



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 08:01 pm GMT

PDB ID : 1TI3
Title : Solution structure of the Thioredoxin h1 from poplar, a CPPC active site variant
Authors : Coudeville, 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

<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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

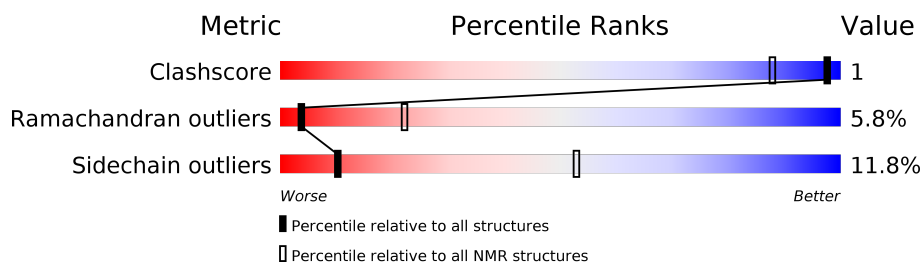
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	 52% 40% . . .

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)	0.27	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.

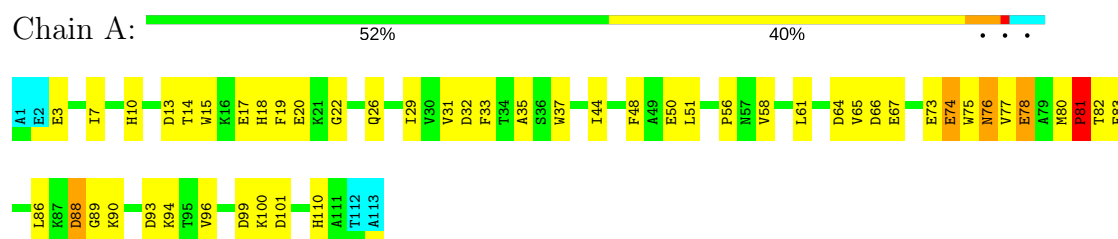
Mol	Chain	Residues	Atoms						Trace
1	A	113	Total	C	H	N	O	S	0
			1766	569	890	140	162	5	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA 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: thioredoxin H

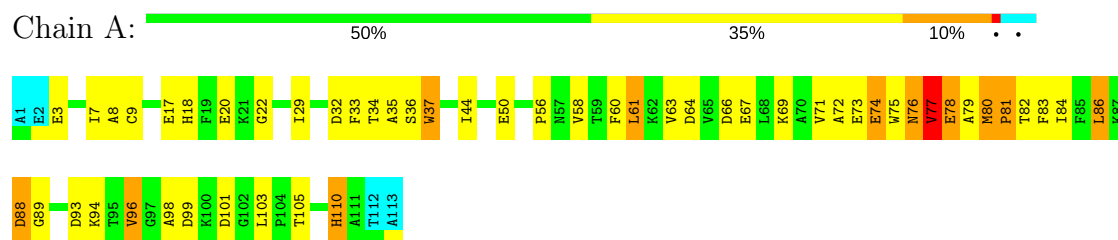


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

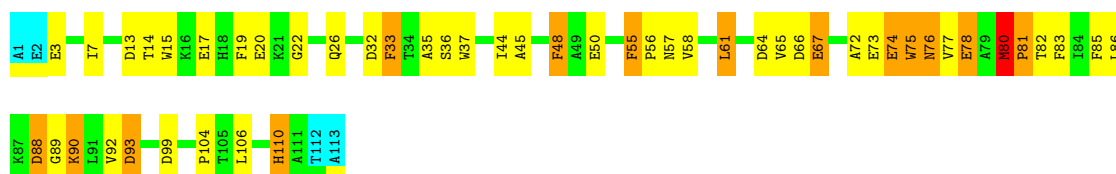
- Molecule 1: thioredoxin H



4.2.2 Score per residue for model 2

- Molecule 1: thioredoxin H

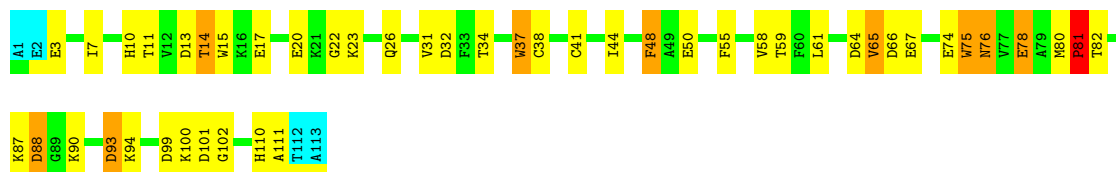




4.2.3 Score per residue for model 3

- Molecule 1: thioredoxin H

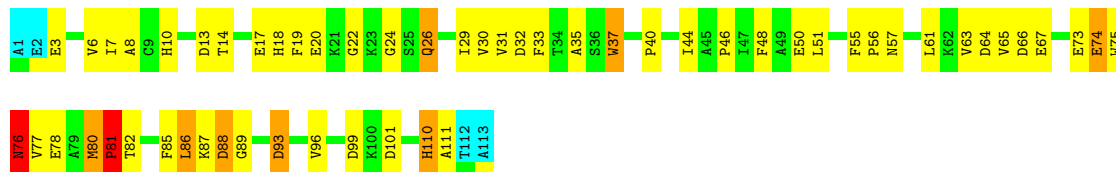
Chain A: 55% 33% 8%



4.2.4 Score per residue for model 4

- Molecule 1: thioredoxin H

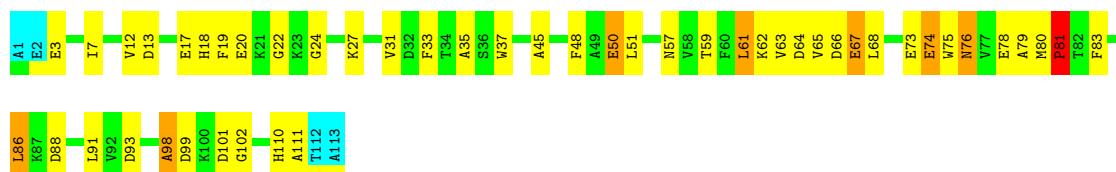
Chain A: 47% 41% 7%



4.2.5 Score per residue for model 5

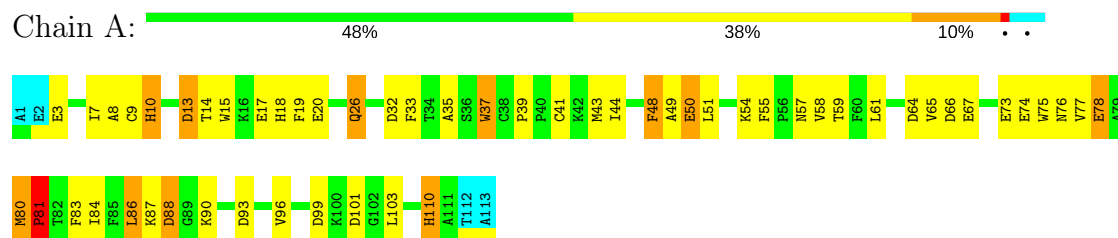
- Molecule 1: thioredoxin H

Chain A: 54% 35% 6%



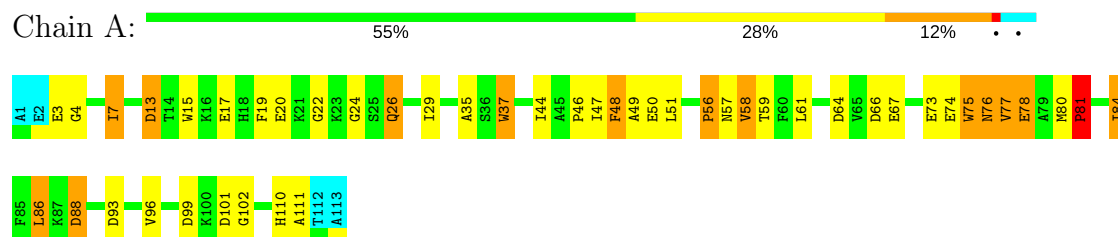
4.2.6 Score per residue for model 6

- Molecule 1: thioredoxin H



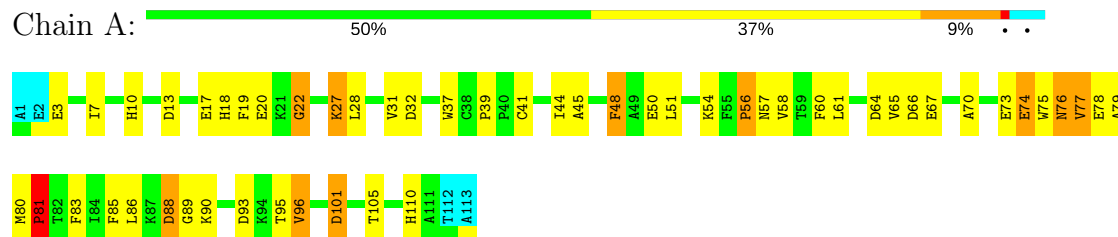
4.2.7 Score per residue for model 7

- Molecule 1: thioredoxin H



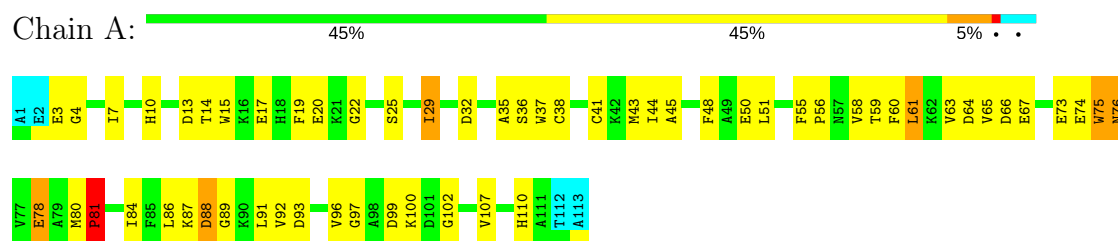
4.2.8 Score per residue for model 8

- Molecule 1: thioredoxin H



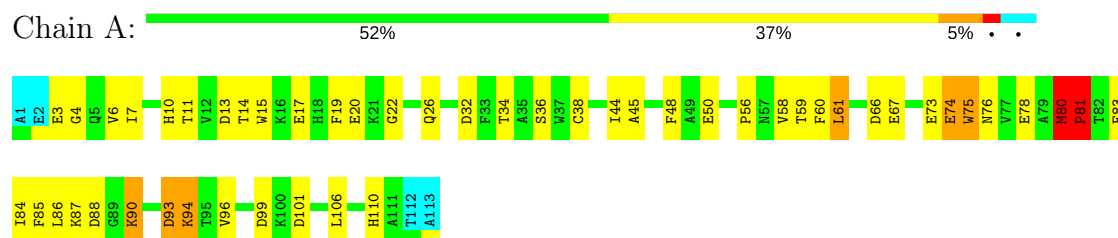
4.2.9 Score per residue for model 9

- Molecule 1: thioredoxin H



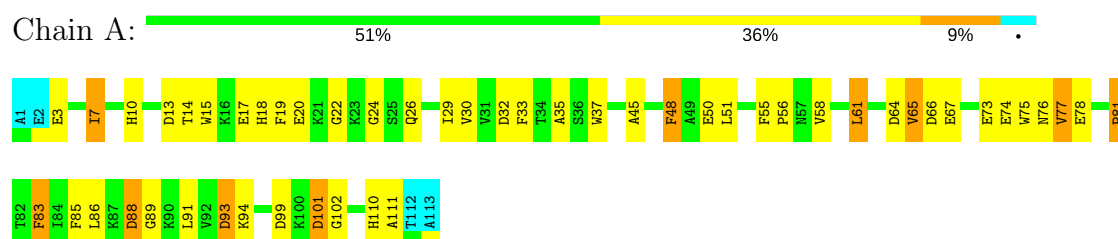
4.2.14 Score per residue for model 14

- Molecule 1: thioredoxin H



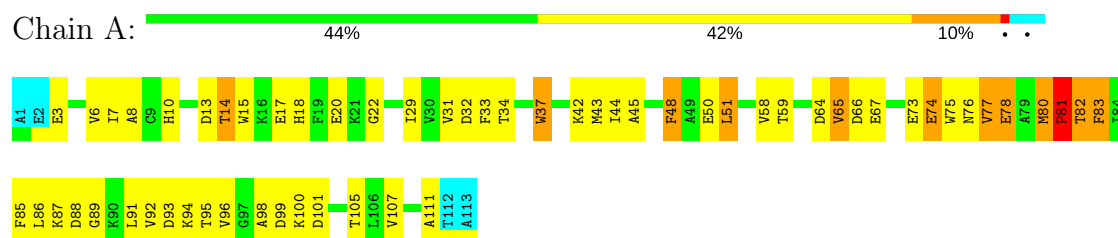
4.2.15 Score per residue for model 15

- Molecule 1: thioredoxin H



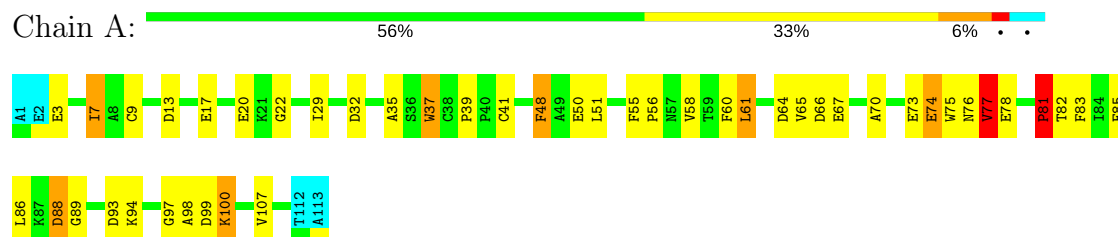
4.2.16 Score per residue for model 16

- Molecule 1: thioredoxin H



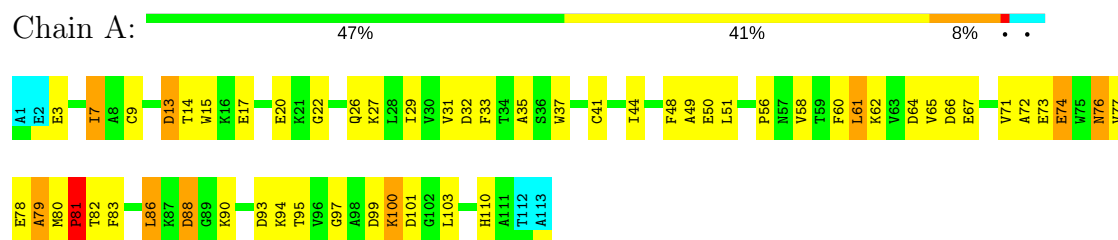
4.2.17 Score per residue for model 17

- Molecule 1: thioredoxin H



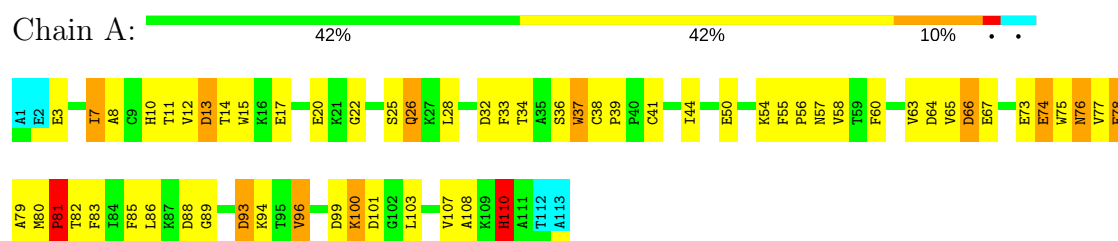
4.2.18 Score per residue for model 18

- Molecule 1: thioredoxin H



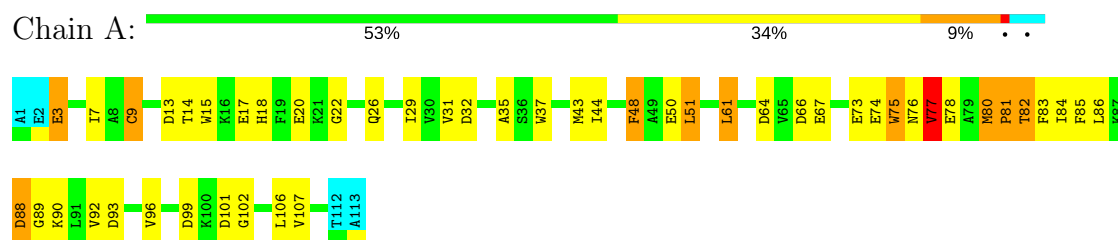
4.2.19 Score per residue for model 19

- Molecule 1: thioredoxin H



4.2.20 Score per residue for model 20

- Molecule 1: thioredoxin H



5 Refinement protocol and experimental data overview

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. 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	2.14±0.05	21±3/871 (2.4±0.4%)	2.31±0.05	40±4/1182 (3.4±0.4%)
All	All	2.14	421/17420 (2.4%)	2.31	805/23640 (3.4%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	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	78	GLU	CD-OE2	20.50	1.48	1.25	11	20
1	A	17	GLU	CD-OE2	16.32	1.43	1.25	10	20
1	A	67	GLU	CD-OE2	16.31	1.43	1.25	16	20
1	A	73	GLU	CD-OE2	15.49	1.42	1.25	11	19
1	A	50	GLU	CD-OE2	14.78	1.42	1.25	12	20
1	A	20	GLU	CD-OE2	14.67	1.41	1.25	17	20
1	A	3	GLU	CD-OE2	13.90	1.41	1.25	20	20
1	A	74	GLU	CD-OE2	13.13	1.40	1.25	5	20
1	A	32	ASP	CG-OD2	8.53	1.45	1.25	18	10
1	A	88	ASP	CG-OD2	8.36	1.44	1.25	6	12
1	A	99	ASP	CG-OD2	8.31	1.44	1.25	17	14
1	A	17	GLU	CD-OE1	-7.95	1.17	1.25	2	1
1	A	75	TRP	CG-CD1	7.75	1.47	1.36	11	5
1	A	74	GLU	CG-CD	7.65	1.63	1.51	14	1
1	A	74	GLU	CB-CG	7.60	1.66	1.52	16	1
1	A	89	GLY	CA-C	7.50	1.63	1.51	20	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	93	ASP	CG-OD2	7.39	1.42	1.25	6	11
1	A	13	ASP	CG-OD2	7.36	1.42	1.25	6	9
1	A	56	PRO	CA-C	7.31	1.67	1.52	14	2
1	A	78	GLU	CB-CG	7.27	1.66	1.52	7	1
1	A	18	HIS	CG-CD2	7.25	1.48	1.35	6	2
1	A	37	TRP	CG-CD1	7.24	1.46	1.36	11	5
1	A	101	ASP	CG-OD2	7.16	1.41	1.25	15	12
1	A	15	TRP	CD2-CE3	7.16	1.51	1.40	9	1
1	A	75	TRP	CD2-CE2	7.09	1.49	1.41	3	2
1	A	64	ASP	CG-OD2	7.08	1.41	1.25	6	13
1	A	75	TRP	CG-CD2	-7.05	1.31	1.43	12	3
1	A	15	TRP	CG-CD2	-6.94	1.31	1.43	9	3
1	A	78	GLU	CD-OE1	-6.94	1.18	1.25	1	2
1	A	50	GLU	CB-CG	6.89	1.65	1.52	5	1
1	A	74	GLU	CD-OE1	-6.82	1.18	1.25	15	1
1	A	24	GLY	CA-C	6.80	1.62	1.51	7	3
1	A	15	TRP	NE1-CE2	6.79	1.46	1.37	13	4
1	A	25	SER	CB-OG	-6.77	1.33	1.42	9	1
1	A	66	ASP	CG-OD2	6.75	1.40	1.25	2	13
1	A	80	MET	N-CA	6.72	1.59	1.46	1	1
1	A	33	PHE	CB-CG	6.65	1.62	1.51	12	1
1	A	10	HIS	CG-CD2	6.65	1.47	1.35	3	4
1	A	81	PRO	N-CD	-6.61	1.38	1.47	3	2
1	A	110	HIS	CG-CD2	6.58	1.47	1.35	7	3
1	A	75	TRP	NE1-CE2	6.54	1.46	1.37	11	3
1	A	43	MET	N-CA	6.48	1.59	1.46	9	1
1	A	3	GLU	CD-OE1	-6.47	1.18	1.25	15	2
1	A	80	MET	C-N	6.44	1.46	1.34	1	4
1	A	75	TRP	CZ2-CH2	6.43	1.49	1.37	17	2
1	A	15	TRP	CG-CD1	6.33	1.45	1.36	3	7
1	A	81	PRO	N-CA	6.29	1.57	1.47	20	1
1	A	72	ALA	N-CA	6.28	1.58	1.46	11	1
1	A	67	GLU	CD-OE1	-6.26	1.18	1.25	14	4
1	A	74	GLU	C-O	6.19	1.35	1.23	11	1
1	A	75	TRP	CD2-CE3	5.98	1.49	1.40	20	1
1	A	22	GLY	CA-C	5.97	1.61	1.51	8	2
1	A	81	PRO	CA-CB	5.95	1.65	1.53	1	2
1	A	36	SER	CA-CB	5.94	1.61	1.52	9	2
1	A	104	PRO	CA-C	5.92	1.64	1.52	2	1
1	A	83	PHE	CB-CG	5.92	1.61	1.51	17	2
1	A	37	TRP	CB-CG	5.87	1.60	1.50	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	79	ALA	CA-C	5.85	1.68	1.52	5	1
1	A	78	GLU	N-CA	5.83	1.58	1.46	11	1
1	A	61	LEU	CA-CB	5.80	1.67	1.53	2	1
1	A	39	PRO	CA-C	5.77	1.64	1.52	17	3
1	A	88	ASP	CA-C	5.75	1.68	1.52	15	1
1	A	95	THR	CB-OG1	-5.74	1.31	1.43	18	1
1	A	75	TRP	CB-CG	5.74	1.60	1.50	10	1
1	A	36	SER	N-CA	5.71	1.57	1.46	14	1
1	A	37	TRP	CG-CD2	-5.71	1.33	1.43	15	4
1	A	110	HIS	CB-CG	5.69	1.60	1.50	3	1
1	A	40	PRO	N-CA	5.67	1.56	1.47	12	1
1	A	80	MET	CA-CB	5.65	1.66	1.53	20	1
1	A	83	PHE	CG-CD2	5.64	1.47	1.38	19	1
1	A	93	ASP	N-CA	5.63	1.57	1.46	15	1
1	A	102	GLY	CA-C	5.63	1.60	1.51	9	2
1	A	39	PRO	N-CD	5.57	1.55	1.47	19	1
1	A	66	ASP	N-CA	5.52	1.57	1.46	3	1
1	A	46	PRO	CA-C	5.51	1.63	1.52	4	1
1	A	48	PHE	CB-CG	5.51	1.60	1.51	20	1
1	A	63	VAL	CA-C	5.49	1.67	1.52	12	1
1	A	33	PHE	C-O	5.47	1.33	1.23	2	1
1	A	37	TRP	N-CA	5.46	1.57	1.46	17	1
1	A	36	SER	CB-OG	5.46	1.49	1.42	19	1
1	A	73	GLU	CD-OE1	-5.44	1.19	1.25	2	1
1	A	85	PHE	CE1-CZ	5.44	1.47	1.37	4	1
1	A	15	TRP	CD1-NE1	5.43	1.47	1.38	19	2
1	A	83	PHE	N-CA	5.42	1.57	1.46	14	2
1	A	63	VAL	CB-CG1	5.41	1.64	1.52	4	1
1	A	93	ASP	CB-CG	5.41	1.63	1.51	19	1
1	A	31	VAL	N-CA	5.40	1.57	1.46	5	1
1	A	17	GLU	CG-CD	5.40	1.60	1.51	19	1
1	A	85	PHE	CG-CD1	5.37	1.46	1.38	14	2
1	A	3	GLU	CG-CD	5.35	1.59	1.51	15	1
1	A	75	TRP	CD1-NE1	5.34	1.47	1.38	17	1
1	A	75	TRP	CA-CB	5.32	1.65	1.53	6	1
1	A	65	VAL	CB-CG2	5.29	1.64	1.52	4	1
1	A	72	ALA	CA-CB	5.27	1.63	1.52	1	1
1	A	20	GLU	CD-OE1	-5.26	1.19	1.25	13	2
1	A	37	TRP	NE1-CE2	5.24	1.44	1.37	15	1
1	A	82	THR	CA-C	5.23	1.66	1.52	10	1
1	A	102	GLY	N-CA	5.23	1.53	1.46	20	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	97	GLY	N-CA	5.22	1.53	1.46	9	1
1	A	33	PHE	N-CA	5.18	1.56	1.46	11	1
1	A	80	MET	CA-C	5.18	1.66	1.52	12	1
1	A	58	VAL	CB-CG1	-5.18	1.42	1.52	8	1
1	A	81	PRO	CA-C	5.18	1.63	1.52	11	1
1	A	81	PRO	C-N	5.16	1.46	1.34	20	1
1	A	19	PHE	CB-CG	5.15	1.60	1.51	8	1
1	A	76	ASN	N-CA	5.15	1.56	1.46	8	1
1	A	107	VAL	CB-CG2	5.12	1.63	1.52	9	1
1	A	35	ALA	CA-CB	5.12	1.63	1.52	4	1
1	A	64	ASP	N-CA	5.11	1.56	1.46	19	1
1	A	31	VAL	CA-C	5.10	1.66	1.52	4	1
1	A	88	ASP	N-CA	5.09	1.56	1.46	13	1
1	A	37	TRP	CZ2-CH2	5.08	1.47	1.37	11	1
1	A	37	TRP	CD2-CE3	5.07	1.48	1.40	5	1
1	A	4	GLY	N-CA	5.07	1.53	1.46	7	1
1	A	70	ALA	N-CA	5.06	1.56	1.46	17	1
1	A	76	ASN	CB-CG	5.06	1.62	1.51	4	1
1	A	78	GLU	CA-C	5.05	1.66	1.52	17	1
1	A	43	MET	CA-C	5.05	1.66	1.52	20	1
1	A	82	THR	N-CA	5.05	1.56	1.46	1	1
1	A	31	VAL	CA-CB	5.05	1.65	1.54	3	1
1	A	37	TRP	CE3-CZ3	5.04	1.47	1.38	3	1
1	A	96	VAL	CA-CB	5.04	1.65	1.54	7	1
1	A	14	THR	N-CA	5.01	1.56	1.46	3	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	83	PHE	CB-CG-CD2	-16.13	109.51	120.80	20	8
1	A	64	ASP	CB-CG-OD1	14.65	131.48	118.30	3	14
1	A	66	ASP	CB-CG-OD1	13.82	130.74	118.30	9	12
1	A	99	ASP	CB-CG-OD2	-13.71	105.96	118.30	2	13
1	A	66	ASP	CB-CG-OD2	-12.86	106.73	118.30	20	14
1	A	64	ASP	CB-CG-OD2	-12.77	106.81	118.30	4	16
1	A	93	ASP	CB-CG-OD2	-12.74	106.84	118.30	5	17
1	A	13	ASP	CB-CG-OD1	12.65	129.68	118.30	19	12
1	A	83	PHE	CB-CG-CD1	12.59	129.62	120.80	11	8
1	A	99	ASP	CB-CG-OD1	12.45	129.50	118.30	4	16
1	A	80	MET	CG-SD-CE	12.21	119.73	100.20	13	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	55	PHE	CB-CG-CD1	-12.08	112.34	120.80	15	6
1	A	81	PRO	N-CA-CB	-11.80	89.14	103.30	12	13
1	A	55	PHE	CB-CG-CD2	11.49	128.85	120.80	15	5
1	A	93	ASP	CB-CG-OD1	11.09	128.28	118.30	17	12
1	A	101	ASP	CB-CG-OD1	10.91	128.12	118.30	18	14
1	A	32	ASP	CB-CG-OD1	10.61	127.85	118.30	9	8
1	A	75	TRP	CD1-NE1-CE2	-10.56	99.50	109.00	8	13
1	A	101	ASP	CB-CG-OD2	-10.42	108.92	118.30	5	13
1	A	81	PRO	N-CD-CG	-10.04	88.13	103.20	19	4
1	A	13	ASP	CB-CG-OD2	-10.01	109.29	118.30	8	14
1	A	19	PHE	CB-CG-CD2	-9.54	114.12	120.80	6	4
1	A	95	THR	CA-CB-CG2	9.49	125.69	112.40	16	2
1	A	92	VAL	CA-CB-CG2	9.47	125.11	110.90	16	5
1	A	32	ASP	CB-CG-OD2	-9.35	109.88	118.30	4	14
1	A	60	PHE	CB-CG-CD2	-9.19	114.36	120.80	9	5
1	A	48	PHE	CB-CG-CD2	-8.99	114.51	120.80	10	5
1	A	96	VAL	CA-CB-CG2	8.98	124.37	110.90	7	2
1	A	37	TRP	CD1-NE1-CE2	-8.94	100.95	109.00	2	14
1	A	45	ALA	CB-CA-C	8.90	123.46	110.10	16	8
1	A	85	PHE	CB-CG-CD2	-8.89	114.58	120.80	19	5
1	A	96	VAL	CA-CB-CG1	8.74	124.02	110.90	19	3
1	A	77	VAL	CA-CB-CG2	8.64	123.85	110.90	20	4
1	A	88	ASP	CB-CG-OD2	-8.57	110.59	118.30	15	14
1	A	75	TRP	CB-CG-CD2	8.53	137.69	126.60	9	3
1	A	35	ALA	N-CA-CB	-8.53	98.16	110.10	18	12
1	A	31	VAL	CA-CB-CG1	8.44	123.55	110.90	16	5
1	A	15	TRP	CD1-NE1-CE2	-8.27	101.56	109.00	14	10
1	A	81	PRO	O-C-N	8.19	135.80	122.70	20	2
1	A	61	LEU	CB-CA-C	8.15	125.68	110.20	20	7
1	A	60	PHE	CB-CG-CD1	-8.07	115.15	120.80	11	7
1	A	33	PHE	CB-CG-CD1	-7.96	115.23	120.80	18	6
1	A	59	THR	CA-CB-CG2	7.90	123.46	112.40	5	6
1	A	58	VAL	CB-CA-C	7.88	126.38	111.40	10	8
1	A	77	VAL	CA-C-N	-7.81	100.02	117.20	17	1
1	A	82	THR	N-CA-CB	7.77	125.06	110.30	11	1
1	A	88	ASP	CB-CG-OD1	7.73	125.26	118.30	11	11
1	A	103	LEU	CB-CA-C	7.70	124.84	110.20	6	4
1	A	19	PHE	CB-CG-CD1	-7.69	115.42	120.80	4	2
1	A	10	HIS	CG-ND1-CE1	-7.67	95.73	105.70	19	4
1	A	98	ALA	N-CA-CB	-7.63	99.41	110.10	1	4
1	A	76	ASN	N-CA-CB	7.62	124.31	110.60	2	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	TRP	CB-CG-CD1	-7.61	117.11	127.00	7	2
1	A	11	THR	CA-CB-CG2	7.57	122.99	112.40	10	3
1	A	83	PHE	O-C-N	7.52	134.73	122.70	8	1
1	A	56	PRO	N-CA-C	7.50	131.61	112.10	7	15
1	A	75	TRP	CD1-CG-CD2	-7.50	100.30	106.30	10	2
1	A	110	HIS	CG-ND1-CE1	-7.49	95.96	105.70	14	10
1	A	81	PRO	CA-N-CD	-7.49	101.02	111.50	14	1
1	A	75	TRP	CG-CD1-NE1	7.45	117.55	110.10	14	3
1	A	33	PHE	CB-CG-CD2	7.44	126.01	120.80	1	4
1	A	75	TRP	NE1-CE2-CZ2	-7.29	122.39	130.40	3	3
1	A	84	ILE	CB-CA-C	7.25	126.11	111.60	1	3
1	A	80	MET	CB-CA-C	7.19	124.78	110.40	2	3
1	A	82	THR	O-C-N	7.17	134.18	122.70	2	3
1	A	34	THR	CA-CB-CG2	7.17	122.43	112.40	3	1
1	A	65	VAL	CA-CB-CG1	7.16	121.65	110.90	3	3
1	A	58	VAL	CA-CB-CG1	7.15	121.63	110.90	9	11
1	A	18	HIS	CA-CB-CG	7.11	125.69	113.60	20	5
1	A	82	THR	CA-CB-CG2	7.08	122.31	112.40	11	3
1	A	29	ILE	CA-CB-CG1	7.07	124.44	111.00	17	4
1	A	107	VAL	CA-CB-CG1	7.01	121.42	110.90	20	2
1	A	20	GLU	N-CA-CB	6.99	123.18	110.60	9	1
1	A	18	HIS	CG-ND1-CE1	-6.89	96.75	105.70	12	4
1	A	18	HIS	N-CA-CB	-6.86	98.25	110.60	10	1
1	A	90	LYS	CB-CA-C	6.82	124.04	110.40	2	4
1	A	77	VAL	CA-CB-CG1	6.82	121.12	110.90	13	2
1	A	38	CYS	CA-CB-SG	-6.81	101.73	114.00	19	2
1	A	105	THR	CA-CB-CG2	6.65	121.71	112.40	12	2
1	A	81	PRO	CA-C-N	-6.63	102.61	117.20	1	9
1	A	87	LYS	N-CA-CB	-6.62	98.68	110.60	10	4
1	A	81	PRO	CA-C-O	6.61	136.05	120.20	1	3
1	A	79	ALA	N-CA-CB	6.59	119.33	110.10	8	3
1	A	78	GLU	CA-CB-CG	6.57	127.86	113.40	17	1
1	A	33	PHE	N-CA-C	-6.55	93.32	111.00	16	3
1	A	14	THR	CA-CB-CG2	6.53	121.53	112.40	3	4
1	A	51	LEU	CB-CA-C	6.51	122.57	110.20	13	4
1	A	62	LYS	N-CA-CB	6.50	122.31	110.60	5	1
1	A	75	TRP	CB-CG-CD1	-6.49	118.56	127.00	5	2
1	A	37	TRP	CG-CD2-CE3	-6.49	128.06	133.90	8	2
1	A	10	HIS	ND1-CE1-NE2	6.48	124.16	109.90	8	5
1	A	18	HIS	ND1-CE1-NE2	6.46	124.11	109.90	15	5
1	A	28	LEU	CB-CA-C	6.46	122.46	110.20	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	83	PHE	N-CA-C	-6.45	93.60	111.00	14	1
1	A	15	TRP	NE1-CE2-CD2	6.43	113.73	107.30	7	2
1	A	75	TRP	CH2-CZ2-CE2	6.40	123.80	117.40	20	1
1	A	40	PRO	N-CA-CB	6.40	110.98	103.30	4	1
1	A	85	PHE	CB-CG-CD1	6.39	125.28	120.80	19	2
1	A	110	HIS	ND1-CE1-NE2	6.39	123.95	109.90	19	10
1	A	86	LEU	CB-CG-CD1	6.36	121.82	111.00	1	2
1	A	37	TRP	CH2-CZ2-CE2	6.34	123.74	117.40	3	1
1	A	48	PHE	CB-CG-CD1	-6.33	116.37	120.80	3	4
1	A	76	ASN	CA-CB-CG	6.32	127.31	113.40	18	1
1	A	57	ASN	CA-CB-CG	6.31	127.27	113.40	11	1
1	A	82	THR	CA-CB-OG1	6.30	122.24	109.00	4	2
1	A	73	GLU	CG-CD-OE1	6.26	130.83	118.30	16	2
1	A	75	TRP	NE1-CE2-CD2	6.25	113.55	107.30	11	3
1	A	82	THR	CA-C-N	-6.23	103.50	117.20	20	2
1	A	77	VAL	CG1-CB-CG2	-6.20	100.98	110.90	1	4
1	A	27	LYS	CB-CA-C	6.20	122.80	110.40	8	1
1	A	6	VAL	CA-CB-CG2	6.20	120.19	110.90	16	3
1	A	111	ALA	N-CA-CB	-6.18	101.44	110.10	15	5
1	A	94	LYS	CB-CG-CD	6.16	127.62	111.60	14	1
1	A	62	LYS	CA-CB-CG	6.16	126.94	113.40	18	1
1	A	59	THR	N-CA-CB	-6.14	98.63	110.30	7	1
1	A	31	VAL	CB-CA-C	6.10	122.99	111.40	18	1
1	A	81	PRO	N-CA-C	6.06	127.85	112.10	9	1
1	A	79	ALA	CB-CA-C	6.05	119.18	110.10	18	1
1	A	27	LYS	CA-CB-CG	6.04	126.70	113.40	5	1
1	A	82	THR	OG1-CB-CG2	-6.02	96.15	110.00	17	1
1	A	8	ALA	N-CA-CB	-6.01	101.69	110.10	4	5
1	A	51	LEU	N-CA-CB	-5.97	98.45	110.40	13	3
1	A	70	ALA	CB-CA-C	5.95	119.02	110.10	11	2
1	A	48	PHE	N-CA-CB	-5.93	99.93	110.60	7	4
1	A	100	LYS	CA-CB-CG	5.91	126.41	113.40	19	3
1	A	49	ALA	O-C-N	-5.91	113.24	122.70	18	1
1	A	37	TRP	CA-CB-CG	5.89	124.90	113.70	17	4
1	A	86	LEU	N-CA-C	-5.89	95.10	111.00	11	3
1	A	39	PRO	N-CA-CB	5.88	110.36	103.30	6	1
1	A	17	GLU	N-CA-C	5.83	126.74	111.00	8	1
1	A	83	PHE	CA-CB-CG	5.83	127.89	113.90	1	2
1	A	103	LEU	CB-CG-CD1	5.81	120.88	111.00	19	1
1	A	37	TRP	NE1-CE2-CD2	5.79	113.09	107.30	5	2
1	A	74	GLU	CG-CD-OE1	5.77	129.85	118.30	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	TRP	N-CA-CB	5.77	120.99	110.60	13	2
1	A	75	TRP	CA-CB-CG	5.75	124.63	113.70	2	2
1	A	35	ALA	CB-CA-C	5.71	118.67	110.10	1	3
1	A	84	ILE	CA-CB-CG2	5.70	122.30	110.90	13	1
1	A	84	ILE	O-C-N	5.70	131.82	122.70	12	1
1	A	50	GLU	CB-CA-C	5.68	121.76	110.40	2	1
1	A	106	LEU	CB-CG-CD1	5.68	120.66	111.00	2	1
1	A	96	VAL	CB-CA-C	5.68	122.19	111.40	20	4
1	A	100	LYS	N-CA-CB	5.67	120.81	110.60	18	1
1	A	43	MET	CA-CB-CG	5.67	122.94	113.30	13	2
1	A	86	LEU	CB-CA-C	5.64	120.92	110.20	4	1
1	A	74	GLU	CA-CB-CG	5.64	125.80	113.40	9	4
1	A	30	VAL	CG1-CB-CG2	-5.64	101.88	110.90	11	1
1	A	66	ASP	CB-CA-C	5.63	121.66	110.40	12	1
1	A	72	ALA	N-CA-CB	5.63	117.98	110.10	2	2
1	A	105	THR	N-CA-CB	-5.63	99.61	110.30	16	2
1	A	41	CYS	N-CA-CB	5.62	120.72	110.60	18	1
1	A	34	THR	N-CA-CB	5.62	120.97	110.30	16	2
1	A	78	GLU	OE1-CD-OE2	5.60	130.02	123.30	16	1
1	A	78	GLU	CB-CA-C	5.59	121.58	110.40	2	1
1	A	80	MET	CA-CB-CG	-5.59	103.80	113.30	20	1
1	A	63	VAL	CA-CB-CG1	5.58	119.27	110.90	5	2
1	A	110	HIS	CE1-NE2-CD2	-5.58	92.65	106.60	19	1
1	A	87	LYS	CB-CA-C	5.56	121.52	110.40	11	1
1	A	10	HIS	CA-CB-CG	5.53	123.00	113.60	19	1
1	A	12	VAL	CA-CB-CG2	5.52	119.18	110.90	19	1
1	A	9	CYS	CA-CB-SG	-5.51	104.07	114.00	20	1
1	A	74	GLU	CG-CD-OE2	-5.51	107.27	118.30	18	2
1	A	15	TRP	CG-CD1-NE1	5.49	115.59	110.10	2	1
1	A	49	ALA	N-CA-CB	-5.48	102.42	110.10	6	1
1	A	7	ILE	CA-CB-CG2	5.48	121.86	110.90	17	1
1	A	86	LEU	CA-C-O	5.48	131.60	120.10	7	2
1	A	67	GLU	CG-CD-OE2	-5.46	107.37	118.30	12	2
1	A	43	MET	CG-SD-CE	5.46	108.94	100.20	6	1
1	A	34	THR	CA-C-O	5.46	131.56	120.10	19	1
1	A	32	ASP	C-N-CA	5.46	135.34	121.70	2	1
1	A	37	TRP	CG-CD1-NE1	5.45	115.55	110.10	8	1
1	A	78	GLU	N-CA-CB	-5.43	100.82	110.60	2	1
1	A	99	ASP	CB-CA-C	5.41	121.22	110.40	12	1
1	A	20	GLU	CG-CD-OE2	-5.40	107.49	118.30	9	2
1	A	15	TRP	CG-CD2-CE3	-5.40	129.04	133.90	19	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	ILE	CA-C-N	-5.39	105.34	117.20	12	1
1	A	19	PHE	CB-CA-C	5.38	121.17	110.40	15	1
1	A	30	VAL	CA-CB-CG1	5.38	118.97	110.90	11	3
1	A	42	LYS	CD-CE-NZ	5.38	124.07	111.70	10	1
1	A	3	GLU	CG-CD-OE2	-5.38	107.55	118.30	17	1
1	A	37	TRP	CD1-CG-CD2	-5.37	102.00	106.30	8	1
1	A	108	ALA	N-CA-CB	-5.37	102.58	110.10	19	1
1	A	107	VAL	CG1-CB-CG2	-5.37	102.31	110.90	17	1
1	A	37	TRP	CB-CA-C	5.36	121.12	110.40	20	1
1	A	4	GLY	N-CA-C	-5.35	99.72	113.10	9	1
1	A	78	GLU	CG-CD-OE1	5.35	129.00	118.30	14	1
1	A	46	PRO	N-CA-C	5.33	125.95	112.10	7	1
1	A	26	GLN	CB-CA-C	5.32	121.05	110.40	19	1
1	A	73	GLU	CG-CD-OE2	-5.32	107.66	118.30	4	2
1	A	7	ILE	CB-CA-C	5.32	122.24	111.60	7	4
1	A	25	SER	N-CA-CB	-5.31	102.54	110.50	10	2
1	A	74	GLU	N-CA-CB	5.31	120.15	110.60	6	1
1	A	37	TRP	CB-CG-CD2	5.30	133.50	126.60	7	1
1	A	78	GLU	N-CA-C	5.30	125.31	111.00	15	1
1	A	68	LEU	CA-C-O	5.29	131.21	120.10	5	1
1	A	32	ASP	CA-CB-CG	5.28	125.02	113.40	3	2
1	A	48	PHE	CB-CA-C	5.28	120.97	110.40	3	2
1	A	111	ALA	N-CA-C	5.28	125.25	111.00	3	1
1	A	80	MET	N-CA-CB	-5.27	101.11	110.60	4	1
1	A	26	GLN	CB-CG-CD	5.27	125.30	111.60	7	1
1	A	83	PHE	CG-CD1-CE1	-5.26	115.01	120.80	6	1
1	A	101	ASP	CB-CA-C	5.25	120.90	110.40	18	1
1	A	71	VAL	CA-CB-CG1	5.24	118.76	110.90	1	1
1	A	100	LYS	C-N-CA	5.20	134.70	121.70	3	1
1	A	12	VAL	CG1-CB-CG2	-5.19	102.59	110.90	5	2
1	A	36	SER	CB-CA-C	5.18	119.95	110.10	2	1
1	A	78	GLU	CG-CD-OE2	-5.18	107.94	118.30	18	1
1	A	19	PHE	N-CA-C	5.18	124.98	111.00	5	1
1	A	75	TRP	CB-CA-C	-5.17	100.06	110.40	13	1
1	A	86	LEU	CA-CB-CG	5.16	127.17	115.30	13	1
1	A	65	VAL	CG1-CB-CG2	5.16	119.16	110.90	16	1
1	A	82	THR	CA-C-O	5.16	130.94	120.10	11	1
1	A	85	PHE	N-CA-C	-5.16	97.08	111.00	16	1
1	A	69	LYS	CB-CG-CD	5.15	125.00	111.60	12	1
1	A	91	LEU	CB-CG-CD1	5.15	119.75	111.00	5	2
1	A	111	ALA	CB-CA-C	5.15	117.82	110.10	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	100	LYS	N-CA-C	5.14	124.89	111.00	11	1
1	A	60	PHE	N-CA-CB	5.14	119.85	110.60	19	1
1	A	74	GLU	O-C-N	-5.14	114.48	122.70	2	1
1	A	84	ILE	CG1-CB-CG2	-5.14	100.10	111.40	7	1
1	A	17	GLU	CG-CD-OE2	-5.14	108.03	118.30	18	1
1	A	103	LEU	N-CA-CB	-5.13	100.13	110.40	1	1
1	A	58	VAL	CA-CB-CG2	5.12	118.59	110.90	3	1
1	A	92	VAL	CB-CA-C	5.12	121.14	111.40	16	1
1	A	17	GLU	C-N-CA	5.12	134.50	121.70	13	1
1	A	42	LYS	CB-CA-C	5.12	120.63	110.40	16	1
1	A	15	TRP	N-CA-CB	5.11	119.81	110.60	18	1
1	A	41	CYS	N-CA-C	5.11	124.79	111.00	8	1
1	A	73	GLU	CA-C-O	-5.11	109.37	120.10	13	1
1	A	47	ILE	CA-CB-CG2	5.10	121.10	110.90	7	1
1	A	106	LEU	CB-CA-C	5.09	119.88	110.20	14	2
1	A	81	PRO	C-N-CA	5.09	134.42	121.70	8	1
1	A	69	LYS	CA-C-O	-5.08	109.44	120.10	1	1
1	A	15	TRP	CD2-CE2-CZ2	-5.07	116.21	122.30	7	1
1	A	88	ASP	N-CA-C	5.07	124.69	111.00	3	1
1	A	45	ALA	CA-C-N	5.06	131.28	117.10	5	1
1	A	54	LYS	N-CA-CB	-5.05	101.52	110.60	19	1
1	A	24	GLY	CA-C-N	-5.04	106.11	117.20	5	1
1	A	49	ALA	N-CA-C	5.04	124.61	111.00	7	1
1	A	77	VAL	N-CA-C	-5.04	97.40	111.00	11	1
1	A	102	GLY	N-CA-C	5.04	125.69	113.10	5	1
1	A	80	MET	CA-C-O	-5.04	109.53	120.10	16	1
1	A	74	GLU	OE1-CD-OE2	5.03	129.34	123.30	18	1
1	A	110	HIS	CB-CA-C	5.03	120.46	110.40	1	1
1	A	88	ASP	CA-CB-CG	5.02	124.45	113.40	12	1
1	A	51	LEU	CA-C-O	-5.02	109.55	120.10	16	1
1	A	67	GLU	N-CA-C	5.02	124.56	111.00	16	1
1	A	64	ASP	CB-CA-C	5.02	120.44	110.40	16	1
1	A	56	PRO	CA-N-CD	-5.01	104.48	111.50	15	1
1	A	75	TRP	CG-CD2-CE3	-5.00	129.40	133.90	4	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

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	48	PHE	Sidechain	11
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	33	PHE	Sidechain	2
1	A	63	VAL	Peptide	2
1	A	80	MET	Mainchain	2
1	A	18	HIS	Sidechain	2
1	A	79	ALA	Peptide	2
1	A	19	PHE	Sidechain	2
1	A	54	LYS	Mainchain,Peptide	2
1	A	10	HIS	Sidechain	2
1	A	9	CYS	Peptide	2
1	A	85	PHE	Sidechain	2
1	A	36	SER	Peptide	1
1	A	4	GLY	Mainchain	1
1	A	58	VAL	Peptide	1
1	A	78	GLU	Sidechain	1
1	A	98	ALA	Mainchain	1
1	A	55	PHE	Sidechain	1
1	A	74	GLU	Mainchain	1
1	A	71	VAL	Mainchain	1
1	A	35	ALA	Mainchain	1
1	A	27	LYS	Peptide	1
1	A	82	THR	Mainchain	1
1	A	31	VAL	Peptide	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	849	864	862	1±1
All	All	16980	17280	17240	20

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: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:N	1:A:80:MET:SD	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:29:ILE:HG12	1:A:86:LEU:O	0.40	2.16	18	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	109/113 (96%)	85±3 (78±2%)	18±2 (16±2%)	6±1 (6±1%)	4	22
All	All	2180/2260 (96%)	1699 (78%)	354 (16%)	127 (6%)	4	22

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	81	PRO	20
1	A	76	ASN	20
1	A	88	ASP	19
1	A	22	GLY	18
1	A	26	GLN	12
1	A	89	GLY	10
1	A	37	TRP	9

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Mol	Chain	Res	Type	Models (Total)
1	A	77	VAL	5
1	A	90	LYS	4
1	A	91	LEU	3
1	A	97	GLY	2
1	A	102	GLY	2
1	A	98	ALA	1
1	A	23	LYS	1
1	A	57	ASN	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/94 (98%)	81±2 (88±2%)	11±2 (12±2%)	10	53
All	All	1840/1880 (98%)	1623 (88%)	217 (12%)	10	53

All 36 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	86	LEU	19
1	A	44	ILE	15
1	A	14	THR	14
1	A	74	GLU	14
1	A	65	VAL	13
1	A	61	LEU	13
1	A	94	LYS	11
1	A	80	MET	10
1	A	78	GLU	10
1	A	51	LEU	9
1	A	96	VAL	8
1	A	93	ASP	6
1	A	29	ILE	6
1	A	48	PHE	5
1	A	84	ILE	5
1	A	100	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	13	ASP	4
1	A	81	PRO	3
1	A	50	GLU	3
1	A	101	ASP	3
1	A	90	LYS	2
1	A	67	GLU	2
1	A	19	PHE	2
1	A	26	GLN	2
1	A	3	GLU	2
1	A	56	PRO	2
1	A	31	VAL	2
1	A	23	LYS	1
1	A	41	CYS	1
1	A	105	THR	1
1	A	11	THR	1
1	A	27	LYS	1
1	A	76	ASN	1
1	A	66	ASP	1
1	A	36	SER	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 carbohydrates 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