	A	149	VAL	CA-CB	6.77	1.69	1.54	19	1
1	A	40	ASP	CB-CG	6.76	1.66	1.51	19	2
1	A	13	ASN	CA-CB	6.75	1.70	1.53	1	1
1	A	24	GLU	C-O	-6.75	1.10	1.23	1	1
1	A	141	SER	N-CA	6.74	1.59	1.46	19	1
1	A	34	LEU	C-N	-6.73	1.18	1.34	19	1
1	A	74	HIS	CB-CG	6.71	1.62	1.50	19	1
1	A	194	GLY	C-O	6.71	1.34	1.23	20	1
1	A	35	PHE	CE1-CZ	6.70	1.50	1.37	19	1
1	A	29	GLN	C-N	6.69	1.49	1.34	1	1
1	A	164	PHE	CD2-CE2	6.68	1.52	1.39	20	2
1	A	56	VAL	CA-CB	-6.68	1.40	1.54	1	1
1	A	65	GLN	CA-CB	6.67	1.68	1.53	1	1
1	A	32	PHE	CB-CG	6.65	1.62	1.51	20	2
1	A	52	GLU	CD-OE1	6.61	1.32	1.25	1	1
1	A	17	LEU	C-O	6.61	1.35	1.23	19	1
1	A	26	VAL	CB-CG1	6.59	1.66	1.52	20	1
1	A	145	GLU	CD-OE1	6.59	1.32	1.25	1	1
1	A	35	PHE	CG-CD1	6.58	1.48	1.38	19	1
1	A	38	TYR	CG-CD1	-6.57	1.30	1.39	20	3
1	A	66	LEU	N-CA	-6.57	1.33	1.46	1	1
1	A	104	THR	CA-CB	6.55	1.70	1.53	20	1
1	A	72	ASN	N-CA	6.55	1.59	1.46	19	2
1	A	24	GLU	CD-OE2	6.55	1.32	1.25	20	1
1	A	43	ARG	CD-NE	6.53	1.57	1.46	1	2
1	A	181	ALA	N-CA	6.52	1.59	1.46	1	1
1	A	203	PHE	C-O	6.50	1.35	1.23	19	1
1	A	52	GLU	CA-C	6.48	1.69	1.52	20	1
1	A	146	ASP	C-N	6.48	1.49	1.34	19	1
1	A	107	TYR	CG-CD1	6.47	1.47	1.39	19	2
1	A	75	LYS	CB-CG	6.46	1.70	1.52	20	2
1	A	35	PHE	CG-CD2	6.44	1.48	1.38	20	1
1	A	82	ARG	CA-CB	6.43	1.68	1.53	20	1
1	A	168	ARG	CZ-NH2	-6.38	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	18	VAL	N-CA	6.38	1.59	1.46	1	2
1	A	159	LYS	CD-CE	6.38	1.67	1.51	19	1
1	A	19	SER	CA-C	-6.37	1.36	1.52	19	1
1	A	61	GLY	CA-C	-6.37	1.41	1.51	20	1
1	A	205	LYS	CD-CE	6.36	1.67	1.51	20	1
1	A	134	HIS	CA-C	6.35	1.69	1.52	19	1
1	A	105	LYS	CD-CE	6.34	1.67	1.51	20	1
1	A	134	HIS	CA-CB	6.34	1.68	1.53	19	1
1	A	128	PRO	CA-CB	-6.32	1.41	1.53	19	1
1	A	40	ASP	CG-OD1	6.31	1.39	1.25	19	1
1	A	91	VAL	CB-CG1	6.30	1.66	1.52	1	1
1	A	202	SER	CA-CB	6.30	1.62	1.52	1	1
1	A	70	HIS	CB-CG	6.29	1.61	1.50	1	1
1	A	134	HIS	C-O	-6.28	1.11	1.23	1	1
1	A	135	LEU	CA-C	6.28	1.69	1.52	20	1
1	A	140	PRO	CA-C	6.28	1.65	1.52	20	1
1	A	151	PHE	CG-CD1	6.27	1.48	1.38	19	1
1	A	41	VAL	CB-CG2	6.27	1.66	1.52	19	1
1	A	63	GLN	CD-OE1	6.25	1.37	1.24	1	1
1	A	40	ASP	CA-C	6.21	1.69	1.52	1	1
1	A	192	ASP	CB-CG	6.18	1.64	1.51	20	1
1	A	106	ASP	N-CA	-6.17	1.34	1.46	1	2
1	A	139	PRO	C-O	6.17	1.35	1.23	19	1
1	A	187	ASP	N-CA	6.16	1.58	1.46	19	1
1	A	133	LEU	N-CA	6.13	1.58	1.46	1	1
1	A	69	SER	CA-CB	6.13	1.62	1.52	19	1
1	A	32	PHE	CA-CB	6.12	1.67	1.53	19	1
1	A	154	ASN	N-CA	-6.12	1.34	1.46	19	1
1	A	18	VAL	C-O	6.12	1.34	1.23	1	1
1	A	164	PHE	CE2-CZ	6.12	1.49	1.37	19	1
1	A	144	GLU	CG-CD	6.10	1.61	1.51	1	1
1	A	147	LEU	C-N	6.10	1.48	1.34	20	2
1	A	180	GLU	CD-OE1	6.09	1.32	1.25	1	1
1	A	13	ASN	C-N	-6.09	1.20	1.34	20	1
1	A	196	ASN	N-CA	-6.08	1.34	1.46	1	1
1	A	189	HIS	CB-CG	6.08	1.61	1.50	19	1
1	A	36	GLY	N-CA	-6.08	1.36	1.46	1	1
1	A	163	PHE	CA-CB	6.06	1.67	1.53	20	1
1	A	197	HIS	CB-CG	-6.06	1.39	1.50	1	1
1	A	126	ILE	CA-CB	6.05	1.68	1.54	19	1
1	A	79	LYS	CD-CE	6.04	1.66	1.51	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	24	GLU	CA-C	6.03	1.68	1.52	19	2
1	A	86	SER	CA-CB	6.03	1.61	1.52	1	1
1	A	52	GLU	CG-CD	-6.03	1.43	1.51	19	2
1	A	26	VAL	CA-C	6.02	1.68	1.52	1	1
1	A	43	ARG	CZ-NH1	6.02	1.40	1.33	19	1
1	A	182	VAL	CB-CG1	6.01	1.65	1.52	1	1
1	A	89	GLN	CG-CD	6.00	1.64	1.51	19	1
1	A	183	GLN	CA-CB	5.98	1.67	1.53	20	1
1	A	131	ALA	C-O	-5.98	1.11	1.23	19	1
1	A	167	ASP	CB-CG	5.97	1.64	1.51	20	1
1	A	30	SER	CB-OG	-5.97	1.34	1.42	20	1
1	A	108	GLY	C-N	5.96	1.47	1.34	1	1
1	A	45	LYS	C-N	-5.96	1.20	1.34	1	1
1	A	164	PHE	CB-CG	-5.96	1.41	1.51	1	1
1	A	59	ALA	C-O	5.95	1.34	1.23	20	1
1	A	167	ASP	CA-C	5.94	1.68	1.52	20	1
1	A	28	PRO	N-CA	5.94	1.57	1.47	19	1
1	A	168	ARG	N-CA	5.93	1.58	1.46	20	1
1	A	105	LYS	CA-CB	5.91	1.67	1.53	19	1
1	A	195	GLU	C-O	-5.90	1.12	1.23	19	1
1	A	81	ILE	N-CA	5.90	1.58	1.46	19	1
1	A	139	PRO	N-CA	5.90	1.57	1.47	19	1
1	A	186	ILE	CA-CB	5.87	1.68	1.54	20	1
1	A	74	HIS	CA-CB	-5.87	1.41	1.53	20	1
1	A	82	ARG	CZ-NH1	5.86	1.40	1.33	19	1
1	A	174	GLN	CA-CB	5.85	1.66	1.53	20	1
1	A	82	ARG	CZ-NH2	-5.85	1.25	1.33	1	2
1	A	14	SER	N-CA	5.85	1.58	1.46	19	2
1	A	148	LYS	C-N	5.84	1.47	1.34	20	1
1	A	205	LYS	N-CA	-5.82	1.34	1.46	19	1
1	A	151	PHE	CA-C	5.81	1.68	1.52	20	1
1	A	106	ASP	C-O	5.79	1.34	1.23	19	1
1	A	39	GLY	N-CA	5.75	1.54	1.46	19	2
1	A	147	LEU	CA-CB	5.75	1.67	1.53	1	2
1	A	183	GLN	CG-CD	5.73	1.64	1.51	19	2
1	A	176	GLY	N-CA	5.72	1.54	1.46	19	1
1	A	189	HIS	CG-ND1	5.72	1.51	1.38	1	1
1	A	188	LEU	CB-CG	5.72	1.69	1.52	1	1
1	A	107	TYR	CB-CG	5.71	1.60	1.51	20	1
1	A	154	ASN	C-O	5.70	1.34	1.23	1	1
1	A	30	SER	C-N	5.69	1.47	1.34	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	16	LEU	CA-CB	5.68	1.66	1.53	19	1
1	A	206	SER	CB-OG	-5.68	1.34	1.42	19	1
1	A	135	LEU	C-O	5.68	1.34	1.23	20	1
1	A	89	GLN	CA-CB	5.67	1.66	1.53	20	1
1	A	165	GLN	N-CA	5.66	1.57	1.46	20	1
1	A	152	SER	N-CA	-5.66	1.35	1.46	19	1
1	A	198	HIS	CA-C	-5.64	1.38	1.52	20	1
1	A	80	PRO	CA-CB	5.64	1.64	1.53	20	1
1	A	108	GLY	N-CA	5.64	1.54	1.46	20	1
1	A	41	VAL	CA-C	5.63	1.67	1.52	1	2
1	A	139	PRO	CA-C	5.63	1.64	1.52	20	1
1	A	84	THR	N-CA	5.62	1.57	1.46	19	1
1	A	146	ASP	CB-CG	5.61	1.63	1.51	1	2
1	A	130	SER	CA-C	5.61	1.67	1.52	20	1
1	A	201	VAL	N-CA	5.61	1.57	1.46	1	1
1	A	77	HIS	ND1-CE1	5.60	1.48	1.34	19	1
1	A	195	GLU	CG-CD	5.59	1.60	1.51	1	1
1	A	163	PHE	CG-CD1	5.58	1.47	1.38	1	2
1	A	106	ASP	C-N	5.57	1.46	1.34	20	1
1	A	87	LYS	CA-C	5.57	1.67	1.52	1	1
1	A	144	GLU	CD-OE1	5.57	1.31	1.25	19	1
1	A	190	ASN	CG-OD1	-5.57	1.11	1.24	20	1
1	A	161	PHE	C-O	5.56	1.33	1.23	1	1
1	A	151	PHE	CE2-CZ	5.56	1.48	1.37	19	1
1	A	168	ARG	NE-CZ	5.55	1.40	1.33	19	1
1	A	164	PHE	C-O	5.54	1.33	1.23	19	1
1	A	39	GLY	C-N	5.53	1.46	1.34	19	1
1	A	80	PRO	CA-C	5.53	1.64	1.52	20	1
1	A	44	VAL	CB-CG2	-5.52	1.41	1.52	20	1
1	A	205	LYS	CE-NZ	-5.51	1.35	1.49	1	1
1	A	37	VAL	CA-CB	5.49	1.66	1.54	20	1
1	A	154	ASN	CB-CG	5.48	1.63	1.51	20	1
1	A	203	PHE	CG-CD2	5.47	1.47	1.38	19	1
1	A	53	ASN	C-O	5.47	1.33	1.23	20	1
1	A	201	VAL	CB-CG2	5.45	1.64	1.52	20	1
1	A	179	GLU	C-N	5.44	1.46	1.34	20	1
1	A	37	VAL	CA-C	5.42	1.67	1.52	19	1
1	A	189	HIS	CA-CB	5.38	1.65	1.53	19	1
1	A	64	ALA	CA-CB	5.38	1.63	1.52	1	1
1	A	19	SER	N-CA	-5.37	1.35	1.46	19	1
1	A	83	ILE	C-N	-5.37	1.21	1.34	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	47	LEU	CA-C	-5.37	1.39	1.52	20	1
1	A	55	LEU	CA-C	-5.36	1.39	1.52	19	1
1	A	127	PHE	CG-CD1	5.36	1.46	1.38	1	1
1	A	165	GLN	CA-CB	5.36	1.65	1.53	1	1
1	A	170	MET	SD-CE	5.33	2.07	1.77	1	1
1	A	33	ILE	CB-CG2	-5.33	1.36	1.52	19	1
1	A	196	ASN	CG-ND2	-5.33	1.19	1.32	19	1
1	A	39	GLY	CA-C	5.33	1.60	1.51	20	1
1	A	155	GLY	C-O	5.32	1.32	1.23	19	1
1	A	108	GLY	C-O	5.31	1.32	1.23	1	1
1	A	144	GLU	CB-CG	5.31	1.62	1.52	1	1
1	A	170	MET	CG-SD	-5.30	1.67	1.81	20	1
1	A	129	PRO	CA-CB	-5.30	1.43	1.53	20	1
1	A	127	PHE	CE2-CZ	5.30	1.47	1.37	1	1
1	A	64	ALA	N-CA	-5.26	1.35	1.46	20	1
1	A	170	MET	C-O	5.25	1.33	1.23	19	1
1	A	90	ASN	CA-C	5.24	1.66	1.52	1	1
1	A	157	VAL	CA-CB	-5.24	1.43	1.54	1	1
1	A	88	HIS	CB-CG	-5.24	1.40	1.50	19	1
1	A	78	GLY	CA-C	5.23	1.60	1.51	19	2
1	A	69	SER	CB-OG	5.22	1.49	1.42	20	1
1	A	42	GLN	CD-OE1	-5.21	1.12	1.24	19	1
1	A	208	ILE	N-CA	5.20	1.56	1.46	20	1
1	A	147	LEU	CA-C	5.20	1.66	1.52	19	1
1	A	172	LEU	N-CA	-5.20	1.35	1.46	19	1
1	A	65	GLN	C-N	-5.20	1.22	1.34	20	1
1	A	141	SER	CB-OG	5.20	1.49	1.42	19	1
1	A	89	GLN	N-CA	5.19	1.56	1.46	1	1
1	A	159	LYS	CA-CB	5.19	1.65	1.53	19	1
1	A	54	ALA	N-CA	-5.17	1.36	1.46	19	1
1	A	69	SER	C-O	5.17	1.33	1.23	20	1
1	A	25	ARG	CZ-NH2	-5.16	1.26	1.33	20	1
1	A	77	HIS	CB-CG	5.16	1.59	1.50	20	1
1	A	185	LEU	CG-CD2	5.15	1.71	1.51	19	1
1	A	32	PHE	N-CA	5.15	1.56	1.46	19	1
1	A	152	SER	CA-CB	5.15	1.60	1.52	19	1
1	A	188	LEU	CA-CB	5.14	1.65	1.53	1	1
1	A	198	HIS	CA-CB	-5.14	1.42	1.53	19	1
1	A	76	LEU	N-CA	-5.13	1.36	1.46	1	2
1	A	183	GLN	N-CA	5.12	1.56	1.46	1	1
1	A	187	ASP	C-O	5.11	1.33	1.23	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	38	TYR	N-CA	-5.11	1.36	1.46	1	1
1	A	198	HIS	CG-CD2	5.10	1.44	1.35	1	1
1	A	145	GLU	CG-CD	-5.08	1.44	1.51	20	1
1	A	21	LEU	C-O	5.08	1.32	1.23	1	1
1	A	173	ILE	N-CA	5.07	1.56	1.46	1	1
1	A	142	VAL	CA-C	5.07	1.66	1.52	19	1
1	A	172	LEU	C-N	-5.06	1.22	1.34	19	1
1	A	62	ASN	CG-OD1	-5.06	1.12	1.24	1	1
1	A	77	HIS	N-CA	5.05	1.56	1.46	20	1
1	A	195	GLU	CB-CG	5.05	1.61	1.52	19	1
1	A	163	PHE	C-O	5.03	1.32	1.23	20	1
1	A	56	VAL	CA-C	5.03	1.66	1.52	1	1
1	A	23	PRO	N-CD	5.03	1.54	1.47	20	1
1	A	38	TYR	CB-CG	-5.02	1.44	1.51	20	1
1	A	127	PHE	CE1-CZ	5.01	1.46	1.37	1	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	43	ARG	NE-CZ-NH2	27.77	134.18	120.30	20	6
1	A	188	LEU	CB-CG-CD1	22.11	148.58	111.00	19	2
1	A	107	TYR	CB-CG-CD2	22.01	134.21	121.00	20	3
1	A	163	PHE	CB-CG-CD1	-20.51	106.45	120.80	20	2
1	A	32	PHE	CB-CG-CD1	19.39	134.37	120.80	1	2
1	A	107	TYR	CB-CG-CD1	-19.29	109.43	121.00	20	2
1	A	32	PHE	CB-CG-CD2	-19.22	107.35	120.80	1	2
1	A	200	ARG	NE-CZ-NH1	-18.83	110.89	120.30	19	7
1	A	151	PHE	CB-CG-CD1	-18.56	107.81	120.80	19	2
1	A	168	ARG	NE-CZ-NH2	-17.37	111.61	120.30	20	2
1	A	43	ARG	NH1-CZ-NH2	-16.77	100.95	119.40	20	2
1	A	37	VAL	CA-CB-CG2	16.36	135.44	110.90	1	1
1	A	82	ARG	NE-CZ-NH2	16.26	128.43	120.30	19	3
1	A	187	ASP	CB-CG-OD1	-16.25	103.68	118.30	1	2
1	A	182	VAL	CA-CB-CG1	14.97	133.35	110.90	1	19
1	A	14	SER	O-C-N	-14.66	99.24	122.70	1	2
1	A	135	LEU	CB-CG-CD1	14.35	135.39	111.00	19	1
1	A	139	PRO	N-CA-CB	13.80	119.86	103.30	20	1
1	A	82	ARG	NE-CZ-NH1	-13.71	113.45	120.30	19	7
1	A	149	VAL	CA-CB-CG1	13.62	131.33	110.90	20	1
1	A	40	ASP	CB-CG-OD1	13.46	130.41	118.30	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	184	ALA	CB-CA-C	13.44	130.26	110.10	19	1
1	A	67	ALA	CB-CA-C	13.31	130.07	110.10	1	13
1	A	25	ARG	NH1-CZ-NH2	-13.28	104.80	119.40	1	2
1	A	35	PHE	CB-CG-CD2	-13.04	111.67	120.80	20	2
1	A	38	TYR	CG-CD2-CE2	13.02	131.71	121.30	19	2
1	A	54	ALA	N-CA-CB	12.91	128.17	110.10	1	1
1	A	21	LEU	CB-CG-CD2	12.88	132.90	111.00	20	2
1	A	91	VAL	CG1-CB-CG2	12.53	130.95	110.90	1	2
1	A	168	ARG	NE-CZ-NH1	12.48	126.54	120.30	19	6
1	A	68	MET	CA-CB-CG	12.29	134.19	113.30	1	1
1	A	200	ARG	NE-CZ-NH2	-12.19	114.21	120.30	20	3
1	A	192	ASP	CB-CG-OD1	12.12	129.21	118.30	1	1
1	A	185	LEU	CB-CA-C	12.05	133.10	110.20	1	1
1	A	52	GLU	OE1-CD-OE2	-12.01	108.89	123.30	1	3
1	A	66	LEU	CB-CG-CD2	-11.95	90.68	111.00	1	2
1	A	74	HIS	O-C-N	-11.92	103.63	122.70	19	1
1	A	21	LEU	CB-CG-CD1	11.62	130.75	111.00	1	3
1	A	40	ASP	CB-CG-OD2	-11.35	108.08	118.30	1	2
1	A	150	LEU	CB-CG-CD2	-11.35	91.71	111.00	1	1
1	A	21	LEU	CA-CB-CG	11.32	141.34	115.30	1	1
1	A	88	HIS	CB-CA-C	11.30	133.00	110.40	19	1
1	A	178	VAL	CA-CB-CG2	11.24	127.76	110.90	20	2
1	A	35	PHE	CZ-CE2-CD2	-11.23	106.63	120.10	1	1
1	A	44	VAL	CG1-CB-CG2	-11.17	93.03	110.90	1	2
1	A	142	VAL	CA-CB-CG1	11.12	127.58	110.90	19	2
1	A	139	PRO	N-CD-CG	10.99	119.68	103.20	20	1
1	A	147	LEU	O-C-N	-10.96	105.16	122.70	19	1
1	A	158	VAL	CA-CB-CG2	10.96	127.33	110.90	1	2
1	A	186	ILE	O-C-N	-10.90	105.26	122.70	1	1
1	A	45	LYS	CB-CA-C	10.84	132.08	110.40	19	1
1	A	167	ASP	CB-CG-OD1	10.73	127.95	118.30	19	2
1	A	42	GLN	O-C-N	-10.71	105.56	122.70	1	1
1	A	139	PRO	CA-N-CD	-10.71	96.50	111.50	20	1
1	A	43	ARG	CB-CA-C	-10.56	89.28	110.40	19	1
1	A	56	VAL	CA-CB-CG1	-10.54	95.08	110.90	1	1
1	A	161	PHE	CB-CG-CD2	-10.52	113.44	120.80	1	2
1	A	25	ARG	NE-CZ-NH1	10.50	125.55	120.30	19	6
1	A	35	PHE	CD1-CE1-CZ	-10.44	107.58	120.10	1	1
1	A	47	LEU	CB-CG-CD2	10.36	128.61	111.00	19	3
1	A	164	PHE	CB-CG-CD2	-10.35	113.56	120.80	19	12
1	A	168	ARG	NH1-CZ-NH2	-10.33	108.04	119.40	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	133	LEU	CA-CB-CG	10.32	139.03	115.30	19	8
1	A	65	GLN	O-C-N	10.31	139.19	122.70	1	1
1	A	33	ILE	O-C-N	-10.28	106.26	122.70	19	2
1	A	184	ALA	N-CA-CB	-10.24	95.77	110.10	19	1
1	A	79	LYS	CB-CG-CD	10.15	137.99	111.60	20	3
1	A	203	PHE	CD1-CE1-CZ	-10.13	107.94	120.10	19	1
1	A	163	PHE	CB-CG-CD2	10.12	127.89	120.80	20	2
1	A	86	SER	N-CA-CB	10.12	125.68	110.50	19	2
1	A	43	ARG	NE-CZ-NH1	10.07	125.33	120.30	5	14
1	A	82	ARG	NH1-CZ-NH2	-10.06	108.33	119.40	1	2
1	A	26	VAL	CG1-CB-CG2	-10.06	94.80	110.90	1	2
1	A	34	LEU	CB-CG-CD2	10.00	128.01	111.00	1	1
1	A	35	PHE	CE1-CZ-CE2	9.98	137.96	120.00	1	1
1	A	196	ASN	CB-CG-OD1	9.97	141.54	121.60	1	3
1	A	47	LEU	C-N-CA	9.94	146.54	121.70	1	1
1	A	144	GLU	OE1-CD-OE2	-9.93	111.38	123.30	1	1
1	A	164	PHE	CG-CD1-CE1	-9.90	109.91	120.80	19	1
1	A	75	LYS	CB-CG-CD	9.90	137.33	111.60	1	1
1	A	28	PRO	N-CD-CG	9.89	118.04	103.20	20	2
1	A	25	ARG	NE-CZ-NH2	-9.88	115.36	120.30	20	2
1	A	175	MET	N-CA-CB	-9.88	92.82	110.60	1	2
1	A	132	THR	CA-CB-OG1	9.79	129.56	109.00	1	1
1	A	41	VAL	CA-CB-CG1	9.71	125.47	110.90	20	7
1	A	156	GLY	N-CA-C	9.63	137.19	113.10	1	2
1	A	28	PRO	CA-N-CD	-9.53	98.16	111.50	19	1
1	A	157	VAL	CA-CB-CG2	9.51	125.17	110.90	1	2
1	A	128	PRO	N-CD-CG	9.49	117.43	103.20	20	2
1	A	46	ILE	CA-CB-CG1	-9.44	93.07	111.00	1	1
1	A	82	ARG	CD-NE-CZ	9.44	136.81	123.60	19	1
1	A	151	PHE	CG-CD1-CE1	-9.43	110.43	120.80	19	2
1	A	170	MET	CG-SD-CE	-9.43	85.11	100.20	20	2
1	A	169	LYS	C-N-CA	9.39	145.17	121.70	19	1
1	A	172	LEU	CB-CG-CD2	9.37	126.94	111.00	20	1
1	A	134	HIS	CA-CB-CG	9.33	129.46	113.60	1	2
1	A	131	ALA	O-C-N	-9.30	107.82	122.70	19	1
1	A	22	ASN	OD1-CG-ND2	-9.30	100.52	121.90	20	1
1	A	88	HIS	CA-CB-CG	9.28	129.38	113.60	19	2
1	A	186	ILE	CB-CA-C	9.22	130.04	111.60	19	2
1	A	38	TYR	CZ-CE2-CD2	-9.21	111.51	119.80	19	1
1	A	35	PHE	CB-CG-CD1	9.21	127.25	120.80	20	1
1	A	197	HIS	CB-CG-CD2	-9.19	102.30	130.80	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	21	LEU	O-C-N	-9.14	108.08	122.70	19	1
1	A	151	PHE	CD1-CE1-CZ	-9.11	109.17	120.10	20	2
1	A	60	ASP	CB-CG-OD1	-9.07	110.13	118.30	20	1
1	A	106	ASP	CB-CA-C	9.07	128.53	110.40	1	2
1	A	203	PHE	CB-CG-CD2	-9.05	114.46	120.80	20	3
1	A	13	ASN	N-CA-CB	-9.04	94.33	110.60	1	2
1	A	195	GLU	C-N-CA	9.02	144.25	121.70	19	4
1	A	38	TYR	CB-CA-C	9.02	128.44	110.40	19	1
1	A	23	PRO	C-N-CA	8.98	144.15	121.70	19	1
1	A	151	PHE	CB-CG-CD2	-8.97	114.52	120.80	20	2
1	A	207	THR	CA-CB-OG1	8.97	127.84	109.00	20	2
1	A	157	VAL	CA-CB-CG1	-8.96	97.45	110.90	1	1
1	A	77	HIS	N-CA-CB	8.94	126.69	110.60	1	1
1	A	141	SER	N-CA-CB	-8.94	97.09	110.50	20	1
1	A	52	GLU	CG-CD-OE1	8.81	135.92	118.30	20	1
1	A	137	ASN	CB-CG-OD1	8.81	139.21	121.60	19	1
1	A	151	PHE	CG-CD2-CE2	-8.79	111.13	120.80	19	2
1	A	44	VAL	CA-CB-CG2	8.76	124.04	110.90	1	1
1	A	129	PRO	O-C-N	8.75	136.71	122.70	1	1
1	A	128	PRO	CA-CB-CG	8.75	121.43	104.80	19	1
1	A	196	ASN	CB-CA-C	8.71	127.81	110.40	1	1
1	A	201	VAL	CA-CB-CG1	8.70	123.95	110.90	19	2
1	A	130	SER	CB-CA-C	-8.69	93.59	110.10	1	2
1	A	27	THR	CA-CB-CG2	8.67	124.54	112.40	1	2
1	A	58	MET	CA-CB-CG	8.67	128.03	113.30	1	1
1	A	105	LYS	CB-CA-C	-8.64	93.11	110.40	1	1
1	A	148	LYS	CB-CG-CD	8.64	134.05	111.60	20	1
1	A	155	GLY	C-N-CA	-8.63	104.17	122.30	19	1
1	A	63	GLN	O-C-N	8.60	136.46	122.70	1	1
1	A	29	GLN	O-C-N	8.55	136.38	122.70	19	1
1	A	46	ILE	CG1-CB-CG2	8.54	130.19	111.40	19	2
1	A	177	SER	N-CA-CB	-8.52	97.72	110.50	1	1
1	A	75	LYS	CA-CB-CG	8.52	132.14	113.40	19	1
1	A	129	PRO	CA-N-CD	-8.52	99.58	111.50	1	2
1	A	72	ASN	OD1-CG-ND2	-8.48	102.39	121.90	1	1
1	A	75	LYS	C-N-CA	8.47	142.87	121.70	19	4
1	A	195	GLU	OE1-CD-OE2	8.47	133.46	123.30	1	1
1	A	203	PHE	CG-CD1-CE1	-8.45	111.51	120.80	20	1
1	A	64	ALA	CB-CA-C	8.40	122.70	110.10	20	1
1	A	55	LEU	CA-CB-CG	8.39	134.59	115.30	1	2
1	A	200	ARG	CA-CB-CG	8.38	131.84	113.40	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	54	ALA	O-C-N	-8.36	109.33	122.70	1	1
1	A	105	LYS	CB-CG-CD	-8.31	90.00	111.60	19	1
1	A	202	SER	CA-CB-OG	-8.31	88.77	111.20	19	1
1	A	142	VAL	CG1-CB-CG2	8.29	124.16	110.90	20	2
1	A	107	TYR	CG-CD1-CE1	-8.27	114.68	121.30	19	1
1	A	47	LEU	CB-CG-CD1	-8.20	97.06	111.00	1	1
1	A	89	GLN	CB-CA-C	-8.19	94.02	110.40	20	1
1	A	187	ASP	CB-CG-OD2	8.17	125.65	118.30	1	2
1	A	186	ILE	CA-CB-CG2	8.16	127.23	110.90	19	2
1	A	55	LEU	O-C-N	8.14	135.72	122.70	1	1
1	A	85	LEU	CB-CG-CD1	8.13	124.81	111.00	1	2
1	A	166	LYS	O-C-N	8.12	135.69	122.70	1	1
1	A	14	SER	CA-C-N	8.11	135.04	117.20	1	1
1	A	143	SER	CA-CB-OG	8.11	133.09	111.20	19	1
1	A	177	SER	CA-CB-OG	8.09	133.05	111.20	1	1
1	A	188	LEU	CB-CG-CD2	8.07	124.72	111.00	1	10
1	A	143	SER	N-CA-CB	8.02	122.54	110.50	1	2
1	A	127	PHE	CB-CG-CD2	-8.02	115.19	120.80	1	1
1	A	151	PHE	CD1-CG-CD2	8.02	128.73	118.30	19	1
1	A	174	GLN	OE1-CD-NE2	-8.02	103.46	121.90	1	1
1	A	68	MET	CG-SD-CE	-8.02	87.37	100.20	1	1
1	A	199	LEU	CB-CG-CD2	-7.98	97.44	111.00	19	2
1	A	190	ASN	CB-CG-OD1	7.95	137.49	121.60	19	2
1	A	13	ASN	CA-C-N	7.94	134.67	117.20	19	1
1	A	87	LYS	CG-CD-CE	-7.94	88.09	111.90	1	2
1	A	38	TYR	CD1-CG-CD2	-7.93	109.17	117.90	1	1
1	A	18	VAL	CA-CB-CG2	-7.92	99.02	110.90	1	2
1	A	23	PRO	O-C-N	-7.91	110.04	122.70	19	1
1	A	57	GLN	OE1-CD-NE2	-7.91	103.72	121.90	20	1
1	A	208	ILE	CB-CG1-CD1	7.90	136.02	113.90	20	1
1	A	196	ASN	O-C-N	-7.89	110.07	122.70	1	1
1	A	87	LYS	CB-CA-C	7.87	126.13	110.40	1	2
1	A	145	GLU	OE1-CD-OE2	-7.86	113.87	123.30	19	2
1	A	32	PHE	CB-CA-C	7.83	126.06	110.40	19	1
1	A	19	SER	N-CA-CB	-7.80	98.79	110.50	1	1
1	A	76	LEU	CA-C-N	-7.80	100.03	117.20	1	2
1	A	169	LYS	CA-CB-CG	7.80	130.56	113.40	1	1
1	A	190	ASN	N-CA-CB	7.77	124.58	110.60	1	2
1	A	166	LYS	CB-CG-CD	7.76	131.77	111.60	20	2
1	A	53	ASN	OD1-CG-ND2	-7.74	104.09	121.90	19	2
1	A	162	LYS	CA-CB-CG	7.73	130.41	113.40	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	VAL	CA-CB-CG1	-7.73	99.30	110.90	19	1
1	A	187	ASP	OD1-CG-OD2	-7.72	108.62	123.30	19	1
1	A	175	MET	CA-CB-CG	-7.72	100.18	113.30	1	2
1	A	85	LEU	CA-CB-CG	7.71	133.03	115.30	1	1
1	A	104	THR	CA-CB-OG1	7.70	125.16	109.00	20	1
1	A	80	PRO	C-N-CA	7.69	140.93	121.70	20	1
1	A	182	VAL	CA-C-N	7.68	134.09	117.20	19	1
1	A	14	SER	CA-CB-OG	7.66	131.88	111.20	20	2
1	A	32	PHE	CG-CD1-CE1	-7.65	112.38	120.80	19	1
1	A	173	ILE	CG1-CB-CG2	-7.65	94.57	111.40	19	2
1	A	205	LYS	C-N-CA	7.65	140.82	121.70	19	1
1	A	43	ARG	O-C-N	-7.63	110.48	122.70	1	1
1	A	58	MET	CA-C-O	-7.63	104.08	120.10	19	2
1	A	159	LYS	CB-CA-C	-7.62	95.17	110.40	19	1
1	A	65	GLN	CA-C-O	-7.61	104.11	120.10	1	2
1	A	140	PRO	CA-N-CD	-7.61	100.84	111.50	19	2
1	A	157	VAL	C-N-CA	7.61	140.73	121.70	19	2
1	A	72	ASN	O-C-N	7.60	136.12	123.20	19	1
1	A	20	ASN	O-C-N	-7.60	110.54	122.70	1	1
1	A	21	LEU	CD1-CG-CD2	-7.58	87.77	110.50	20	1
1	A	156	GLY	CA-C-O	7.58	134.24	120.60	20	1
1	A	161	PHE	CG-CD2-CE2	-7.53	112.51	120.80	1	1
1	A	146	ASP	CB-CG-OD1	7.53	125.08	118.30	20	1
1	A	182	VAL	N-CA-CB	7.53	128.07	111.50	1	1
1	A	206	SER	C-N-CA	7.49	140.43	121.70	20	1
1	A	149	VAL	CG1-CB-CG2	-7.45	98.97	110.90	20	3
1	A	72	ASN	CA-C-N	-7.45	101.30	116.20	19	2
1	A	38	TYR	CB-CG-CD2	7.44	125.46	121.00	1	1
1	A	16	LEU	CB-CG-CD1	-7.43	98.37	111.00	1	1
1	A	133	LEU	CB-CG-CD2	7.41	123.60	111.00	1	2
1	A	64	ALA	N-CA-CB	-7.41	99.72	110.10	19	1
1	A	151	PHE	CB-CA-C	7.40	125.19	110.40	19	1
1	A	66	LEU	CB-CA-C	-7.40	96.15	110.20	1	2
1	A	107	TYR	CD1-CG-CD2	7.38	126.02	117.90	19	1
1	A	153	SER	CB-CA-C	-7.38	96.09	110.10	1	1
1	A	82	ARG	CB-CG-CD	-7.36	92.47	111.60	1	1
1	A	135	LEU	O-C-N	-7.34	110.96	122.70	19	1
1	A	152	SER	CA-CB-OG	-7.34	91.39	111.20	20	2
1	A	192	ASP	CB-CA-C	7.33	125.06	110.40	20	2
1	A	138	ILE	CA-CB-CG2	-7.33	96.25	110.90	19	1
1	A	24	GLU	CA-C-O	7.29	135.41	120.10	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	87	LYS	N-CA-CB	7.29	123.72	110.60	20	1
1	A	140	PRO	N-CD-CG	7.26	114.09	103.20	1	1
1	A	170	MET	O-C-N	-7.25	111.11	122.70	20	1
1	A	23	PRO	N-CA-C	7.24	130.93	112.10	20	1
1	A	15	VAL	CA-CB-CG2	7.22	121.73	110.90	20	1
1	A	85	LEU	N-CA-C	7.20	130.44	111.00	19	2
1	A	78	GLY	C-N-CA	7.17	139.62	121.70	19	1
1	A	42	GLN	CA-C-O	7.15	135.11	120.10	1	1
1	A	34	LEU	O-C-N	7.14	134.13	122.70	20	2
1	A	208	ILE	CA-CB-CG2	-7.14	96.62	110.90	19	1
1	A	31	LEU	CD1-CG-CD2	7.13	131.90	110.50	19	1
1	A	147	LEU	N-CA-CB	-7.12	96.15	110.40	1	1
1	A	182	VAL	O-C-N	-7.11	111.32	122.70	20	2
1	A	81	ILE	O-C-N	7.11	134.07	122.70	1	1
1	A	61	GLY	O-C-N	-7.11	111.33	122.70	1	1
1	A	76	LEU	CA-C-O	7.10	135.00	120.10	20	1
1	A	197	HIS	CG-CD2-NE2	-7.10	95.72	109.20	20	1
1	A	35	PHE	C-N-CA	7.09	137.20	122.30	20	1
1	A	179	GLU	CG-CD-OE1	7.09	132.49	118.30	1	2
1	A	74	HIS	CB-CA-C	-7.09	96.23	110.40	19	2
1	A	71	LEU	CB-CG-CD2	7.07	123.02	111.00	19	1
1	A	59	ALA	N-CA-CB	-7.07	100.21	110.10	19	2
1	A	197	HIS	C-N-CA	7.06	139.34	121.70	1	1
1	A	202	SER	O-C-N	-7.06	111.41	122.70	20	1
1	A	76	LEU	CB-CG-CD2	7.05	122.99	111.00	19	1
1	A	161	PHE	CB-CG-CD1	7.03	125.72	120.80	1	3
1	A	44	VAL	N-CA-CB	-7.02	96.05	111.50	19	2
1	A	55	LEU	CB-CA-C	7.01	123.51	110.20	19	1
1	A	80	PRO	N-CD-CG	7.00	113.69	103.20	19	1
1	A	195	GLU	O-C-N	-6.99	111.51	122.70	1	1
1	A	158	VAL	CA-C-N	-6.98	101.84	117.20	1	1
1	A	126	ILE	CA-C-N	-6.97	101.86	117.20	20	1
1	A	148	LYS	CB-CA-C	6.97	124.34	110.40	20	1
1	A	192	ASP	CB-CG-OD2	-6.96	112.03	118.30	20	1
1	A	162	LYS	CB-CA-C	-6.95	96.49	110.40	19	1
1	A	38	TYR	O-C-N	6.95	135.01	123.20	1	1
1	A	164	PHE	O-C-N	6.94	133.81	122.70	20	2
1	A	22	ASN	CA-C-O	-6.94	105.53	120.10	20	1
1	A	34	LEU	CA-CB-CG	6.92	131.23	115.30	1	1
1	A	63	GLN	C-N-CA	6.92	139.01	121.70	19	1
1	A	52	GLU	C-N-CA	6.92	139.00	121.70	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	193	LEU	N-CA-CB	-6.92	96.57	110.40	20	1
1	A	159	LYS	O-C-N	6.91	134.95	123.20	19	1
1	A	91	VAL	CA-CB-CG1	6.90	121.26	110.90	20	2
1	A	168	ARG	CB-CA-C	6.90	124.21	110.40	19	1
1	A	75	LYS	CB-CA-C	6.90	124.20	110.40	20	3
1	A	56	VAL	CB-CA-C	6.90	124.51	111.40	20	1
1	A	37	VAL	CG1-CB-CG2	-6.89	99.88	110.90	1	1
1	A	144	GLU	CA-C-O	-6.88	105.65	120.10	1	2
1	A	162	LYS	N-CA-CB	-6.88	98.22	110.60	19	1
1	A	62	ASN	CA-CB-CG	6.87	128.52	113.40	1	1
1	A	202	SER	N-CA-CB	-6.87	100.19	110.50	20	1
1	A	145	GLU	CB-CA-C	6.87	124.14	110.40	19	1
1	A	69	SER	CB-CA-C	-6.86	97.07	110.10	20	1
1	A	53	ASN	CA-CB-CG	6.85	128.47	113.40	1	1
1	A	57	GLN	C-N-CA	6.85	138.82	121.70	19	1
1	A	192	ASP	OD1-CG-OD2	-6.85	110.29	123.30	1	2
1	A	183	GLN	C-N-CA	6.84	138.81	121.70	1	1
1	A	160	GLY	CA-C-N	6.84	132.25	117.20	20	2
1	A	43	ARG	N-CA-CB	-6.83	98.31	110.60	19	2
1	A	104	THR	OG1-CB-CG2	-6.81	94.34	110.00	20	2
1	A	45	LYS	CA-CB-CG	6.79	128.34	113.40	20	1
1	A	20	ASN	CA-C-O	6.79	134.35	120.10	1	1
1	A	161	PHE	CD1-CE1-CZ	6.78	128.23	120.10	19	2
1	A	74	HIS	C-N-CA	6.78	138.64	121.70	19	1
1	A	164	PHE	N-CA-C	6.77	129.29	111.00	1	1
1	A	46	ILE	CA-C-O	-6.76	105.90	120.10	1	2
1	A	203	PHE	CD1-CG-CD2	6.74	127.06	118.30	20	2
1	A	208	ILE	CA-C-O	6.73	134.24	120.10	19	1
1	A	162	LYS	CA-C-O	6.73	134.23	120.10	1	1
1	A	130	SER	C-N-CA	6.73	138.52	121.70	1	1
1	A	179	GLU	CA-CB-CG	-6.73	98.60	113.40	20	1
1	A	17	LEU	C-N-CA	6.72	138.50	121.70	1	1
1	A	107	TYR	CG-CD2-CE2	-6.70	115.94	121.30	19	1
1	A	196	ASN	N-CA-C	6.70	129.08	111.00	19	1
1	A	91	VAL	C-N-CA	6.70	138.44	121.70	1	3
1	A	58	MET	CA-C-N	6.69	131.91	117.20	19	1
1	A	83	ILE	CA-CB-CG2	6.67	124.23	110.90	1	1
1	A	193	LEU	C-N-CA	6.66	136.29	122.30	1	1
1	A	55	LEU	N-CA-CB	-6.66	97.07	110.40	20	1
1	A	58	MET	N-CA-CB	-6.66	98.61	110.60	20	1
1	A	34	LEU	CB-CG-CD1	-6.66	99.69	111.00	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	22	ASN	O-C-N	-6.65	108.46	121.10	1	2
1	A	53	ASN	CB-CG-OD1	-6.65	108.30	121.60	20	2
1	A	164	PHE	CD1-CE1-CZ	-6.63	112.15	120.10	1	1
1	A	148	LYS	O-C-N	-6.62	112.11	122.70	1	1
1	A	43	ARG	CD-NE-CZ	-6.61	114.34	123.60	1	9
1	A	133	LEU	CB-CG-CD1	-6.61	99.76	111.00	20	3
1	A	186	ILE	CA-C-O	6.61	133.97	120.10	1	1
1	A	196	ASN	OD1-CG-ND2	-6.60	106.72	121.90	1	2
1	A	199	LEU	CB-CA-C	6.59	122.72	110.20	19	1
1	A	107	TYR	CD1-CE1-CZ	6.58	125.72	119.80	1	1
1	A	58	MET	O-C-N	6.58	133.22	122.70	1	1
1	A	104	THR	CA-CB-CG2	-6.57	103.20	112.40	1	1
1	A	140	PRO	O-C-N	6.56	133.19	122.70	1	1
1	A	167	ASP	CA-CB-CG	6.55	127.81	113.40	1	1
1	A	61	GLY	CA-C-N	6.54	131.58	117.20	1	1
1	A	77	HIS	CB-CA-C	-6.53	97.34	110.40	1	1
1	A	68	MET	O-C-N	-6.51	112.29	122.70	1	2
1	A	189	HIS	N-CA-CB	-6.51	98.89	110.60	20	1
1	A	180	GLU	O-C-N	-6.50	112.30	122.70	19	1
1	A	17	LEU	CB-CG-CD2	-6.50	99.95	111.00	20	1
1	A	46	ILE	C-N-CA	-6.48	105.50	121.70	20	1
1	A	135	LEU	CB-CA-C	-6.47	97.91	110.20	19	2
1	A	168	ARG	CD-NE-CZ	-6.47	114.55	123.60	1	1
1	A	177	SER	C-N-CA	-6.46	105.54	121.70	1	1
1	A	107	TYR	CB-CA-C	6.45	123.30	110.40	20	2
1	A	60	ASP	CB-CA-C	-6.45	97.51	110.40	20	1
1	A	158	VAL	C-N-CA	6.44	137.81	121.70	20	1
1	A	164	PHE	CD1-CG-CD2	6.43	126.66	118.30	1	2
1	A	164	PHE	CB-CG-CD1	-6.42	116.31	120.80	1	1
1	A	129	PRO	N-CD-CG	6.42	112.83	103.20	19	1
1	A	24	GLU	OE1-CD-OE2	6.42	131.00	123.30	20	1
1	A	149	VAL	C-N-CA	6.41	137.72	121.70	19	1
1	A	188	LEU	CB-CA-C	6.41	122.37	110.20	19	1
1	A	127	PHE	CB-CA-C	6.40	123.19	110.40	1	1
1	A	14	SER	C-N-CA	6.38	137.66	121.70	1	1
1	A	23	PRO	CA-C-N	6.38	131.23	117.20	19	1
1	A	86	SER	O-C-N	-6.38	112.50	122.70	1	1
1	A	104	THR	O-C-N	-6.37	112.51	122.70	20	2
1	A	150	LEU	CA-CB-CG	6.36	129.94	115.30	19	1
1	A	108	GLY	O-C-N	6.36	132.88	122.70	20	1
1	A	31	LEU	O-C-N	-6.36	112.52	122.70	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	22	ASN	N-CA-CB	6.35	122.03	110.60	20	1
1	A	24	GLU	C-N-CA	6.34	137.55	121.70	20	1
1	A	69	SER	C-N-CA	6.34	137.54	121.70	19	1
1	A	79	LYS	O-C-N	-6.33	109.07	121.10	20	1
1	A	31	LEU	CB-CA-C	6.33	122.23	110.20	1	1
1	A	153	SER	N-CA-C	6.33	128.08	111.00	1	2
1	A	26	VAL	CA-CB-CG2	6.32	120.39	110.90	1	1
1	A	199	LEU	CA-C-O	6.32	133.37	120.10	1	1
1	A	200	ARG	NH1-CZ-NH2	-6.31	112.45	119.40	20	1
1	A	183	GLN	CB-CA-C	-6.31	97.78	110.40	19	1
1	A	69	SER	N-CA-CB	6.31	119.97	110.50	20	1
1	A	22	ASN	CA-CB-CG	6.31	127.27	113.40	1	1
1	A	138	ILE	N-CA-CB	6.30	125.29	110.80	1	1
1	A	21	LEU	N-CA-CB	-6.29	97.82	110.40	1	2
1	A	153	SER	N-CA-CB	6.29	119.93	110.50	20	1
1	A	198	HIS	CA-CB-CG	6.29	124.29	113.60	19	1
1	A	185	LEU	N-CA-C	-6.28	94.04	111.00	1	1
1	A	19	SER	N-CA-C	-6.28	94.04	111.00	20	1
1	A	207	THR	CA-CB-CG2	-6.27	103.62	112.40	1	1
1	A	67	ALA	N-CA-CB	6.27	118.88	110.10	19	1
1	A	132	THR	OG1-CB-CG2	6.26	124.40	110.00	19	2
1	A	29	GLN	CA-C-O	-6.26	106.96	120.10	19	1
1	A	84	THR	O-C-N	6.25	132.71	122.70	19	1
1	A	76	LEU	CB-CG-CD1	6.25	121.63	111.00	1	1
1	A	193	LEU	CB-CG-CD1	-6.24	100.39	111.00	20	1
1	A	144	GLU	C-N-CA	6.24	137.29	121.70	19	1
1	A	62	ASN	CB-CG-OD1	-6.23	109.14	121.60	20	2
1	A	199	LEU	N-CA-CB	-6.22	97.96	110.40	20	1
1	A	38	TYR	CG-CD1-CE1	-6.21	116.33	121.30	19	2
1	A	17	LEU	O-C-N	-6.21	112.77	122.70	19	2
1	A	165	GLN	N-CA-C	6.20	127.75	111.00	20	1
1	A	85	LEU	C-N-CA	6.20	137.21	121.70	20	1
1	A	161	PHE	N-CA-CB	6.20	121.76	110.60	1	1
1	A	188	LEU	O-C-N	-6.20	112.78	122.70	1	1
1	A	206	SER	O-C-N	-6.20	112.78	122.70	20	1
1	A	24	GLU	N-CA-CB	-6.20	99.45	110.60	1	1
1	A	17	LEU	CA-C-O	6.18	133.08	120.10	1	1
1	A	164	PHE	CZ-CE2-CD2	-6.17	112.69	120.10	19	1
1	A	194	GLY	CA-C-N	-6.17	103.62	117.20	19	1
1	A	149	VAL	CA-CB-CG2	-6.17	101.65	110.90	20	1
1	A	82	ARG	O-C-N	6.16	132.56	122.70	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	129	PRO	N-CA-CB	6.16	110.70	103.30	20	1
1	A	160	GLY	C-N-CA	6.16	137.11	121.70	20	1
1	A	170	MET	N-CA-C	6.16	127.63	111.00	19	1
1	A	60	ASP	N-CA-CB	6.16	121.69	110.60	20	1
1	A	81	ILE	CA-C-N	-6.16	103.66	117.20	1	1
1	A	23	PRO	N-CA-CB	-6.16	95.83	102.60	20	1
1	A	141	SER	CA-CB-OG	6.15	127.80	111.20	20	1
1	A	39	GLY	CA-C-N	6.15	130.72	117.20	19	1
1	A	40	ASP	CA-C-O	6.13	132.98	120.10	20	1
1	A	133	LEU	CB-CA-C	6.13	121.84	110.20	1	1
1	A	31	LEU	CA-C-O	6.13	132.97	120.10	19	1
1	A	106	ASP	OD1-CG-OD2	-6.12	111.67	123.30	1	1
1	A	197	HIS	ND1-CG-CD2	-6.12	97.43	106.00	19	1
1	A	128	PRO	O-C-N	-6.11	109.49	121.10	1	1
1	A	29	GLN	N-CA-CB	6.10	121.59	110.60	20	1
1	A	195	GLU	CG-CD-OE1	-6.10	106.10	118.30	1	1
1	A	185	LEU	CB-CG-CD1	6.08	121.34	111.00	20	1
1	A	145	GLU	CG-CD-OE1	6.08	130.46	118.30	19	1
1	A	187	ASP	C-N-CA	6.07	136.88	121.70	19	1
1	A	59	ALA	CB-CA-C	6.06	119.19	110.10	1	1
1	A	106	ASP	CB-CG-OD1	6.05	123.75	118.30	1	1
1	A	15	VAL	O-C-N	-6.05	113.01	122.70	19	1
1	A	58	MET	CG-SD-CE	-6.04	90.54	100.20	1	1
1	A	196	ASN	N-CA-CB	-6.04	99.73	110.60	1	1
1	A	207	THR	N-CA-CB	-6.04	98.83	110.30	20	1
1	A	172	LEU	CA-C-N	6.03	130.46	117.20	19	1
1	A	135	LEU	CB-CG-CD2	6.02	121.24	111.00	20	1
1	A	163	PHE	CG-CD1-CE1	-6.02	114.18	120.80	1	1
1	A	19	SER	O-C-N	-6.01	113.08	122.70	19	1
1	A	157	VAL	CB-CA-C	-6.01	99.98	111.40	19	1
1	A	152	SER	N-CA-CB	-6.01	101.49	110.50	20	1
1	A	86	SER	CB-CA-C	6.00	121.51	110.10	20	2
1	A	191	HIS	N-CA-CB	5.99	121.39	110.60	1	1
1	A	76	LEU	CB-CA-C	-5.98	98.84	110.20	1	1
1	A	89	GLN	CG-CD-NE2	5.97	131.03	116.70	19	1
1	A	70	HIS	N-CA-CB	-5.96	99.87	110.60	19	1
1	A	44	VAL	CA-CB-CG1	5.95	119.82	110.90	1	1
1	A	173	ILE	CA-CB-CG1	5.95	122.30	111.00	1	1
1	A	149	VAL	O-C-N	-5.94	113.19	122.70	1	1
1	A	133	LEU	O-C-N	5.94	132.21	122.70	19	1
1	A	81	ILE	C-N-CA	5.94	136.55	121.70	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	ILE	CA-C-N	5.93	130.24	117.20	19	1
1	A	38	TYR	CA-C-O	-5.93	107.65	120.10	1	1
1	A	22	ASN	CB-CG-ND2	-5.93	102.48	116.70	20	1
1	A	88	HIS	N-CA-CB	-5.92	99.94	110.60	19	1
1	A	150	LEU	CD1-CG-CD2	-5.92	92.73	110.50	20	1
1	A	31	LEU	CB-CG-CD2	-5.92	100.94	111.00	19	1
1	A	24	GLU	N-CA-C	5.91	126.97	111.00	19	1
1	A	130	SER	O-C-N	-5.91	113.24	122.70	1	1
1	A	89	GLN	CA-CB-CG	5.91	126.39	113.40	19	1
1	A	18	VAL	O-C-N	5.90	132.15	122.70	20	1
1	A	74	HIS	CB-CG-ND1	5.90	137.96	123.20	20	1
1	A	150	LEU	CA-C-O	-5.89	107.72	120.10	1	1
1	A	71	LEU	N-CA-CB	-5.89	98.61	110.40	20	1
1	A	27	THR	CB-CA-C	5.89	127.51	111.60	1	1
1	A	17	LEU	CB-CG-CD1	-5.89	100.99	111.00	1	1
1	A	40	ASP	N-CA-C	-5.88	95.12	111.00	20	1
1	A	82	ARG	CA-CB-CG	5.85	126.27	113.40	1	1
1	A	45	LYS	N-CA-CB	-5.85	100.08	110.60	19	3
1	A	159	LYS	CD-CE-NZ	-5.84	98.27	111.70	19	1
1	A	46	ILE	CA-C-N	5.84	130.04	117.20	1	1
1	A	126	ILE	C-N-CA	5.83	136.28	121.70	1	1
1	A	136	SER	CA-CB-OG	5.83	126.95	111.20	1	1
1	A	179	GLU	OE1-CD-OE2	-5.83	116.30	123.30	1	1
1	A	66	LEU	CD1-CG-CD2	-5.83	93.01	110.50	19	1
1	A	201	VAL	CB-CA-C	-5.82	100.34	111.40	20	2
1	A	126	ILE	CA-CB-CG1	-5.82	99.95	111.00	20	2
1	A	56	VAL	N-CA-CB	-5.81	98.71	111.50	19	1
1	A	70	HIS	CB-CA-C	-5.81	98.78	110.40	20	1
1	A	126	ILE	CB-CG1-CD1	-5.81	97.63	113.90	19	1
1	A	66	LEU	O-C-N	-5.78	113.45	122.70	1	1
1	A	19	SER	CA-C-O	5.78	132.25	120.10	19	1
1	A	75	LYS	CA-C-N	-5.78	104.48	117.20	19	1
1	A	127	PHE	CD1-CE1-CZ	-5.78	113.17	120.10	1	1
1	A	80	PRO	CA-C-N	-5.78	104.49	117.20	19	1
1	A	193	LEU	CB-CG-CD2	5.78	120.82	111.00	20	1
1	A	157	VAL	N-CA-CB	5.77	124.20	111.50	19	1
1	A	145	GLU	N-CA-CB	-5.77	100.22	110.60	19	1
1	A	18	VAL	C-N-CA	5.76	136.09	121.70	19	2
1	A	155	GLY	O-C-N	5.76	132.99	123.20	19	2
1	A	179	GLU	CG-CD-OE2	-5.75	106.79	118.30	1	2
1	A	83	ILE	CB-CA-C	-5.75	100.09	111.60	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	104	THR	C-N-CA	5.75	136.08	121.70	20	1
1	A	199	LEU	O-C-N	-5.75	113.50	122.70	1	1
1	A	60	ASP	CA-CB-CG	5.74	126.03	113.40	1	1
1	A	194	GLY	O-C-N	5.74	131.88	122.70	1	1
1	A	70	HIS	CG-ND1-CE1	5.74	116.23	108.20	1	1
1	A	58	MET	CB-CA-C	5.72	121.85	110.40	19	1
1	A	13	ASN	O-C-N	-5.72	113.55	122.70	19	1
1	A	44	VAL	C-N-CA	5.71	135.99	121.70	1	1
1	A	108	GLY	C-N-CA	5.71	135.98	121.70	19	1
1	A	21	LEU	CB-CA-C	5.71	121.05	110.20	20	1
1	A	128	PRO	N-CA-CB	5.70	110.14	103.30	20	1
1	A	70	HIS	O-C-N	-5.70	113.58	122.70	1	1
1	A	38	TYR	CB-CG-CD1	5.69	124.41	121.00	1	3
1	A	70	HIS	CE1-NE2-CD2	-5.68	92.39	106.60	19	1
1	A	130	SER	CA-CB-OG	5.68	126.54	111.20	20	1
1	A	171	ALA	N-CA-CB	5.67	118.05	110.10	1	1
1	A	42	GLN	C-N-CA	5.66	135.85	121.70	19	1
1	A	82	ARG	CG-CD-NE	-5.63	99.97	111.80	1	1
1	A	38	TYR	CD1-CE1-CZ	-5.63	114.73	119.80	20	2
1	A	203	PHE	CG-CD2-CE2	-5.63	114.61	120.80	19	1
1	A	105	LYS	CA-CB-CG	5.63	125.78	113.40	20	1
1	A	179	GLU	CB-CG-CD	-5.62	99.02	114.20	1	1
1	A	178	VAL	O-C-N	5.62	131.68	122.70	20	2
1	A	198	HIS	N-CA-CB	-5.61	100.50	110.60	1	1
1	A	13	ASN	C-N-CA	5.61	135.73	121.70	19	1
1	A	138	ILE	CB-CA-C	-5.61	100.38	111.60	19	1
1	A	39	GLY	CA-C-O	-5.61	110.51	120.60	19	1
1	A	192	ASP	CA-C-O	5.61	131.88	120.10	20	1
1	A	18	VAL	N-CA-CB	-5.60	99.18	111.50	19	1
1	A	168	ARG	CA-C-N	-5.60	104.88	117.20	20	1
1	A	150	LEU	C-N-CA	5.60	135.70	121.70	19	1
1	A	34	LEU	N-CA-CB	-5.59	99.21	110.40	1	1
1	A	62	ASN	C-N-CA	5.59	135.68	121.70	20	1
1	A	18	VAL	CA-CB-CG1	5.58	119.26	110.90	1	1
1	A	47	LEU	N-CA-C	-5.57	95.96	111.00	1	2
1	A	132	THR	CA-CB-CG2	-5.56	104.61	112.40	20	2
1	A	201	VAL	CA-C-N	-5.54	105.00	117.20	19	1
1	A	137	ASN	O-C-N	-5.54	113.84	122.70	1	1
1	A	153	SER	CA-C-N	-5.54	105.02	117.20	19	2
1	A	140	PRO	CB-CA-C	5.54	125.84	112.00	19	1
1	A	205	LYS	CB-CG-CD	5.53	125.98	111.60	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	GLN	OE1-CD-NE2	-5.53	109.19	121.90	19	1
1	A	26	VAL	CA-CB-CG1	5.52	119.18	110.90	1	1
1	A	183	GLN	O-C-N	-5.52	113.87	122.70	20	1
1	A	142	VAL	O-C-N	5.50	131.51	122.70	20	1
1	A	188	LEU	N-CA-CB	-5.50	99.40	110.40	20	1
1	A	171	ALA	CB-CA-C	5.50	118.34	110.10	20	1
1	A	72	ASN	CB-CG-OD1	-5.49	110.63	121.60	19	2
1	A	57	GLN	CA-CB-CG	-5.48	101.34	113.40	1	1
1	A	41	VAL	O-C-N	-5.48	113.93	122.70	19	1
1	A	137	ASN	CB-CG-ND2	-5.47	103.56	116.70	19	1
1	A	54	ALA	CA-C-N	-5.47	105.17	117.20	20	1
1	A	88	HIS	CB-CG-ND1	5.46	136.86	123.20	19	1
1	A	126	ILE	CA-C-O	5.46	131.57	120.10	20	1
1	A	41	VAL	C-N-CA	5.45	135.33	121.70	19	1
1	A	165	GLN	CG-CD-OE1	-5.45	110.70	121.60	1	1
1	A	80	PRO	O-C-N	-5.45	113.99	122.70	1	1
1	A	202	SER	CA-C-O	5.44	131.52	120.10	20	1
1	A	57	GLN	CA-C-N	-5.43	105.26	117.20	1	1
1	A	195	GLU	CB-CG-CD	-5.42	99.56	114.20	19	1
1	A	90	ASN	CB-CA-C	5.42	121.25	110.40	1	1
1	A	72	ASN	CB-CA-C	5.42	121.25	110.40	20	1
1	A	105	LYS	O-C-N	5.42	131.37	122.70	1	1
1	A	86	SER	C-N-CA	5.42	135.24	121.70	19	1
1	A	90	ASN	CB-CG-OD1	5.40	132.40	121.60	1	1
1	A	167	ASP	CA-C-N	5.39	129.07	117.20	1	1
1	A	104	THR	CB-CA-C	-5.38	97.06	111.60	19	1
1	A	133	LEU	CA-C-O	-5.38	108.79	120.10	19	1
1	A	37	VAL	C-N-CA	5.38	135.15	121.70	20	1
1	A	127	PHE	CZ-CE2-CD2	-5.38	113.65	120.10	20	1
1	A	187	ASP	O-C-N	-5.37	114.10	122.70	19	1
1	A	76	LEU	N-CA-CB	-5.37	99.66	110.40	20	1
1	A	158	VAL	CA-CB-CG1	5.37	118.95	110.90	19	1
1	A	21	LEU	C-N-CA	5.37	135.12	121.70	19	1
1	A	68	MET	CB-CG-SD	5.36	128.48	112.40	1	1
1	A	91	VAL	CA-C-N	-5.36	105.41	117.20	1	1
1	A	43	ARG	N-CA-C	-5.36	96.53	111.00	20	1
1	A	13	ASN	N-CA-C	5.35	125.44	111.00	1	1
1	A	150	LEU	O-C-N	5.34	131.25	122.70	1	1
1	A	189	HIS	CG-ND1-CE1	-5.34	98.76	105.70	1	1
1	A	105	LYS	CA-C-N	-5.33	105.47	117.20	19	1
1	A	62	ASN	CA-C-N	-5.31	105.51	117.20	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	195	GLU	CA-C-O	5.31	131.25	120.10	1	1
1	A	201	VAL	O-C-N	-5.31	114.20	122.70	1	1
1	A	29	GLN	C-N-CA	-5.31	108.43	121.70	19	1
1	A	74	HIS	CG-ND1-CE1	5.31	115.63	108.20	19	1
1	A	174	GLN	N-CA-CB	5.30	120.15	110.60	19	1
1	A	27	THR	C-N-CD	5.30	139.53	128.40	1	1
1	A	130	SER	CA-C-O	5.30	131.23	120.10	1	1
1	A	151	PHE	N-CA-CB	-5.30	101.07	110.60	1	1
1	A	86	SER	CA-CB-OG	5.29	125.48	111.20	1	1
1	A	155	GLY	CA-C-N	-5.29	105.62	116.20	19	1
1	A	159	LYS	CA-CB-CG	-5.29	101.77	113.40	19	1
1	A	164	PHE	CA-C-N	-5.29	105.57	117.20	20	1
1	A	175	MET	CG-SD-CE	-5.27	91.76	100.20	1	2
1	A	37	VAL	N-CA-CB	5.27	123.10	111.50	19	1
1	A	149	VAL	CA-C-N	5.27	128.80	117.20	1	1
1	A	178	VAL	CG1-CB-CG2	-5.26	102.48	110.90	20	1
1	A	42	GLN	CB-CG-CD	5.26	125.28	111.60	19	1
1	A	162	LYS	CG-CD-CE	5.26	127.67	111.90	1	1
1	A	37	VAL	O-C-N	5.25	131.10	122.70	19	1
1	A	46	ILE	CB-CA-C	5.25	122.09	111.60	19	1
1	A	131	ALA	C-N-CA	5.24	134.80	121.70	1	1
1	A	83	ILE	N-CA-C	-5.23	96.89	111.00	1	1
1	A	190	ASN	CB-CA-C	5.23	120.86	110.40	19	1
1	A	189	HIS	C-N-CA	5.22	134.76	121.70	20	1
1	A	31	LEU	CB-CG-CD1	5.22	119.88	111.00	20	1
1	A	22	ASN	CA-C-N	5.22	131.71	117.10	1	1
1	A	84	THR	CA-CB-OG1	5.22	119.95	109.00	19	1
1	A	190	ASN	CA-CB-CG	5.21	124.87	113.40	19	1
1	A	77	HIS	CA-C-O	5.21	131.05	120.10	1	1
1	A	133	LEU	C-N-CA	5.21	134.73	121.70	20	1
1	A	198	HIS	CB-CA-C	5.21	120.81	110.40	1	1
1	A	202	SER	CB-CA-C	-5.20	100.22	110.10	1	1
1	A	43	ARG	C-N-CA	5.19	134.69	121.70	1	1
1	A	167	ASP	C-N-CA	5.19	134.67	121.70	19	2
1	A	83	ILE	CB-CG1-CD1	5.17	128.39	113.90	19	1
1	A	36	GLY	CA-C-N	5.17	128.57	117.20	1	1
1	A	68	MET	CA-C-O	5.16	130.93	120.10	20	1
1	A	126	ILE	CA-CB-CG2	-5.16	100.59	110.90	19	1
1	A	160	GLY	N-CA-C	-5.15	100.23	113.10	19	1
1	A	45	LYS	CG-CD-CE	5.14	127.33	111.90	1	1
1	A	52	GLU	CB-CA-C	5.14	120.69	110.40	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	167	ASP	CA-C-O	5.14	130.89	120.10	19	1
1	A	74	HIS	CA-CB-CG	-5.14	104.87	113.60	1	1
1	A	173	ILE	CB-CG1-CD1	5.14	128.29	113.90	19	1
1	A	147	LEU	CA-C-O	5.14	130.89	120.10	20	1
1	A	35	PHE	CA-CB-CG	5.13	126.22	113.90	20	1
1	A	90	ASN	N-CA-CB	-5.13	101.37	110.60	1	1
1	A	129	PRO	C-N-CA	-5.13	108.88	121.70	1	1
1	A	41	VAL	N-CA-C	5.12	124.83	111.00	1	1
1	A	87	LYS	CD-CE-NZ	5.12	123.48	111.70	1	1
1	A	32	PHE	CG-CD2-CE2	5.12	126.43	120.80	19	1
1	A	62	ASN	OD1-CG-ND2	-5.11	110.15	121.90	1	1
1	A	192	ASP	C-N-CA	-5.11	108.93	121.70	19	1
1	A	188	LEU	N-CA-C	5.11	124.79	111.00	20	1
1	A	25	ARG	CA-C-O	-5.10	109.39	120.10	19	1
1	A	190	ASN	O-C-N	-5.10	114.54	122.70	1	1
1	A	208	ILE	CG1-CB-CG2	-5.09	100.19	111.40	1	2
1	A	18	VAL	CB-CA-C	-5.09	101.74	111.40	1	1
1	A	170	MET	N-CA-CB	5.08	119.74	110.60	19	1
1	A	33	ILE	CA-CB-CG1	-5.07	101.36	111.00	1	1
1	A	174	GLN	CG-CD-NE2	-5.07	104.53	116.70	20	1
1	A	27	THR	OG1-CB-CG2	-5.07	98.34	110.00	20	1
1	A	147	LEU	CA-C-N	5.06	128.34	117.20	19	1
1	A	203	PHE	CB-CA-C	-5.06	100.28	110.40	1	1
1	A	42	GLN	CG-CD-NE2	5.06	128.84	116.70	19	1
1	A	162	LYS	O-C-N	-5.06	114.61	122.70	1	1
1	A	174	GLN	CA-CB-CG	-5.06	102.28	113.40	20	1
1	A	136	SER	C-N-CA	5.05	134.33	121.70	20	1
1	A	31	LEU	CA-C-N	5.04	128.29	117.20	1	1
1	A	181	ALA	O-C-N	-5.04	114.63	122.70	1	1
1	A	29	GLN	CA-CB-CG	5.04	124.48	113.40	19	1
1	A	16	LEU	N-CA-C	5.04	124.60	111.00	1	1
1	A	36	GLY	O-C-N	-5.03	114.66	122.70	1	1
1	A	163	PHE	O-C-N	-5.02	114.66	122.70	1	1
1	A	170	MET	CB-CG-SD	5.02	127.47	112.40	1	1
1	A	20	ASN	CA-C-N	5.02	128.25	117.20	19	1
1	A	20	ASN	CA-CB-CG	5.02	124.44	113.40	19	1
1	A	106	ASP	O-C-N	5.02	130.73	122.70	19	1
1	A	197	HIS	CE1-NE2-CD2	-5.02	94.05	106.60	19	1
1	A	184	ALA	CA-C-N	-5.01	106.17	117.20	19	1
1	A	153	SER	CA-CB-OG	5.01	124.73	111.20	19	1
1	A	203	PHE	CZ-CE2-CD2	-5.01	114.09	120.10	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	166	LYS	N-CA-C	5.01	124.53	111.00	19	1
1	A	89	GLN	C-N-CA	5.00	134.21	121.70	19	1
1	A	74	HIS	CA-C-N	5.00	128.20	117.20	19	1
1	A	151	PHE	CA-CB-CG	5.00	125.90	113.90	19	1
1	A	156	GLY	CA-C-N	-5.00	106.20	117.20	20	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	70	HIS	Sidechain,Mainchain	3
1	A	200	ARG	Sidechain	3
1	A	163	PHE	Sidechain,Mainchain	3
1	A	74	HIS	Sidechain,Mainchain	3
1	A	38	TYR	Sidechain	3
1	A	77	HIS	Sidechain	3
1	A	79	LYS	Mainchain	2
1	A	133	LEU	Mainchain	2
1	A	161	PHE	Sidechain	2
1	A	134	HIS	Sidechain	2
1	A	179	GLU	Sidechain,Mainchain	2
1	A	86	SER	Mainchain	2
1	A	151	PHE	Sidechain,Mainchain	2
1	A	168	ARG	Sidechain,Mainchain	2
1	A	137	ASN	Mainchain	2
1	A	181	ALA	Mainchain	2
1	A	53	ASN	Sidechain	2
1	A	104	THR	Mainchain	2
1	A	159	LYS	Mainchain	2
1	A	197	HIS	Sidechain	2
1	A	25	ARG	Sidechain,Mainchain	2
1	A	127	PHE	Sidechain	2
1	A	60	ASP	Mainchain	2
1	A	32	PHE	Sidechain,Mainchain	2
1	A	185	LEU	Mainchain	2
1	A	189	HIS	Mainchain,Sidechain	2
1	A	82	ARG	Sidechain	2
1	A	206	SER	Mainchain	2
1	A	107	TYR	Sidechain	2
1	A	43	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	191	HIS	Sidechain	2
1	A	128	PRO	Peptide,Mainchain	2
1	A	58	MET	Mainchain	1
1	A	198	HIS	Mainchain	1
1	A	78	GLY	Mainchain	1
1	A	193	LEU	Mainchain	1
1	A	57	GLN	Sidechain	1
1	A	39	GLY	Mainchain	1
1	A	171	ALA	Mainchain	1
1	A	14	SER	Mainchain	1
1	A	47	LEU	Mainchain	1
1	A	143	SER	Mainchain	1
1	A	87	LYS	Mainchain	1
1	A	203	PHE	Sidechain	1
1	A	195	GLU	Mainchain	1
1	A	145	GLU	Sidechain	1
1	A	31	LEU	Mainchain	1
1	A	69	SER	Mainchain	1
1	A	180	GLU	Sidechain,Mainchain	1
1	A	33	ILE	Mainchain	1
1	A	158	VAL	Mainchain	1
1	A	135	LEU	Mainchain	1
1	A	65	GLN	Mainchain	1
1	A	182	VAL	Mainchain	1
1	A	54	ALA	Mainchain	1
1	A	46	ILE	Mainchain	1
1	A	18	VAL	Mainchain	1
1	A	55	LEU	Mainchain	1
1	A	68	MET	Mainchain	1
1	A	71	LEU	Mainchain	1
1	A	186	ILE	Mainchain	1
1	A	146	ASP	Sidechain	1
1	A	62	ASN	Mainchain	1
1	A	183	GLN	Sidechain	1
1	A	19	SER	Mainchain	1
1	A	22	ASN	Sidechain	1
1	A	131	ALA	Mainchain	1
1	A	20	ASN	Sidechain,Mainchain	1
1	A	72	ASN	Sidechain	1
1	A	24	GLU	Sidechain,Mainchain	1
1	A	187	ASP	Sidechain	1
1	A	152	SER	Mainchain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	45	LYS	Mainchain	1
1	A	170	MET	Mainchain	1
1	A	149	VAL	Mainchain	1
1	A	165	GLN	Mainchain	1
1	A	13	ASN	Mainchain	1
1	A	36	GLY	Mainchain	1
1	A	157	VAL	Mainchain	1
1	A	105	LYS	Mainchain	1
1	A	66	LEU	Mainchain	1
1	A	188	LEU	Mainchain	1
1	A	164	PHE	Sidechain	1
1	A	130	SER	Mainchain	1
1	A	192	ASP	Sidechain,Mainchain	1
1	A	153	SER	Mainchain	1
1	A	88	HIS	Sidechain	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	1285	11±15
All	All	25440	25820	25801	218

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 4.

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:CG	1:A:58:MET:SD	1.47	2.01	19	1
1:A:170:MET:SD	1:A:170:MET:CE	1.43	2.07	1	1
1:A:140:PRO:CA	1:A:140:PRO:N	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	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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:81:ILE:HD13	1:A:81:ILE:H	0.73	1.41	2	3
1:A:21:LEU:HD13	1:A:52:GLU:O	0.69	1.87	19	1
1:A:133:LEU:HD23	1:A:133:LEU:H	0.69	1.47	20	2
1:A:66:LEU:C	1:A:66:LEU:HD23	0.69	2.08	1	1
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	3
1:A:166:LYS:CG	1:A:166:LYS:CE	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:58:MET:SD	1:A:58:MET:CB	0.62	2.86	19	1
1:A:21:LEU:HD13	1:A:26:VAL:HG21	0.62	1.70	1	1
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:17:LEU:HD21	1:A:53:ASN:CG	0.61	2.16	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:140:PRO:C	1:A:140:PRO:N	0.58	2.52	19	1
1:A:57:GLN:HE22	1:A:90:ASN:ND2	0.57	1.96	19	1
1:A:81:ILE:CD1	1:A:81:ILE:H	0.56	2.13	2	1
1:A:17:LEU:HD23	1:A:18:VAL:N	0.55	2.16	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:N	1:A:81:ILE:HD13	0.54	2.17	20	2
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:81:ILE:HD13	1:A:81:ILE:N	0.53	2.16	3	2
1:A:14:SER:HB3	1:A:60:ASP:HA	0.53	1.80	1	1
1:A:138:ILE:O	1:A:138:ILE:CG1	0.52	2.57	19	1
1:A:73:GLY:H	1:A:81:ILE:HG12	0.52	1.64	1	1
1:A:33:ILE:HG21	1:A:186:ILE:HG22	0.52	1.82	20	2
1:A:73:GLY:N	1:A:81:ILE:HD11	0.52	2.20	1	1
1:A:151:PHE:CE2	1:A:188:LEU:HD23	0.51	2.40	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:HD11	1:A:169:LYS:O	0.51	2.06	1	1
1:A:66:LEU:C	1:A:66:LEU:CD2	0.51	2.79	1	1
1:A:166:LYS:CD	1:A:166:LYS:NZ	0.50	2.65	1	1
1:A:40:ASP:N	1:A:63:GLN:OE1	0.50	2.44	19	1
1:A:21:LEU:HD13	1:A:26:VAL:CG2	0.50	2.36	1	1
1:A:57:GLN:HE22	1:A:90:ASN:HD21	0.50	1.50	19	1
1:A:185:LEU:O	1:A:186:ILE:C	0.50	2.47	1	1
1:A:59:ALA:HB3	1:A:63:GLN:HG3	0.50	1.81	2	2
1:A:58:MET:CE	1:A:58:MET:CG	0.50	2.84	19	1
1:A:170:MET:CB	1:A:170:MET:CE	0.50	2.90	1	1
1:A:165:GLN:HG2	1:A:166:LYS:H	0.49	1.66	20	1
1:A:189:HIS:N	1:A:201:VAL:CG1	0.49	2.76	19	1
1:A:145:GLU:HG2	1:A:145:GLU:O	0.49	2.07	19	1
1:A:134:HIS:O	1:A:135:LEU:HD13	0.49	2.07	20	1
1:A:134:HIS:CD2	1:A:134:HIS:C	0.48	2.87	1	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: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:31:LEU:HD11	1:A:44:VAL:CG1	0.47	2.39	13	2
1:A:139:PRO:C	1:A:140:PRO:CA	0.47	2.66	19	1
1:A:81:ILE:N	1:A:81:ILE:CD1	0.47	2.78	20	3
1:A:45:LYS:CE	1:A:91:VAL:HG11	0.47	2.40	1	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:131:ALA:O	1:A:174:GLN:HG2	0.46	2.10	1	1
1:A:22:ASN:O	1:A:26:VAL:HG22	0.46	2.11	5	1
1:A:66:LEU:HD23	1:A:66:LEU:O	0.46	2.09	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:28:PRO:HG3	1:A:46:ILE:HD12	0.45	1.87	1	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:133:LEU:N	1:A:133:LEU:CD2	0.45	2.79	20	1
1:A:16:LEU:HD21	1:A:64:ALA:HB1	0.45	1.88	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

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:GLN:HB2	1:A:57:GLN:HB3	0.45	1.88	19	1
1:A:15:VAL:HG11	1:A:88:HIS: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: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	1
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:58:MET:HG3	1:A:59:ALA:N	0.44	2.27	1	1
1:A:138:ILE:HG13	1:A:138:ILE:O	0.43	2.12	19	1
1:A:55:LEU:C	1:A:55:LEU:CD1	0.43	2.86	20	1
1:A:31:LEU:C	1:A:31:LEU:HD12	0.43	2.33	15	2
1:A:18:VAL:HB	1:A:54:ALA:HB3	0.43	1.90	20	1
1:A:58:MET:CE	1:A:58:MET:HA	0.43	2.43	19	1
1:A:133:LEU:HD22	1:A:173:ILE:HG22	0.43	1.90	10	2
1:A:175:MET:N	1:A:175:MET:SD	0.43	2.91	1	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:45:LYS:C	1:A:46:ILE:HD12	0.42	2.34	19	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:29:GLN:C	1:A:29:GLN:HE21	0.42	2.16	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:133:LEU:HD12	1:A:151:PHE:HE1	0.42	1.75	19	1
1:A:190:ASN:HA	1:A:199:LEU:O	0.42	2.15	1	1
1:A:132:THR:HG21	1:A:206:SER:O	0.42	2.15	19	1
1:A:17:LEU:C	1:A:18:VAL:HG23	0.42	2.35	19	1
1:A:19:SER:O	1:A:20:ASN:CB	0.42	2.68	20	1
1:A:76:LEU:O	1:A:79:LYS:HE2	0.42	2.14	16	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:148:LYS:HB2	1:A:161:PHE:CD2	0.41	2.49	19	1
1:A:136:SER:N	1:A:200:ARG:O	0.41	2.53	19	1
1:A:57:GLN:HE22	1:A:91:VAL:HG12	0.41	1.75	17	1
1:A:133:LEU:CD2	1:A:133:LEU:H	0.41	2.27	1	1
1:A:66:LEU:O	1:A:67:ALA:C	0.41	2.54	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:ILE:HD12	1:A:186:ILE:HA	0.41	1.91	1	1
1:A:45:LYS:HD3	1:A:104:THR:CG2	0.41	2.45	19	1
1:A:186:ILE:HG21	1:A:186:ILE:HD13	0.41	1.72	1	1
1:A:145:GLU:CG	1:A:145:GLU:O	0.41	2.69	20	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:20:ASN:CG	1:A:20:ASN:O	0.41	2.58	20	1
1:A:127:PHE:CE2	1:A:205:LYS:HB3	0.41	2.51	20	1
1:A:16:LEU:HD11	1:A:64:ALA:O	0.41	2.16	1	1
1:A:178:VAL:C	1:A:180:GLU:N	0.41	2.75	1	1
1:A:133:LEU:HD21	1:A:181:ALA:HB1	0.40	1.93	15	2
1:A:170:MET:HB2	1:A:170:MET:CE	0.40	2.46	1	1
1:A:151:PHE:HA	1:A:154:ASN:ND2	0.40	2.31	1	1
1:A:68:MET:HG3	1:A:69:SER:N	0.40	2.32	19	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

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

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	165	GLN	14
1	A	15	VAL	14
1	A	61	GLY	13
1	A	14	SER	12
1	A	197	HIS	10
1	A	20	ASN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	196	ASN	10
1	A	157	VAL	9
1	A	78	GLY	9
1	A	140	PRO	6
1	A	72	ASN	6
1	A	87	LYS	6
1	A	166	LYS	6
1	A	156	GLY	5
1	A	126	ILE	5
1	A	81	ILE	5
1	A	90	ASN	4
1	A	108	GLY	4
1	A	75	LYS	4
1	A	164	PHE	4
1	A	195	GLU	4
1	A	129	PRO	4
1	A	191	HIS	4
1	A	80	PRO	3
1	A	76	LEU	3
1	A	88	HIS	3
1	A	59	ALA	3
1	A	198	HIS	3
1	A	192	ASP	2
1	A	207	THR	2
1	A	60	ASP	2
1	A	168	ARG	2
1	A	41	VAL	2
1	A	47	LEU	2
1	A	77	HIS	2
1	A	137	ASN	2
1	A	175	MET	1
1	A	128	PRO	1
1	A	28	PRO	1
1	A	170	MET	1
1	A	63	GLN	1
1	A	179	GLU	1
1	A	150	LEU	1
1	A	151	PHE	1
1	A	89	GLN	1
1	A	82	ARG	1
1	A	154	ASN	1
1	A	39	GLY	1

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Mol	Chain	Res	Type	Models (Total)
1	A	167	ASP	1
1	A	23	PRO	1
1	A	32	PHE	1
1	A	131	ALA	1
1	A	147	LEU	1
1	A	21	LEU	1
1	A	13	ASN	1
1	A	142	VAL	1
1	A	187	ASP	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	144/197 (73%)	114±10 (79±7%)	30±10 (21±7%)	4	33
All	All	2880/3940 (73%)	2273 (79%)	607 (21%)	4	33

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	79	LYS	20
1	A	188	LEU	20
1	A	133	LEU	20
1	A	135	LEU	20
1	A	75	LYS	19
1	A	70	HIS	19
1	A	34	LEU	19
1	A	71	LEU	19
1	A	185	LEU	19
1	A	170	MET	18
1	A	13	ASN	18
1	A	196	ASN	18
1	A	164	PHE	15
1	A	58	MET	15
1	A	157	VAL	15
1	A	41	VAL	14

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Mol	Chain	Res	Type	Models (Total)
1	A	45	LYS	13
1	A	189	HIS	13
1	A	186	ILE	13
1	A	169	LYS	13
1	A	55	LEU	12
1	A	132	THR	12
1	A	137	ASN	11
1	A	81	ILE	11
1	A	20	ASN	10
1	A	202	SER	10
1	A	53	ASN	9
1	A	167	ASP	9
1	A	175	MET	8
1	A	32	PHE	8
1	A	76	LEU	8
1	A	165	GLN	7
1	A	205	LYS	7
1	A	46	ILE	6
1	A	33	ILE	6
1	A	90	ASN	5
1	A	89	GLN	5
1	A	154	ASN	5
1	A	87	LYS	5
1	A	127	PHE	4
1	A	193	LEU	4
1	A	168	ARG	4
1	A	26	VAL	4
1	A	126	ILE	4
1	A	85	LEU	3
1	A	27	THR	3
1	A	21	LEU	3
1	A	192	ASP	3
1	A	144	GLU	3
1	A	158	VAL	3
1	A	29	GLN	3
1	A	17	LEU	3
1	A	31	LEU	3
1	A	25	ARG	2
1	A	178	VAL	2
1	A	88	HIS	2
1	A	191	HIS	2
1	A	172	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	187	ASP	2
1	A	166	LYS	2
1	A	134	HIS	2
1	A	147	LEU	2
1	A	138	ILE	2
1	A	66	LEU	2
1	A	206	SER	2
1	A	198	HIS	2
1	A	130	SER	2
1	A	40	ASP	2
1	A	200	ARG	2
1	A	201	VAL	2
1	A	72	ASN	2
1	A	23	PRO	2
1	A	62	ASN	2
1	A	74	HIS	1
1	A	35	PHE	1
1	A	140	PRO	1
1	A	177	SER	1
1	A	142	VAL	1
1	A	146	ASP	1
1	A	207	THR	1
1	A	68	MET	1
1	A	159	LYS	1
1	A	57	GLN	1
1	A	128	PRO	1
1	A	15	VAL	1
1	A	190	ASN	1
1	A	28	PRO	1
1	A	150	LEU	1
1	A	204	SER	1
1	A	183	GLN	1
1	A	43	ARG	1
1	A	105	LYS	1
1	A	42	GLN	1
1	A	197	HIS	1
1	A	195	GLU	1
1	A	91	VAL	1
1	A	19	SER	1
1	A	14	SER	1
1	A	65	GLN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided