



Full wwPDB NMR Structure Validation Report ⓘ

Mar 26, 2026 – 08:46 PM UTC

PDB ID : 1N5G / pdb_00001n5g
Title : NMR Structures of the Zinc Finger Domain of Human DNA Polymerase-alpha
Authors : Evanics, F.; Maurmann, L.; Yang, W.W.; Bose, R.N.
Deposited on : 2002-11-05

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

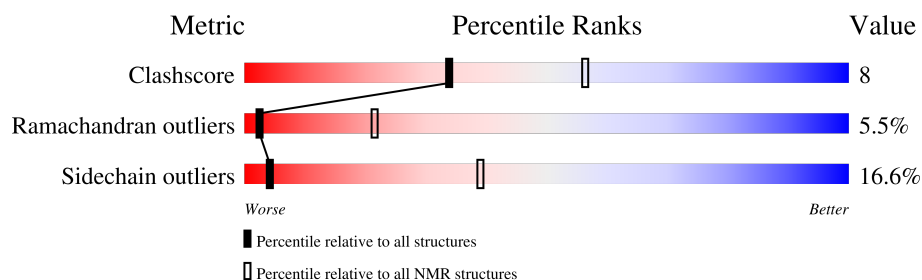
1 Overall quality at a glance

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	38	

2 Ensemble composition and analysis

This entry contains 29 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 14 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:4-A:38 (35)	0.56	14

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 1 single-model cluster was found.

Cluster number	Models
1	8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21
2	1, 2, 3, 4, 5, 6, 7, 29
3	24, 25, 26, 27
4	22, 23
Single-model clusters	28

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 615 atoms, of which 310 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 38-mer of DNA polymerase alpha catalytic subunit.

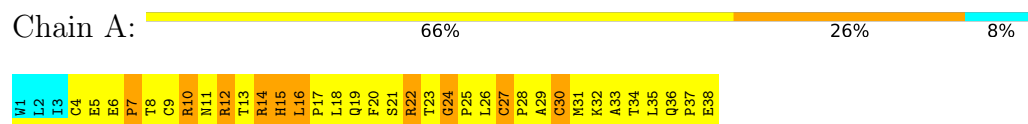
Mol	Chain	Residues	Atoms						Trace
1	A	38	Total	C	H	N	O	S	0
			615	190	310	57	53	5	

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: 38-mer of DNA polymerase alpha catalytic subunit



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

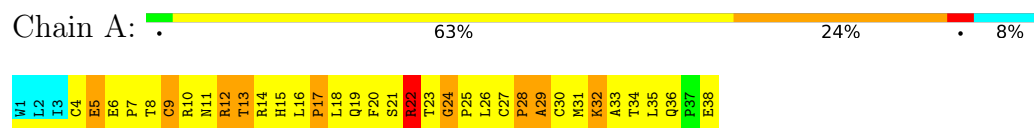
4.2.1 Score per residue for model 1

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



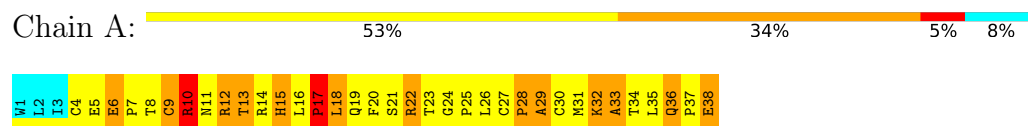
4.2.2 Score per residue for model 2

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



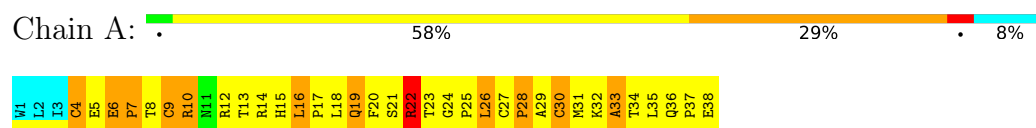
4.2.3 Score per residue for model 3

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



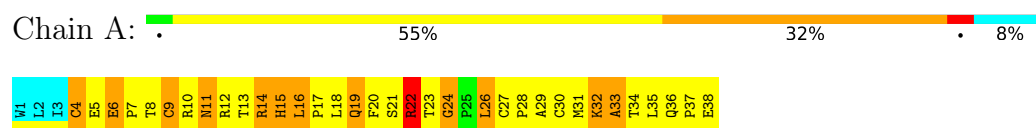
4.2.4 Score per residue for model 4

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



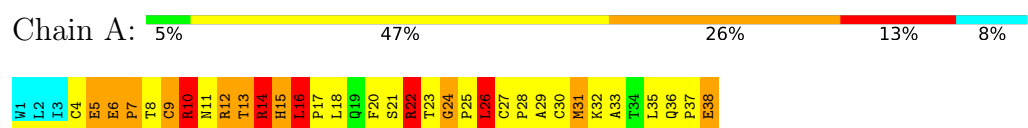
4.2.5 Score per residue for model 5

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



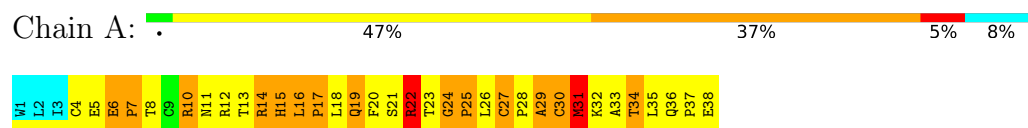
4.2.6 Score per residue for model 6

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



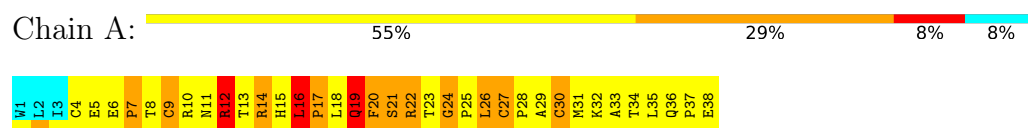
4.2.7 Score per residue for model 7

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



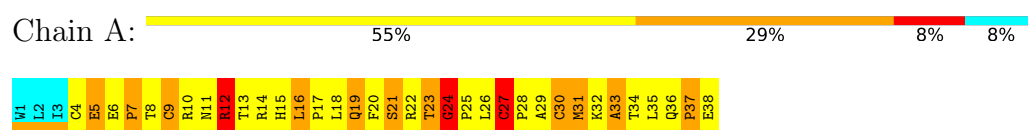
4.2.8 Score per residue for model 8

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



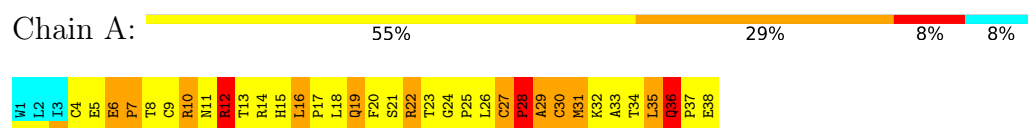
4.2.9 Score per residue for model 9

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



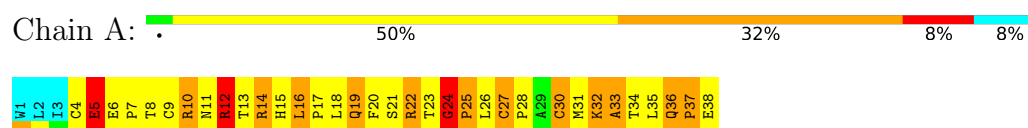
4.2.10 Score per residue for model 10

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



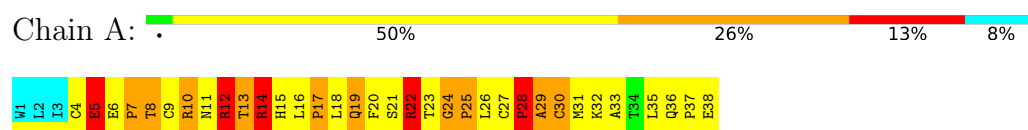
4.2.11 Score per residue for model 11

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



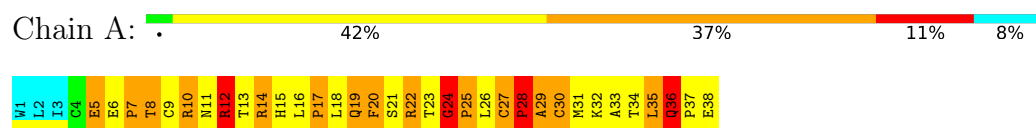
4.2.12 Score per residue for model 12

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



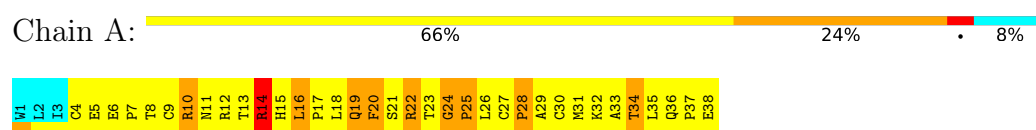
4.2.13 Score per residue for model 13

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



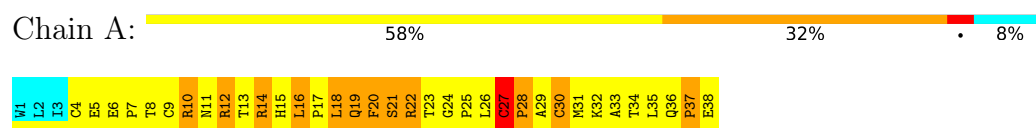
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



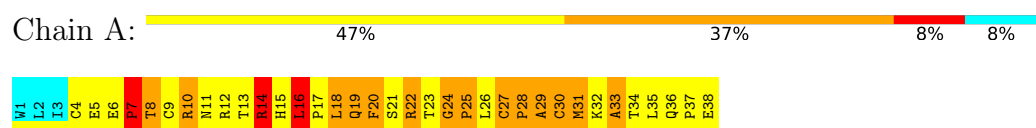
4.2.15 Score per residue for model 15

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



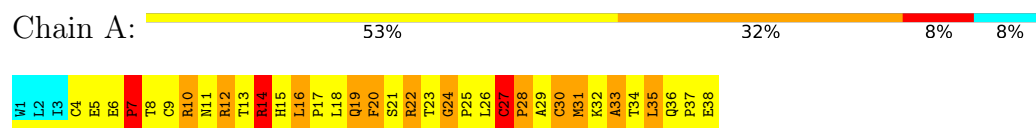
4.2.16 Score per residue for model 16

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



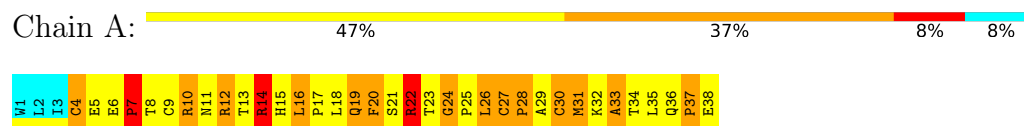
4.2.17 Score per residue for model 17

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



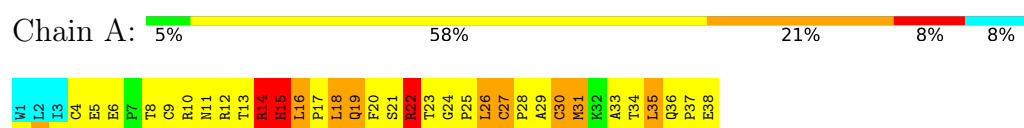
4.2.18 Score per residue for model 18

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



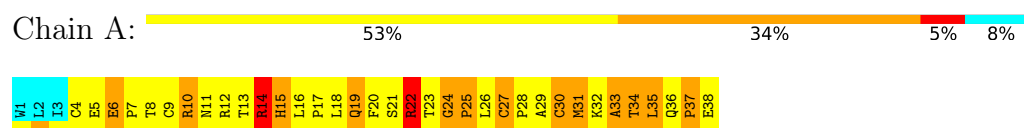
4.2.19 Score per residue for model 19

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



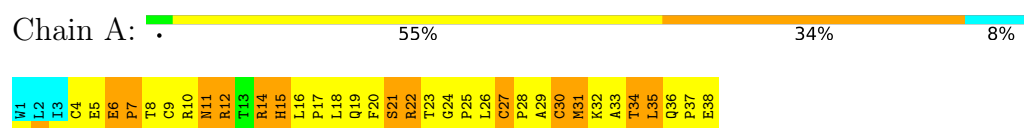
4.2.20 Score per residue for model 20

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



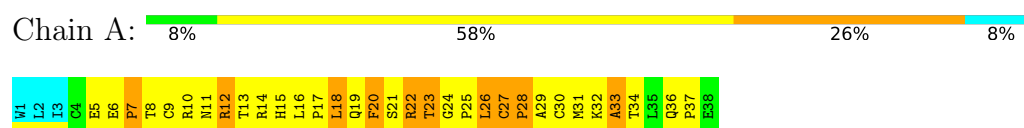
4.2.21 Score per residue for model 21

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



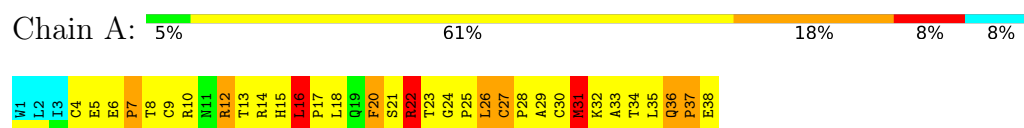
4.2.22 Score per residue for model 22

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



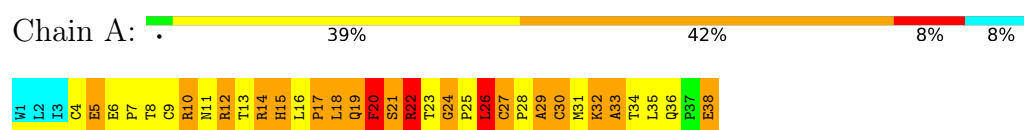
4.2.23 Score per residue for model 23

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



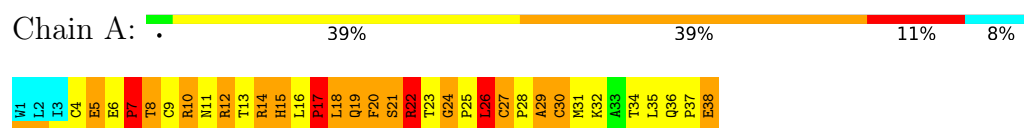
4.2.24 Score per residue for model 24

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



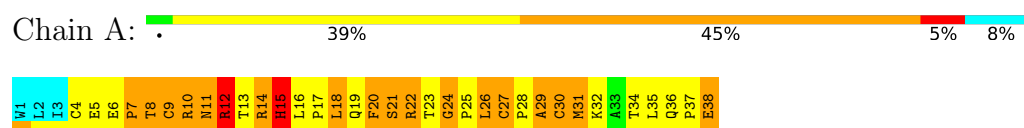
4.2.25 Score per residue for model 25

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



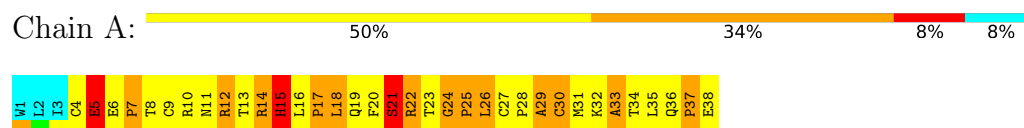
4.2.26 Score per residue for model 26

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



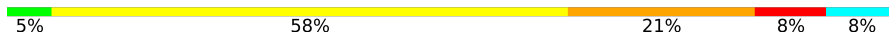
4.2.27 Score per residue for model 27

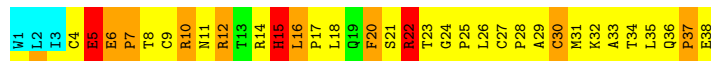
- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit



4.2.28 Score per residue for model 28

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit

Chain A:  5% 58% 21% 8% 8%



4.2.29 Score per residue for model 29

- Molecule 1: 38-mer of DNA polymerase alpha catalytic subunit

Chain A:  58% 24% 11% 8%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing and constrained molecular dynamics simulations*.

Of the 100 calculated structures, 29 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
Discover	refinement	97.0

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	4.20±0.63	52±13/281 (18.3± 4.8%)	3.49±0.40	53±13/379 (13.9± 3.4%)
All	All	4.25	1495/8149 (18.3%)	3.52	1525/10991 (13.9%)

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	4.8±2.1
All	All	0	140

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	16	LEU	N-CA	34.76	1.85	1.46	6	16
1	A	15	HIS	CA-C	27.70	1.90	1.52	7	14
1	A	36	GLN	N-CA	26.18	1.71	1.46	10	15
1	A	29	ALA	CA-C	24.47	1.84	1.53	10	18
1	A	26	LEU	CA-C	23.38	1.69	1.52	17	15
1	A	16	LEU	CA-C	22.18	1.75	1.52	19	14
1	A	12	ARG	CA-C	20.47	1.80	1.52	10	8
1	A	13	THR	CA-C	20.40	1.80	1.52	2	16
1	A	27	CYS	CA-C	19.27	1.70	1.52	10	12
1	A	33	ALA	N-CA	19.11	1.69	1.46	24	13
1	A	30	CYS	N-CA	19.11	1.70	1.46	4	9
1	A	15	HIS	CG-CD2	18.87	1.56	1.35	6	20
1	A	14	ARG	CA-C	18.41	1.77	1.52	8	13
1	A	28	PRO	N-CA	17.77	1.65	1.47	7	12
1	A	7	PRO	CA-C	17.65	1.77	1.52	25	7
1	A	11	ASN	N-CA	16.86	1.67	1.46	9	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	23	THR	CA-C	16.74	1.68	1.53	20	18
1	A	25	PRO	CA-C	16.59	1.73	1.53	15	11
1	A	25	PRO	N-CA	16.55	1.68	1.47	20	9
1	A	31	MET	N-CA	16.29	1.66	1.46	7	7
1	A	4	CYS	CA-C	16.12	1.73	1.52	9	12
1	A	24	GLY	N-CA	16.06	1.66	1.44	27	10
1	A	34	THR	CA-C	16.02	1.74	1.52	22	18
1	A	6	GLU	N-CA	15.94	1.57	1.46	21	19
1	A	6	GLU	CA-C	15.83	1.69	1.52	14	9
1	A	15	HIS	CB-CG	15.74	1.72	1.50	28	6
1	A	8	THR	CA-C	15.69	1.72	1.52	14	10
1	A	32	LYS	CA-C	15.56	1.72	1.52	17	11
1	A	23	THR	C-N	15.46	1.56	1.33	4	5
1	A	21	SER	CA-C	15.41	1.70	1.53	2	11
1	A	22	ARG	NE-CZ	15.31	1.49	1.33	14	15
1	A	37	PRO	CA-CB	15.24	1.75	1.53	15	10
1	A	36	GLN	CA-C	15.18	1.69	1.52	14	24
1	A	12	ARG	N-CA	15.02	1.65	1.46	16	8
1	A	28	PRO	CA-C	14.55	1.73	1.52	4	18
1	A	5	GLU	N-CA	14.47	1.63	1.46	10	15
1	A	18	LEU	N-CA	14.38	1.64	1.46	11	22
1	A	10	ARG	N-CA	14.36	1.63	1.46	21	12
1	A	17	PRO	C-N	14.28	1.52	1.33	8	8
1	A	23	THR	N-CA	14.26	1.64	1.46	17	4
1	A	7	PRO	N-CA	14.16	1.65	1.47	7	10
1	A	20	PHE	N-CA	14.15	1.64	1.46	13	14
1	A	19	GLN	CA-C	14.11	1.69	1.52	2	11
1	A	35	LEU	N-CA	13.91	1.63	1.46	5	6
1	A	13	THR	N-CA	13.80	1.63	1.46	4	12
1	A	9	CYS	CA-C	13.49	1.70	1.52	20	9
1	A	26	LEU	N-CA	13.48	1.61	1.46	28	8
1	A	35	LEU	CA-C	13.46	1.71	1.52	6	11
1	A	34	THR	N-CA	13.46	1.62	1.46	15	11
1	A	27	CYS	N-CA	13.41	1.60	1.46	23	8
1	A	18	LEU	CA-C	13.29	1.70	1.52	12	16
1	A	30	CYS	CA-C	13.27	1.70	1.52	16	12
1	A	32	LYS	C-N	13.26	1.50	1.33	9	6
1	A	17	PRO	N-CD	13.24	1.66	1.47	15	8
1	A	32	LYS	N-CA	13.24	1.62	1.46	2	11
1	A	22	ARG	N-CA	13.06	1.62	1.46	28	9
1	A	5	GLU	CA-C	13.04	1.70	1.52	27	11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	26	LEU	CA-CB	13.03	1.75	1.53	4	11
1	A	17	PRO	CA-C	12.82	1.71	1.52	14	10
1	A	29	ALA	N-CA	12.75	1.65	1.46	9	7
1	A	37	PRO	C-N	12.62	1.51	1.33	27	9
1	A	33	ALA	CA-C	12.47	1.69	1.52	13	5
1	A	14	ARG	NE-CZ	12.47	1.46	1.33	19	8
1	A	25	PRO	CA-CB	12.46	1.61	1.53	16	6
1	A	26	LEU	CB-CG	12.41	1.78	1.53	8	4
1	A	15	HIS	ND1-CE1	12.32	1.44	1.32	20	14
1	A	31	MET	CA-C	12.31	1.68	1.52	22	11
1	A	11	ASN	CA-C	12.10	1.68	1.52	15	8
1	A	36	GLN	CA-CB	12.02	1.69	1.53	27	9
1	A	4	CYS	C-N	11.99	1.48	1.33	18	12
1	A	4	CYS	N-CA	11.99	1.60	1.46	19	5
1	A	15	HIS	N-CA	11.96	1.61	1.46	15	7
1	A	35	LEU	CA-CB	11.94	1.72	1.53	10	6
1	A	16	LEU	CB-CG	11.74	1.76	1.53	18	5
1	A	12	ARG	CZ-NH1	11.72	1.49	1.32	3	6
1	A	28	PRO	CA-CB	11.64	1.65	1.53	21	7
1	A	12	ARG	NE-CZ	11.50	1.45	1.33	28	10
1	A	12	ARG	CA-CB	11.43	1.72	1.53	6	5
1	A	6	GLU	CA-CB	11.41	1.67	1.53	19	9
1	A	23	THR	CA-CB	11.39	1.71	1.53	2	16
1	A	24	GLY	CA-C	11.29	1.68	1.51	14	13
1	A	20	PHE	C-N	11.27	1.46	1.33	22	6
1	A	8	THR	CA-CB	11.24	1.71	1.53	4	13
1	A	15	HIS	CE1-NE2	11.23	1.43	1.32	25	11
1	A	10	ARG	CA-C	11.21	1.67	1.52	7	11
1	A	19	GLN	CA-CB	11.19	1.68	1.54	3	7
1	A	36	GLN	C-N	11.00	1.50	1.33	19	6
1	A	14	ARG	N-CA	10.97	1.59	1.46	15	13
1	A	8	THR	N-CA	10.83	1.59	1.46	17	9
1	A	19	GLN	N-CA	10.82	1.60	1.46	14	7
1	A	29	ALA	CA-CB	10.80	1.68	1.53	13	8
1	A	5	GLU	CA-CB	10.78	1.70	1.53	24	4
1	A	9	CYS	N-CA	10.74	1.59	1.46	27	10
1	A	12	ARG	CD-NE	10.72	1.61	1.46	9	2
1	A	10	ARG	CD-NE	10.70	1.61	1.46	6	5
1	A	37	PRO	CA-C	10.69	1.71	1.52	11	8
1	A	22	ARG	CD-NE	10.64	1.61	1.46	5	7
1	A	12	ARG	C-N	10.52	1.48	1.34	3	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	22	ARG	CZ-NH2	10.43	1.47	1.33	15	4
1	A	31	MET	C-N	10.43	1.48	1.34	3	7
1	A	11	ASN	C-N	10.42	1.47	1.34	28	2
1	A	16	LEU	CA-CB	10.41	1.66	1.53	26	8
1	A	21	SER	C-N	10.29	1.46	1.33	12	6
1	A	15	HIS	CG-ND1	10.28	1.49	1.38	16	10
1	A	17	PRO	CA-CB	10.27	1.68	1.53	17	7
1	A	20	PHE	CA-C	10.20	1.67	1.52	8	10
1	A	28	PRO	C-N	10.16	1.46	1.33	12	9
1	A	21	SER	CA-CB	10.12	1.68	1.53	18	5
1	A	22	ARG	CA-C	9.99	1.66	1.52	4	13
1	A	26	LEU	C-N	9.93	1.43	1.33	22	8
1	A	31	MET	CA-CB	9.93	1.69	1.53	28	5
1	A	18	LEU	CA-CB	9.92	1.68	1.53	13	5
1	A	28	PRO	N-CD	9.85	1.61	1.47	5	6
1	A	14	ARG	C-O	9.85	1.36	1.24	25	9
1	A	22	ARG	CZ-NH1	9.83	1.46	1.32	23	8
1	A	17	PRO	N-CA	9.81	1.60	1.47	10	13
1	A	10	ARG	CA-CB	9.48	1.68	1.53	26	4
1	A	13	THR	CB-OG1	9.39	1.58	1.43	17	6
1	A	15	HIS	C-N	9.34	1.45	1.33	13	5
1	A	7	PRO	C-N	9.19	1.44	1.33	16	7
1	A	27	CYS	C-N	8.84	1.44	1.33	22	4
1	A	13	THR	CA-CB	8.79	1.67	1.53	16	4
1	A	5	GLU	CD-OE2	8.76	1.42	1.25	4	5
1	A	10	ARG	NE-CZ	8.75	1.42	1.33	22	3
1	A	22	ARG	C-O	8.74	1.35	1.24	3	6
1	A	34	THR	CA-CB	8.73	1.67	1.53	26	6
1	A	38	GLU	CA-C	8.69	1.71	1.52	10	9
1	A	10	ARG	C-N	8.58	1.45	1.33	22	3
1	A	8	THR	C-N	8.54	1.45	1.34	23	6
1	A	15	HIS	CD2-NE2	8.50	1.47	1.37	25	7
1	A	14	ARG	C-N	8.40	1.45	1.34	20	5
1	A	21	SER	N-CA	8.32	1.56	1.46	9	7
1	A	5	GLU	CD-OE1	8.28	1.41	1.25	5	6
1	A	38	GLU	CG-CD	8.24	1.72	1.52	24	2
1	A	38	GLU	CD-OE1	8.23	1.41	1.25	6	4
1	A	4	CYS	CA-CB	-8.12	1.43	1.53	6	5
1	A	33	ALA	CA-CB	8.07	1.66	1.53	6	4
1	A	27	CYS	CA-CB	7.99	1.65	1.53	11	6
1	A	20	PHE	C-O	7.99	1.35	1.23	20	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	31	MET	CG-SD	7.97	2.00	1.80	3	2
1	A	24	GLY	C-N	7.88	1.40	1.33	21	3
1	A	9	CYS	C-O	7.86	1.33	1.24	24	7
1	A	19	GLN	C-N	7.78	1.45	1.33	14	3
1	A	16	LEU	C-O	7.76	1.32	1.24	20	4
1	A	25	PRO	N-CD	7.75	1.58	1.47	25	2
1	A	5	GLU	C-N	7.70	1.49	1.33	9	4
1	A	9	CYS	C-N	7.69	1.44	1.33	4	7
1	A	34	THR	C-N	7.67	1.43	1.33	26	6
1	A	36	GLN	C-O	-7.65	1.17	1.24	23	3
1	A	19	GLN	CG-CD	7.62	1.71	1.52	20	5
1	A	6	GLU	C-O	-7.62	1.18	1.24	7	5
1	A	32	LYS	CA-CB	7.60	1.65	1.53	27	5
1	A	11	ASN	CA-CB	7.58	1.66	1.53	10	3
1	A	11	ASN	C-O	7.57	1.32	1.24	24	3
1	A	7	PRO	N-CD	7.54	1.58	1.47	6	3
1	A	22	ARG	C-N	7.49	1.43	1.33	14	6
1	A	17	PRO	CG-CD	7.39	1.75	1.50	27	3
1	A	22	ARG	CA-CB	7.39	1.65	1.53	20	3
1	A	14	ARG	CD-NE	7.34	1.56	1.46	18	2
1	A	16	LEU	CG-CD2	7.34	1.76	1.52	16	2
1	A	37	PRO	N-CD	-7.31	1.37	1.47	8	3
1	A	25	PRO	C-N	7.21	1.43	1.33	26	5
1	A	16	LEU	C-N	7.19	1.43	1.33	20	4
1	A	14	ARG	CZ-NH1	7.19	1.42	1.32	3	3
1	A	35	LEU	CB-CG	7.17	1.67	1.53	23	3
1	A	30	CYS	C-N	7.16	1.43	1.33	27	5
1	A	6	GLU	CG-CD	7.12	1.69	1.52	7	2
1	A	32	LYS	CB-CG	7.07	1.73	1.52	25	2
1	A	20	PHE	CG-CD2	7.04	1.53	1.38	21	1
1	A	38	GLU	N-CA	6.98	1.59	1.46	20	3
1	A	14	ARG	CZ-NH2	-6.96	1.24	1.33	28	4
1	A	6	GLU	CD-OE1	6.93	1.38	1.25	5	6
1	A	4	CYS	C-O	6.92	1.32	1.24	12	1
1	A	13	THR	C-N	6.92	1.43	1.34	20	2
1	A	37	PRO	N-CA	6.88	1.56	1.47	27	4
1	A	27	CYS	C-O	6.86	1.31	1.24	4	1
1	A	10	ARG	CZ-NH1	6.83	1.42	1.32	3	2
1	A	28	PRO	CB-CG	6.81	1.83	1.49	22	1
1	A	36	GLN	CG-CD	6.80	1.69	1.52	21	1
1	A	18	LEU	C-N	6.77	1.42	1.33	10	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	18	LEU	CB-CG	6.76	1.67	1.53	19	1
1	A	20	PHE	CG-CD1	6.73	1.52	1.38	28	2
1	A	15	HIS	C-O	-6.64	1.15	1.24	27	1
1	A	29	ALA	C-N	-6.59	1.24	1.33	22	3
1	A	30	CYS	CA-CB	6.52	1.64	1.53	15	2
1	A	12	ARG	CZ-NH2	-6.50	1.25	1.33	28	3
1	A	8	THR	C-O	6.38	1.31	1.24	20	3
1	A	26	LEU	C-O	-6.37	1.17	1.23	28	3
1	A	5	GLU	C-O	6.36	1.31	1.24	21	3
1	A	15	HIS	CA-CB	-6.36	1.43	1.53	2	4
1	A	6	GLU	C-N	6.34	1.48	1.33	5	3
1	A	28	PRO	CG-CD	6.31	1.72	1.50	14	1
1	A	13	THR	C-O	6.28	1.31	1.24	7	1
1	A	35	LEU	C-N	6.27	1.44	1.34	26	4
1	A	7	PRO	CG-CD	6.24	1.72	1.50	22	1
1	A	38	GLU	C-OXT	-6.24	1.11	1.23	29	2
1	A	12	ARG	C-O	6.22	1.31	1.24	14	3
1	A	20	PHE	CA-CB	6.19	1.62	1.54	14	2
1	A	38	GLU	CD-OE2	6.16	1.37	1.25	7	3
1	A	38	GLU	CA-CB	6.13	1.65	1.53	14	5
1	A	6	GLU	CD-OE2	6.09	1.36	1.25	29	3
1	A	28	PRO	C-O	6.09	1.31	1.24	25	1
1	A	29	ALA	C-O	5.91	1.32	1.23	18	2
1	A	20	PHE	CB-CG	5.84	1.64	1.50	7	2
1	A	10	ARG	CB-CG	5.74	1.69	1.52	23	1
1	A	14	ARG	CB-CG	5.72	1.69	1.52	16	2
1	A	11	ASN	CB-CG	5.65	1.66	1.52	26	1
1	A	33	ALA	C-N	-5.55	1.26	1.33	13	3
1	A	19	GLN	C-O	-5.54	1.17	1.24	25	1
1	A	14	ARG	CA-CB	5.52	1.62	1.53	6	1
1	A	4	CYS	CB-SG	5.49	1.99	1.81	24	1
1	A	5	GLU	CG-CD	5.49	1.65	1.52	24	2
1	A	7	PRO	CA-CB	5.47	1.61	1.53	15	1
1	A	6	GLU	CB-CG	5.41	1.68	1.52	28	1
1	A	37	PRO	C-O	5.41	1.31	1.24	23	1
1	A	23	THR	CB-OG1	-5.39	1.35	1.43	17	2
1	A	19	GLN	CD-OE1	5.37	1.33	1.23	15	1
1	A	24	GLY	C-O	5.35	1.31	1.24	9	1
1	A	9	CYS	CA-CB	-5.21	1.45	1.53	5	1
1	A	8	THR	CB-OG1	5.18	1.52	1.43	18	2
1	A	33	ALA	C-O	-5.16	1.18	1.24	28	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	36	GLN	CB-CG	5.11	1.67	1.52	20	1
1	A	21	SER	C-O	5.08	1.30	1.24	4	1
1	A	22	ARG	CB-CG	5.07	1.67	1.52	12	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	15	HIS	ND1-CE1-NE2	22.39	130.79	108.40	18	28
1	A	25	PRO	N-CA-CB	-22.10	88.01	102.81	16	6
1	A	15	HIS	CE1-NE2-CD2	-19.14	89.86	109.00	23	26
1	A	28	PRO	O-C-N	-18.36	109.70	122.73	7	4
1	A	15	HIS	CA-CB-CG	17.32	131.12	113.80	6	18
1	A	19	GLN	N-CA-C	16.87	133.12	113.38	8	11
1	A	31	MET	CA-C-O	-15.73	102.78	120.24	4	11
1	A	20	PHE	CA-CB-CG	14.58	128.38	113.80	11	18
1	A	22	ARG	NE-CZ-NH2	-14.19	106.43	119.20	22	7
1	A	19	GLN	OE1-CD-NE2	-13.79	108.81	122.60	21	11
1	A	22	ARG	NE-CZ-NH1	13.36	134.86	121.50	17	12
1	A	27	CYS	CB-CA-C	13.24	125.10	109.47	18	10
1	A	27	CYS	O-C-N	-13.15	111.58	121.84	7	8
1	A	11	ASN	CA-CB-CG	13.09	125.69	112.60	22	12
1	A	16	LEU	CA-C-N	13.05	133.03	119.19	15	13
1	A	16	LEU	C-N-CA	13.05	133.03	119.19	15	13
1	A	6	GLU	O-C-N	-12.59	110.43	120.38	15	11
1	A	27	CYS	CA-C-O	12.53	131.66	119.13	7	11
1	A	36	GLN	CA-C-O	-12.51	107.63	119.13	16	14
1	A	18	LEU	N-CA-CB	12.47	128.09	110.01	22	12
1	A	28	PRO	N-CA-CB	12.20	110.94	102.65	8	9
1	A	22	ARG	N-CA-C	11.99	127.17	112.54	7	10
1	A	29	ALA	CA-C-O	11.98	135.54	121.28	9	2
1	A	26	LEU	N-CA-CB	11.88	126.97	110.10	28	5
1	A	30	CYS	N-CA-CB	-11.82	92.91	110.53	24	19
1	A	8	THR	N-CA-C	11.79	123.87	111.14	4	14
1	A	28	PRO	CA-C-O	11.78	133.83	121.11	7	2
1	A	26	LEU	CA-C-O	-11.63	108.11	120.55	22	4
1	A	12	ARG	CA-C-O	-11.58	106.65	119.97	8	11
1	A	22	ARG	O-C-N	11.58	134.47	122.08	13	8
1	A	6	GLU	CA-C-O	-11.57	108.49	119.13	16	15
1	A	6	GLU	N-CA-CB	-11.54	99.43	110.39	28	2
1	A	17	PRO	CB-CA-C	11.54	131.41	113.06	10	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	32	LYS	O-C-N	-11.39	110.04	122.12	11	6
1	A	16	LEU	CA-C-O	-11.32	108.22	118.63	27	13
1	A	13	THR	N-CA-C	-11.30	98.72	111.71	2	8
1	A	23	THR	CA-C-O	-11.21	108.54	120.42	5	13
1	A	32	LYS	N-CA-C	11.13	123.42	111.28	21	7
1	A	22	ARG	CA-C-O	11.13	132.81	120.90	11	5
1	A	37	PRO	O-C-N	11.10	137.89	122.35	11	5
1	A	33	ALA	N-CA-C	11.04	123.32	111.28	14	13
1	A	8	THR	O-C-N	11.03	134.00	122.09	14	10
1	A	17	PRO	CA-C-O	-11.01	103.15	119.34	11	8
1	A	17	PRO	O-C-N	-10.98	109.61	122.24	2	5
1	A	5	GLU	CA-C-O	-10.94	109.03	121.07	18	8
1	A	36	GLN	OE1-CD-NE2	-10.76	111.84	122.60	19	7
1	A	18	LEU	N-CA-C	10.75	122.57	111.07	23	7
1	A	15	HIS	CG-ND1-CE1	-10.64	91.21	109.30	26	19
1	A	30	CYS	N-CA-C	10.63	125.51	112.54	22	4
1	A	15	HIS	N-CA-CB	10.62	126.58	110.22	7	10
1	A	9	CYS	CB-CA-C	10.49	127.47	110.90	21	8
1	A	6	GLU	CB-CG-CD	10.49	130.43	112.60	10	8
1	A	11	ASN	OD1-CG-ND2	-10.35	112.25	122.60	16	8
1	A	6	GLU	N-CA-C	10.34	126.81	112.75	26	4
1	A	12	ARG	N-CA-C	10.34	123.60	111.71	18	8
1	A	9	CYS	O-C-N	10.32	133.06	122.12	18	3
1	A	34	THR	CA-C-O	-10.26	109.68	120.55	3	3
1	A	37	PRO	N-CD-CG	10.25	118.57	103.20	14	6
1	A	34	THR	O-C-N	10.11	132.83	122.12	8	3
1	A	35	LEU	CA-C-O	-10.10	109.72	120.63	28	11
1	A	25	PRO	N-CA-C	10.05	126.27	114.20	19	6
1	A	14	ARG	CA-C-O	-10.05	108.74	120.10	19	7
1	A	23	THR	N-CA-C	10.00	126.36	112.45	22	8
1	A	16	LEU	O-C-N	-10.00	109.82	121.32	2	11
1	A	8	THR	CA-C-O	9.98	130.98	120.70	3	9
1	A	36	GLN	O-C-N	9.98	127.15	120.27	16	13
1	A	26	LEU	O-C-N	9.85	133.08	121.76	17	5
1	A	10	ARG	CA-C-O	-9.77	110.19	120.55	3	12
1	A	35	LEU	O-C-N	-9.71	111.60	122.09	27	4
1	A	24	GLY	O-C-N	-9.70	112.07	121.77	13	5
1	A	11	ASN	CB-CA-C	9.65	126.24	110.81	24	1
1	A	33	ALA	CA-C-O	-9.58	110.29	120.63	5	11
1	A	14	ARG	N-CA-CB	9.54	125.07	110.28	8	7
1	A	21	SER	CB-CA-C	9.50	124.35	111.14	13	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	ARG	NE-CZ-NH1	9.45	130.95	121.50	22	3
1	A	31	MET	N-CA-C	9.43	124.04	112.54	25	9
1	A	32	LYS	CA-C-N	9.40	132.88	120.28	11	7
1	A	32	LYS	C-N-CA	9.40	132.88	120.28	11	7
1	A	18	LEU	CA-C-O	9.40	130.38	120.42	11	6
1	A	15	HIS	CG-CD2-NE2	9.39	116.59	107.20	5	12
1	A	4	CYS	O-C-N	9.37	132.15	122.03	28	4
1	A	4	CYS	CA-C-O	-9.37	111.17	121.00	26	6
1	A	9	CYS	CA-C-O	-9.32	110.67	120.55	18	4
1	A	31	MET	CG-SD-CE	9.31	121.39	100.90	16	5
1	A	22	ARG	N-CA-CB	9.27	124.24	110.33	19	1
1	A	4	CYS	N-CA-C	9.24	122.29	111.02	20	5
1	A	4	CYS	N-CA-CB	9.18	123.29	109.98	28	7
1	A	35	LEU	N-CA-C	9.16	121.26	111.28	8	6
1	A	15	HIS	CA-C-O	-9.16	109.75	120.10	3	6
1	A	8	THR	CA-C-N	9.12	133.24	120.29	13	7
1	A	8	THR	C-N-CA	9.12	133.24	120.29	13	7
1	A	5	GLU	N-CA-CB	9.12	123.68	109.82	16	4
1	A	36	GLN	CA-C-N	9.11	129.16	119.05	23	9
1	A	36	GLN	C-N-CA	9.11	129.16	119.05	23	9
1	A	37	PRO	N-CA-C	9.11	125.23	114.03	12	5
1	A	13	THR	CA-C-O	-9.09	110.91	120.55	17	6
1	A	28	PRO	N-CA-C	9.09	131.19	112.47	13	4
1	A	37	PRO	N-CA-CB	9.08	112.78	103.25	7	8
1	A	5	GLU	CB-CA-C	9.05	125.31	110.92	13	4
1	A	29	ALA	N-CA-C	9.00	121.44	110.91	28	4
1	A	9	CYS	N-CA-C	9.00	121.09	111.28	18	4
1	A	33	ALA	O-C-N	8.95	131.29	122.07	2	6
1	A	31	MET	N-CA-CB	8.95	123.54	110.20	4	7
1	A	35	LEU	CB-CA-C	8.93	127.15	110.63	2	6
1	A	24	GLY	CA-C-O	-8.89	108.81	121.52	3	14
1	A	14	ARG	O-C-N	8.85	132.57	122.22	16	5
1	A	27	CYS	N-CA-CB	8.83	127.08	110.65	7	2
1	A	22	ARG	CB-CA-C	8.81	124.90	110.81	17	5
1	A	12	ARG	CB-CA-C	8.78	125.61	110.68	2	7
1	A	10	ARG	N-CA-C	8.78	121.64	111.11	15	8
1	A	21	SER	CA-C-N	8.75	132.34	120.44	27	4
1	A	21	SER	C-N-CA	8.75	132.34	120.44	27	4
1	A	14	ARG	NE-CZ-NH2	-8.71	111.36	119.20	13	8
1	A	13	THR	O-C-N	8.70	132.11	122.20	5	6
1	A	22	ARG	CA-CB-CG	8.68	131.46	114.10	14	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	22	ARG	NH1-CZ-NH2	-8.64	108.07	119.30	12	8
1	A	20	PHE	N-CA-CB	8.59	122.02	110.59	18	2
1	A	11	ASN	CA-C-O	-8.54	111.76	120.90	24	6
1	A	33	ALA	N-CA-CB	-8.52	97.54	110.16	28	5
1	A	34	THR	CA-CB-CG2	8.52	124.98	110.50	20	4
1	A	15	HIS	O-C-N	-8.48	112.30	122.22	17	6
1	A	5	GLU	N-CA-C	8.46	120.19	110.97	10	10
1	A	38	GLU	CA-CB-CG	8.45	130.99	114.10	28	6
1	A	5	GLU	O-C-N	-8.44	113.38	122.07	12	7
1	A	25	PRO	CA-C-O	8.43	128.53	118.92	21	2
1	A	17	PRO	N-CA-C	8.41	126.00	113.81	7	2
1	A	13	THR	CA-CB-OG1	-8.39	97.02	109.60	3	4
1	A	6	GLU	CB-CA-C	8.38	126.68	110.17	6	9
1	A	36	GLN	N-CA-CB	8.33	122.72	110.30	6	5
1	A	34	THR	N-CA-C	8.25	121.31	111.33	26	3
1	A	28	PRO	CB-CA-C	-8.24	97.97	111.56	4	3
1	A	22	ARG	CB-CG-CD	8.22	130.20	111.30	28	3
1	A	20	PHE	CB-CA-C	8.20	123.92	110.24	19	6
1	A	19	GLN	CG-CD-NE2	8.18	128.66	116.40	11	2
1	A	16	LEU	CB-CA-C	8.17	126.27	110.17	2	2
1	A	4	CYS	CB-CA-C	-8.17	98.05	110.88	24	6
1	A	36	GLN	CB-CG-CD	-8.16	98.72	112.60	13	11
1	A	30	CYS	O-C-N	8.11	131.77	122.20	3	3
1	A	18	LEU	O-C-N	8.09	130.69	122.12	10	4
1	A	14	ARG	N-CA-C	-8.03	102.50	111.82	8	3
1	A	30	CYS	CA-C-O	-8.01	110.18	119.56	19	6
1	A	33	ALA	CB-CA-C	8.00	124.45	110.85	24	6
1	A	18	LEU	CB-CA-C	7.99	123.53	110.90	17	5
1	A	17	PRO	N-CD-CG	7.98	115.17	103.20	6	2
1	A	7	PRO	CA-C-N	7.96	131.27	120.44	21	3
1	A	7	PRO	C-N-CA	7.96	131.27	120.44	21	3
1	A	11	ASN	N-CA-CB	7.94	121.79	110.12	11	2
1	A	38	GLU	N-CA-CB	7.92	123.96	110.50	12	5
1	A	23	THR	CA-CB-CG2	7.87	123.87	110.50	4	4
1	A	33	ALA	CA-C-N	7.86	130.81	120.28	4	6
1	A	33	ALA	C-N-CA	7.86	130.81	120.28	4	6
1	A	23	THR	CA-CB-OG1	7.85	121.37	109.60	22	1
1	A	21	SER	CA-C-O	7.83	131.71	120.51	14	4
1	A	20	PHE	N-CA-C	7.80	123.56	113.18	23	4
1	A	32	LYS	CB-CA-C	7.78	123.09	110.88	7	3
1	A	10	ARG	N-CA-CB	-7.74	98.78	110.01	26	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	12	ARG	CA-C-N	7.73	131.66	120.38	7	2
1	A	12	ARG	C-N-CA	7.73	131.66	120.38	7	2
1	A	27	CYS	CA-C-N	7.70	129.46	119.84	12	4
1	A	27	CYS	C-N-CA	7.70	129.46	119.84	12	4
1	A	32	LYS	CA-C-O	-7.67	110.62	119.60	26	5
1	A	23	THR	O-C-N	7.67	132.24	122.19	7	2
1	A	13	THR	N-CA-CB	7.66	122.01	110.22	2	3
1	A	27	CYS	N-CA-C	-7.58	98.69	110.14	15	2
1	A	25	PRO	O-C-N	-7.57	112.42	122.64	2	2
1	A	5	GLU	CB-CG-CD	7.55	125.44	112.60	5	5
1	A	26	LEU	CB-CA-C	-7.53	95.43	110.42	3	6
1	A	10	ARG	NE-CZ-NH2	-7.52	112.43	119.20	24	4
1	A	15	HIS	CA-C-N	7.52	132.10	120.97	26	3
1	A	15	HIS	C-N-CA	7.52	132.10	120.97	26	3
1	A	30	CYS	CA-CB-SG	7.50	131.65	114.40	4	2
1	A	28	PRO	CA-C-N	7.47	133.39	122.63	14	1
1	A	28	PRO	C-N-CA	7.47	133.39	122.63	14	1
1	A	34	THR	CA-CB-OG1	7.46	120.79	109.60	25	5
1	A	15	HIS	CB-CG-ND1	-7.46	111.52	122.70	4	4
1	A	19	GLN	CB-CA-C	7.44	122.98	112.11	24	5
1	A	31	MET	O-C-N	-7.43	114.00	122.03	6	3
1	A	29	ALA	O-C-N	7.42	132.46	122.59	19	3
1	A	4	CYS	CA-CB-SG	-7.42	97.34	114.40	3	7
1	A	21	SER	N-CA-C	7.40	122.31	112.25	8	4
1	A	38	GLU	CB-CA-C	7.39	124.14	110.10	19	8
1	A	14	ARG	CB-CA-C	7.38	123.23	110.68	13	2
1	A	9	CYS	N-CA-CB	-7.37	99.26	110.16	17	6
1	A	7	PRO	CA-C-O	-7.34	107.23	120.60	9	2
1	A	30	CYS	CA-C-N	7.32	130.09	120.28	16	5
1	A	30	CYS	C-N-CA	7.32	130.09	120.28	16	5
1	A	32	LYS	CA-CB-CG	7.30	128.69	114.10	12	3
1	A	7	PRO	N-CA-CB	7.27	110.88	103.25	4	3
1	A	36	GLN	CG-CD-NE2	7.27	127.30	116.40	19	2
1	A	19	GLN	CB-CG-CD	7.26	124.95	112.60	5	2
1	A	9	CYS	CA-CB-SG	-7.24	97.75	114.40	22	5
1	A	12	ARG	NE-CZ-NH2	-7.23	112.69	119.20	6	2
1	A	15	HIS	CB-CG-CD2	-7.21	121.82	131.20	13	5
1	A	30	CYS	CB-CA-C	7.20	124.28	109.95	7	4
1	A	18	LEU	CA-C-N	7.20	133.11	122.74	5	2
1	A	18	LEU	C-N-CA	7.20	133.11	122.74	5	2
1	A	12	ARG	CG-CD-NE	7.18	127.80	112.00	27	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	31	MET	CB-CA-C	7.17	122.22	110.90	2	4
1	A	28	PRO	CA-N-CD	-7.16	101.97	112.00	8	2
1	A	29	ALA	CB-CA-C	-7.15	101.08	112.09	10	5
1	A	34	THR	CA-C-N	7.14	130.18	120.54	20	8
1	A	34	THR	C-N-CA	7.14	130.18	120.54	20	8
1	A	19	GLN	CA-C-O	-7.09	112.07	120.57	5	4
1	A	15	HIS	ND1-CG-CD2	7.07	113.17	106.10	4	3
1	A	37	PRO	CA-C-O	-7.04	108.85	119.55	26	4
1	A	36	GLN	CB-CA-C	-7.03	102.53	113.57	18	1
1	A	8	THR	CA-CB-OG1	-6.99	99.12	109.60	4	7
1	A	12	ARG	N-CA-CB	6.98	120.38	110.12	26	7
1	A	11	ASN	O-C-N	-6.98	114.72	122.12	15	7
1	A	24	GLY	CA-C-N	6.94	128.51	119.84	7	1
1	A	24	GLY	C-N-CA	6.94	128.51	119.84	7	1
1	A	32	LYS	CB-CG-CD	6.93	127.23	111.30	28	1
1	A	10	ARG	CB-CA-C	-6.91	99.75	110.81	15	8
1	A	32	LYS	N-CA-CB	6.85	120.76	110.22	13	3
1	A	15	HIS	N-CA-C	-6.84	103.84	111.71	20	4
1	A	37	PRO	CA-N-CD	-6.82	102.45	112.00	6	2
1	A	22	ARG	CA-C-N	6.82	129.71	120.44	4	3
1	A	22	ARG	C-N-CA	6.82	129.71	120.44	4	3
1	A	6	GLU	CA-CB-CG	6.81	127.71	114.10	21	6
1	A	10	ARG	NE-CZ-NH1	6.79	128.29	121.50	12	6
1	A	12	ARG	O-C-N	6.75	129.28	122.12	2	5
1	A	26	LEU	N-CA-C	-6.75	96.42	110.80	9	4
1	A	37	PRO	CB-CA-C	6.70	123.67	112.62	27	2
1	A	7	PRO	O-C-N	-6.67	113.63	122.64	22	3
1	A	14	ARG	CB-CG-CD	6.67	126.63	111.30	10	1
1	A	7	PRO	CB-CA-C	6.66	122.55	111.56	18	4
1	A	21	SER	CA-CB-OG	6.64	124.39	111.10	7	1
1	A	14	ARG	CA-CB-CG	6.59	127.27	114.10	7	1
1	A	10	ARG	CA-C-N	-6.56	109.01	121.54	22	1
1	A	10	ARG	C-N-CA	-6.56	109.01	121.54	22	1
1	A	38	GLU	CB-CG-CD	6.54	123.72	112.60	8	6
1	A	25	PRO	CA-C-N	6.53	130.13	121.90	15	2
1	A	25	PRO	C-N-CA	6.53	130.13	121.90	15	2
1	A	26	LEU	CA-C-N	6.52	130.35	121.74	28	2
1	A	26	LEU	C-N-CA	6.52	130.35	121.74	28	2
1	A	6	GLU	CA-C-N	6.51	127.97	119.84	20	3
1	A	6	GLU	C-N-CA	6.51	127.97	119.84	20	3
1	A	20	PHE	CA-C-O	-6.50	111.41	119.28	10	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	14	ARG	NH1-CZ-NH2	6.48	127.72	119.30	21	3
1	A	21	SER	O-C-N	-6.43	114.04	122.59	15	3
1	A	23	THR	CB-CA-C	6.42	123.49	112.00	8	3
1	A	37	PRO	CA-CB-CG	6.39	116.63	104.50	13	1
1	A	21	SER	N-CA-CB	-6.38	99.71	110.49	12	6
1	A	12	ARG	CA-CB-CG	6.33	126.75	114.10	21	5
1	A	17	PRO	N-CA-CB	6.32	109.89	103.25	27	4
1	A	17	PRO	CA-CB-CG	6.31	116.48	104.50	10	1
1	A	28	PRO	N-CD-CG	6.23	112.54	103.20	24	4
1	A	29	ALA	N-CA-CB	-6.22	103.02	112.47	6	2
1	A	34	THR	N-CA-CB	-6.21	100.74	110.06	26	3
1	A	36	GLN	N-CA-C	6.17	120.56	112.17	14	5
1	A	14	ARG	NE-CZ-NH1	6.13	127.63	121.50	10	2
1	A	18	LEU	CD1-CG-CD2	-6.12	97.33	110.80	23	2
1	A	35	LEU	CD1-CG-CD2	6.11	124.23	110.80	8	3
1	A	10	ARG	CA-CB-CG	6.10	126.29	114.10	9	3
1	A	7	PRO	N-CA-C	6.09	125.02	112.47	24	1
1	A	20	PHE	O-C-N	6.06	130.45	122.33	6	1
1	A	13	THR	CA-C-N	6.06	129.00	120.28	19	3
1	A	13	THR	C-N-CA	6.06	129.00	120.28	19	3
1	A	14	ARG	CD-NE-CZ	6.04	132.86	124.40	28	1
1	A	16	LEU	N-CA-C	6.02	121.82	113.45	24	2
1	A	25	PRO	CA-N-CD	-6.01	103.58	112.00	4	3
1	A	8	THR	CA-CB-CG2	5.99	120.68	110.50	6	2
1	A	7	PRO	N-CD-CG	5.95	112.12	103.20	20	4
1	A	17	PRO	CA-N-CD	-5.90	103.74	112.00	6	3
1	A	25	PRO	CA-CB-CG	5.87	115.65	104.50	20	2
1	A	11	ASN	CB-CG-ND2	5.82	125.13	116.40	8	2
1	A	17	PRO	CA-C-N	5.80	127.98	120.44	19	1
1	A	17	PRO	C-N-CA	5.80	127.98	120.44	19	1
1	A	5	GLU	CA-C-N	5.78	126.25	119.83	7	2
1	A	5	GLU	C-N-CA	5.78	126.25	119.83	7	2
1	A	19	GLN	O-C-N	-5.76	114.93	122.59	25	2
1	A	28	PRO	CA-CB-CG	5.76	115.44	104.50	5	2
1	A	6	GLU	CG-CD-OE2	5.66	131.42	118.40	3	1
1	A	6	GLU	CG-CD-OE1	5.66	131.41	118.40	20	2
1	A	24	GLY	N-CA-C	5.62	123.80	112.34	6	3
1	A	31	MET	CA-CB-CG	-5.61	102.87	114.10	28	3
1	A	5	GLU	CA-CB-CG	5.61	125.32	114.10	28	1
1	A	25	PRO	N-CD-CG	5.58	111.57	103.20	12	1
1	A	29	ALA	CA-C-N	5.58	131.56	121.92	16	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	ALA	C-N-CA	5.58	131.56	121.92	16	1
1	A	35	LEU	N-CA-CB	5.57	119.79	110.32	6	1
1	A	14	ARG	CA-C-N	5.56	128.28	120.28	21	1
1	A	14	ARG	C-N-CA	5.56	128.28	120.28	21	1
1	A	9	CYS	CA-C-N	5.52	127.95	120.38	17	3
1	A	9	CYS	C-N-CA	5.52	127.95	120.38	17	3
1	A	19	GLN	N-CA-CB	-5.48	103.68	111.84	13	2
1	A	13	THR	CA-CB-CG2	5.47	119.80	110.50	5	1
1	A	16	LEU	CB-CG-CD1	5.46	127.07	110.70	16	1
1	A	19	GLN	CG-CD-OE1	-5.44	109.91	120.80	11	1
1	A	12	ARG	NH1-CZ-NH2	-5.39	112.29	119.30	22	2
1	A	22	ARG	CD-NE-CZ	5.33	131.86	124.40	7	3
1	A	13	THR	CB-CA-C	5.28	119.56	110.79	13	2
1	A	36	GLN	CA-CB-CG	5.27	124.64	114.10	10	1
1	A	38	GLU	CG-CD-OE1	5.25	130.47	118.40	23	1
1	A	23	THR	N-CA-CB	5.24	117.55	110.10	18	1
1	A	12	ARG	CD-NE-CZ	-5.23	117.08	124.40	2	1
1	A	10	ARG	CB-CG-CD	-5.23	99.27	111.30	3	1
1	A	10	ARG	CG-CD-NE	5.21	123.47	112.00	10	1
1	A	32	LYS	CG-CD-CE	5.19	123.24	111.30	24	1
1	A	22	ARG	CG-CD-NE	-5.17	100.63	112.00	9	1
1	A	11	ASN	N-CA-C	5.12	116.94	111.36	5	2
1	A	36	GLN	CG-CD-OE1	5.07	130.94	120.80	25	1
1	A	18	LEU	CB-CG-CD1	5.06	125.89	110.70	23	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	10	ARG	Sidechain	17
1	A	14	ARG	Mainchain,Sidechain	15
1	A	22	ARG	Mainchain,Sidechain	14
1	A	20	PHE	Sidechain	13
1	A	15	HIS	Sidechain,Mainchain	6
1	A	38	GLU	Sidechain	5
1	A	12	ARG	Mainchain,Sidechain	5
1	A	17	PRO	Mainchain	5
1	A	29	ALA	Mainchain	5
1	A	19	GLN	Mainchain,Sidechain	5
1	A	33	ALA	Mainchain	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	26	LEU	Mainchain	5
1	A	27	CYS	Mainchain	5
1	A	32	LYS	Mainchain	4
1	A	5	GLU	Mainchain	3
1	A	28	PRO	Mainchain	3
1	A	11	ASN	Sidechain,Mainchain	3
1	A	24	GLY	Mainchain	3
1	A	21	SER	Mainchain	3
1	A	4	CYS	Mainchain	2
1	A	16	LEU	Mainchain	2
1	A	31	MET	Mainchain	2
1	A	36	GLN	Mainchain	2
1	A	13	THR	Mainchain	1
1	A	23	THR	Mainchain	1
1	A	6	GLU	Mainchain	1
1	A	35	LEU	Mainchain	1
1	A	7	PRO	Mainchain	1
1	A	9	CYS	Mainchain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	275	273	275	5±2
All	All	7975	8001	7975	131

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:CA	1:A:26:LEU:CB	1.63	1.75	4	1
1:A:27:CYS:CA	1:A:27:CYS:C	1.58	1.76	11	1
1:A:16:LEU:CB	1:A:16:LEU:CG	1.58	1.76	18	1
1:A:29:ALA:C	1:A:29:ALA:CA	1.57	1.74	12	3
1:A:17:PRO:CD	1:A:17:PRO:CG	1.56	1.74	25	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PRO:CA	1:A:7:PRO:C	1.56	1.77	26	2
1:A:13:THR:CA	1:A:13:THR:C	1.55	1.75	6	2
1:A:33:ALA:N	1:A:33:ALA:CA	1.55	1.69	24	1
1:A:16:LEU:C	1:A:16:LEU:CA	1.55	1.75	19	1
1:A:26:LEU:CB	1:A:26:LEU:CG	1.55	1.78	8	1
1:A:14:ARG:C	1:A:14:ARG:CA	1.53	1.77	8	1
1:A:16:LEU:CA	1:A:16:LEU:N	1.53	1.70	5	2
1:A:36:GLN:N	1:A:36:GLN:CA	1.53	1.68	13	2
1:A:16:LEU:CG	1:A:16:LEU:CD2	1.53	1.76	16	1
1:A:12:ARG:CA	1:A:12:ARG:C	1.53	1.80	10	1
1:A:37:PRO:CA	1:A:37:PRO:CB	1.52	1.75	15	1
1:A:30:CYS:N	1:A:30:CYS:CA	1.51	1.70	4	1
1:A:15:HIS:CA	1:A:15:HIS:C	1.44	1.90	7	1
1:A:25:PRO:CA	1:A:25:PRO:N	1.44	1.68	20	1
1:A:28:PRO:CB	1:A:28:PRO:CG	1.44	1.83	22	1
1:A:26:LEU:CB	1:A:26:LEU:C	0.86	2.48	4	1
1:A:16:LEU:CD2	1:A:16:LEU:CB	0.83	2.56	16	1
1:A:16:LEU:CB	1:A:16:LEU:CD1	0.82	2.58	18	1
1:A:30:CYS:N	1:A:30:CYS:CB	0.81	2.42	4	1
1:A:16:LEU:CB	1:A:16:LEU:CD2	0.80	2.58	18	1
1:A:16:LEU:CD2	1:A:16:LEU:CD1	0.79	2.61	16	1
1:A:16:LEU:CG	1:A:16:LEU:CA	0.75	2.65	18	1
1:A:35:LEU:C	1:A:36:GLN:CA	0.73	2.61	13	2
1:A:36:GLN:N	1:A:36:GLN:CB	0.72	2.51	13	1
1:A:29:ALA:C	1:A:30:CYS:CA	0.71	2.62	4	1
1:A:29:ALA:C	1:A:29:ALA:CB	0.71	2.63	10	2
1:A:13:THR:C	1:A:13:THR:N	0.69	2.50	2	1
1:A:27:CYS:SG	1:A:30:CYS:HB3	0.67	2.29	19	14
1:A:7:PRO:C	1:A:7:PRO:CB	0.67	2.67	26	2
1:A:29:ALA:CA	1:A:30:CYS:N	0.66	2.58	10	3
1:A:32:LYS:C	1:A:33:ALA:CA	0.64	2.68	24	1
1:A:33:ALA:N	1:A:33:ALA:CB	0.63	2.59	24	1
1:A:24:GLY:C	1:A:25:PRO:CA	0.62	2.69	20	1
1:A:16:LEU:N	1:A:16:LEU:CB	0.61	2.59	5	2
1:A:27:CYS:SG	1:A:30:CYS:CB	0.61	2.88	17	8
1:A:13:THR:C	1:A:13:THR:CB	0.61	2.67	2	2
1:A:26:LEU:CG	1:A:26:LEU:CA	0.60	2.74	8	1
1:A:27:CYS:O	1:A:27:CYS:SG	0.58	2.60	22	2
1:A:31:MET:SD	1:A:31:MET:C	0.57	2.88	7	1
1:A:27:CYS:SG	1:A:30:CYS:HB2	0.56	2.41	16	3
1:A:26:LEU:CB	1:A:26:LEU:CD1	0.55	2.76	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:HIS:C	1:A:15:HIS:CB	0.55	2.78	7	1
1:A:22:ARG:HD3	1:A:22:ARG:H	0.55	1.61	24	2
1:A:27:CYS:C	1:A:27:CYS:CB	0.54	2.75	11	1
1:A:15:HIS:C	1:A:15:HIS:N	0.52	2.64	7	1
1:A:14:ARG:C	1:A:14:ARG:N	0.52	2.63	8	1
1:A:33:ALA:O	1:A:37:PRO:HD2	0.51	2.05	27	4
1:A:6:GLU:HB3	1:A:7:PRO:HD3	0.50	1.84	28	1
1:A:9:CYS:SG	1:A:12:ARG:NE	0.50	2.81	9	2
1:A:36:GLN:HB2	1:A:37:PRO:HD3	0.49	1.84	23	1
1:A:15:HIS:HB3	1:A:18:LEU:HD11	0.49	1.83	27	1
1:A:16:LEU:CD2	1:A:16:LEU:HB3	0.49	2.37	16	1
1:A:15:HIS:C	1:A:16:LEU:CA	0.48	2.74	5	2
1:A:5:GLU:HB3	1:A:30:CYS:SG	0.48	2.49	13	3
1:A:12:ARG:HH12	1:A:26:LEU:HD13	0.47	1.69	6	1
1:A:12:ARG:O	1:A:15:HIS:HB2	0.47	2.10	26	4
1:A:29:ALA:C	1:A:29:ALA:N	0.46	2.62	10	1
1:A:33:ALA:N	1:A:33:ALA:C	0.45	2.65	24	1
1:A:18:LEU:HD12	1:A:19:GLN:N	0.45	2.27	25	2
1:A:5:GLU:HA	1:A:9:CYS:HB2	0.45	1.88	6	1
1:A:37:PRO:CB	1:A:37:PRO:C	0.44	2.80	15	1
1:A:16:LEU:CD1	1:A:31:MET:HE1	0.44	2.43	23	1
1:A:16:LEU:C	1:A:16:LEU:N	0.44	2.64	19	1
1:A:6:GLU:O	1:A:10:ARG:HB2	0.43	2.13	3	2
1:A:10:ARG:O	1:A:13:THR:HB	0.43	2.14	6	1
1:A:14:ARG:CA	1:A:14:ARG:O	0.43	2.54	8	1
1:A:33:ALA:O	1:A:37:PRO:CD	0.43	2.67	20	1
1:A:5:GLU:OE1	1:A:37:PRO:HG2	0.42	2.15	28	1
1:A:33:ALA:O	1:A:36:GLN:HB2	0.42	2.15	3	1
1:A:15:HIS:O	1:A:18:LEU:HG	0.41	2.15	19	3
1:A:28:PRO:O	1:A:29:ALA:HB3	0.41	2.16	4	1
1:A:36:GLN:N	1:A:36:GLN:HA	0.41	2.05	10	1
1:A:7:PRO:CA	1:A:8:THR:N	0.40	2.67	25	1
1:A:27:CYS:SG	1:A:27:CYS:O	0.40	2.79	26	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	34/38 (89%)	25±1 (75±4%)	7±1 (20±4%)	2±1 (5±4%)	2	21
All	All	986/1102 (89%)	735 (75%)	197 (20%)	54 (5%)	2	21

All 7 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	24	GLY	18
1	A	7	PRO	17
1	A	25	PRO	7
1	A	28	PRO	5
1	A	29	ALA	4
1	A	5	GLU	2
1	A	17	PRO	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	32/35 (91%)	27±2 (83±6%)	5±2 (17±6%)	4	39
All	All	928/1015 (91%)	774 (83%)	154 (17%)	4	39

All 26 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	22	ARG	27
1	A	12	ARG	14
1	A	19	GLN	13
1	A	16	LEU	12
1	A	14	ARG	11
1	A	31	MET	10
1	A	21	SER	7
1	A	26	LEU	7
1	A	9	CYS	6
1	A	6	GLU	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	28	PRO	5
1	A	17	PRO	4
1	A	34	THR	4
1	A	8	THR	4
1	A	5	GLU	4
1	A	38	GLU	4
1	A	18	LEU	3
1	A	7	PRO	3
1	A	35	LEU	3
1	A	25	PRO	2
1	A	36	GLN	1
1	A	13	THR	1
1	A	4	CYS	1
1	A	23	THR	1
1	A	20	PHE	1
1	A	15	HIS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided