Full wwPDB NMR Structure Validation Report (i)

Feb 16, 2022 – 10:05 AM EST

PDB ID	:	1N5G
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 (i) symbol.

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

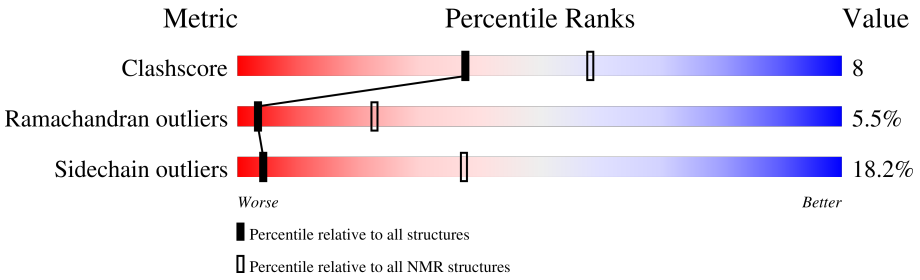
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	38	74% 16% • 8%

2 Ensemble composition and analysis (i)

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)	0.32	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
			Total	C	H	N	O	S	
1	A	38	615	190	310	57	53	5	0

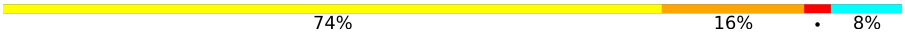
4 Residue-property plots

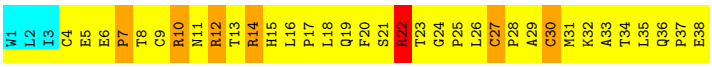
4.1 Average score per residue in the NMR ensemble

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

Chain A:





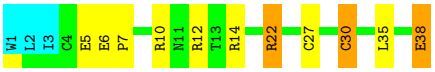
4.2 Scores per residue for each member of the ensemble

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

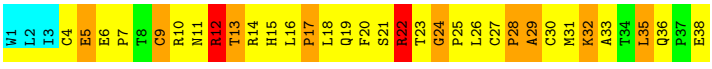
Chain A:



4.2.2 Score per residue for model 2

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

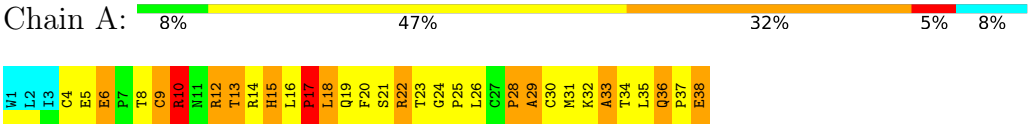
Chain A:



4.2.3 Score per residue for model 3

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

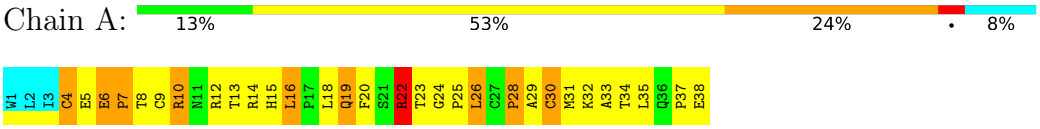
Chain A:



4.2.4 Score per residue for model 4

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

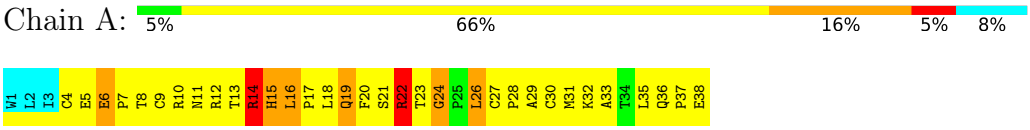
Chain A:



4.2.5 Score per residue for model 5

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

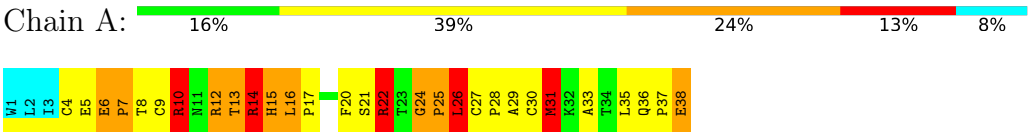
Chain A:



4.2.6 Score per residue for model 6

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

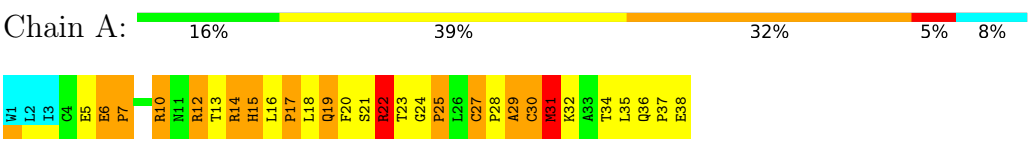
Chain A:



4.2.7 Score per residue for model 7

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

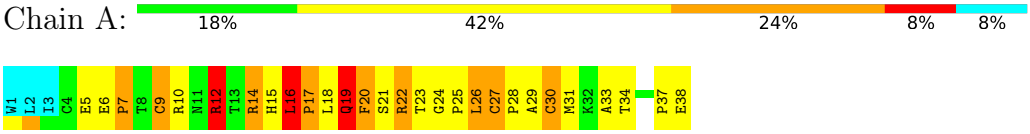
Chain A:



4.2.8 Score per residue for model 8

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

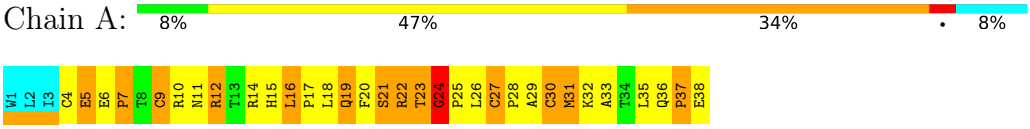
Chain A:



4.2.9 Score per residue for model 9

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

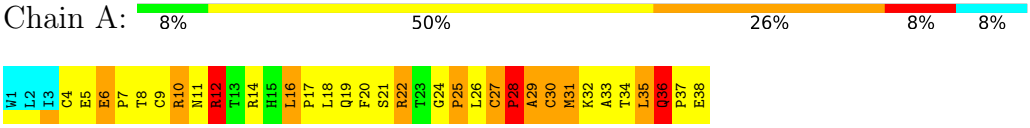
Chain A:



4.2.10 Score per residue for model 10

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

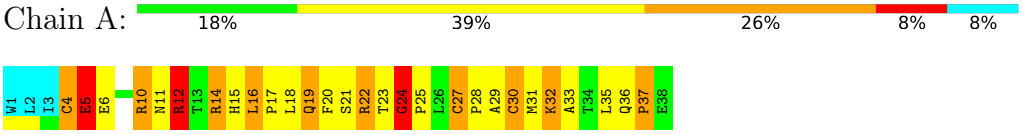
Chain A:



4.2.11 Score per residue for model 11

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

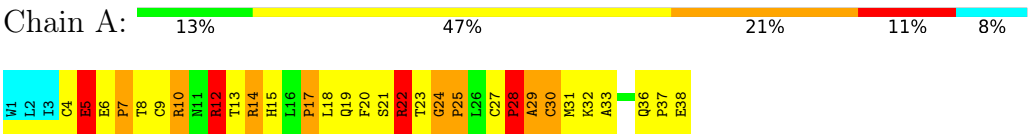
Chain A:



4.2.12 Score per residue for model 12

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

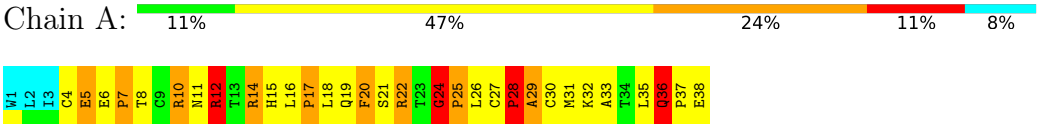
Chain A:



4.2.13 Score per residue for model 13

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

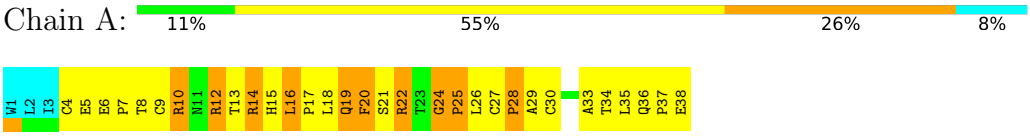
Chain A:



4.2.14 Score per residue for model 14 (medoid)

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

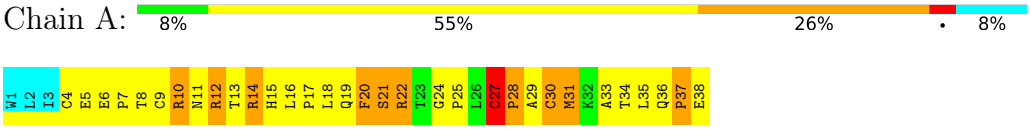
Chain A:



4.2.15 Score per residue for model 15

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

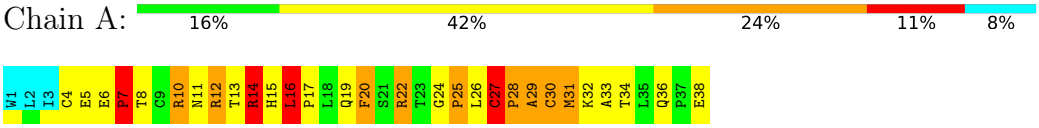
Chain A:



4.2.16 Score per residue for model 16

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

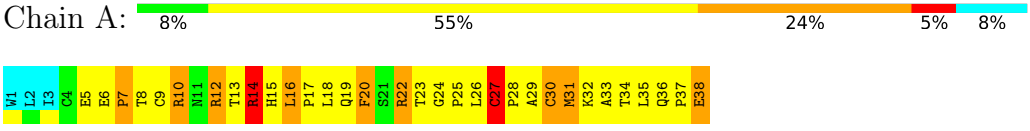
Chain A:



4.2.17 Score per residue for model 17

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

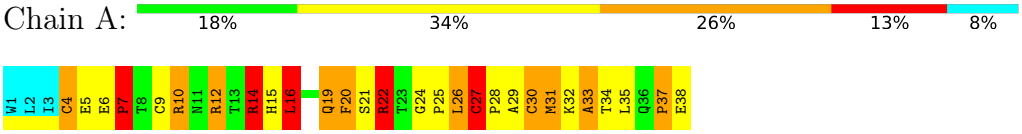
Chain A:



4.2.18 Score per residue for model 18

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

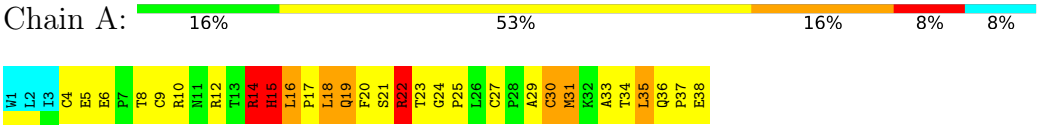
Chain A:



4.2.19 Score per residue for model 19

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

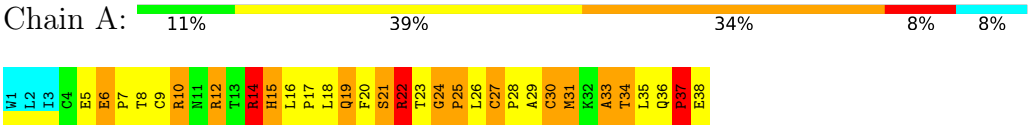
Chain A:



4.2.20 Score per residue for model 20

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

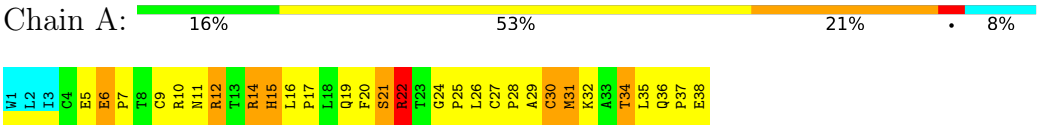
Chain A:



4.2.21 Score per residue for model 21

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

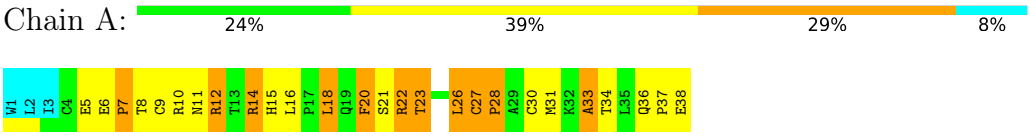
Chain A:



4.2.22 Score per residue for model 22

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

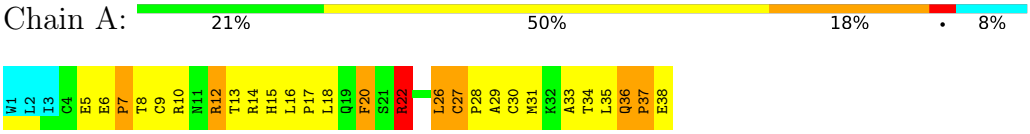
Chain A:



4.2.23 Score per residue for model 23

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

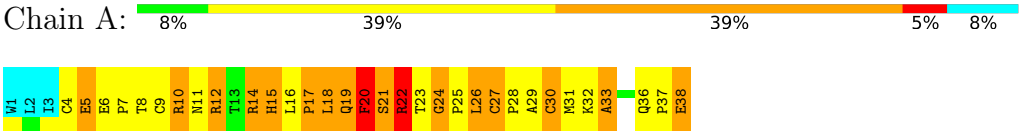
Chain A:



4.2.24 Score per residue for model 24

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

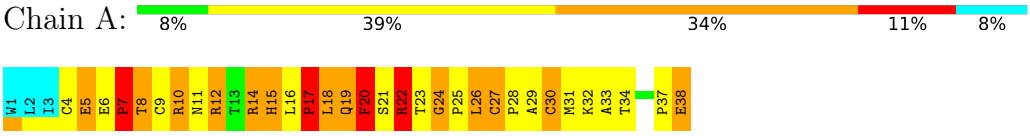
Chain A:



4.2.25 Score per residue for model 25

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

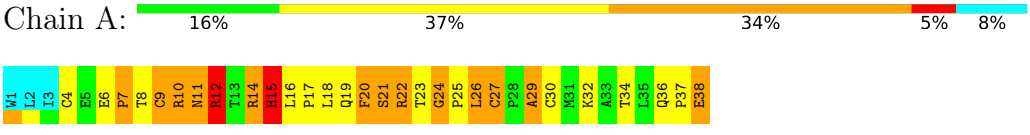
Chain A:



4.2.26 Score per residue for model 26

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

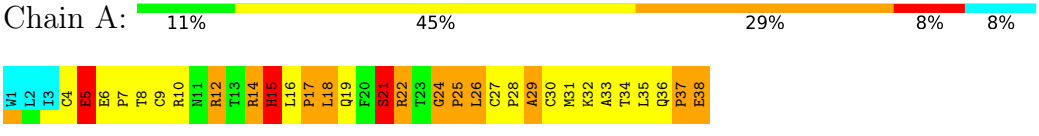
Chain A:



4.2.27 Score per residue for model 27

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

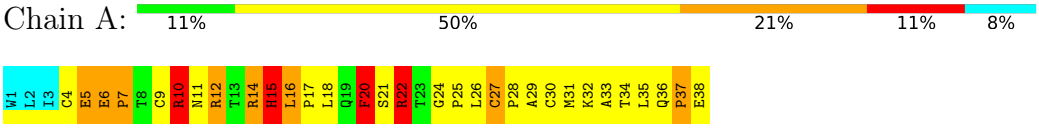
Chain A:



4.2.28 Score per residue for model 28

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

Chain A:



4.2.29 Score per residue for model 29

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

Chain A:

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 (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.95±0.38	25±7/281 (9.0± 2.6%)	2.88±0.32	28±7/379 (7.3± 1.7%)
All	All	2.98	737/8149 (9.0%)	2.90	805/10991 (7.3%)

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	19.53	1.85	1.46	6	7
1	A	5	GLU	CD-OE2	14.86	1.42	1.25	4	12
1	A	15	HIS	CA-C	14.39	1.90	1.52	7	7
1	A	5	GLU	CD-OE1	14.03	1.41	1.25	5	14
1	A	38	GLU	CD-OE1	13.94	1.41	1.25	6	10
1	A	38	GLU	CG-CD	13.79	1.72	1.51	24	10
1	A	24	GLY	N-CA	13.77	1.66	1.46	27	7
1	A	17	PRO	N-CD	13.17	1.66	1.47	15	8
1	A	23	THR	C-N	13.04	1.56	1.33	4	5
1	A	22	ARG	NE-CZ	12.96	1.49	1.33	14	14
1	A	36	GLN	N-CA	12.57	1.71	1.46	10	6
1	A	25	PRO	N-CA	12.50	1.68	1.47	20	9
1	A	12	ARG	CZ-NH1	12.39	1.49	1.33	3	8
1	A	7	PRO	CA-C	12.31	1.77	1.52	25	3
1	A	15	HIS	CB-CG	12.30	1.72	1.50	28	3
1	A	15	HIS	CG-CD2	12.27	1.56	1.35	6	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	29	ALA	CA-C	12.00	1.84	1.52	10	8
1	A	6	GLU	CG-CD	11.93	1.69	1.51	7	5
1	A	30	CYS	N-CA	11.86	1.70	1.46	4	4
1	A	33	ALA	N-CA	11.76	1.69	1.46	24	6
1	A	6	GLU	CD-OE1	11.70	1.38	1.25	5	12
1	A	28	PRO	N-CA	11.32	1.66	1.47	2	8
1	A	37	PRO	CA-CB	10.80	1.75	1.53	15	7
1	A	22	ARG	CZ-NH2	10.74	1.47	1.33	15	4
1	A	7	PRO	N-CA	10.70	1.65	1.47	7	6
1	A	13	THR	CA-C	10.57	1.80	1.52	2	6
1	A	12	ARG	CA-C	10.55	1.80	1.52	10	2
1	A	14	ARG	NE-CZ	10.55	1.46	1.33	19	5
1	A	11	ASN	N-CA	10.37	1.67	1.46	9	2
1	A	38	GLU	CD-OE2	10.37	1.37	1.25	7	9
1	A	22	ARG	CZ-NH1	10.36	1.46	1.33	23	8
1	A	6	GLU	CD-OE2	10.24	1.36	1.25	29	8
1	A	31	MET	N-CA	10.24	1.66	1.46	7	6
1	A	25	PRO	CA-C	10.13	1.73	1.52	15	6
1	A	24	GLY	CA-C	10.12	1.68	1.51	14	10
1	A	21	SER	CA-CB	10.12	1.68	1.52	18	6
1	A	28	PRO	CA-C	10.11	1.73	1.52	4	9
1	A	4	CYS	CB-SG	10.07	1.99	1.82	24	5
1	A	20	PHE	CG-CD2	9.92	1.53	1.38	21	3
1	A	28	PRO	N-CD	9.78	1.61	1.47	5	6
1	A	12	ARG	NE-CZ	9.73	1.45	1.33	28	8
1	A	17	PRO	CA-C	9.50	1.71	1.52	14	3
1	A	20	PHE	CG-CD1	9.49	1.52	1.38	28	5
1	A	14	ARG	CA-C	9.48	1.77	1.52	8	4
1	A	26	LEU	CA-CB	9.46	1.75	1.53	4	4
1	A	29	ALA	N-CA	9.45	1.65	1.46	9	4
1	A	12	ARG	N-CA	9.38	1.65	1.46	16	8
1	A	5	GLU	CG-CD	9.21	1.65	1.51	24	8
1	A	20	PHE	N-CA	9.19	1.64	1.46	13	5
1	A	23	THR	N-CA	9.12	1.64	1.46	17	1
1	A	27	CYS	CB-SG	9.11	1.97	1.82	8	4
1	A	27	CYS	C-N	9.10	1.51	1.34	26	4
1	A	37	PRO	CA-C	9.05	1.71	1.52	11	6
1	A	10	ARG	N-CA	8.98	1.64	1.46	18	6
1	A	27	CYS	CA-C	8.88	1.76	1.52	11	4
1	A	26	LEU	CB-CG	8.87	1.78	1.52	8	2
1	A	18	LEU	N-CA	8.85	1.64	1.46	11	14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	9	CYS	CB-SG	8.81	1.97	1.82	10	6
1	A	29	ALA	CA-CB	8.78	1.70	1.52	19	7
1	A	13	THR	N-CA	8.73	1.63	1.46	4	3
1	A	19	GLN	CG-CD	8.72	1.71	1.51	20	7
1	A	12	ARG	CD-NE	8.71	1.61	1.46	9	1
1	A	6	GLU	CB-CG	8.70	1.68	1.52	28	3
1	A	10	ARG	CD-NE	8.69	1.61	1.46	6	5
1	A	35	LEU	N-CA	8.68	1.63	1.46	5	2
1	A	22	ARG	CD-NE	8.65	1.61	1.46	5	2
1	A	36	GLN	C-N	8.54	1.50	1.34	19	4
1	A	16	LEU	CA-C	8.47	1.75	1.52	19	2
1	A	5	GLU	N-CA	8.46	1.63	1.46	10	4
1	A	16	LEU	CB-CG	8.41	1.76	1.52	18	2
1	A	35	LEU	CA-CB	8.32	1.72	1.53	4	2
1	A	34	THR	N-CA	8.28	1.62	1.46	15	5
1	A	32	LYS	N-CA	8.26	1.62	1.46	2	3
1	A	34	THR	CA-C	8.24	1.74	1.52	22	7
1	A	12	ARG	CA-CB	8.23	1.72	1.53	6	3
1	A	22	ARG	N-CA	8.22	1.62	1.46	28	3
1	A	17	PRO	N-CA	7.93	1.60	1.47	10	8
1	A	36	GLN	CG-CD	7.82	1.69	1.51	21	2
1	A	17	PRO	C-N	7.82	1.52	1.34	8	2
1	A	32	LYS	CB-CG	7.82	1.73	1.52	25	2
1	A	13	THR	CB-OG1	7.76	1.58	1.43	17	5
1	A	4	CYS	CA-C	7.75	1.73	1.52	9	2
1	A	25	PRO	N-CD	7.68	1.58	1.47	25	2
1	A	32	LYS	CA-C	7.66	1.72	1.52	17	5
1	A	17	PRO	CG-CD	7.64	1.75	1.50	27	3
1	A	5	GLU	CA-CB	7.62	1.70	1.53	24	2
1	A	6	GLU	C-N	7.59	1.48	1.34	5	3
1	A	30	CYS	CB-SG	-7.56	1.69	1.82	20	2
1	A	8	THR	CA-C	7.56	1.72	1.52	14	2
1	A	26	LEU	C-N	7.54	1.51	1.34	14	2
1	A	7	PRO	N-CD	-7.53	1.37	1.47	14	3
1	A	14	ARG	CZ-NH1	7.51	1.42	1.33	3	4
1	A	31	MET	CG-SD	7.50	2.00	1.81	3	1
1	A	20	PHE	CB-CG	7.49	1.64	1.51	7	2
1	A	26	LEU	N-CA	7.48	1.61	1.46	28	3
1	A	15	HIS	N-CA	7.46	1.61	1.46	15	4
1	A	10	ARG	NE-CZ	7.40	1.42	1.33	22	3
1	A	37	PRO	N-CD	-7.39	1.37	1.47	8	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	28	PRO	CA-CB	7.38	1.68	1.53	13	5
1	A	37	PRO	C-N	7.37	1.51	1.34	27	6
1	A	17	PRO	CA-CB	7.33	1.68	1.53	17	3
1	A	32	LYS	C-N	7.25	1.50	1.34	9	2
1	A	26	LEU	CA-C	7.22	1.71	1.52	8	8
1	A	35	LEU	CA-C	7.19	1.71	1.52	6	2
1	A	10	ARG	CZ-NH1	7.12	1.42	1.33	3	2
1	A	36	GLN	CA-CB	7.10	1.69	1.53	27	3
1	A	4	CYS	N-CA	7.09	1.60	1.46	19	3
1	A	27	CYS	N-CA	7.04	1.60	1.46	23	6
1	A	23	THR	CA-CB	7.04	1.71	1.53	2	3
1	A	38	GLU	CA-C	7.02	1.71	1.52	10	5
1	A	38	GLU	CB-CG	7.00	1.65	1.52	27	4
1	A	4	CYS	C-N	6.99	1.50	1.34	25	3
1	A	19	GLN	N-CA	6.90	1.60	1.46	14	5
1	A	36	GLN	CA-C	6.89	1.70	1.52	5	5
1	A	14	ARG	C-O	6.87	1.36	1.23	25	1
1	A	31	MET	CA-CB	6.86	1.69	1.53	28	2
1	A	8	THR	CA-CB	6.83	1.71	1.53	4	4
1	A	14	ARG	N-CA	6.83	1.60	1.46	8	4
1	A	28	PRO	CB-CG	6.75	1.83	1.50	22	1
1	A	19	GLN	CA-CB	6.74	1.68	1.53	3	2
1	A	16	LEU	CG-CD2	6.74	1.76	1.51	16	2
1	A	33	ALA	CA-CB	6.72	1.66	1.52	6	3
1	A	5	GLU	C-N	6.72	1.49	1.34	9	1
1	A	21	SER	CA-C	6.70	1.70	1.52	2	4
1	A	14	ARG	CZ-NH2	-6.66	1.24	1.33	28	4
1	A	5	GLU	CA-C	6.65	1.70	1.52	27	1
1	A	9	CYS	CA-C	6.64	1.70	1.52	20	2
1	A	30	CYS	CA-C	6.61	1.70	1.52	16	4
1	A	9	CYS	N-CA	6.61	1.59	1.46	27	4
1	A	38	GLU	N-CA	6.58	1.59	1.46	20	2
1	A	11	ASN	CB-CG	6.58	1.66	1.51	26	2
1	A	18	LEU	CA-C	6.57	1.70	1.52	13	4
1	A	18	LEU	CA-CB	6.53	1.68	1.53	13	1
1	A	28	PRO	CG-CD	6.53	1.72	1.50	14	1
1	A	5	GLU	CB-CG	6.53	1.64	1.52	8	1
1	A	8	THR	N-CA	6.52	1.59	1.46	5	4
1	A	22	ARG	C-O	6.46	1.35	1.23	3	1
1	A	7	PRO	CG-CD	6.46	1.72	1.50	22	2
1	A	38	GLU	C-OXT	-6.46	1.11	1.23	29	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	16	LEU	CA-CB	6.43	1.68	1.53	20	3
1	A	6	GLU	CA-C	6.43	1.69	1.52	14	2
1	A	10	ARG	CA-CB	6.41	1.68	1.53	26	3
1	A	19	GLN	CA-C	6.41	1.69	1.52	2	3
1	A	33	ALA	CA-C	6.40	1.69	1.52	13	1
1	A	20	PHE	CE1-CZ	6.35	1.49	1.37	14	3
1	A	10	ARG	CB-CG	6.34	1.69	1.52	23	1
1	A	20	PHE	C-O	6.32	1.35	1.23	20	1
1	A	14	ARG	CB-CG	6.31	1.69	1.52	16	2
1	A	24	GLY	C-N	6.29	1.46	1.34	13	3
1	A	6	GLU	CA-CB	6.28	1.67	1.53	19	3
1	A	12	ARG	CZ-NH2	-6.19	1.25	1.33	28	3
1	A	12	ARG	C-N	6.09	1.48	1.34	3	5
1	A	6	GLU	N-CA	6.06	1.58	1.46	24	7
1	A	31	MET	C-N	6.04	1.48	1.34	3	1
1	A	31	MET	CA-C	6.02	1.68	1.52	23	3
1	A	11	ASN	CA-C	5.98	1.68	1.52	15	2
1	A	23	THR	CA-C	5.97	1.68	1.52	20	2
1	A	11	ASN	C-N	5.95	1.47	1.34	28	1
1	A	14	ARG	CD-NE	5.93	1.56	1.46	18	2
1	A	10	ARG	CA-C	5.74	1.67	1.52	7	1
1	A	25	PRO	CA-CB	5.67	1.64	1.53	19	2
1	A	32	LYS	CD-CE	5.67	1.65	1.51	4	1
1	A	27	CYS	CA-CB	5.64	1.66	1.53	14	2
1	A	36	GLN	CB-CG	5.64	1.67	1.52	20	1
1	A	22	ARG	CG-CD	5.63	1.66	1.51	16	1
1	A	12	ARG	CG-CD	5.61	1.66	1.51	7	2
1	A	22	ARG	CB-CG	5.59	1.67	1.52	12	1
1	A	21	SER	CB-OG	5.59	1.49	1.42	7	2
1	A	37	PRO	N-CA	5.56	1.56	1.47	27	4
1	A	28	PRO	C-N	5.55	1.46	1.34	12	1
1	A	13	THR	CA-CB	5.53	1.67	1.53	16	1
1	A	21	SER	C-N	5.53	1.46	1.34	12	1
1	A	16	LEU	C-N	5.47	1.44	1.34	8	2
1	A	20	PHE	CA-C	5.44	1.67	1.52	8	2
1	A	10	ARG	CG-CD	5.37	1.65	1.51	25	2
1	A	38	GLU	CA-CB	5.35	1.65	1.53	14	4
1	A	34	THR	CA-CB	5.32	1.67	1.53	26	1
1	A	14	ARG	CG-CD	5.28	1.65	1.51	17	1
1	A	9	CYS	C-O	5.28	1.33	1.23	24	2
1	A	38	GLU	C-O	5.25	1.33	1.23	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	35	LEU	CB-CG	5.25	1.67	1.52	23	1
1	A	21	SER	N-CA	5.23	1.56	1.46	9	2
1	A	22	ARG	CA-CB	5.21	1.65	1.53	20	1
1	A	32	LYS	CA-CB	5.21	1.65	1.53	27	1
1	A	20	PHE	CD1-CE1	5.18	1.49	1.39	24	1
1	A	37	PRO	CG-CD	5.18	1.67	1.50	4	1
1	A	20	PHE	C-N	5.17	1.46	1.34	22	1
1	A	20	PHE	CD2-CE2	5.15	1.49	1.39	25	1
1	A	8	THR	C-N	5.08	1.45	1.34	23	1
1	A	10	ARG	C-N	5.07	1.45	1.34	22	1
1	A	11	ASN	CA-CB	5.03	1.66	1.53	10	1
1	A	22	ARG	CA-C	5.02	1.66	1.52	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(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	22	ARG	NE-CZ-NH1	29.12	134.86	120.30	17	23
1	A	22	ARG	NE-CZ-NH2	-27.75	106.43	120.30	22	18
1	A	12	ARG	NE-CZ-NH1	21.30	130.95	120.30	22	23
1	A	14	ARG	NE-CZ-NH2	-17.88	111.36	120.30	13	20
1	A	10	ARG	NE-CZ-NH1	15.99	128.29	120.30	12	20
1	A	10	ARG	NE-CZ-NH2	-15.74	112.43	120.30	24	17
1	A	12	ARG	NE-CZ-NH2	-15.22	112.69	120.30	6	14
1	A	14	ARG	NE-CZ-NH1	14.66	127.63	120.30	10	20
1	A	31	MET	CG-SD-CE	13.24	121.39	100.20	16	8
1	A	25	PRO	N-CA-CB	-12.74	88.01	103.30	16	6
1	A	20	PHE	CB-CG-CD2	-11.41	112.82	120.80	3	12
1	A	15	HIS	CG-ND1-CE1	-11.14	91.21	105.70	26	9
1	A	20	PHE	CB-CG-CD1	-10.97	113.12	120.80	26	9
1	A	15	HIS	CA-CB-CG	10.30	131.12	113.60	6	7
1	A	22	ARG	NH1-CZ-NH2	-10.30	108.07	119.40	12	12
1	A	37	PRO	N-CD-CG	10.25	118.57	103.20	14	6
1	A	30	CYS	N-CA-CB	-10.02	92.57	110.60	10	17
1	A	30	CYS	CA-CB-SG	9.80	131.65	114.00	4	5
1	A	33	ALA	CB-CA-C	9.57	124.45	110.10	24	7
1	A	15	HIS	ND1-CE1-NE2	9.49	130.79	109.90	18	14
1	A	37	PRO	O-C-N	9.49	137.89	122.70	11	4
1	A	16	LEU	CB-CG-CD1	9.45	127.07	111.00	16	3
1	A	4	CYS	CA-CB-SG	-9.26	97.34	114.00	3	9
1	A	27	CYS	N-CA-CB	9.15	127.08	110.60	7	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	9	CYS	CA-CB-SG	-9.03	97.75	114.00	22	7
1	A	38	GLU	OE1-CD-OE2	-8.99	112.52	123.30	3	10
1	A	34	THR	CA-CB-CG2	8.99	124.98	112.40	20	5
1	A	33	ALA	N-CA-CB	-8.97	97.54	110.10	28	6
1	A	35	LEU	CB-CA-C	8.92	127.15	110.20	2	5
1	A	15	HIS	N-CA-CB	8.88	126.58	110.60	7	6
1	A	18	LEU	N-CA-CB	8.85	128.09	110.40	22	7
1	A	6	GLU	OE1-CD-OE2	-8.83	112.71	123.30	3	3
1	A	26	LEU	CB-CG-CD1	-8.82	96.00	111.00	22	5
1	A	18	LEU	CB-CG-CD1	8.76	125.89	111.00	23	8
1	A	9	CYS	CB-CA-C	8.53	127.47	110.40	21	8
1	A	16	LEU	CB-CA-C	8.46	126.27	110.20	2	6
1	A	26	LEU	N-CA-CB	8.28	126.97	110.40	28	5
1	A	31	MET	CA-C-O	-8.25	102.78	120.10	4	2
1	A	22	ARG	CA-CB-CG	8.21	131.46	113.40	14	9
1	A	23	THR	CA-CB-CG2	8.20	123.87	112.40	4	4
1	A	19	GLN	N-CA-C	8.19	133.12	111.00	8	3
1	A	17	PRO	O-C-N	-8.18	109.61	122.70	2	4
1	A	6	GLU	CB-CA-C	8.14	126.68	110.40	6	9
1	A	28	PRO	O-C-N	-8.13	109.70	122.70	7	2
1	A	14	ARG	N-CA-CB	8.04	125.07	110.60	8	3
1	A	38	GLU	CA-CB-CG	8.00	130.99	113.40	28	5
1	A	17	PRO	N-CD-CG	7.98	115.17	103.20	6	2
1	A	30	CYS	CA-C-N	7.94	134.66	117.20	23	2
1	A	11	ASN	CB-CA-C	7.92	126.24	110.40	24	1
1	A	32	LYS	O-C-N	-7.91	110.04	122.70	11	3
1	A	37	PRO	N-CA-CB	7.90	112.78	103.30	7	7
1	A	26	LEU	O-C-N	-7.86	110.12	122.70	27	3
1	A	26	LEU	CB-CA-C	-7.77	95.43	110.20	3	6
1	A	17	PRO	CB-CA-C	7.76	131.41	112.00	10	1
1	A	18	LEU	CB-CG-CD2	7.71	124.11	111.00	15	5
1	A	26	LEU	CB-CG-CD2	-7.66	97.98	111.00	26	2
1	A	5	GLU	OE1-CD-OE2	-7.65	114.11	123.30	3	5
1	A	12	ARG	CG-CD-NE	7.62	127.80	111.80	27	1
1	A	12	ARG	CB-CA-C	7.60	125.61	110.40	2	5
1	A	22	ARG	N-CA-CB	7.58	124.24	110.60	19	1
1	A	14	ARG	NH1-CZ-NH2	7.57	127.72	119.40	21	4
1	A	35	LEU	CB-CG-CD1	7.56	123.86	111.00	18	2
1	A	29	ALA	CB-CA-C	7.51	121.37	110.10	8	6
1	A	21	SER	CB-CA-C	7.50	124.35	110.10	13	2
1	A	5	GLU	CB-CA-C	7.46	125.31	110.40	13	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	31	MET	N-CA-CB	-7.45	97.19	110.60	28	6
1	A	38	GLU	N-CA-CB	7.42	123.96	110.60	12	4
1	A	27	CYS	CB-CA-C	7.42	125.24	110.40	2	7
1	A	28	PRO	N-CA-CB	-7.39	94.43	103.30	16	6
1	A	22	ARG	O-C-N	7.36	134.47	122.70	13	1
1	A	29	ALA	CA-C-O	7.35	135.54	120.10	9	1
1	A	28	PRO	N-CA-C	7.34	131.19	112.10	13	4
1	A	18	LEU	CA-CB-CG	7.28	132.05	115.30	2	2
1	A	5	GLU	N-CA-CB	7.26	123.68	110.60	16	3
1	A	22	ARG	CB-CA-C	7.25	124.90	110.40	17	4
1	A	21	SER	N-CA-CB	-7.19	99.71	110.50	12	6
1	A	22	ARG	CA-C-N	-7.17	101.42	117.20	2	4
1	A	22	ARG	CB-CG-CD	7.15	130.20	111.60	28	3
1	A	17	PRO	CA-C-O	-7.10	103.15	120.20	11	2
1	A	8	THR	O-C-N	7.07	134.00	122.70	14	4
1	A	4	CYS	N-CA-CB	7.05	123.29	110.60	28	3
1	A	16	LEU	CB-CG-CD2	7.04	122.97	111.00	3	3
1	A	31	MET	CA-CB-CG	7.02	125.24	113.30	12	6
1	A	18	LEU	CB-CA-C	7.01	123.53	110.20	17	5
1	A	32	LYS	CA-CB-CG	6.95	128.69	113.40	12	1
1	A	30	CYS	CB-CA-C	6.94	124.28	110.40	7	3
1	A	35	LEU	O-C-N	-6.94	111.60	122.70	27	1
1	A	38	GLU	CB-CA-C	6.87	124.14	110.40	19	7
1	A	28	PRO	CA-N-CD	-6.80	101.97	111.50	8	2
1	A	20	PHE	CB-CA-C	6.76	123.92	110.40	19	5
1	A	36	GLN	N-CA-CB	6.73	122.72	110.60	6	2
1	A	15	HIS	CE1-NE2-CD2	-6.70	89.86	106.60	23	2
1	A	35	LEU	CA-C-N	6.69	131.92	117.20	9	3
1	A	14	ARG	CD-NE-CZ	6.62	132.86	123.60	28	1
1	A	10	ARG	N-CA-CB	-6.56	98.78	110.60	26	1
1	A	6	GLU	CG-CD-OE2	6.56	131.42	118.30	3	1
1	A	6	GLU	CG-CD-OE1	6.56	131.41	118.30	20	3
1	A	24	GLY	CA-C-O	-6.55	108.81	120.60	3	8
1	A	6	GLU	CA-CB-CG	6.50	127.71	113.40	21	6
1	A	15	HIS	O-C-N	-6.50	112.30	122.70	17	2
1	A	9	CYS	O-C-N	6.48	133.06	122.70	18	2
1	A	12	ARG	NH1-CZ-NH2	-6.47	112.29	119.40	22	2
1	A	37	PRO	CA-N-CD	-6.46	102.45	111.50	6	2
1	A	25	PRO	O-C-N	-6.43	112.42	122.70	2	1
1	A	14	ARG	CB-CA-C	6.41	123.23	110.40	13	2
1	A	12	ARG	CA-C-O	-6.40	106.65	120.10	8	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	32	LYS	CB-CA-C	6.35	123.09	110.40	7	3
1	A	20	PHE	N-CA-CB	6.34	122.02	110.60	18	2
1	A	34	THR	O-C-N	6.33	132.83	122.70	8	1
1	A	7	PRO	N-CA-CB	6.32	110.88	103.30	4	2
1	A	14	ARG	CA-CB-CG	6.31	127.27	113.40	7	1
1	A	9	CYS	N-CA-CB	-6.30	99.26	110.60	17	4
1	A	19	GLN	CB-CA-C	6.30	122.99	110.40	25	5
1	A	35	LEU	CB-CG-CD2	-6.28	100.32	111.00	11	5
1	A	11	ASN	CA-C-N	6.27	130.99	117.20	15	1
1	A	38	GLU	CA-C-O	-6.26	106.95	120.10	16	2
1	A	28	PRO	N-CD-CG	6.23	112.54	103.20	24	4
1	A	37	PRO	CA-CB-CG	6.23	116.63	104.80	13	1
1	A	27	CYS	CA-CB-SG	6.22	125.19	114.00	5	6
1	A	11	ASN	N-CA-CB	6.21	121.79	110.60	11	1
1	A	6	GLU	N-CA-CB	-6.21	99.43	110.60	28	2
1	A	4	CYS	CB-CA-C	-6.18	98.05	110.40	24	1
1	A	14	ARG	O-C-N	6.17	132.57	122.70	16	2
1	A	25	PRO	CA-N-CD	6.17	120.33	111.70	28	3
1	A	13	THR	N-CA-CB	6.16	122.01	110.30	2	1
1	A	17	PRO	CA-CB-CG	6.15	116.48	104.80	10	1
1	A	8	THR	CA-C-N	-6.15	103.67	117.20	19	3
1	A	29	ALA	O-C-N	6.10	132.46	122.70	19	2
1	A	38	GLU	CG-CD-OE1	6.08	130.47	118.30	23	2
1	A	12	ARG	CA-CB-CG	6.07	126.75	113.40	21	5
1	A	22	ARG	CA-C-O	6.05	132.81	120.10	11	1
1	A	20	PHE	CA-CB-CG	6.03	128.38	113.90	11	4
1	A	23	THR	CA-C-N	6.03	128.26	116.20	19	2
1	A	32	LYS	CB-CG-CD	6.01	127.23	111.60	28	1
1	A	6	GLU	CB-CG-CD	6.01	130.43	114.20	10	1
1	A	22	ARG	N-CA-C	5.99	127.17	111.00	7	2
1	A	24	GLY	CA-C-N	5.98	133.85	117.10	4	3
1	A	7	PRO	N-CD-CG	5.95	112.12	103.20	20	4
1	A	36	GLN	CA-C-O	-5.94	107.63	120.10	16	4
1	A	16	LEU	O-C-N	-5.94	109.82	121.10	2	2
1	A	8	THR	CA-CB-CG2	5.92	120.68	112.40	6	1
1	A	31	MET	CB-CA-C	5.91	122.22	110.40	2	2
1	A	27	CYS	CA-C-O	-5.91	107.69	120.10	23	4
1	A	17	PRO	CA-C-N	-5.91	104.21	117.20	28	2
1	A	4	CYS	O-C-N	5.91	132.15	122.70	28	1
1	A	22	ARG	CD-NE-CZ	5.90	131.86	123.60	7	3
1	A	23	THR	CA-CB-OG1	5.89	121.37	109.00	22	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	13	THR	O-C-N	5.88	132.11	122.70	5	2
1	A	35	LEU	CA-CB-CG	-5.88	101.78	115.30	14	1
1	A	16	LEU	CA-C-O	-5.86	107.79	120.10	9	4
1	A	10	ARG	CA-CB-CG	5.86	126.29	113.40	9	3
1	A	6	GLU	N-CA-C	5.86	126.81	111.00	26	2
1	A	19	GLN	CG-CD-OE1	-5.84	109.91	121.60	11	1
1	A	23	THR	O-C-N	-5.83	113.29	123.20	25	2
1	A	5	GLU	O-C-N	-5.82	113.38	122.70	12	3
1	A	27	CYS	CA-C-N	5.81	133.37	117.10	27	1
1	A	14	ARG	CB-CG-CD	5.78	126.63	111.60	10	1
1	A	6	GLU	CA-C-N	5.76	133.23	117.10	25	3
1	A	26	LEU	CA-C-O	-5.71	108.11	120.10	22	2
1	A	25	PRO	CA-CB-CG	5.71	115.65	104.80	20	2
1	A	14	ARG	CA-C-N	5.71	129.76	117.20	27	2
1	A	13	THR	CA-CB-OG1	-5.71	97.02	109.00	3	1
1	A	19	GLN	OE1-CD-NE2	-5.69	108.81	121.90	21	1
1	A	23	THR	N-CA-C	5.69	126.36	111.00	22	1
1	A	28	PRO	CA-C-O	5.68	133.83	120.20	7	1
1	A	30	CYS	O-C-N	5.67	131.77	122.70	3	2
1	A	7	PRO	O-C-N	-5.67	113.63	122.70	22	1
1	A	37	PRO	CA-C-N	5.67	129.67	117.20	24	2
1	A	32	LYS	N-CA-CB	5.65	120.76	110.60	13	2
1	A	36	GLN	CA-C-N	5.63	132.88	117.10	23	2
1	A	6	GLU	O-C-N	-5.62	110.43	121.10	15	1
1	A	34	THR	CA-CB-OG1	5.62	120.79	109.00	25	1
1	A	28	PRO	CB-CA-C	-5.61	97.97	112.00	4	1
1	A	28	PRO	CA-CB-CG	5.60	115.44	104.80	5	1
1	A	29	ALA	N-CA-C	5.59	126.10	111.00	19	1
1	A	11	ASN	CA-CB-CG	5.59	125.69	113.40	22	2
1	A	25	PRO	N-CD-CG	5.58	111.57	103.20	12	1
1	A	10	ARG	CG-CD-NE	5.56	123.47	111.80	10	1
1	A	29	ALA	N-CA-CB	-5.55	102.33	110.10	18	4
1	A	17	PRO	CA-N-CD	-5.54	103.74	111.50	6	1
1	A	6	GLU	CA-C-O	-5.53	108.49	120.10	16	2
1	A	21	SER	CA-C-O	5.53	131.71	120.10	14	1
1	A	23	THR	CA-C-O	-5.50	108.54	120.10	5	1
1	A	10	ARG	NH1-CZ-NH2	-5.49	113.36	119.40	28	2
1	A	17	PRO	N-CA-CB	5.49	109.89	103.30	27	1
1	A	25	PRO	N-CA-C	5.45	126.27	112.10	19	3
1	A	29	ALA	CA-C-N	-5.44	105.22	117.20	9	2
1	A	31	MET	O-C-N	-5.43	114.00	122.70	6	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	12	ARG	N-CA-CB	5.43	120.38	110.60	26	1
1	A	26	LEU	CA-C-N	5.42	129.12	117.20	23	1
1	A	5	GLU	CA-CB-CG	5.42	125.32	113.40	28	1
1	A	21	SER	O-C-N	-5.41	114.04	122.70	15	1
1	A	14	ARG	CA-C-O	-5.41	108.74	120.10	19	2
1	A	36	GLN	CB-CG-CD	5.40	125.64	111.60	7	1
1	A	7	PRO	CA-C-O	-5.40	107.23	120.20	9	2
1	A	26	LEU	N-CA-C	-5.40	96.42	111.00	9	1
1	A	25	PRO	CA-C-N	-5.38	105.36	117.20	10	1
1	A	36	GLN	O-C-N	-5.38	110.88	121.10	13	1
1	A	30	CYS	N-CA-C	5.37	125.51	111.00	22	1
1	A	33	ALA	O-C-N	5.37	131.29	122.70	2	2
1	A	17	PRO	N-CA-C	5.34	126.00	112.10	7	1
1	A	10	ARG	CB-CA-C	-5.32	99.75	110.40	15	2
1	A	22	ARG	CG-CD-NE	-5.32	100.63	111.80	9	1
1	A	14	ARG	CG-CD-NE	5.29	122.90	111.80	10	1
1	A	13	THR	CA-CB-CG2	5.29	119.80	112.40	5	1
1	A	5	GLU	CA-C-O	-5.27	109.03	120.10	18	1
1	A	28	PRO	CA-C-N	-5.26	105.62	117.20	24	1
1	A	12	ARG	CD-NE-CZ	5.25	130.95	123.60	5	1
1	A	23	THR	N-CA-CB	5.24	120.25	110.30	9	1
1	A	18	LEU	O-C-N	-5.23	114.33	122.70	24	1
1	A	5	GLU	CA-C-N	5.21	128.67	117.20	28	1
1	A	11	ASN	O-C-N	-5.20	114.37	122.70	26	1
1	A	8	THR	CA-C-O	5.18	130.98	120.10	3	1
1	A	8	THR	CA-CB-OG1	5.17	119.85	109.00	25	1
1	A	19	GLN	CB-CG-CD	5.13	124.95	111.60	5	1
1	A	36	GLN	CA-CB-CG	5.11	124.64	113.40	10	1
1	A	5	GLU	CG-CD-OE1	5.10	128.50	118.30	27	1
1	A	16	LEU	CA-C-N	5.08	131.31	117.10	2	2
1	A	10	ARG	C-N-CA	-5.08	109.01	121.70	22	1
1	A	37	PRO	N-CA-C	5.05	125.23	112.10	12	1
1	A	34	THR	N-CA-CB	-5.03	100.74	110.30	26	1
1	A	27	CYS	O-C-N	-5.01	111.58	121.10	7	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
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
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 (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	275	273	275	4±3
All	All	7975	8001	7975	129

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:16:LEU:CB	1:A:16:LEU:CG	1.58	1.76	18	1
1:A:17:PRO:CD	1:A:17:PRO:CG	1.56	1.74	25	2
1:A:33:ALA:N	1:A:33:ALA:CA	1.55	1.69	24	1
1:A:26:LEU:CB	1:A:26:LEU:CG	1.55	1.78	8	1
1:A:29:ALA:C	1:A:29:ALA:CA	1.54	1.74	12	3
1:A:27:CYS:CA	1:A:27:CYS:C	1.54	1.76	11	1
1:A:13:THR:CA	1:A:13:THR:C	1.53	1.75	6	2
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:14:ARG:C	1:A:14:ARG:CA	1.52	1.77	8	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:7:PRO:CA	1:A:7:PRO:C	1.51	1.77	26	2
1:A:16:LEU:C	1:A:16:LEU:CA	1.50	1.75	19	1
1:A:12:ARG:CA	1:A:12:ARG:C	1.48	1.80	10	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:15:HIS:CA	1:A:15:HIS:C	1.40	1.90	7	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:26:LEU:CB	1:A:26:LEU:C	0.81	2.48	4	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:36:GLN:N	1:A:36:GLN:CB	0.72	2.51	13	1
1:A:35:LEU:C	1:A:36:GLN:CA	0.68	2.61	13	2
1:A:27:CYS:SG	1:A:30:CYS:HB3	0.67	2.29	19	14
1:A:29:ALA:CA	1:A:30:CYS:N	0.66	2.58	10	3
1:A:29:ALA:C	1:A:30:CYS:CA	0.66	2.62	4	1
1:A:29:ALA:C	1:A:29:ALA:CB	0.66	2.63	10	1
1:A:13:THR:C	1:A:13:THR:N	0.64	2.50	2	1
1:A:33:ALA:N	1:A:33:ALA:CB	0.63	2.59	24	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: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:27:CYS:SG	1:A:30:CYS:HB2	0.56	2.41	16	3
1:A:7:PRO:C	1:A:7:PRO:CB	0.56	2.67	26	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:26:LEU:CB	1:A:26:LEU:CD1	0.55	2.76	8	1
1:A:22:ARG:HD3	1:A:22:ARG:H	0.55	1.61	24	2
1:A:24:GLY:C	1:A:25:PRO:CA	0.53	2.69	20	1
1:A:32:LYS:C	1:A:33:ALA:CA	0.53	2.68	24	1
1:A:31:MET:SD	1:A:31:MET:C	0.52	2.88	7	1
1:A:13:THR:C	1:A:13:THR:CB	0.51	2.67	2	2
1:A:33:ALA:O	1:A:37:PRO:HD2	0.51	2.05	27	4
1:A:16:LEU:CA	1:A:16:LEU:O	0.50	2.48	19	1
1:A:6:GLU:HB3	1:A:7:PRO:HD3	0.50	1.84	28	1
1:A:27:CYS:C	1:A:27:CYS:CB	0.50	2.75	11	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:13:THR:CA	1:A:14:ARG:N	0.48	2.67	6	1
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:14:ARG:C	1:A:14:ARG:N	0.47	2.63	8	1
1:A:12:ARG:O	1:A:15:HIS:HB2	0.47	2.10	26	4
1:A:7:PRO:CA	1:A:8:THR:N	0.45	2.67	25	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:15:HIS:C	1:A:15:HIS:CB	0.44	2.78	7	1
1:A:6:GLU:O	1:A:10:ARG:HB2	0.43	2.13	3	2
1:A:15:HIS:C	1:A:16:LEU:CA	0.43	2.74	5	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:29:ALA:C	1:A:29:ALA:N	0.42	2.62	10	1
1:A:15:HIS:C	1:A:15:HIS:N	0.42	2.64	7	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:33:ALA:N	1:A:33:ALA:C	0.41	2.65	24	1
1:A:27:CYS:SG	1:A:27:CYS:O	0.40	2.79	26	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	34/38 (89%)	25±1 (75±4%)	7±1 (20±4%)	2±1 (5±4%)	3 23
All	All	986/1102 (89%)	735 (75%)	197 (20%)	54 (5%)	3 23

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 (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	32/35 (91%)	26±2 (82±7%)	6±2 (18±7%)	4 37
All	All	928/1015 (91%)	759 (82%)	169 (18%)	4 37

All 28 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	29
1	A	12	ARG	19
1	A	19	GLN	13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	14	ARG	12
1	A	31	MET	11
1	A	16	LEU	11
1	A	21	SER	9
1	A	35	LEU	6
1	A	6	GLU	5
1	A	28	PRO	5
1	A	26	LEU	5
1	A	9	CYS	4
1	A	17	PRO	4
1	A	34	THR	4
1	A	20	PHE	4
1	A	8	THR	4
1	A	38	GLU	4
1	A	25	PRO	3
1	A	7	PRO	3
1	A	5	GLU	3
1	A	4	CYS	2
1	A	27	CYS	2
1	A	37	PRO	2
1	A	36	GLN	1
1	A	18	LEU	1
1	A	23	THR	1
1	A	10	ARG	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 monosaccharides 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