



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 10:02 AM UTC

PDB ID : 1TI3 / pdb_00001ti3
Title : Solution structure of the Thioredoxin h1 from poplar, a CPPC active site variant
Authors : Coudevylle, N.; Thureau, A.; Hemmerlin, C.; Gelhaye, E.; Jacquot, J.P.; Cung, M.T.
Deposited on : 2004-06-02

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

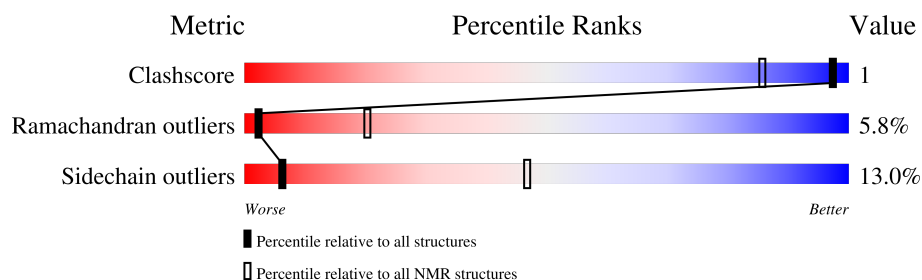
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

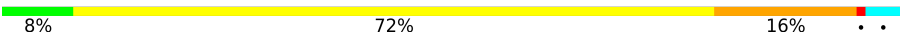
The overall completeness of chemical shifts assignment was not calculated.

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 ≥ 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	113	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:3-A:111 (109)	0.47	1

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1766 atoms, of which 890 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called thioredoxin H.

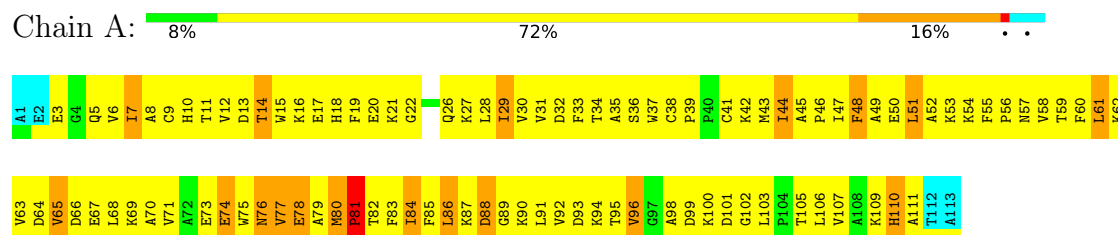
Mol	Chain	Residues	Atoms						Trace
1	A	113	Total	C	H	N	O	S	0
			1766	569	890	140	162	5	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: thioredoxin H

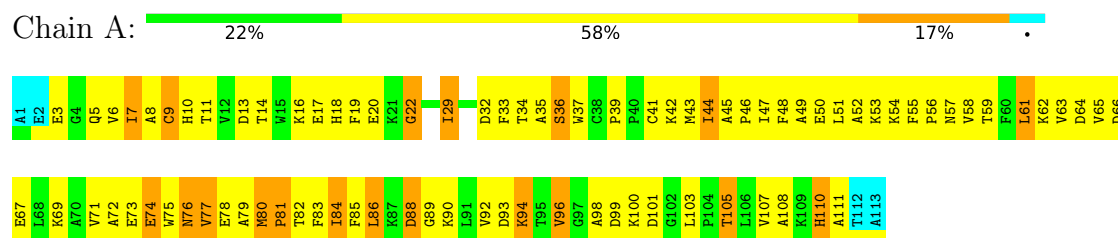


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

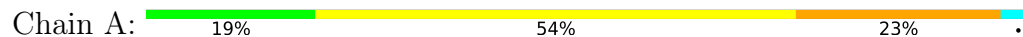
4.2.1 Score per residue for model 1 (medoid)

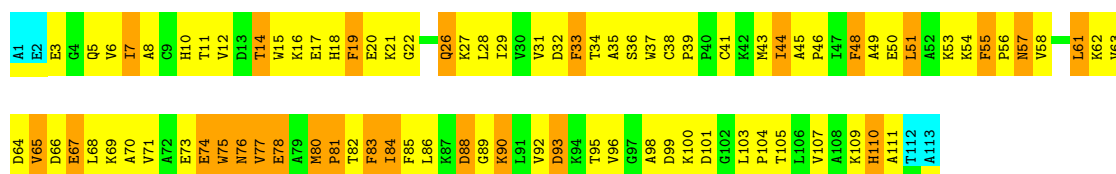
- Molecule 1: thioredoxin H



4.2.2 Score per residue for model 2

- Molecule 1: thioredoxin H

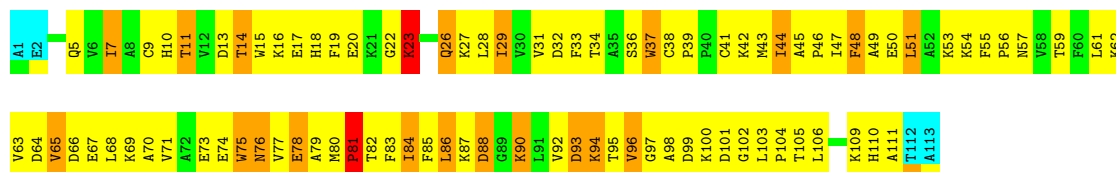




4.2.3 Score per residue for model 3

- Molecule 1: thioredoxin H

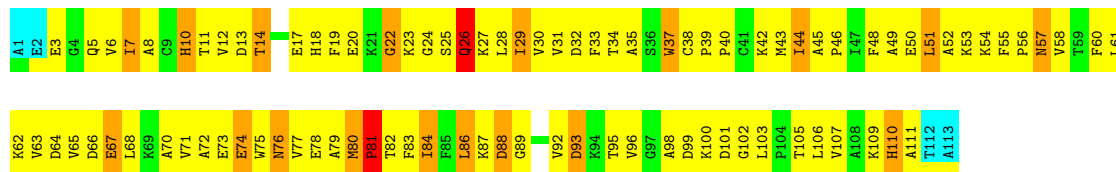
Chain A: 17% 60% 18% . .



4.2.4 Score per residue for model 4

- Molecule 1: thioredoxin H

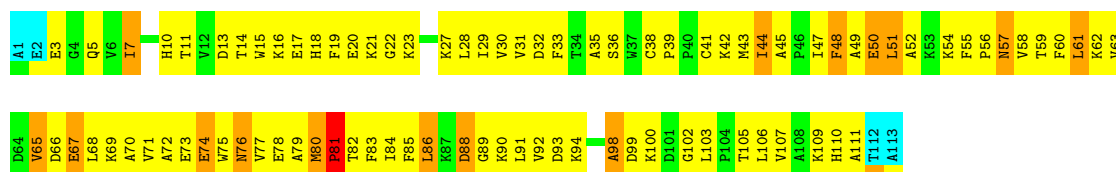
Chain A: 15% 64% 16% . .



4.2.5 Score per residue for model 5

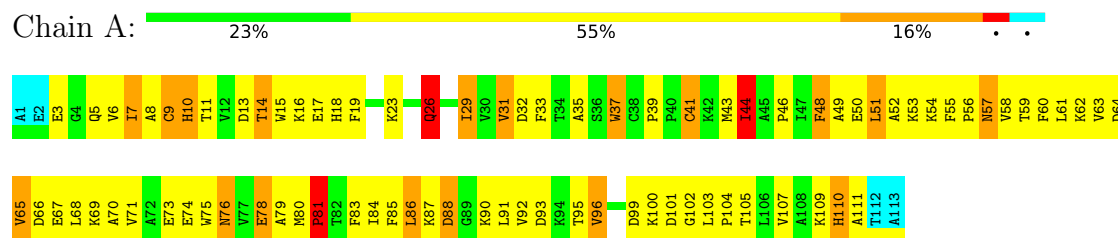
- Molecule 1: thioredoxin H

Chain A: 19% 64% 13% . .



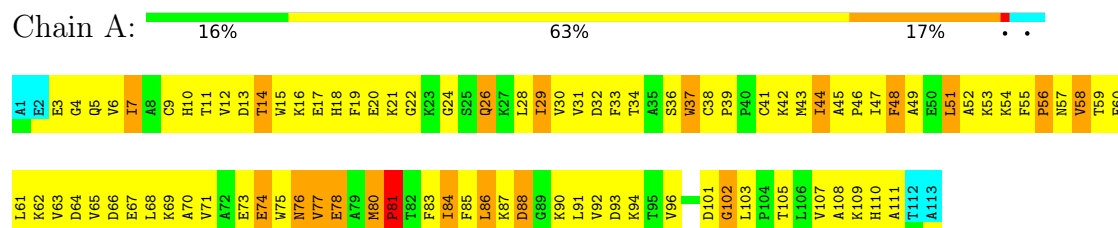
4.2.6 Score per residue for model 6

- Molecule 1: thioredoxin H



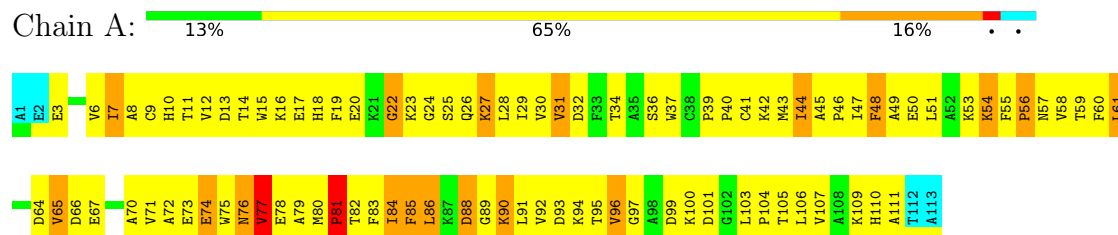
4.2.7 Score per residue for model 7

- Molecule 1: thioredoxin H



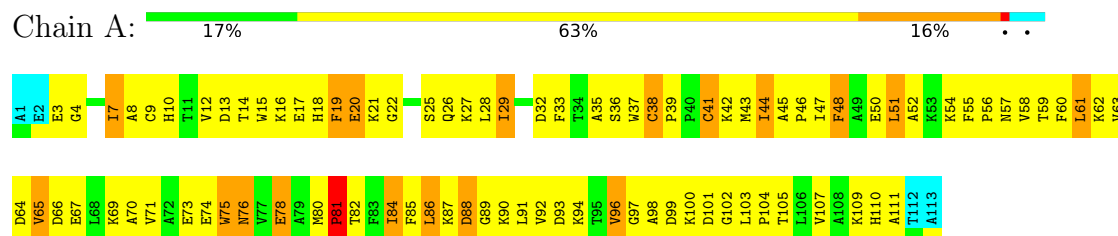
4.2.8 Score per residue for model 8

- Molecule 1: thioredoxin H



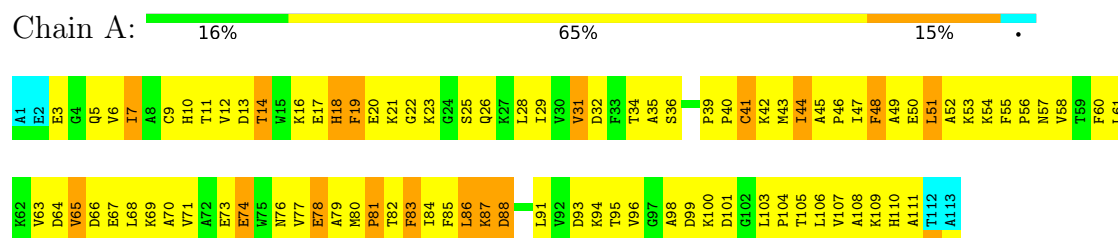
4.2.9 Score per residue for model 9

- Molecule 1: thioredoxin H



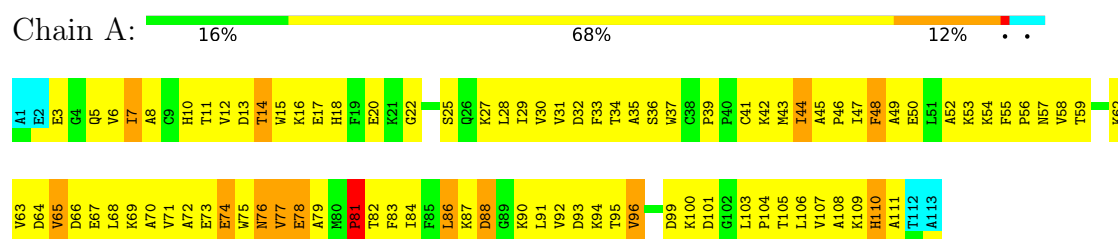
4.2.10 Score per residue for model 10

- Molecule 1: thioredoxin H



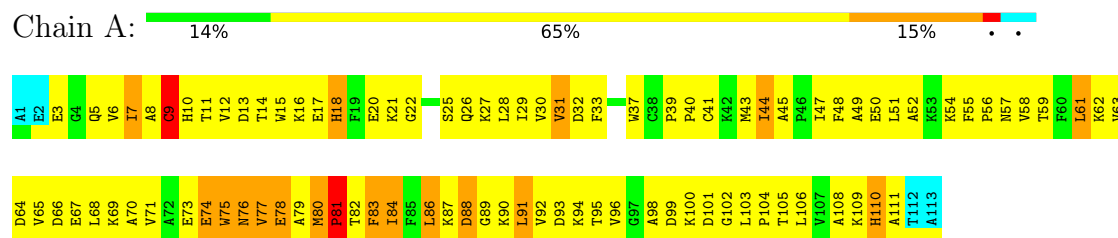
4.2.11 Score per residue for model 11

- Molecule 1: thioredoxin H



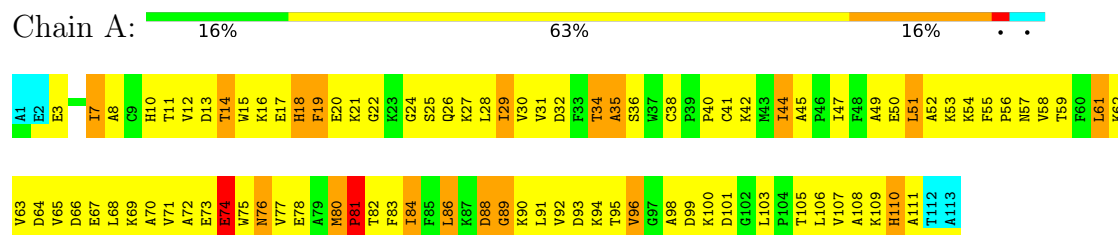
4.2.12 Score per residue for model 12

- Molecule 1: thioredoxin H



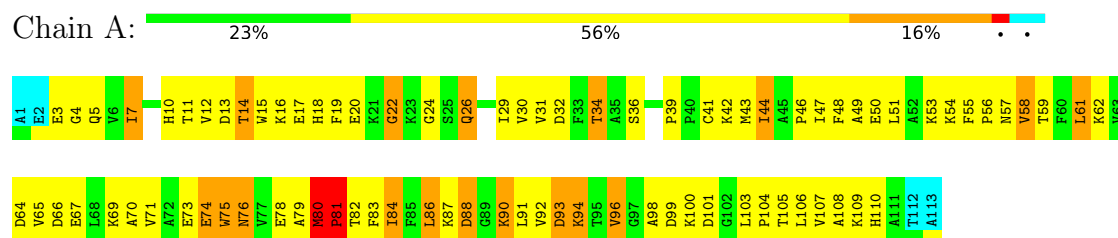
4.2.13 Score per residue for model 13

- Molecule 1: thioredoxin H



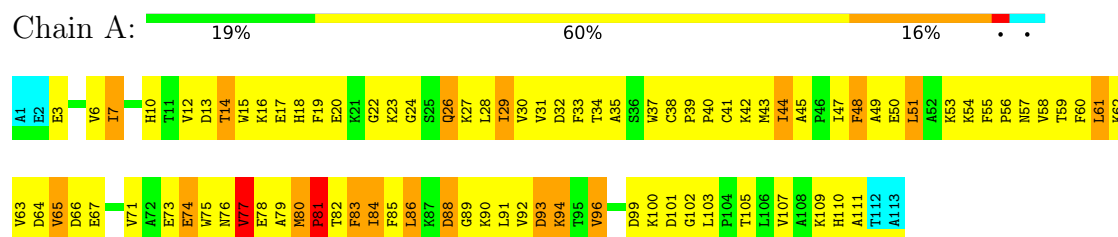
4.2.14 Score per residue for model 14

- Molecule 1: thioredoxin H



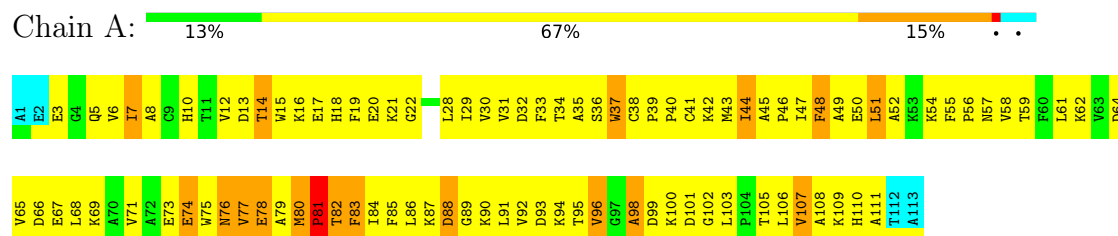
4.2.15 Score per residue for model 15

- Molecule 1: thioredoxin H



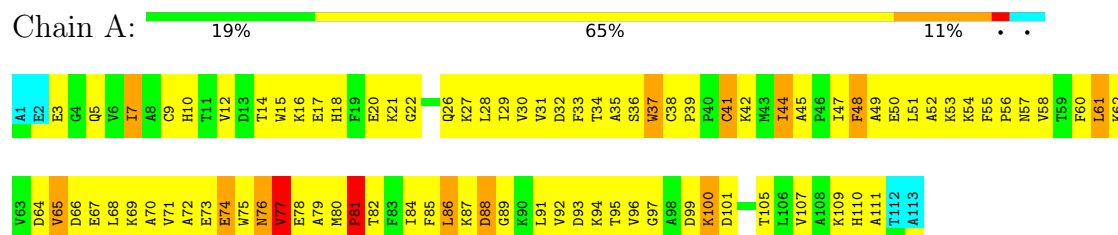
4.2.16 Score per residue for model 16

- Molecule 1: thioredoxin H



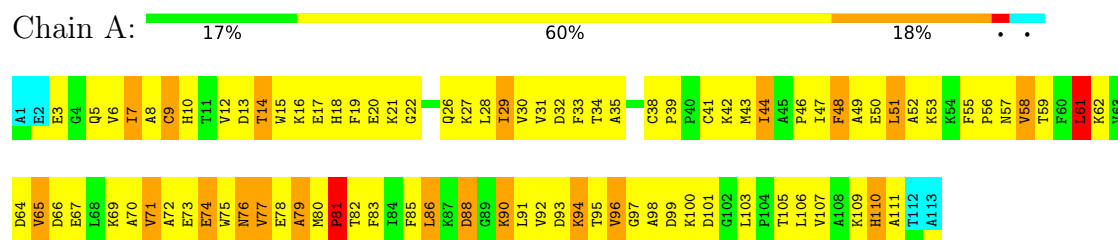
4.2.17 Score per residue for model 17

- Molecule 1: thioredoxin H



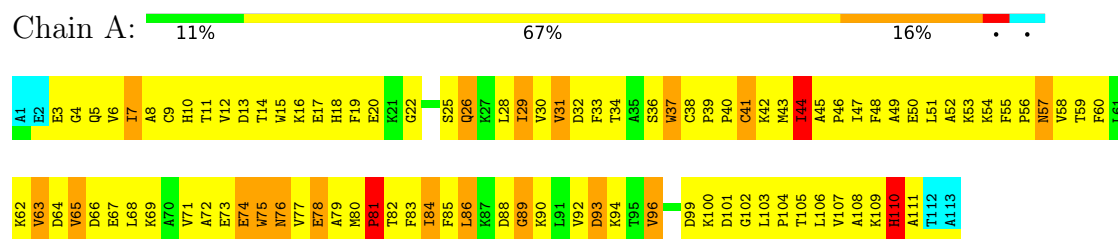
4.2.18 Score per residue for model 18

- Molecule 1: thioredoxin H



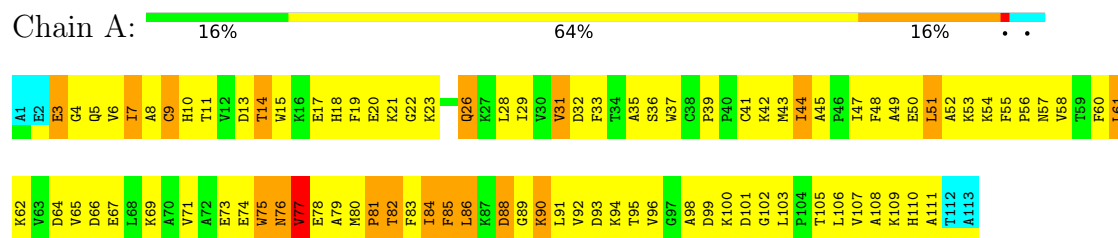
4.2.19 Score per residue for model 19

- Molecule 1: thioredoxin H



4.2.20 Score per residue for model 20

- Molecule 1: thioredoxin H



5 Refinement protocol and experimental data overview [i](#)

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
DIANA	structure solution	
Discover	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.78±0.04	76±6/871 (8.7± 0.7%)	3.07±0.07	109±11/1182 (9.2± 0.9%)
All	All	2.78	1515/17420 (8.7%)	3.08	2181/23640 (9.2%)

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	5.3±2.0
All	All	0	106

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	39	PRO	CA-C	13.15	1.64	1.52	17	17
1	A	79	ALA	CA-C	13.07	1.68	1.52	5	8
1	A	78	GLU	CD-OE2	12.03	1.48	1.25	11	15
1	A	80	MET	CA-C	11.93	1.66	1.52	12	10
1	A	63	VAL	CA-C	11.78	1.67	1.52	12	4
1	A	55	PHE	CA-C	11.43	1.66	1.52	10	14
1	A	10	HIS	ND1-CE1	11.30	1.43	1.32	9	14
1	A	88	ASP	CA-C	11.29	1.68	1.52	15	9
1	A	82	THR	CA-C	11.15	1.66	1.52	10	7
1	A	18	HIS	CG-CD2	11.11	1.48	1.35	6	10
1	A	86	LEU	CA-C	11.04	1.65	1.52	20	8
1	A	18	HIS	CE1-NE2	10.91	1.43	1.32	9	12
1	A	43	MET	N-CA	10.79	1.59	1.46	9	8
1	A	31	VAL	CA-C	10.63	1.66	1.52	4	8
1	A	78	GLU	CA-C	10.61	1.66	1.53	17	7
1	A	110	HIS	CE1-NE2	10.47	1.43	1.32	11	10

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	58	VAL	CA-C	10.37	1.66	1.52	20	7
1	A	32	ASP	CG-OD2	10.33	1.45	1.25	18	17
1	A	72	ALA	N-CA	10.26	1.58	1.46	11	4
1	A	10	HIS	CG-CD2	10.19	1.47	1.35	3	13
1	A	84	ILE	CA-C	10.13	1.64	1.52	13	10
1	A	88	ASP	CG-OD2	10.11	1.44	1.25	6	16
1	A	110	HIS	CG-CD2	10.08	1.47	1.35	7	12
1	A	99	ASP	CG-OD2	10.06	1.44	1.25	17	17
1	A	56	PRO	CA-C	9.98	1.67	1.52	14	7
1	A	45	ALA	CA-C	9.91	1.65	1.52	15	10
1	A	77	VAL	CA-C	9.88	1.65	1.52	5	8
1	A	43	MET	CA-C	9.87	1.66	1.52	20	6
1	A	55	PHE	CA-CB	9.76	1.63	1.53	8	3
1	A	8	ALA	CA-C	9.69	1.65	1.52	19	1
1	A	76	ASN	CA-C	9.67	1.65	1.52	19	7
1	A	35	ALA	CA-C	9.62	1.65	1.52	11	4
1	A	17	GLU	CD-OE2	9.61	1.43	1.25	10	16
1	A	67	GLU	CD-OE2	9.60	1.43	1.25	16	19
1	A	10	HIS	CE1-NE2	9.53	1.42	1.32	11	8
1	A	63	VAL	CA-CB	9.53	1.64	1.53	6	4
1	A	68	LEU	CA-CB	9.52	1.63	1.53	17	4
1	A	93	ASP	N-CA	9.43	1.57	1.46	15	5
1	A	74	GLU	C-O	9.39	1.35	1.24	11	2
1	A	96	VAL	CA-C	9.37	1.63	1.52	9	8
1	A	36	SER	N-CA	9.33	1.57	1.46	14	6
1	A	83	PHE	N-CA	9.20	1.57	1.46	14	2
1	A	50	GLU	CA-C	9.17	1.65	1.52	17	5
1	A	6	VAL	CA-CB	9.14	1.64	1.54	7	2
1	A	73	GLU	CD-OE2	9.13	1.42	1.25	11	14
1	A	6	VAL	CA-C	9.10	1.63	1.52	15	7
1	A	12	VAL	CA-C	9.02	1.64	1.52	4	8
1	A	37	TRP	CA-C	9.02	1.64	1.52	19	6
1	A	66	ASP	N-CA	9.02	1.57	1.46	3	8
1	A	18	HIS	ND1-CE1	9.01	1.41	1.32	12	11
1	A	7	ILE	CA-C	9.00	1.64	1.52	5	13
1	A	93	ASP	CG-OD2	8.95	1.42	1.25	6	15
1	A	54	LYS	CA-C	8.95	1.65	1.52	9	9
1	A	13	ASP	CG-OD2	8.91	1.42	1.25	6	16
1	A	78	GLU	N-CA	8.88	1.58	1.46	11	3
1	A	57	ASN	CA-C	8.85	1.64	1.52	12	7
1	A	93	ASP	CA-C	8.85	1.63	1.52	14	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	61	LEU	CA-C	8.84	1.63	1.52	13	4
1	A	85	PHE	CA-C	8.82	1.62	1.52	15	6
1	A	62	LYS	CA-C	8.81	1.62	1.52	13	6
1	A	83	PHE	CA-C	8.81	1.62	1.52	15	6
1	A	31	VAL	N-CA	8.79	1.57	1.46	5	2
1	A	81	PRO	C-N	8.77	1.46	1.33	20	1
1	A	70	ALA	CA-C	8.75	1.64	1.52	12	5
1	A	27	LYS	CA-C	8.74	1.63	1.52	8	9
1	A	50	GLU	CD-OE2	8.71	1.42	1.25	12	18
1	A	95	THR	CA-C	8.69	1.63	1.52	18	9
1	A	101	ASP	CG-OD2	8.67	1.41	1.25	15	17
1	A	20	GLU	CD-OE2	8.65	1.41	1.25	17	17
1	A	104	PRO	CA-C	8.65	1.64	1.52	2	4
1	A	78	GLU	C-N	8.64	1.44	1.33	16	7
1	A	51	LEU	CA-C	8.62	1.64	1.52	6	7
1	A	68	LEU	CA-C	8.61	1.64	1.53	2	6
1	A	34	THR	CA-C	8.60	1.63	1.52	18	6
1	A	37	TRP	N-CA	8.59	1.57	1.46	17	5
1	A	64	ASP	CG-OD2	8.56	1.41	1.25	6	18
1	A	80	MET	N-CA	8.56	1.59	1.46	1	2
1	A	47	ILE	CA-C	8.54	1.62	1.52	17	4
1	A	92	VAL	CA-CB	8.52	1.64	1.54	17	4
1	A	91	LEU	CA-C	8.49	1.64	1.52	20	4
1	A	89	GLY	CA-C	8.49	1.63	1.51	20	4
1	A	30	VAL	CA-C	8.48	1.63	1.52	8	5
1	A	109	LYS	CA-C	8.47	1.63	1.52	4	7
1	A	100	LYS	CA-C	8.45	1.64	1.52	6	9
1	A	47	ILE	N-CA	8.41	1.56	1.46	18	7
1	A	66	ASP	CA-C	8.39	1.64	1.52	2	2
1	A	14	THR	CA-C	8.38	1.64	1.52	3	7
1	A	16	LYS	CA-C	8.37	1.63	1.52	8	7
1	A	10	HIS	CA-C	8.36	1.62	1.52	13	7
1	A	29	ILE	CA-C	8.34	1.63	1.52	16	8
1	A	33	PHE	C-O	8.30	1.33	1.24	2	4
1	A	61	LEU	N-CA	8.25	1.55	1.46	14	2
1	A	69	LYS	N-CA	8.23	1.56	1.46	17	1
1	A	31	VAL	CA-CB	8.22	1.65	1.54	3	2
1	A	3	GLU	CD-OE2	8.21	1.41	1.25	20	18
1	A	66	ASP	CG-OD2	8.17	1.40	1.25	2	17
1	A	96	VAL	CA-CB	8.15	1.65	1.53	11	4
1	A	14	THR	N-CA	8.15	1.56	1.46	3	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	15	TRP	NE1-CE2	8.12	1.46	1.37	13	5
1	A	76	ASN	N-CA	8.10	1.56	1.46	8	4
1	A	61	LEU	CA-CB	8.10	1.67	1.53	2	1
1	A	36	SER	CA-C	8.10	1.64	1.52	3	4
1	A	101	ASP	CA-C	8.08	1.63	1.52	17	6
1	A	74	GLU	N-CA	8.07	1.55	1.46	17	6
1	A	53	LYS	CA-C	8.05	1.63	1.52	6	5
1	A	87	LYS	N-CA	8.04	1.55	1.45	3	2
1	A	90	LYS	CA-C	8.04	1.64	1.53	6	14
1	A	88	ASP	N-CA	8.02	1.56	1.46	13	3
1	A	28	LEU	CA-C	7.99	1.63	1.52	13	6
1	A	70	ALA	N-CA	7.97	1.56	1.46	17	5
1	A	64	ASP	N-CA	7.95	1.56	1.46	19	3
1	A	75	TRP	CA-CB	7.94	1.65	1.53	6	2
1	A	82	THR	N-CA	7.92	1.56	1.46	1	5
1	A	33	PHE	N-CA	7.92	1.56	1.46	11	1
1	A	110	HIS	ND1-CE1	7.84	1.40	1.32	18	10
1	A	75	TRP	NE1-CE2	7.83	1.46	1.37	11	3
1	A	67	GLU	CA-C	7.82	1.62	1.52	6	8
1	A	18	HIS	N-CA	7.78	1.55	1.46	15	3
1	A	59	THR	CA-C	7.76	1.62	1.52	18	5
1	A	74	GLU	CD-OE2	7.76	1.40	1.25	5	17
1	A	19	PHE	CA-C	7.71	1.62	1.52	7	8
1	A	24	GLY	CA-C	7.69	1.62	1.51	7	3
1	A	105	THR	N-CA	7.69	1.55	1.46	15	8
1	A	71	VAL	CA-C	7.68	1.62	1.52	17	7
1	A	46	PRO	CA-C	7.68	1.63	1.52	4	4
1	A	38	CYS	C-N	7.67	1.42	1.33	17	5
1	A	15	TRP	CA-C	7.67	1.63	1.52	16	4
1	A	32	ASP	N-CA	7.63	1.55	1.45	11	2
1	A	49	ALA	CA-C	7.62	1.62	1.52	13	6
1	A	48	PHE	N-CA	7.61	1.55	1.46	18	3
1	A	44	ILE	N-CA	7.60	1.55	1.46	4	3
1	A	82	THR	CA-CB	7.59	1.64	1.53	4	1
1	A	103	LEU	CA-C	7.53	1.61	1.52	3	14
1	A	90	LYS	N-CA	7.53	1.55	1.46	9	7
1	A	95	THR	CB-OG1	-7.49	1.31	1.43	18	1
1	A	40	PRO	N-CA	7.47	1.56	1.47	12	1
1	A	105	THR	CA-C	7.46	1.62	1.52	13	8
1	A	106	LEU	CA-C	7.46	1.62	1.52	8	4
1	A	94	LYS	CA-C	7.46	1.62	1.52	5	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	106	LEU	N-CA	7.45	1.54	1.46	4	3
1	A	78	GLU	C-O	-7.44	1.14	1.24	19	2
1	A	50	GLU	N-CA	7.41	1.54	1.46	14	4
1	A	15	TRP	N-CA	7.41	1.55	1.46	17	5
1	A	48	PHE	CA-C	7.40	1.62	1.52	5	4
1	A	63	VAL	N-CA	7.39	1.54	1.46	10	3
1	A	74	GLU	CA-C	7.39	1.63	1.52	17	4
1	A	107	VAL	N-CA	7.36	1.55	1.46	8	4
1	A	69	LYS	CA-C	7.31	1.62	1.52	20	4
1	A	53	LYS	N-CA	7.30	1.55	1.46	7	3
1	A	99	ASP	CA-C	7.28	1.60	1.52	6	6
1	A	35	ALA	CA-CB	7.28	1.63	1.53	4	1
1	A	21	LYS	CA-C	7.26	1.61	1.52	13	6
1	A	110	HIS	CB-CG	7.25	1.60	1.50	3	2
1	A	92	VAL	CA-C	7.23	1.61	1.52	12	3
1	A	92	VAL	C-N	7.22	1.42	1.33	3	3
1	A	67	GLU	C-N	7.20	1.41	1.33	17	1
1	A	52	ALA	CA-C	7.18	1.62	1.52	6	2
1	A	21	LYS	N-CA	7.17	1.54	1.46	2	4
1	A	23	LYS	CA-C	7.16	1.62	1.52	6	3
1	A	17	GLU	CA-C	7.15	1.62	1.52	6	5
1	A	79	ALA	N-CA	7.12	1.54	1.46	19	3
1	A	9	CYS	CA-C	7.11	1.61	1.52	9	9
1	A	107	VAL	CA-C	7.09	1.61	1.52	13	2
1	A	26	GLN	C-N	7.09	1.42	1.33	20	2
1	A	110	HIS	CD2-NE2	-7.08	1.30	1.37	6	4
1	A	87	LYS	CA-C	7.05	1.62	1.53	14	2
1	A	71	VAL	CA-CB	7.03	1.62	1.54	13	1
1	A	75	TRP	CA-C	7.02	1.61	1.52	15	4
1	A	38	CYS	CA-C	7.00	1.61	1.52	7	5
1	A	80	MET	CA-CB	6.99	1.64	1.52	19	4
1	A	71	VAL	N-CA	6.99	1.54	1.46	11	3
1	A	92	VAL	N-CA	6.98	1.54	1.46	14	2
1	A	77	VAL	N-CA	6.97	1.55	1.46	8	3
1	A	33	PHE	CA-C	6.97	1.60	1.52	16	6
1	A	94	LYS	N-CA	6.97	1.54	1.46	9	2
1	A	98	ALA	CA-C	6.95	1.62	1.52	4	4
1	A	17	GLU	N-CA	6.93	1.54	1.46	20	4
1	A	3	GLU	CA-C	6.92	1.60	1.52	1	3
1	A	57	ASN	N-CA	6.91	1.55	1.46	2	4
1	A	34	THR	N-CA	6.90	1.54	1.45	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	79	ALA	C-O	-6.88	1.15	1.23	16	1
1	A	110	HIS	CA-C	6.88	1.61	1.52	7	6
1	A	11	THR	CA-CB	6.86	1.63	1.53	3	6
1	A	65	VAL	CA-C	6.84	1.62	1.52	18	6
1	A	32	ASP	CA-C	6.82	1.61	1.52	2	5
1	A	16	LYS	N-CA	6.82	1.54	1.46	8	2
1	A	7	ILE	N-CA	6.82	1.54	1.46	12	1
1	A	73	GLU	C-N	6.81	1.42	1.33	4	5
1	A	103	LEU	N-CA	6.79	1.53	1.46	3	2
1	A	34	THR	C-N	-6.78	1.24	1.33	16	2
1	A	15	TRP	CD2-CE3	6.77	1.51	1.40	9	1
1	A	30	VAL	N-CA	6.76	1.54	1.46	14	1
1	A	22	GLY	CA-C	6.76	1.61	1.51	8	4
1	A	54	LYS	C-N	6.75	1.38	1.33	13	2
1	A	13	ASP	CA-C	6.73	1.61	1.52	6	1
1	A	97	GLY	CA-C	6.72	1.59	1.51	8	2
1	A	75	TRP	CG-CD2	-6.72	1.31	1.43	12	2
1	A	58	VAL	CA-CB	6.71	1.63	1.54	8	2
1	A	77	VAL	CA-CB	6.70	1.63	1.54	13	4
1	A	89	GLY	C-N	6.70	1.43	1.33	5	1
1	A	19	PHE	N-CA	6.69	1.54	1.46	16	2
1	A	25	SER	CA-C	6.68	1.60	1.52	8	4
1	A	84	ILE	N-CA	6.64	1.54	1.46	15	3
1	A	65	VAL	CA-CB	6.63	1.63	1.54	2	3
1	A	4	GLY	N-CA	6.62	1.53	1.45	7	2
1	A	87	LYS	CA-CB	6.61	1.63	1.53	10	2
1	A	37	TRP	CA-CB	6.61	1.63	1.52	20	1
1	A	15	TRP	CG-CD2	-6.61	1.31	1.43	9	3
1	A	11	THR	CA-C	6.61	1.61	1.52	12	7
1	A	81	PRO	N-CD	-6.61	1.38	1.47	3	2
1	A	26	GLN	N-CA	6.57	1.54	1.46	17	4
1	A	101	ASP	N-CA	6.54	1.54	1.46	18	4
1	A	29	ILE	N-CA	6.51	1.54	1.46	7	2
1	A	81	PRO	CA-CB	6.50	1.65	1.53	1	2
1	A	75	TRP	CZ2-CH2	6.49	1.49	1.37	17	2
1	A	72	ALA	CA-CB	6.48	1.63	1.53	1	1
1	A	15	TRP	CA-CB	6.48	1.63	1.53	3	1
1	A	60	PHE	CA-C	6.48	1.60	1.52	4	3
1	A	7	ILE	C-O	6.48	1.30	1.24	13	2
1	A	65	VAL	N-CA	6.45	1.54	1.46	8	4
1	A	80	MET	C-N	6.44	1.46	1.34	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	50	GLU	C-N	6.39	1.42	1.33	6	1
1	A	57	ASN	C-O	6.39	1.32	1.24	3	1
1	A	97	GLY	N-CA	6.37	1.53	1.45	9	2
1	A	102	GLY	CA-C	6.36	1.60	1.51	9	3
1	A	68	LEU	N-CA	6.36	1.55	1.46	11	1
1	A	84	ILE	C-O	6.36	1.30	1.24	4	1
1	A	96	VAL	C-N	6.35	1.39	1.33	6	3
1	A	105	THR	CA-CB	6.33	1.63	1.53	5	1
1	A	108	ALA	CA-C	6.32	1.60	1.52	14	2
1	A	103	LEU	CA-CB	6.31	1.61	1.53	15	2
1	A	44	ILE	CA-C	6.31	1.62	1.52	20	5
1	A	99	ASP	N-CA	6.30	1.53	1.46	18	2
1	A	20	GLU	N-CA	6.29	1.53	1.46	16	3
1	A	81	PRO	N-CA	6.29	1.57	1.47	20	1
1	A	40	PRO	CA-C	6.29	1.61	1.52	8	3
1	A	37	TRP	NE1-CE2	6.29	1.44	1.37	15	1
1	A	38	CYS	CA-CB	6.27	1.63	1.53	4	1
1	A	82	THR	CB-OG1	-6.25	1.33	1.43	1	1
1	A	57	ASN	C-N	6.25	1.42	1.33	9	1
1	A	18	HIS	CD2-NE2	6.25	1.44	1.37	11	1
1	A	111	ALA	CA-C	6.24	1.60	1.52	1	4
1	A	82	THR	C-N	-6.24	1.25	1.33	16	1
1	A	27	LYS	N-CA	6.24	1.53	1.45	2	1
1	A	85	PHE	C-N	6.23	1.41	1.33	2	1
1	A	18	HIS	CA-C	6.23	1.61	1.52	20	5
1	A	38	CYS	N-CA	6.21	1.54	1.46	7	3
1	A	110	HIS	N-CA	6.20	1.53	1.46	15	2
1	A	109	LYS	N-CA	6.19	1.53	1.46	3	1
1	A	59	THR	N-CA	6.18	1.53	1.46	13	2
1	A	5	GLN	CA-C	6.18	1.59	1.52	14	8
1	A	73	GLU	CA-C	6.17	1.60	1.52	2	4
1	A	98	ALA	N-CA	6.15	1.54	1.46	10	4
1	A	26	GLN	CA-C	6.14	1.61	1.52	7	5
1	A	85	PHE	N-CA	6.14	1.54	1.46	19	3
1	A	27	LYS	C-O	6.12	1.31	1.23	17	1
1	A	91	LEU	N-CA	6.12	1.54	1.46	17	1
1	A	44	ILE	CA-CB	6.11	1.62	1.54	1	3
1	A	47	ILE	CA-CB	6.11	1.61	1.54	10	4
1	A	73	GLU	C-O	-6.08	1.17	1.24	2	1
1	A	12	VAL	N-CA	6.06	1.54	1.46	8	5
1	A	83	PHE	CA-CB	6.04	1.62	1.53	12	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	18	HIS	CB-CG	6.03	1.58	1.50	19	2
1	A	54	LYS	CA-CB	6.03	1.62	1.53	12	1
1	A	85	PHE	CA-CB	6.03	1.62	1.53	18	2
1	A	42	LYS	CA-C	6.02	1.60	1.52	10	4
1	A	41	CYS	N-CA	6.01	1.54	1.46	16	1
1	A	75	TRP	N-CA	6.00	1.53	1.46	2	3
1	A	42	LYS	N-CA	6.00	1.53	1.46	4	5
1	A	28	LEU	CA-CB	5.99	1.62	1.53	9	2
1	A	95	THR	C-N	-5.97	1.26	1.33	10	2
1	A	111	ALA	N-CA	5.96	1.53	1.46	2	5
1	A	12	VAL	CA-CB	5.94	1.63	1.54	13	2
1	A	62	LYS	CA-CB	5.91	1.60	1.52	9	2
1	A	6	VAL	N-CA	5.90	1.52	1.46	1	1
1	A	84	ILE	CA-CB	5.89	1.63	1.54	2	3
1	A	29	ILE	CA-CB	5.88	1.63	1.54	6	4
1	A	102	GLY	N-CA	5.88	1.53	1.45	20	4
1	A	108	ALA	C-N	5.87	1.41	1.33	13	1
1	A	86	LEU	CA-CB	5.87	1.64	1.53	5	2
1	A	10	HIS	CD2-NE2	5.86	1.44	1.37	13	1
1	A	109	LYS	CA-CB	5.84	1.62	1.53	20	3
1	A	3	GLU	N-CA	5.81	1.54	1.46	9	2
1	A	73	GLU	N-CA	5.79	1.53	1.46	2	1
1	A	20	GLU	CA-C	5.77	1.60	1.52	19	3
1	A	62	LYS	N-CA	5.76	1.53	1.46	1	2
1	A	59	THR	CA-CB	5.74	1.62	1.53	5	1
1	A	10	HIS	CB-CG	5.73	1.58	1.50	4	3
1	A	42	LYS	C-N	5.73	1.41	1.33	4	2
1	A	59	THR	CB-OG1	-5.72	1.34	1.43	14	1
1	A	100	LYS	N-CA	5.72	1.53	1.46	15	3
1	A	34	THR	CA-CB	5.72	1.63	1.53	2	1
1	A	64	ASP	C-N	-5.70	1.26	1.33	3	1
1	A	74	GLU	C-N	5.70	1.41	1.33	12	3
1	A	33	PHE	C-N	5.69	1.41	1.33	17	1
1	A	103	LEU	C-N	5.68	1.41	1.33	13	2
1	A	55	PHE	N-CA	5.68	1.52	1.46	11	1
1	A	75	TRP	CD2-CE3	5.67	1.49	1.40	20	1
1	A	39	PRO	N-CD	5.64	1.55	1.47	19	1
1	A	76	ASN	CA-CB	5.63	1.62	1.53	6	1
1	A	95	THR	CA-CB	5.63	1.62	1.52	12	1
1	A	51	LEU	N-CA	5.62	1.53	1.46	1	1
1	A	35	ALA	N-CA	5.61	1.53	1.45	18	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	43	MET	C-N	-5.61	1.27	1.34	20	1
1	A	96	VAL	C-O	5.60	1.30	1.24	20	1
1	A	73	GLU	CA-CB	5.59	1.62	1.53	14	1
1	A	7	ILE	CA-CB	5.58	1.61	1.54	10	2
1	A	39	PRO	C-N	5.56	1.41	1.33	4	1
1	A	95	THR	N-CA	5.55	1.52	1.46	20	1
1	A	64	ASP	C-O	5.52	1.30	1.24	15	1
1	A	71	VAL	C-N	5.51	1.40	1.33	4	1
1	A	55	PHE	C-N	5.49	1.41	1.34	7	2
1	A	36	SER	CA-CB	5.49	1.61	1.53	9	1
1	A	25	SER	C-N	5.46	1.41	1.33	10	1
1	A	30	VAL	C-O	5.45	1.29	1.24	8	1
1	A	52	ALA	N-CA	5.45	1.53	1.46	11	1
1	A	28	LEU	N-CA	5.45	1.53	1.45	20	2
1	A	37	TRP	CG-CD2	-5.45	1.33	1.43	15	4
1	A	107	VAL	C-O	-5.44	1.17	1.24	2	1
1	A	72	ALA	C-O	-5.42	1.17	1.24	17	1
1	A	84	ILE	CB-CG1	5.37	1.64	1.53	7	1
1	A	109	LYS	C-N	5.37	1.40	1.33	14	2
1	A	90	LYS	CA-CB	5.36	1.62	1.53	13	1
1	A	57	ASN	CA-CB	5.35	1.62	1.53	15	2
1	A	46	PRO	C-N	5.35	1.40	1.34	10	1
1	A	32	ASP	C-N	5.35	1.41	1.33	13	1
1	A	108	ALA	N-CA	5.33	1.52	1.46	14	1
1	A	74	GLU	CA-CB	5.33	1.62	1.53	15	1
1	A	98	ALA	C-N	5.30	1.40	1.33	16	4
1	A	13	ASP	N-CA	5.29	1.52	1.46	7	1
1	A	10	HIS	C-N	5.28	1.39	1.33	3	2
1	A	83	PHE	C-O	5.28	1.30	1.24	7	1
1	A	41	CYS	C-N	5.27	1.40	1.33	19	1
1	A	11	THR	N-CA	5.25	1.52	1.45	4	1
1	A	96	VAL	N-CA	5.24	1.53	1.46	20	2
1	A	69	LYS	C-N	5.24	1.40	1.33	7	1
1	A	30	VAL	C-N	5.23	1.40	1.33	7	2
1	A	92	VAL	C-O	-5.23	1.18	1.24	11	1
1	A	12	VAL	C-N	5.23	1.40	1.33	15	1
1	A	33	PHE	CB-CG	5.22	1.62	1.50	12	1
1	A	80	MET	C-O	5.21	1.30	1.24	13	1
1	A	50	GLU	CA-CB	5.20	1.61	1.53	20	1
1	A	81	PRO	CA-C	5.18	1.63	1.52	11	1
1	A	5	GLN	N-CA	5.15	1.52	1.46	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	18	HIS	CG-ND1	5.13	1.43	1.38	6	1
1	A	37	TRP	CZ2-CH2	5.13	1.47	1.37	11	1
1	A	53	LYS	C-N	5.13	1.40	1.34	8	1
1	A	91	LEU	CA-CB	5.10	1.62	1.53	12	1
1	A	41	CYS	CA-C	5.10	1.59	1.52	6	2
1	A	71	VAL	C-O	5.08	1.29	1.24	13	1
1	A	14	THR	CA-CB	5.07	1.61	1.53	6	1
1	A	65	VAL	C-N	5.07	1.40	1.33	2	2
1	A	32	ASP	CA-CB	5.04	1.61	1.53	18	1
1	A	31	VAL	C-N	5.04	1.40	1.33	13	1
1	A	101	ASP	CA-CB	5.03	1.61	1.53	4	1
1	A	45	ALA	N-CA	5.03	1.50	1.46	20	1
1	A	18	HIS	CA-CB	5.03	1.61	1.53	15	1
1	A	77	VAL	C-N	5.02	1.40	1.33	15	1
1	A	75	TRP	CD2-CE2	5.01	1.49	1.41	3	1
1	A	11	THR	C-N	5.00	1.40	1.33	4	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	110	HIS	CE1-NE2-CD2	-16.35	92.65	109.00	19	20
1	A	10	HIS	ND1-CE1-NE2	15.76	124.16	108.40	8	20
1	A	18	HIS	ND1-CE1-NE2	15.71	124.11	108.40	15	20
1	A	110	HIS	ND1-CE1-NE2	15.55	123.95	108.40	19	20
1	A	76	ASN	CA-CB-CG	14.71	127.31	112.60	18	7
1	A	57	ASN	CA-CB-CG	14.67	127.27	112.60	11	8
1	A	17	GLU	N-CA-C	14.47	126.74	110.97	8	9
1	A	10	HIS	CE1-NE2-CD2	-14.46	94.55	109.00	8	20
1	A	83	PHE	CA-CB-CG	14.09	127.89	113.80	1	9
1	A	18	HIS	CE1-NE2-CD2	-13.66	95.34	109.00	15	20
1	A	71	VAL	N-CA-C	13.54	123.41	110.42	6	18
1	A	81	PRO	N-CD-CG	-13.05	88.13	103.80	19	6
1	A	55	PHE	CA-C-N	13.02	133.04	118.85	17	20
1	A	55	PHE	C-N-CA	13.02	133.04	118.85	17	20
1	A	56	PRO	N-CA-C	13.01	131.61	113.53	7	19
1	A	19	PHE	N-CA-C	12.85	124.98	110.97	5	13
1	A	49	ALA	N-CA-C	12.65	124.61	111.07	7	17
1	A	32	ASP	CA-CB-CG	12.42	125.02	112.60	3	12
1	A	92	VAL	N-CA-C	12.38	123.22	110.72	15	10
1	A	81	PRO	N-CA-CB	-12.24	89.14	102.60	12	13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	58	VAL	CB-CA-C	12.07	124.17	110.41	6	15
1	A	18	HIS	CA-CB-CG	11.89	125.69	113.80	20	10
1	A	88	ASP	CA-CB-CG	11.85	124.45	112.60	12	13
1	A	93	ASP	CA-CB-CG	11.74	124.34	112.60	1	10
1	A	111	ALA	N-CA-C	11.68	124.01	111.28	15	12
1	A	48	PHE	CA-CB-CG	11.57	125.37	113.80	4	13
1	A	80	MET	CA-C-O	-11.50	109.53	119.76	16	7
1	A	41	CYS	N-CA-C	11.37	124.79	111.71	8	18
1	A	110	HIS	N-CA-C	11.27	123.13	111.07	11	14
1	A	67	GLU	N-CA-C	11.18	124.56	111.71	16	17
1	A	44	ILE	N-CA-C	11.15	123.33	110.62	13	17
1	A	39	PRO	N-CA-C	11.05	124.18	110.70	17	13
1	A	101	ASP	CA-CB-CG	10.89	123.49	112.60	15	12
1	A	100	LYS	N-CA-C	10.89	124.30	111.02	2	17
1	A	74	GLU	N-CA-C	10.79	124.06	111.11	13	11
1	A	73	GLU	CA-C-O	-10.77	109.37	120.90	13	10
1	A	47	ILE	N-CA-C	10.74	121.40	110.23	12	7
1	A	109	LYS	N-CA-C	10.50	122.72	111.28	15	12
1	A	17	GLU	CA-C-N	10.49	134.50	120.65	13	6
1	A	17	GLU	C-N-CA	10.49	134.50	120.65	13	6
1	A	107	VAL	N-CA-C	10.37	121.25	110.36	13	13
1	A	51	LEU	CA-C-O	-10.38	109.55	120.55	16	3
1	A	69	LYS	CA-C-O	-10.36	109.44	120.42	1	5
1	A	78	GLU	N-CA-C	10.25	125.31	113.01	15	9
1	A	43	MET	N-CA-C	10.20	122.39	111.28	8	15
1	A	60	PHE	CA-CB-CG	10.18	123.98	113.80	10	7
1	A	75	TRP	N-CA-C	10.07	123.50	111.82	14	6
1	A	69	LYS	N-CA-C	10.04	123.15	111.11	18	13
1	A	16	LYS	N-CA-C	9.96	122.14	111.28	14	12
1	A	45	ALA	CA-C-O	-9.91	109.67	119.08	5	1
1	A	42	LYS	N-CA-C	9.89	122.06	111.28	1	6
1	A	71	VAL	CA-C-O	-9.82	110.76	121.17	16	5
1	A	101	ASP	N-CA-C	9.79	121.55	111.07	10	5
1	A	18	HIS	CB-CG-CD2	-9.75	118.53	131.20	10	8
1	A	83	PHE	O-C-N	9.69	134.73	123.29	8	2
1	A	7	ILE	CB-CA-C	9.67	122.24	110.73	7	11
1	A	110	HIS	CB-CG-CD2	-9.65	118.66	131.20	13	9
1	A	96	VAL	CB-CA-C	9.63	122.19	110.73	20	9
1	A	66	ASP	CA-CB-CG	9.60	122.20	112.60	5	12
1	A	13	ASP	CA-C-O	-9.56	110.42	120.55	13	3
1	A	92	VAL	CA-C-O	-9.50	109.65	120.96	14	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	82	THR	CA-C-O	9.48	130.94	120.70	11	7
1	A	34	THR	CA-C-O	9.44	131.56	120.99	19	7
1	A	84	ILE	CB-CA-C	9.42	126.11	110.95	1	10
1	A	36	SER	CA-C-O	-9.39	110.85	120.90	19	2
1	A	99	ASP	CA-CB-CG	9.36	121.96	112.60	13	6
1	A	18	HIS	N-CA-C	9.36	122.43	111.02	9	5
1	A	86	LEU	CA-C-O	9.30	130.64	120.32	6	11
1	A	102	GLY	CA-C-N	9.29	130.15	119.83	4	3
1	A	102	GLY	C-N-CA	9.29	130.15	119.83	4	3
1	A	80	MET	CB-CA-C	9.27	124.78	109.85	2	6
1	A	106	LEU	N-CA-C	9.21	120.92	111.07	14	7
1	A	10	HIS	CA-CB-CG	9.20	123.00	113.80	19	7
1	A	82	THR	O-C-N	9.14	134.18	123.30	2	3
1	A	18	HIS	CG-CD2-NE2	9.10	116.30	107.20	9	12
1	A	76	ASN	OD1-CG-ND2	-9.09	113.51	122.60	12	4
1	A	83	PHE	N-CA-C	-9.09	93.60	108.41	14	3
1	A	85	PHE	CA-CB-CG	9.08	122.88	113.80	5	6
1	A	13	ASP	CA-CB-CG	8.99	121.59	112.60	11	7
1	A	95	THR	CA-CB-CG2	8.94	125.69	110.50	16	2
1	A	20	GLU	N-CA-C	8.89	120.97	111.28	1	8
1	A	20	GLU	N-CA-CB	8.88	123.18	110.12	9	5
1	A	29	ILE	CA-C-O	8.86	130.38	120.90	16	4
1	A	13	ASP	N-CA-C	8.83	122.02	111.33	5	9
1	A	96	VAL	O-C-N	8.78	131.22	122.71	17	1
1	A	65	VAL	N-CA-C	8.76	119.55	110.62	10	14
1	A	53	LYS	N-CA-C	8.74	120.81	111.28	14	10
1	A	33	PHE	CA-CB-CG	-8.66	105.14	113.80	15	3
1	A	83	PHE	CA-C-O	8.65	129.86	120.43	12	6
1	A	92	VAL	CA-CB-CG2	8.65	125.11	110.40	16	5
1	A	10	HIS	CB-CG-CD2	-8.64	119.97	131.20	4	7
1	A	32	ASP	CA-C-N	8.61	135.34	123.11	2	8
1	A	32	ASP	C-N-CA	8.61	135.34	123.11	2	8
1	A	74	GLU	CA-C-O	-8.60	111.61	121.07	20	2
1	A	111	ALA	CA-C-N	8.59	132.32	120.63	19	1
1	A	111	ALA	C-N-CA	8.59	132.32	120.63	19	1
1	A	80	MET	CG-SD-CE	8.56	119.73	100.90	13	1
1	A	110	HIS	CG-CD2-NE2	8.53	115.73	107.20	19	5
1	A	81	PRO	CA-C-N	8.48	134.42	122.72	8	6
1	A	81	PRO	C-N-CA	8.48	134.42	122.72	8	6
1	A	82	THR	CA-CB-OG1	8.43	122.24	109.60	4	4
1	A	19	PHE	CA-CB-CG	-8.42	105.38	113.80	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	33	PHE	N-CA-C	-8.37	93.32	107.80	16	4
1	A	46	PRO	N-CA-C	8.37	125.95	113.81	7	9
1	A	111	ALA	CA-C-O	-8.31	112.01	120.90	20	5
1	A	54	LYS	N-CA-C	8.29	121.24	111.71	11	9
1	A	84	ILE	CA-C-O	8.29	129.14	120.36	4	6
1	A	38	CYS	CA-C-N	8.28	128.90	120.38	9	5
1	A	38	CYS	C-N-CA	8.28	128.90	120.38	9	5
1	A	49	ALA	O-C-N	-8.26	113.24	122.08	18	1
1	A	29	ILE	CA-CB-CG1	8.26	124.44	110.40	17	8
1	A	75	TRP	CA-C-O	-8.26	112.15	120.82	2	4
1	A	100	LYS	CA-C-N	8.26	134.70	120.58	3	8
1	A	100	LYS	C-N-CA	8.26	134.70	120.58	3	8
1	A	21	LYS	N-CA-C	8.24	119.95	110.97	9	3
1	A	96	VAL	CA-CB-CG2	8.22	124.37	110.40	7	2
1	A	62	LYS	CA-C-N	8.20	132.62	122.37	18	10
1	A	62	LYS	C-N-CA	8.20	132.62	122.37	18	10
1	A	76	ASN	N-CA-CB	8.18	124.31	110.49	2	11
1	A	82	THR	N-CA-CB	8.18	125.06	110.83	11	2
1	A	68	LEU	CA-C-N	8.17	131.89	120.29	4	7
1	A	68	LEU	C-N-CA	8.17	131.89	120.29	4	7
1	A	96	VAL	CA-CB-CG1	8.01	124.02	110.40	19	3
1	A	10	HIS	CG-ND1-CE1	-7.98	95.73	109.30	19	14
1	A	84	ILE	O-C-N	7.98	131.82	123.20	12	2
1	A	35	ALA	N-CA-CB	-7.98	98.16	110.29	18	11
1	A	42	LYS	CA-C-O	-7.96	112.47	120.82	8	2
1	A	71	VAL	O-C-N	7.95	129.70	121.91	16	5
1	A	51	LEU	N-CA-CB	-7.93	98.45	110.12	13	6
1	A	48	PHE	CA-C-N	7.93	131.22	120.44	1	4
1	A	48	PHE	C-N-CA	7.93	131.22	120.44	1	4
1	A	86	LEU	N-CA-C	-7.93	95.10	108.26	11	7
1	A	52	ALA	N-CA-C	7.92	119.54	111.07	12	13
1	A	93	ASP	N-CA-C	7.92	120.16	108.60	19	2
1	A	77	VAL	CA-CB-CG2	7.91	123.85	110.40	20	4
1	A	31	VAL	O-C-N	7.91	130.09	122.97	19	1
1	A	103	LEU	CA-C-O	-7.91	111.57	119.08	9	4
1	A	75	TRP	O-C-N	7.90	130.31	122.09	13	4
1	A	10	HIS	CG-CD2-NE2	7.88	115.08	107.20	8	6
1	A	105	THR	N-CA-C	7.88	120.56	111.11	17	6
1	A	57	ASN	OD1-CG-ND2	-7.85	114.75	122.60	16	4
1	A	110	HIS	CG-ND1-CE1	-7.85	95.96	109.30	14	15
1	A	50	GLU	N-CA-C	7.83	120.51	111.11	18	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	ASP	CA-C-N	7.82	131.17	120.46	14	6
1	A	64	ASP	C-N-CA	7.82	131.17	120.46	14	6
1	A	82	THR	CB-CA-C	7.81	122.63	109.75	8	1
1	A	14	THR	N-CA-C	7.79	119.78	111.28	1	11
1	A	78	GLU	CB-CG-CD	7.79	125.84	112.60	17	4
1	A	75	TRP	CB-CG-CD2	7.78	137.69	126.80	9	2
1	A	72	ALA	N-CA-C	7.76	120.43	111.11	4	3
1	A	59	THR	N-CA-CB	-7.76	98.63	110.04	7	1
1	A	80	MET	O-C-N	-7.75	114.95	121.23	19	5
1	A	82	THR	CA-C-N	7.75	134.19	122.65	4	8
1	A	82	THR	C-N-CA	7.75	134.19	122.65	4	8
1	A	103	LEU	N-CA-C	7.75	123.32	113.25	15	2
1	A	81	PRO	O-C-N	7.74	135.80	121.10	20	2
1	A	31	VAL	CA-CB-CG1	7.74	123.55	110.40	16	5
1	A	54	LYS	CA-C-N	7.73	131.49	122.52	7	4
1	A	54	LYS	C-N-CA	7.73	131.49	122.52	7	4
1	A	83	PHE	CA-C-N	7.71	133.71	123.06	16	7
1	A	83	PHE	C-N-CA	7.71	133.71	123.06	16	7
1	A	8	ALA	N-CA-C	7.70	121.39	110.23	11	8
1	A	77	VAL	CA-C-O	7.63	130.32	120.78	18	3
1	A	59	THR	CA-CB-CG2	7.62	123.46	110.50	5	7
1	A	18	HIS	N-CA-CB	-7.61	98.25	109.82	10	2
1	A	28	LEU	CB-CA-C	7.58	122.46	109.51	8	5
1	A	105	THR	O-C-N	7.58	129.91	122.03	9	3
1	A	94	LYS	CA-C-O	7.56	129.46	120.99	14	1
1	A	48	PHE	CA-C-O	-7.56	112.45	120.92	14	3
1	A	39	PRO	CA-C-N	7.51	127.06	119.24	4	7
1	A	39	PRO	C-N-CA	7.51	127.06	119.24	4	7
1	A	106	LEU	CA-C-N	7.51	130.09	120.70	10	5
1	A	106	LEU	C-N-CA	7.51	130.09	120.70	10	5
1	A	39	PRO	N-CA-CB	7.50	110.36	103.08	6	1
1	A	3	GLU	CA-C-O	7.49	129.25	121.23	14	2
1	A	81	PRO	CA-N-CD	-7.49	101.02	111.50	14	1
1	A	26	GLN	CB-CG-CD	7.47	125.30	112.60	7	6
1	A	92	VAL	CB-CA-C	7.46	121.14	111.81	16	4
1	A	5	GLN	OE1-CD-NE2	-7.44	115.16	122.60	7	5
1	A	75	TRP	N-CA-CB	7.42	120.99	109.94	13	4
1	A	45	ALA	CA-C-N	7.41	127.77	119.32	5	6
1	A	45	ALA	C-N-CA	7.41	127.77	119.32	5	6
1	A	108	ALA	N-CA-C	7.41	118.99	111.07	19	7
1	A	39	PRO	CB-CA-C	7.39	119.94	110.92	3	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	LYS	CA-C-O	-7.39	113.24	121.00	12	1
1	A	18	HIS	CG-ND1-CE1	-7.38	96.75	109.30	12	11
1	A	85	PHE	CA-C-O	7.36	128.13	120.40	16	3
1	A	29	ILE	N-CA-C	-7.36	98.64	108.35	3	3
1	A	87	LYS	N-CA-CB	-7.35	98.68	110.51	10	6
1	A	11	THR	CA-CB-CG2	7.35	122.99	110.50	10	4
1	A	105	THR	CA-C-N	7.33	129.97	120.44	14	8
1	A	105	THR	C-N-CA	7.33	129.97	120.44	14	8
1	A	104	PRO	CA-C-N	7.33	130.32	120.65	3	3
1	A	104	PRO	C-N-CA	7.33	130.32	120.65	3	3
1	A	74	GLU	O-C-N	-7.32	114.48	122.09	2	3
1	A	103	LEU	CB-CA-C	7.32	124.58	110.17	1	4
1	A	61	LEU	CB-CA-C	7.31	124.16	109.68	14	7
1	A	62	LYS	N-CA-CB	7.31	122.31	110.90	5	1
1	A	65	VAL	CA-C-O	-7.30	112.76	120.57	18	1
1	A	99	ASP	CA-C-N	7.22	130.29	120.54	14	5
1	A	99	ASP	C-N-CA	7.22	130.29	120.54	14	5
1	A	12	VAL	N-CA-C	7.21	121.92	112.76	8	5
1	A	41	CYS	N-CA-CB	7.21	120.72	110.12	18	3
1	A	36	SER	O-C-N	7.20	129.58	122.09	19	3
1	A	40	PRO	N-CA-CB	7.18	110.98	103.15	4	2
1	A	31	VAL	CA-C-O	7.17	126.60	120.22	2	4
1	A	19	PHE	CA-C-N	7.17	129.76	120.44	5	6
1	A	19	PHE	C-N-CA	7.17	129.76	120.44	5	6
1	A	66	ASP	N-CA-C	7.16	119.70	111.11	8	5
1	A	47	ILE	CB-CA-C	7.14	121.11	111.97	15	3
1	A	31	VAL	CB-CA-C	7.14	122.99	111.29	18	7
1	A	60	PHE	CA-C-O	7.14	129.16	120.60	15	3
1	A	94	LYS	CB-CG-CD	7.10	127.62	111.30	14	1
1	A	51	LEU	CB-CA-C	7.09	122.57	110.79	13	4
1	A	57	ASN	N-CA-C	7.08	121.37	112.87	5	1
1	A	45	ALA	O-C-N	-7.08	113.17	121.32	8	1
1	A	105	THR	N-CA-CB	7.04	120.52	109.82	8	2
1	A	32	ASP	N-CA-C	7.04	120.43	110.23	12	3
1	A	6	VAL	CB-CA-C	7.03	120.61	110.98	12	2
1	A	107	VAL	CA-C-O	-7.02	113.72	121.17	16	3
1	A	34	THR	CA-CB-CG2	7.02	122.43	110.50	3	2
1	A	5	GLN	CA-C-N	7.01	131.88	122.90	12	6
1	A	5	GLN	C-N-CA	7.01	131.88	122.90	12	6
1	A	48	PHE	O-C-N	7.01	129.55	122.12	17	1
1	A	86	LEU	CB-CA-C	7.00	120.92	110.14	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	28	LEU	O-C-N	-6.99	115.23	123.06	16	1
1	A	53	LYS	CA-C-N	6.98	130.92	120.31	1	6
1	A	53	LYS	C-N-CA	6.98	130.92	120.31	1	6
1	A	70	ALA	N-CA-C	6.97	118.56	110.97	5	4
1	A	3	GLU	CA-C-N	6.95	128.38	120.53	4	2
1	A	3	GLU	C-N-CA	6.95	128.38	120.53	4	2
1	A	82	THR	CA-CB-CG2	6.95	122.31	110.50	11	2
1	A	84	ILE	CA-CB-CG2	6.94	122.30	110.50	13	2
1	A	53	LYS	CA-C-O	6.92	127.89	120.55	8	2
1	A	86	LEU	O-C-N	-6.92	114.91	123.36	7	1
1	A	78	GLU	CA-CB-CG	6.88	127.86	114.10	17	1
1	A	74	GLU	N-CA-CB	6.85	120.15	109.94	6	1
1	A	50	GLU	CA-C-O	6.85	128.03	120.63	19	1
1	A	19	PHE	CA-C-O	-6.85	113.81	121.00	20	3
1	A	90	LYS	CB-CA-C	6.84	124.04	110.42	2	3
1	A	109	LYS	O-C-N	-6.82	114.89	122.12	19	2
1	A	50	GLU	CB-CA-C	6.82	121.76	110.92	2	2
1	A	91	LEU	CA-C-N	6.81	130.48	120.74	14	6
1	A	91	LEU	C-N-CA	6.81	130.48	120.74	14	6
1	A	29	ILE	N-CA-CB	6.81	121.08	111.82	13	3
1	A	66	ASP	CB-CA-C	6.78	121.66	110.81	12	1
1	A	32	ASP	CA-C-O	6.78	128.95	121.56	3	2
1	A	70	ALA	CA-C-N	6.77	129.34	120.60	7	3
1	A	70	ALA	C-N-CA	6.77	129.34	120.60	7	3
1	A	105	THR	CA-C-O	-6.77	113.66	120.90	13	2
1	A	97	GLY	CA-C-O	6.76	128.66	121.08	8	1
1	A	48	PHE	N-CA-CB	-6.75	99.93	110.06	7	5
1	A	30	VAL	N-CA-CB	6.75	122.37	111.23	16	3
1	A	62	LYS	CA-C-O	6.73	128.61	120.27	9	6
1	A	33	PHE	CA-C-O	6.72	127.65	120.46	17	2
1	A	99	ASP	CB-CA-C	6.72	121.22	109.80	12	1
1	A	75	TRP	CB-CA-C	-6.72	100.06	110.81	13	1
1	A	7	ILE	CA-CB-CG2	6.68	121.86	110.50	17	4
1	A	110	HIS	ND1-CG-CD2	6.68	112.78	106.10	7	5
1	A	47	ILE	CA-C-N	6.67	129.76	120.29	10	5
1	A	47	ILE	C-N-CA	6.67	129.76	120.29	10	5
1	A	68	LEU	CA-C-O	6.66	127.86	121.67	17	3
1	A	72	ALA	O-C-N	6.66	129.01	122.09	4	3
1	A	26	GLN	CA-C-O	6.65	130.02	120.51	2	3
1	A	62	LYS	CB-CA-C	6.63	120.30	110.62	2	3
1	A	19	PHE	CB-CA-C	6.63	121.17	110.96	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	65	VAL	CA-CB-CG1	6.62	121.65	110.40	3	3
1	A	58	VAL	CA-CB-CG1	6.61	121.63	110.40	9	9
1	A	81	PRO	CA-C-O	6.61	136.05	120.20	1	3
1	A	105	THR	CA-CB-CG2	6.59	121.71	110.50	12	2
1	A	28	LEU	CA-C-N	6.59	132.20	122.71	17	3
1	A	28	LEU	C-N-CA	6.59	132.20	122.71	17	3
1	A	83	PHE	CB-CG-CD2	-6.58	109.51	120.70	20	2
1	A	106	LEU	CA-C-O	-6.58	114.09	121.00	19	2
1	A	82	THR	OG1-CB-CG2	-6.57	96.15	109.30	17	1
1	A	110	HIS	O-C-N	6.56	128.85	122.03	13	1
1	A	27	LYS	CB-CA-C	6.55	122.80	110.62	8	1
1	A	94	LYS	O-C-N	-6.53	115.97	123.42	18	2
1	A	37	TRP	CB-CG-CD1	-6.53	117.11	126.90	7	1
1	A	100	LYS	N-CA-CB	6.53	120.81	109.72	18	1
1	A	88	ASP	N-CA-C	6.52	124.69	110.80	3	4
1	A	30	VAL	CA-C-O	6.52	126.86	120.27	4	4
1	A	15	TRP	N-CA-CB	6.50	119.81	110.06	18	1
1	A	14	THR	CA-CB-CG2	6.49	121.53	110.50	3	5
1	A	79	ALA	CA-C-O	6.49	128.58	121.06	11	4
1	A	107	VAL	CA-CB-CG1	6.48	121.42	110.40	20	1
1	A	31	VAL	N-CA-C	6.48	118.39	107.18	17	1
1	A	36	SER	N-CA-C	6.46	120.02	111.75	8	8
1	A	16	LYS	CA-C-N	6.46	129.17	120.65	1	5
1	A	16	LYS	C-N-CA	6.46	129.17	120.65	1	5
1	A	52	ALA	CA-C-N	6.43	128.90	120.28	10	2
1	A	52	ALA	C-N-CA	6.43	128.90	120.28	10	2
1	A	62	LYS	CA-CB-CG	6.42	126.94	114.10	18	1
1	A	28	LEU	CA-C-O	6.42	127.92	120.80	11	1
1	A	98	ALA	N-CA-CB	-6.39	99.41	109.51	1	2
1	A	59	THR	CA-C-O	6.34	128.47	121.56	15	3
1	A	66	ASP	CA-C-N	6.33	129.94	120.31	3	3
1	A	66	ASP	C-N-CA	6.33	129.94	120.31	3	3
1	A	44	ILE	N-CA-CB	6.33	118.39	110.47	6	3
1	A	95	THR	CA-C-N	6.31	130.37	122.48	12	2
1	A	95	THR	C-N-CA	6.31	130.37	122.48	12	2
1	A	77	VAL	CA-CB-CG1	6.31	121.12	110.40	13	1
1	A	25	SER	CA-C-O	6.31	127.31	120.43	11	2
1	A	27	LYS	CA-CB-CG	6.30	126.70	114.10	5	1
1	A	6	VAL	CA-C-N	6.29	131.47	123.10	4	4
1	A	6	VAL	C-N-CA	6.29	131.47	123.10	4	4
1	A	110	HIS	CA-CB-CG	-6.27	107.53	113.80	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	76	ASN	CA-C-O	6.27	129.48	120.51	19	1
1	A	20	GLU	CB-CG-CD	6.26	123.25	112.60	4	2
1	A	95	THR	N-CA-C	-6.25	99.54	109.23	2	2
1	A	85	PHE	N-CA-C	-6.25	97.08	108.02	16	1
1	A	47	ILE	CA-CB-CG2	6.24	121.10	110.50	7	2
1	A	10	HIS	ND1-CG-CD2	6.23	112.33	106.10	11	3
1	A	64	ASP	CA-CB-CG	6.23	118.83	112.60	15	2
1	A	59	THR	N-CA-C	6.21	118.79	110.35	7	1
1	A	58	VAL	CA-C-O	6.20	125.74	120.22	12	2
1	A	109	LYS	CA-C-N	6.20	128.87	120.44	10	4
1	A	109	LYS	C-N-CA	6.20	128.87	120.44	10	4
1	A	31	VAL	N-CA-CB	6.19	121.45	111.23	15	1
1	A	55	PHE	O-C-N	-6.19	116.32	121.27	16	1
1	A	15	TRP	CD2-CE2-CZ2	-6.19	116.21	122.40	7	2
1	A	103	LEU	CA-C-N	6.18	127.56	119.84	12	3
1	A	103	LEU	C-N-CA	6.18	127.56	119.84	12	3
1	A	41	CYS	CA-C-N	6.17	129.37	120.79	14	1
1	A	41	CYS	C-N-CA	6.17	129.37	120.79	14	1
1	A	110	HIS	CB-CA-C	6.17	120.46	110.96	1	3
1	A	100	LYS	CA-CB-CG	6.15	126.41	114.10	19	3
1	A	9	CYS	CA-C-O	6.15	128.52	120.21	7	3
1	A	73	GLU	O-C-N	6.15	128.49	122.09	20	4
1	A	39	PRO	CA-C-O	-6.14	111.65	120.56	18	3
1	A	107	VAL	CA-C-N	6.13	128.41	120.44	14	1
1	A	107	VAL	C-N-CA	6.13	128.41	120.44	14	1
1	A	79	ALA	CB-CA-C	6.12	119.18	110.24	18	1
1	A	65	VAL	O-C-N	-6.12	115.94	121.87	14	3
1	A	24	GLY	CA-C-N	6.12	131.62	123.00	14	2
1	A	24	GLY	C-N-CA	6.12	131.62	123.00	14	2
1	A	30	VAL	O-C-N	6.11	129.80	123.20	13	3
1	A	42	LYS	CB-CA-C	6.11	120.63	110.92	16	3
1	A	29	ILE	O-C-N	-6.11	116.00	123.09	16	1
1	A	46	PRO	O-C-N	-6.11	115.22	122.24	8	1
1	A	95	THR	CA-C-O	6.11	127.21	120.31	13	3
1	A	105	THR	CB-CA-C	6.09	120.60	110.92	7	2
1	A	82	THR	N-CA-C	-6.08	99.79	109.76	20	2
1	A	63	VAL	O-C-N	6.06	129.76	123.03	1	3
1	A	15	TRP	O-C-N	6.06	128.55	122.12	20	2
1	A	81	PRO	N-CA-C	6.06	127.85	112.10	9	1
1	A	48	PHE	CB-CA-C	6.05	120.97	110.68	3	3
1	A	73	GLU	CA-C-N	6.05	128.70	120.54	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	73	GLU	C-N-CA	6.05	128.70	120.54	8	1
1	A	42	LYS	O-C-N	6.04	128.52	122.12	18	4
1	A	101	ASP	CB-CA-C	6.02	120.90	110.79	18	2
1	A	11	THR	CA-C-O	-6.01	114.99	121.36	6	2
1	A	12	VAL	CA-C-O	5.99	128.26	120.78	17	1
1	A	13	ASP	N-CA-CB	5.99	118.69	110.01	19	1
1	A	64	ASP	CB-CA-C	5.97	120.44	110.88	16	1
1	A	31	VAL	CA-C-N	5.97	130.32	120.94	10	4
1	A	31	VAL	C-N-CA	5.97	130.32	120.94	10	4
1	A	6	VAL	CA-C-O	5.97	126.96	120.57	6	2
1	A	109	LYS	N-CA-CB	5.97	118.66	110.01	4	1
1	A	29	ILE	CA-CB-CG2	5.96	120.64	110.50	1	1
1	A	52	ALA	O-C-N	5.96	128.44	122.12	6	1
1	A	69	LYS	CB-CG-CD	5.96	125.00	111.30	12	1
1	A	5	GLN	CB-CA-C	5.95	119.31	110.62	1	2
1	A	47	ILE	N-CA-CB	5.95	117.51	110.55	20	3
1	A	37	TRP	CA-CB-CG	5.95	124.90	113.60	17	4
1	A	18	HIS	CA-C-O	5.94	129.00	120.51	20	2
1	A	76	ASN	CA-C-N	5.93	128.60	122.96	19	1
1	A	76	ASN	C-N-CA	5.93	128.60	122.96	19	1
1	A	43	MET	CA-C-N	5.91	128.87	120.53	15	1
1	A	43	MET	C-N-CA	5.91	128.87	120.53	15	1
1	A	111	ALA	N-CA-CB	-5.90	101.44	110.12	15	3
1	A	104	PRO	N-CA-C	5.88	124.59	112.47	12	5
1	A	27	LYS	O-C-N	5.88	129.72	123.42	11	1
1	A	8	ALA	N-CA-CB	-5.88	101.70	110.17	13	4
1	A	110	HIS	CA-C-N	5.88	128.48	120.54	2	3
1	A	110	HIS	C-N-CA	5.88	128.48	120.54	2	3
1	A	95	THR	O-C-N	-5.88	117.33	123.56	11	1
1	A	8	ALA	CA-C-N	5.87	131.75	122.94	9	1
1	A	8	ALA	C-N-CA	5.87	131.75	122.94	9	1
1	A	37	TRP	CB-CA-C	5.87	121.12	111.50	20	2
1	A	79	ALA	N-CA-C	5.87	118.00	108.26	20	1
1	A	37	TRP	CA-C-O	5.86	128.89	120.51	6	1
1	A	74	GLU	CA-CB-CG	5.85	125.80	114.10	9	5
1	A	89	GLY	CA-C-N	5.85	132.71	121.54	19	1
1	A	89	GLY	C-N-CA	5.85	132.71	121.54	19	1
1	A	57	ASN	N-CA-CB	-5.85	102.09	110.57	10	1
1	A	73	GLU	CB-CA-C	5.84	120.21	110.92	17	1
1	A	37	TRP	CG-CD2-CE3	-5.84	128.06	133.90	8	1
1	A	18	HIS	CA-C-N	5.83	128.03	120.44	13	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	HIS	C-N-CA	5.83	128.03	120.44	13	4
1	A	78	GLU	CB-CA-C	5.83	121.58	110.27	2	1
1	A	66	ASP	N-CA-CB	5.83	118.46	110.01	17	1
1	A	71	VAL	CB-CA-C	5.83	119.34	111.88	18	1
1	A	76	ASN	CB-CG-ND2	5.82	125.13	116.40	12	1
1	A	108	ALA	O-C-N	5.82	128.14	122.09	16	1
1	A	51	LEU	N-CA-C	5.82	118.09	111.11	3	3
1	A	75	TRP	CA-CB-CG	5.80	124.63	113.60	2	3
1	A	98	ALA	N-CA-C	5.80	118.76	110.24	12	2
1	A	7	ILE	CA-C-O	5.79	126.47	120.39	3	1
1	A	27	LYS	CG-CD-CE	5.78	124.59	111.30	5	1
1	A	26	GLN	OE1-CD-NE2	-5.78	116.82	122.60	8	1
1	A	6	VAL	CA-CB-CG2	5.76	120.19	110.40	16	2
1	A	23	LYS	CA-C-O	5.76	127.64	121.02	20	2
1	A	103	LEU	N-CA-CB	-5.75	100.13	110.37	1	2
1	A	45	ALA	CB-CA-C	5.75	121.49	110.17	9	3
1	A	58	VAL	N-CA-CB	-5.74	104.87	112.34	6	1
1	A	77	VAL	N-CA-C	-5.74	97.40	109.34	11	2
1	A	59	THR	CA-C-N	5.74	131.97	122.33	9	2
1	A	59	THR	C-N-CA	5.74	131.97	122.33	9	2
1	A	106	LEU	CB-CA-C	5.73	119.88	110.88	14	2
1	A	25	SER	N-CA-C	-5.72	99.91	109.24	11	1
1	A	105	THR	CA-CB-OG1	5.71	118.17	109.60	18	1
1	A	70	ALA	O-C-N	5.71	128.19	122.08	6	1
1	A	79	ALA	O-C-N	5.71	129.53	123.42	16	2
1	A	6	VAL	N-CA-CB	5.71	118.33	111.31	10	1
1	A	102	GLY	N-CA-C	5.71	119.79	112.83	12	3
1	A	86	LEU	CA-C-N	5.69	133.14	123.01	13	1
1	A	86	LEU	C-N-CA	5.69	133.14	123.01	13	1
1	A	73	GLU	N-CA-C	5.69	117.94	111.11	6	1
1	A	15	TRP	N-CA-C	5.69	118.22	111.33	12	1
1	A	44	ILE	CA-C-O	-5.69	115.03	120.95	1	2
1	A	64	ASP	CB-CG-OD1	5.69	131.48	118.40	3	1
1	A	4	GLY	N-CA-C	-5.68	99.72	113.18	9	2
1	A	50	GLU	CA-C-N	5.67	128.20	120.54	4	1
1	A	50	GLU	C-N-CA	5.67	128.20	120.54	4	1
1	A	106	LEU	N-CA-CB	-5.66	101.51	109.94	10	1
1	A	75	TRP	CG-CD1-NE1	5.65	117.55	110.20	14	1
1	A	75	TRP	CD2-CE2-CZ2	-5.65	116.75	122.40	20	2
1	A	54	LYS	N-CA-CB	-5.65	101.52	110.22	19	3
1	A	69	LYS	CA-C-N	5.65	128.64	120.79	20	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	69	LYS	C-N-CA	5.65	128.64	120.79	20	3
1	A	79	ALA	CA-C-N	5.65	129.19	121.74	19	3
1	A	79	ALA	C-N-CA	5.65	129.19	121.74	19	3
1	A	90	LYS	CA-C-O	-5.64	112.44	120.51	20	1
1	A	84	ILE	CA-C-N	5.63	130.16	122.84	4	1
1	A	84	ILE	C-N-CA	5.63	130.16	122.84	4	1
1	A	3	GLU	O-C-N	5.63	129.17	123.26	7	1
1	A	53	LYS	O-C-N	-5.62	116.16	122.12	8	1
1	A	18	HIS	ND1-CG-CD2	5.61	111.71	106.10	17	1
1	A	47	ILE	CA-CB-CG1	5.60	119.92	110.40	3	1
1	A	85	PHE	O-C-N	5.60	130.45	123.28	20	1
1	A	74	GLU	CB-CA-C	5.59	119.76	110.81	4	4
1	A	76	ASN	O-C-N	-5.56	115.19	122.59	11	1
1	A	75	TRP	CB-CG-CD1	-5.56	118.56	126.90	5	2
1	A	66	ASP	CA-C-O	5.56	126.85	120.90	14	1
1	A	42	LYS	CA-C-N	5.55	127.99	120.44	9	1
1	A	42	LYS	C-N-CA	5.55	127.99	120.44	9	1
1	A	14	THR	O-C-N	5.55	128.00	122.12	14	1
1	A	55	PHE	CB-CA-C	5.54	119.19	110.71	12	1
1	A	54	LYS	CB-CA-C	5.54	119.98	110.79	5	2
1	A	85	PHE	N-CA-CB	5.54	119.26	110.84	7	1
1	A	72	ALA	CA-C-N	5.53	127.63	120.44	4	2
1	A	72	ALA	C-N-CA	5.53	127.63	120.44	4	2
1	A	21	LYS	CB-CA-C	5.53	119.47	110.96	18	1
1	A	93	ASP	CA-C-O	-5.53	115.52	121.38	19	1
1	A	36	SER	CB-CA-C	5.52	119.95	110.79	2	1
1	A	7	ILE	CA-C-N	5.52	128.68	120.95	2	1
1	A	7	ILE	C-N-CA	5.52	128.68	120.95	2	1
1	A	42	LYS	N-CA-CB	5.51	118.19	109.82	14	1
1	A	38	CYS	CA-CB-SG	-5.51	101.73	114.40	19	1
1	A	60	PHE	N-CA-CB	5.50	119.85	110.71	19	1
1	A	94	LYS	CB-CA-C	5.49	119.14	109.80	20	1
1	A	91	LEU	CD1-CG-CD2	-5.49	98.72	110.80	6	1
1	A	30	VAL	N-CA-C	-5.48	100.16	108.17	5	1
1	A	28	LEU	N-CA-CB	-5.48	101.78	110.06	13	1
1	A	46	PRO	CA-C-N	5.47	127.45	120.56	19	2
1	A	46	PRO	C-N-CA	5.47	127.45	120.56	19	2
1	A	44	ILE	CA-CB-CG2	5.46	119.79	110.50	9	1
1	A	84	ILE	N-CA-C	-5.46	100.33	108.46	3	1
1	A	80	MET	N-CA-CB	-5.46	101.11	110.01	4	1
1	A	50	GLU	O-C-N	5.45	127.92	122.08	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	78	GLU	N-CA-CB	-5.45	100.82	110.42	2	2
1	A	16	LYS	CB-CG-CD	5.45	123.84	111.30	7	1
1	A	34	THR	N-CA-C	-5.45	100.44	108.99	19	4
1	A	22	GLY	CA-C-N	5.44	131.05	122.34	4	1
1	A	22	GLY	C-N-CA	5.44	131.05	122.34	4	1
1	A	40	PRO	CA-C-N	5.44	128.58	120.31	13	1
1	A	40	PRO	C-N-CA	5.44	128.58	120.31	13	1
1	A	77	VAL	O-C-N	5.44	129.37	122.57	17	2
1	A	71	VAL	N-CA-CB	5.43	116.91	110.55	5	2
1	A	99	ASP	CA-C-O	5.43	126.60	119.98	8	1
1	A	15	TRP	CA-C-O	-5.42	115.13	120.82	11	1
1	A	48	PHE	N-CA-C	5.41	117.93	111.71	1	1
1	A	99	ASP	CB-CG-OD2	-5.41	105.96	118.40	2	1
1	A	59	THR	CA-CB-OG1	5.41	117.72	109.60	8	1
1	A	73	GLU	CG-CD-OE1	5.40	130.83	118.40	16	1
1	A	65	VAL	CA-C-N	5.39	127.51	120.28	10	1
1	A	65	VAL	C-N-CA	5.39	127.51	120.28	10	1
1	A	55	PHE	CA-C-O	-5.39	114.19	120.34	2	1
1	A	62	LYS	CG-CD-CE	5.39	123.69	111.30	13	2
1	A	98	ALA	CA-C-O	-5.38	114.98	120.80	14	2
1	A	92	VAL	O-C-N	-5.37	116.41	121.94	16	1
1	A	56	PRO	CA-N-CD	-5.37	104.48	112.00	15	3
1	A	66	ASP	CB-CG-OD1	5.37	130.74	118.40	9	1
1	A	33	PHE	O-C-N	5.36	130.11	123.14	5	1
1	A	26	GLN	CB-CA-C	5.34	121.05	110.42	19	1
1	A	54	LYS	CA-C-O	5.33	126.17	120.20	9	2
1	A	62	LYS	N-CA-C	5.33	116.89	107.61	13	1
1	A	67	GLU	O-C-N	-5.32	115.72	122.27	3	1
1	A	63	VAL	N-CA-CB	5.32	117.86	111.31	6	2
1	A	90	LYS	N-CA-C	5.32	122.13	110.80	14	2
1	A	20	GLU	CA-C-N	5.32	127.67	120.65	9	1
1	A	20	GLU	C-N-CA	5.32	127.67	120.65	9	1
1	A	93	ASP	N-CA-CB	-5.31	102.84	111.24	17	1
1	A	18	HIS	O-C-N	5.31	127.76	122.08	11	2
1	A	58	VAL	O-C-N	-5.30	118.20	122.97	6	1
1	A	14	THR	CA-C-O	-5.30	114.93	120.55	14	1
1	A	100	LYS	CG-CD-CE	5.30	123.49	111.30	17	1
1	A	55	PHE	N-CA-CB	-5.29	101.71	111.03	12	1
1	A	63	VAL	CB-CA-C	5.29	117.47	110.91	2	2
1	A	25	SER	CB-CA-C	5.29	119.38	109.71	4	1
1	A	29	ILE	CA-C-N	5.28	130.28	122.94	18	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	ILE	C-N-CA	5.28	130.28	122.94	18	3
1	A	34	THR	N-CA-CB	5.28	120.69	111.13	11	2
1	A	20	GLU	CA-C-O	-5.28	115.25	120.90	7	2
1	A	85	PHE	CB-CA-C	5.28	118.32	110.62	1	1
1	A	35	ALA	CB-CA-C	5.28	118.67	109.65	1	2
1	A	37	TRP	CA-C-N	5.28	126.92	122.28	6	1
1	A	37	TRP	C-N-CA	5.28	126.92	122.28	6	1
1	A	49	ALA	N-CA-CB	-5.27	102.42	110.07	6	1
1	A	35	ALA	O-C-N	5.27	128.97	123.06	10	1
1	A	57	ASN	CB-CG-ND2	5.25	124.28	116.40	10	2
1	A	80	MET	N-CA-C	5.25	117.22	109.50	12	1
1	A	83	PHE	CB-CG-CD1	5.24	129.62	120.70	11	1
1	A	23	LYS	N-CA-CB	5.24	119.34	110.49	3	1
1	A	12	VAL	CA-C-N	5.23	127.29	120.28	17	1
1	A	12	VAL	C-N-CA	5.23	127.29	120.28	17	1
1	A	88	ASP	CA-C-N	5.23	131.66	121.41	17	1
1	A	88	ASP	C-N-CA	5.23	131.66	121.41	17	1
1	A	64	ASP	N-CA-CB	-5.23	101.66	110.49	17	1
1	A	75	TRP	CD1-NE1-CE2	-5.22	99.50	108.90	8	1
1	A	95	THR	CA-CB-OG1	5.22	117.43	109.60	11	1
1	A	63	VAL	CA-CB-CG1	5.22	119.27	110.40	5	2
1	A	61	LEU	CA-C-O	5.22	127.30	121.40	20	2
1	A	14	THR	N-CA-CB	5.21	117.87	110.06	7	1
1	A	25	SER	N-CA-CB	5.20	118.01	109.95	19	1
1	A	59	THR	O-C-N	5.20	128.72	122.79	5	2
1	A	18	HIS	CB-CG-ND1	5.20	130.50	122.70	10	1
1	A	68	LEU	N-CA-C	5.19	116.53	110.41	10	1
1	A	11	THR	O-C-N	-5.19	116.85	122.92	11	1
1	A	66	ASP	O-C-N	5.19	127.41	122.07	17	1
1	A	74	GLU	CA-C-N	5.17	127.21	120.28	7	2
1	A	74	GLU	C-N-CA	5.17	127.21	120.28	7	2
1	A	12	VAL	CA-CB-CG2	5.17	119.18	110.40	19	1
1	A	5	GLN	O-C-N	5.16	129.30	123.42	19	1
1	A	80	MET	CA-CB-CG	-5.15	103.80	114.10	20	1
1	A	75	TRP	NE1-CE2-CZ2	-5.14	122.39	130.10	3	1
1	A	40	PRO	N-CA-C	5.14	123.05	112.47	10	1
1	A	56	PRO	CB-CA-C	-5.14	104.56	111.85	10	1
1	A	77	VAL	N-CA-CB	5.13	119.69	111.23	13	1
1	A	111	ALA	O-C-N	5.13	127.57	122.08	18	2
1	A	108	ALA	N-CA-CB	-5.13	102.58	110.01	19	1
1	A	84	ILE	N-CA-CB	5.12	119.83	111.44	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	44	ILE	CB-CA-C	5.11	119.04	112.14	1	1
1	A	80	MET	CA-C-N	-5.11	114.73	127.00	1	1
1	A	80	MET	C-N-CA	-5.11	114.73	127.00	1	1
1	A	29	ILE	CB-CA-C	5.10	117.06	110.12	4	1
1	A	110	HIS	CA-C-O	-5.10	115.46	120.82	14	1
1	A	33	PHE	CB-CA-C	5.10	119.03	111.17	1	2
1	A	87	LYS	CB-CA-C	5.10	121.52	111.22	11	1
1	A	70	ALA	CB-CA-C	5.09	119.02	110.92	11	1
1	A	101	ASP	CA-C-O	-5.09	114.59	120.24	3	1
1	A	12	VAL	O-C-N	-5.09	116.26	122.06	9	1
1	A	24	GLY	O-C-N	5.09	129.31	122.70	8	1
1	A	32	ASP	O-C-N	-5.08	116.62	122.87	12	1
1	A	38	CYS	O-C-N	-5.08	115.48	121.32	16	1
1	A	42	LYS	CB-CG-CD	5.08	122.98	111.30	17	1
1	A	66	ASP	CB-CG-OD2	-5.07	106.73	118.40	20	1
1	A	100	LYS	CA-C-O	5.06	126.94	121.02	18	1
1	A	7	ILE	CA-CB-CG1	5.06	119.00	110.40	14	1
1	A	78	GLU	CA-C-N	5.05	130.52	122.74	4	1
1	A	78	GLU	C-N-CA	5.05	130.52	122.74	4	1
1	A	64	ASP	CB-CG-OD2	-5.04	106.81	118.40	4	1
1	A	30	VAL	CA-CB-CG1	5.04	118.97	110.40	11	1
1	A	102	GLY	O-C-N	-5.04	117.28	122.17	12	1
1	A	88	ASP	CA-C-O	5.03	127.70	120.51	3	1
1	A	93	ASP	CB-CG-OD2	-5.03	106.84	118.40	5	1
1	A	90	LYS	CA-C-N	5.03	131.14	121.54	14	1
1	A	90	LYS	C-N-CA	5.03	131.14	121.54	14	1
1	A	21	LYS	N-CA-CB	5.02	117.24	109.91	16	1
1	A	94	LYS	CA-C-N	5.01	128.34	121.33	14	1
1	A	94	LYS	C-N-CA	5.01	128.34	121.33	14	1
1	A	17	GLU	CB-CG-CD	5.00	121.11	112.60	3	1
1	A	34	THR	O-C-N	-5.00	117.68	123.33	10	1
1	A	102	GLY	CA-C-O	5.00	125.70	120.80	12	1
1	A	47	ILE	CB-CG1-CD1	5.00	124.30	113.80	16	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	81	PRO	Peptide,Mainchain	17
1	A	48	PHE	Sidechain	11

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	77	VAL	Peptide,Mainchain	10
1	A	110	HIS	Sidechain	9
1	A	75	TRP	Peptide	8
1	A	57	ASN	Peptide,Mainchain	6
1	A	83	PHE	Sidechain	5
1	A	87	LYS	Peptide	4
1	A	9	CYS	Peptide	2
1	A	19	PHE	Sidechain	2
1	A	33	PHE	Sidechain	2
1	A	10	HIS	Sidechain	2
1	A	54	LYS	Peptide,Mainchain	2
1	A	85	PHE	Sidechain	2
1	A	63	VAL	Peptide	2
1	A	18	HIS	Sidechain	2
1	A	79	ALA	Peptide	2
1	A	80	MET	Mainchain	2
1	A	36	SER	Peptide	1
1	A	55	PHE	Sidechain	1
1	A	78	GLU	Sidechain	1
1	A	58	VAL	Peptide	1
1	A	31	VAL	Peptide	1
1	A	35	ALA	Mainchain	1
1	A	74	GLU	Mainchain	1
1	A	4	GLY	Mainchain	1
1	A	98	ALA	Mainchain	1
1	A	27	LYS	Peptide	1
1	A	71	VAL	Mainchain	1
1	A	82	THR	Mainchain	1

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	849	864	862	1±1
All	All	16980	17280	17240	22

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:THR:HA	1:A:80:MET:SD	0.61	2.36	14	3
1:A:9:CYS:SG	1:A:61:LEU:HD13	0.60	2.37	17	4
1:A:80:MET:HE2	1:A:80:MET:HA	0.56	1.77	15	1
1:A:9:CYS:SG	1:A:61:LEU:CD1	0.56	2.94	17	1
1:A:38:CYS:SG	1:A:41:CYS:SG	0.55	3.04	3	2
1:A:41:CYS:HA	1:A:44:ILE:HG22	0.50	1.84	19	2
1:A:51:LEU:HD11	1:A:107:VAL:HG11	0.48	1.86	16	1
1:A:77:VAL:HG22	1:A:82:THR:HG21	0.47	1.85	16	1
1:A:9:CYS:SG	1:A:61:LEU:HB2	0.45	2.52	10	1
1:A:80:MET:SD	1:A:80:MET:N	0.43	2.92	2	1
1:A:41:CYS:SG	1:A:81:PRO:CG	0.42	3.07	17	1
1:A:28:LEU:HD21	1:A:110:HIS:HB3	0.41	1.91	19	1
1:A:8:ALA:O	1:A:9:CYS:SG	0.41	2.78	6	1
1:A:80:MET:HA	1:A:80:MET:HE2	0.40	1.93	12	1
1:A:29:ILE:HG12	1:A:86:LEU:O	0.40	2.16	18	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	109/113 (96%)	85±3 (78±2%)	18±2 (16±2%)	6±1 (6±1%)	2	20
All	All	2180/2260 (96%)	1699 (78%)	354 (16%)	127 (6%)	2	20

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

Mol	Chain	Res	Type	Models (Total)
1	A	76	ASN	20
1	A	81	PRO	20
1	A	88	ASP	19
1	A	22	GLY	18
1	A	26	GLN	12
1	A	89	GLY	10

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Mol	Chain	Res	Type	Models (Total)
1	A	37	TRP	9
1	A	77	VAL	5
1	A	90	LYS	4
1	A	91	LEU	3
1	A	102	GLY	2
1	A	97	GLY	2
1	A	23	LYS	1
1	A	98	ALA	1
1	A	57	ASN	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	92/94 (98%)	80±2 (87±2%)	12±2 (13±2%)	6	47
All	All	1840/1880 (98%)	1601 (87%)	239 (13%)	6	47

All 35 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	7	ILE	20
1	A	44	ILE	20
1	A	86	LEU	20
1	A	74	GLU	16
1	A	61	LEU	15
1	A	14	THR	15
1	A	84	ILE	14
1	A	96	VAL	14
1	A	51	LEU	14
1	A	65	VAL	13
1	A	29	ILE	12
1	A	94	LYS	11
1	A	78	GLU	9
1	A	93	ASP	6
1	A	31	VAL	5
1	A	80	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	67	GLU	3
1	A	23	LYS	3
1	A	81	PRO	3
1	A	90	LYS	2
1	A	26	GLN	2
1	A	56	PRO	2
1	A	19	PHE	2
1	A	48	PHE	2
1	A	58	VAL	2
1	A	105	THR	1
1	A	11	THR	1
1	A	50	GLU	1
1	A	27	LYS	1
1	A	20	GLU	1
1	A	41	CYS	1
1	A	36	SER	1
1	A	18	HIS	1
1	A	100	LYS	1
1	A	3	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided