



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 07:42 AM UTC

PDB ID : 1BW3 / pdb_00001bw3
Title : THREE-DIMENSIONAL STRUCTURE IN SOLUTION OF BARWIN, A
PROTEIN FROM BARLEY SEED
Authors : Poulsen, F.M.
Deposited on : 1992-07-06

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

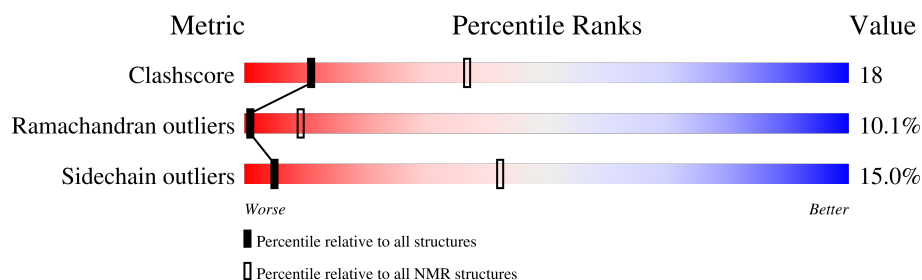
1 Overall quality at a glance

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	125	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:1-A:125 (125)	1.57	6

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1863 atoms, of which 895 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BARWIN, BASIC BARLEY SEED PROTEIN.

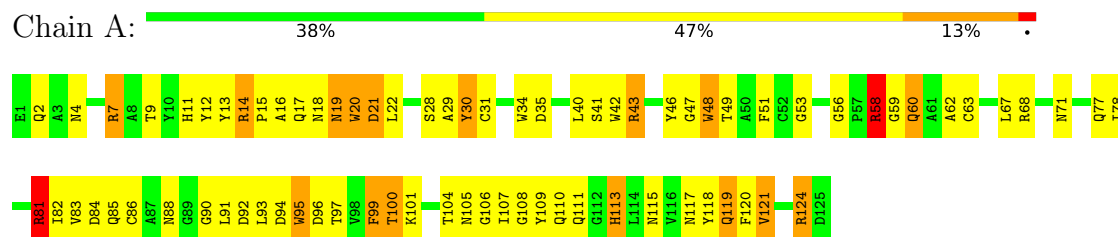
Mol	Chain	Residues	Atoms						Trace
1	A	125	Total	C	H	N	O	S	0
			1863	603	895	175	184	6	

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: BARWIN, BASIC BARLEY SEED PROTEIN

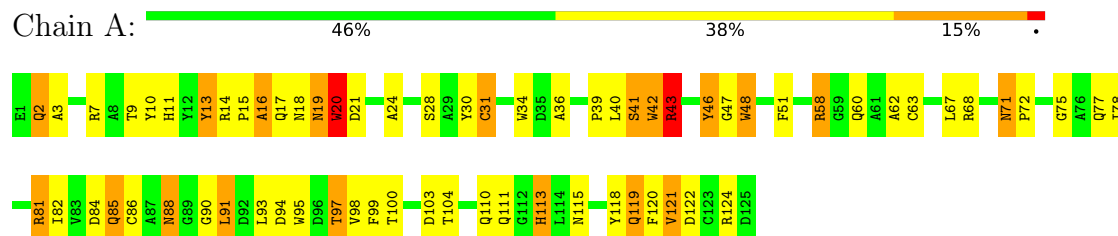


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

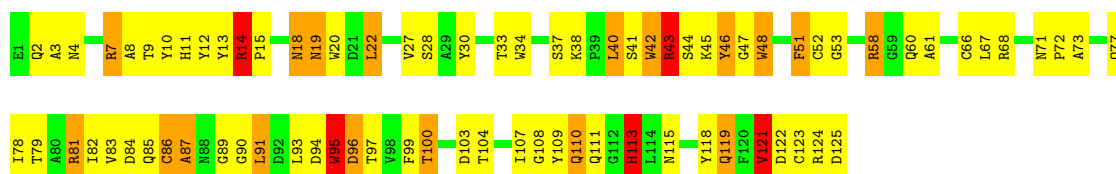
- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

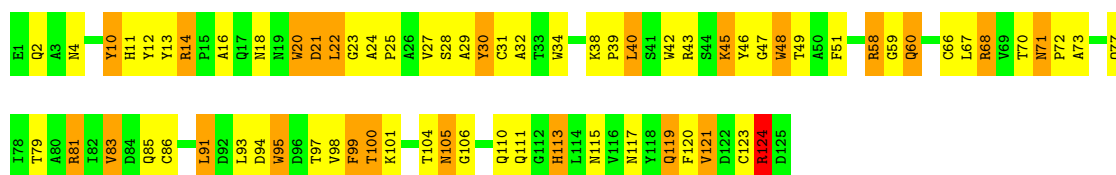




4.2.3 Score per residue for model 3

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

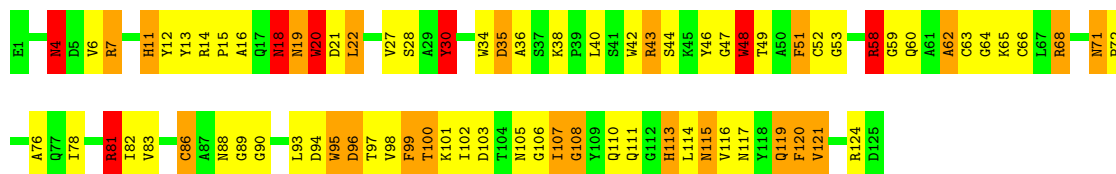
Chain A: 43% 38% 18%



4.2.4 Score per residue for model 4

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

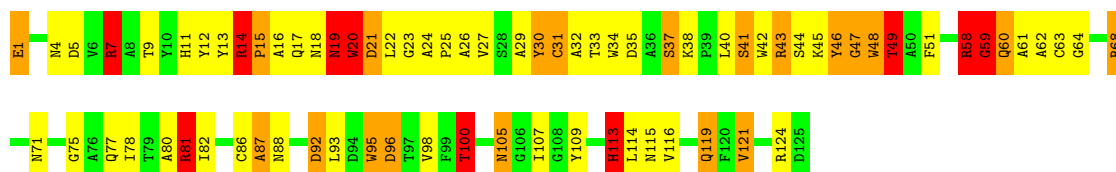
Chain A: 38% 39% 18% 6%



4.2.5 Score per residue for model 5

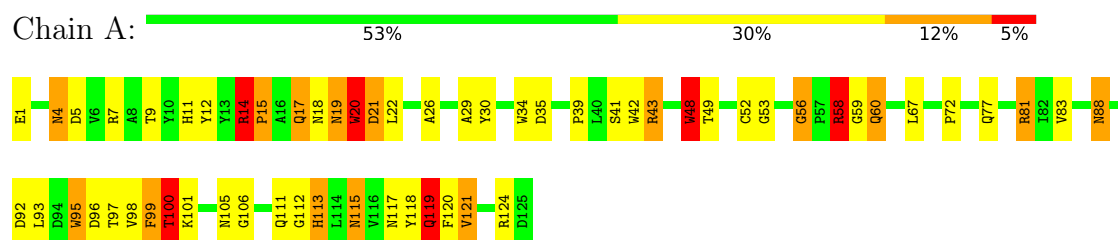
- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN

Chain A: 39% 37% 16% 8%



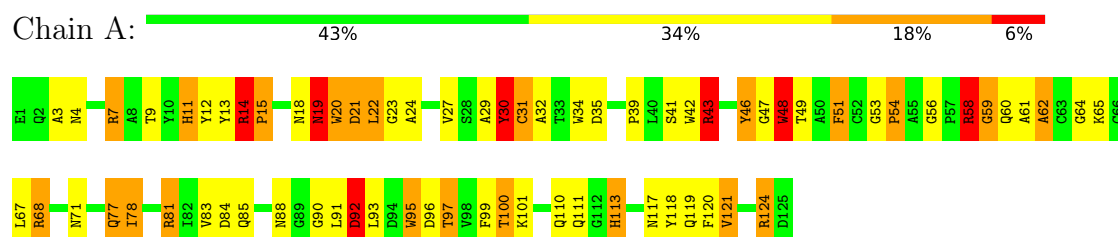
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



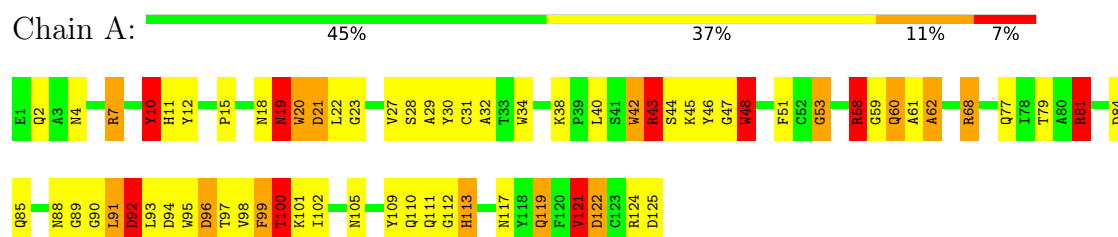
4.2.7 Score per residue for model 7

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



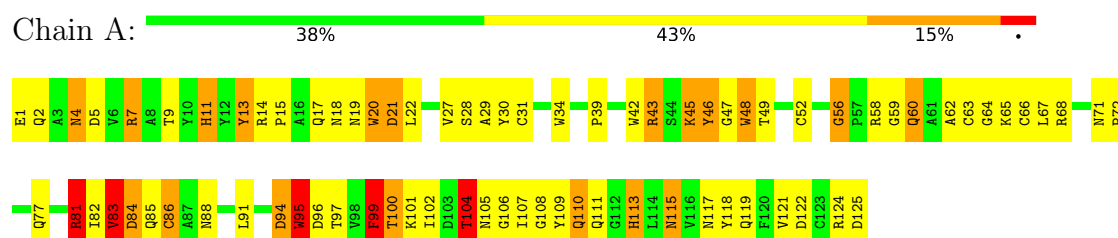
4.2.8 Score per residue for model 8

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



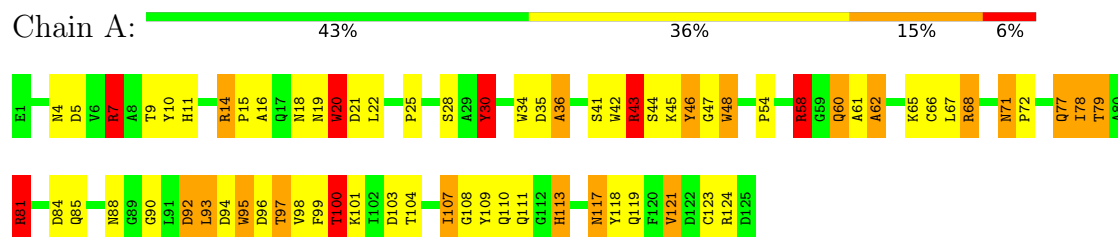
4.2.9 Score per residue for model 9

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



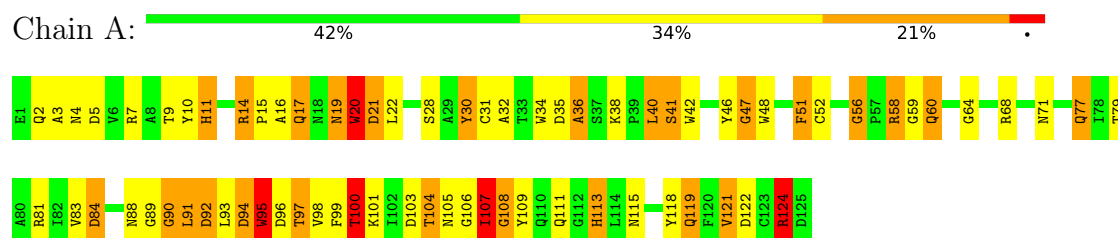
4.2.10 Score per residue for model 10

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



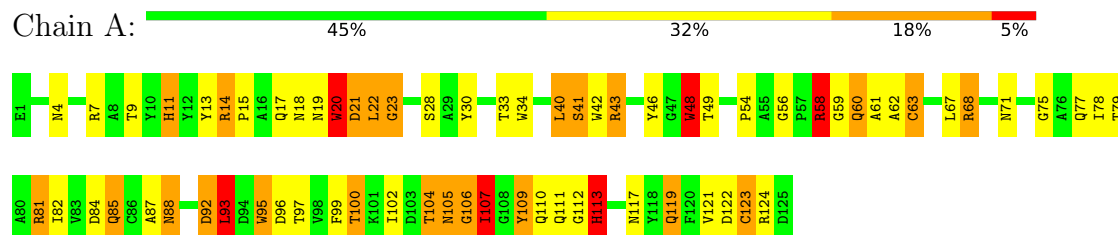
4.2.11 Score per residue for model 11

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



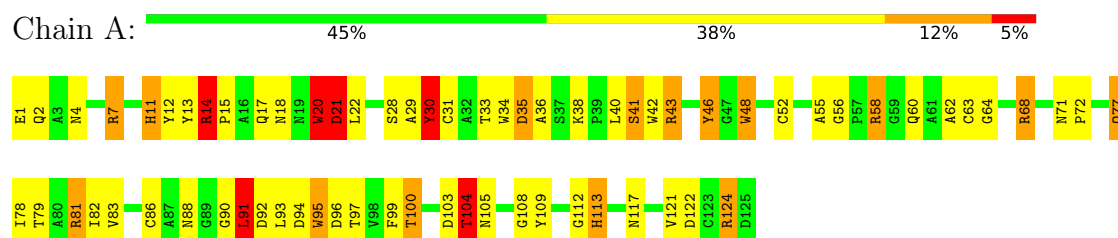
4.2.12 Score per residue for model 12

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



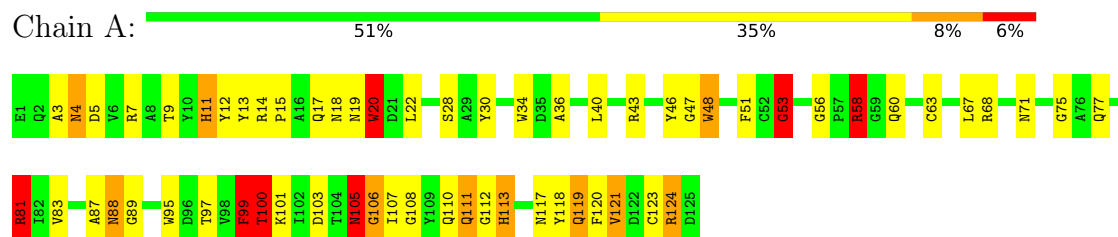
4.2.13 Score per residue for model 13

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



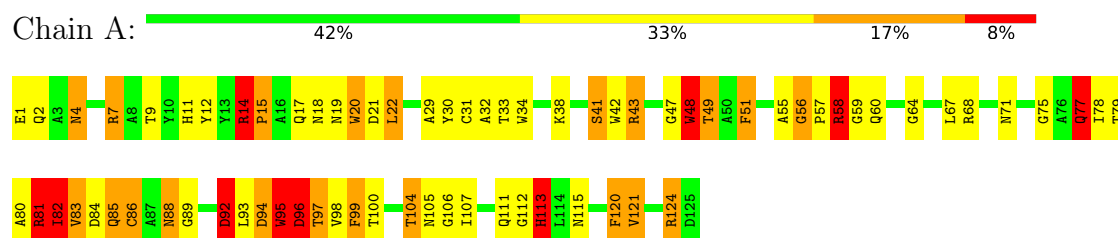
4.2.14 Score per residue for model 14

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



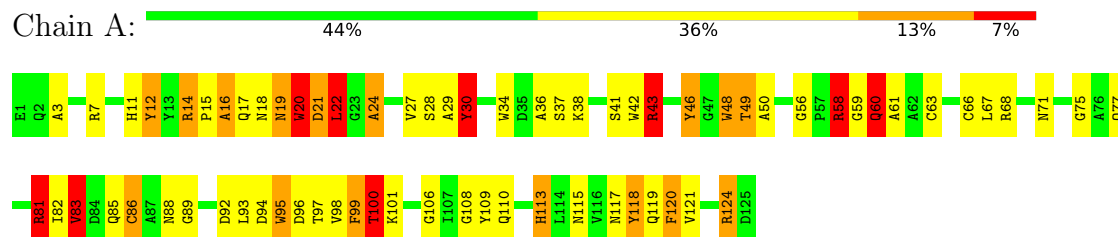
4.2.15 Score per residue for model 15

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



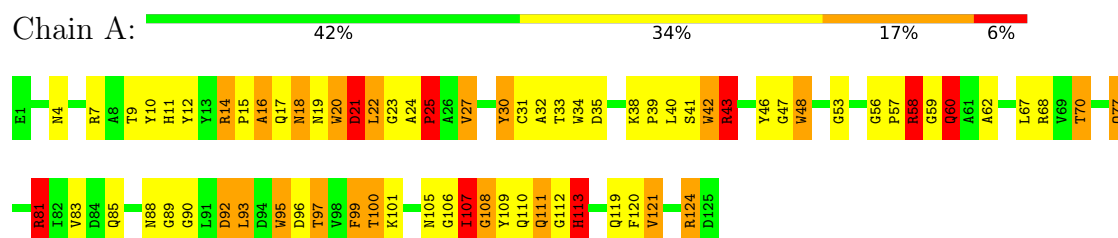
4.2.16 Score per residue for model 16

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



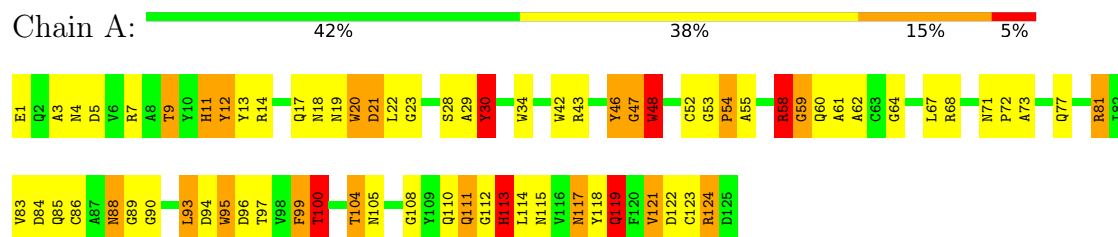
4.2.17 Score per residue for model 17

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



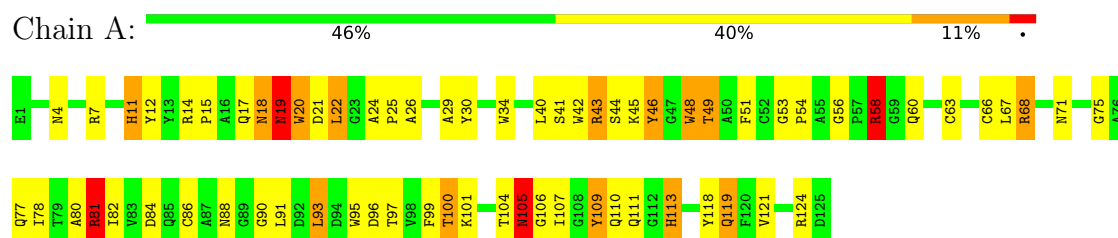
4.2.18 Score per residue for model 18

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



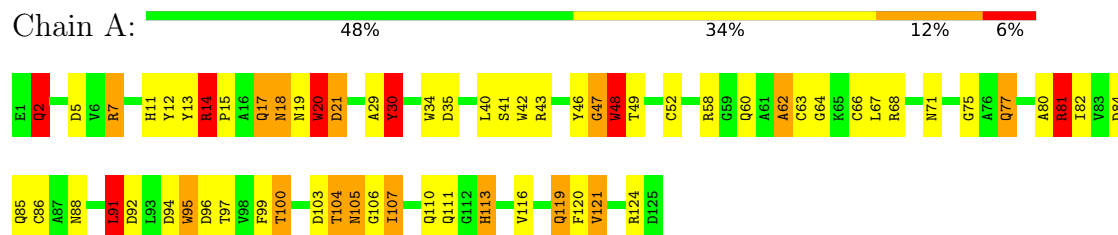
4.2.19 Score per residue for model 19

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



4.2.20 Score per residue for model 20

- Molecule 1: BARWIN, BASIC BARLEY SEED PROTEIN



5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 20 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
X-PLOR	refinement	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	2.12±0.03	16±3/995 (1.6± 0.3%)	1.98±0.04	36±5/1358 (2.7± 0.4%)
All	All	2.12	323/19900 (1.6%)	1.98	725/27160 (2.7%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	6.6±0.7
All	All	0	132

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	48	TRP	CA-CB	13.03	1.71	1.53	5	4
1	A	11	HIS	CG-ND1	-9.13	1.28	1.38	8	20
1	A	113	HIS	CG-ND1	-8.82	1.28	1.38	8	20
1	A	47	GLY	N-CA	8.61	1.51	1.44	20	6
1	A	89	GLY	N-CA	8.55	1.52	1.44	8	5
1	A	105	ASN	CA-C	8.33	1.56	1.52	6	1
1	A	48	TRP	NE1-CE2	-7.29	1.29	1.37	6	15
1	A	48	TRP	CG-CD2	-7.04	1.31	1.43	4	7
1	A	58	ARG	CA-CB	6.72	1.62	1.53	18	1
1	A	90	GLY	N-CA	6.58	1.51	1.45	4	6
1	A	20	TRP	N-CA	6.34	1.54	1.46	10	2
1	A	100	THR	N-CA	6.30	1.54	1.46	10	8
1	A	79	THR	N-CA	6.29	1.53	1.46	10	5
1	A	100	THR	CA-CB	6.25	1.62	1.53	4	2
1	A	56	GLY	N-CA	6.21	1.53	1.44	7	8
1	A	20	TRP	CG-CD2	-6.15	1.32	1.43	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	121	VAL	CA-C	6.09	1.58	1.52	2	4
1	A	93	LEU	CA-CB	6.08	1.60	1.52	4	2
1	A	11	HIS	CD2-NE2	-6.07	1.31	1.37	11	16
1	A	20	TRP	CA-CB	6.02	1.63	1.53	20	2
1	A	48	TRP	CA-C	-6.01	1.45	1.53	10	1
1	A	43	ARG	CZ-NH2	-5.90	1.25	1.33	17	11
1	A	113	HIS	CD2-NE2	-5.86	1.31	1.37	4	18
1	A	81	ARG	CA-CB	-5.86	1.44	1.53	14	2
1	A	81	ARG	NE-CZ	-5.83	1.26	1.33	16	5
1	A	91	LEU	CA-CB	5.82	1.61	1.53	2	1
1	A	96	ASP	N-CA	5.82	1.53	1.46	4	2
1	A	82	ILE	N-CA	5.80	1.53	1.46	20	7
1	A	112	GLY	N-CA	5.79	1.51	1.45	15	3
1	A	80	ALA	N-CA	5.77	1.52	1.45	20	1
1	A	81	ARG	CZ-NH1	-5.77	1.24	1.32	4	1
1	A	58	ARG	NE-CZ	-5.73	1.26	1.33	10	1
1	A	83	VAL	N-CA	5.72	1.52	1.46	3	5
1	A	23	GLY	N-CA	5.72	1.52	1.45	12	3
1	A	20	TRP	NE1-CE2	-5.68	1.31	1.37	3	6
1	A	29	ALA	N-CA	5.62	1.53	1.45	20	3
1	A	49	THR	N-CA	5.60	1.52	1.46	5	4
1	A	5	ASP	N-CA	5.59	1.53	1.46	10	1
1	A	58	ARG	CZ-NH2	-5.56	1.26	1.33	10	4
1	A	46	TYR	N-CA	5.51	1.52	1.45	9	3
1	A	103	ASP	CA-CB	5.50	1.59	1.52	2	1
1	A	93	LEU	N-CA	5.49	1.53	1.46	17	2
1	A	104	THR	N-CA	5.48	1.53	1.46	15	5
1	A	42	TRP	NE1-CE2	-5.46	1.31	1.37	17	2
1	A	91	LEU	N-CA	5.45	1.53	1.46	13	2
1	A	97	THR	N-CA	5.45	1.53	1.46	15	1
1	A	12	TYR	CA-CB	5.44	1.59	1.52	16	1
1	A	116	VAL	N-CA	5.43	1.52	1.46	20	1
1	A	27	VAL	N-CA	5.43	1.53	1.46	17	1
1	A	12	TYR	N-CA	5.43	1.53	1.46	2	2
1	A	99	PHE	N-CA	5.41	1.52	1.46	15	2
1	A	48	TRP	N-CA	5.41	1.53	1.46	1	1
1	A	14	ARG	N-CA	5.41	1.53	1.46	7	2
1	A	36	ALA	N-CA	5.40	1.53	1.46	11	1
1	A	120	PHE	N-CA	5.40	1.52	1.45	6	7
1	A	43	ARG	NE-CZ	-5.38	1.27	1.33	17	3
1	A	7	ARG	CZ-NH2	-5.38	1.26	1.33	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	71	ASN	N-CA	5.38	1.52	1.46	9	3
1	A	43	ARG	N-CA	5.37	1.53	1.46	19	1
1	A	124	ARG	CZ-NH2	-5.34	1.26	1.33	3	2
1	A	44	SER	N-CA	5.33	1.53	1.46	2	2
1	A	45	LYS	N-CA	5.33	1.52	1.46	2	1
1	A	34	TRP	CG-CD2	-5.32	1.34	1.43	6	6
1	A	18	ASN	N-CA	5.32	1.52	1.46	6	2
1	A	70	THR	N-CA	5.31	1.52	1.46	3	1
1	A	117	ASN	N-CA	5.30	1.52	1.46	8	1
1	A	86	CYS	N-CA	5.27	1.51	1.45	9	1
1	A	2	GLN	N-CA	5.26	1.52	1.45	8	1
1	A	113	HIS	N-CA	5.25	1.52	1.46	17	2
1	A	81	ARG	CZ-NH2	-5.24	1.26	1.33	6	5
1	A	10	TYR	N-CA	5.23	1.52	1.45	1	1
1	A	106	GLY	N-CA	5.23	1.52	1.45	9	2
1	A	25	PRO	CA-C	5.22	1.59	1.52	17	1
1	A	110	GLN	N-CA	5.21	1.52	1.46	2	2
1	A	95	TRP	N-CA	5.20	1.52	1.46	17	1
1	A	65	LYS	N-CA	5.18	1.52	1.45	4	1
1	A	59	GLY	N-CA	5.18	1.52	1.45	5	3
1	A	78	ILE	CA-C	5.17	1.58	1.52	10	1
1	A	19	ASN	N-CA	5.16	1.52	1.46	7	2
1	A	11	HIS	N-CA	5.15	1.52	1.46	1	1
1	A	81	ARG	N-CA	5.14	1.52	1.46	12	1
1	A	95	TRP	CG-CD2	-5.14	1.34	1.43	14	1
1	A	68	ARG	NE-CZ	-5.13	1.27	1.33	3	2
1	A	77	GLN	N-CA	5.13	1.52	1.45	13	1
1	A	95	TRP	NE1-CE2	-5.12	1.31	1.37	9	3
1	A	123	CYS	N-CA	5.11	1.52	1.46	12	1
1	A	53	GLY	N-CA	5.11	1.51	1.44	4	3
1	A	51	PHE	CA-C	5.10	1.58	1.52	4	1
1	A	14	ARG	CD-NE	5.09	1.53	1.46	7	1
1	A	46	TYR	CA-CB	5.09	1.60	1.54	19	1
1	A	24	ALA	CA-C	5.08	1.58	1.53	1	1
1	A	92	ASP	N-CA	5.08	1.52	1.46	17	1
1	A	107	ILE	N-CA	5.06	1.52	1.46	17	1
1	A	110	GLN	CA-CB	5.06	1.60	1.53	8	1
1	A	43	ARG	CD-NE	5.04	1.53	1.46	10	1
1	A	122	ASP	N-CA	5.03	1.51	1.45	18	1
1	A	7	ARG	NE-CZ	-5.03	1.27	1.33	7	1
1	A	9	THR	N-CA	5.02	1.52	1.46	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	71	ASN	CA-C	5.00	1.58	1.52	19	2
1	A	68	ARG	CZ-NH2	-5.00	1.26	1.33	8	1
1	A	111	GLN	N-CA	5.00	1.52	1.46	17	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	21	ASP	N-CA-C	-12.67	90.61	109.62	3	1
1	A	24	ALA	N-CA-C	11.78	135.85	109.81	17	2
1	A	10	TYR	N-CA-C	11.46	129.06	107.75	8	1
1	A	89	GLY	N-CA-C	11.26	139.87	113.18	2	1
1	A	81	ARG	NE-CZ-NH1	-11.03	110.47	121.50	4	4
1	A	95	TRP	N-CA-C	-10.99	94.22	109.71	20	1
1	A	81	ARG	NE-CZ-NH2	-10.72	109.55	119.20	9	3
1	A	51	PHE	CA-CB-CG	-10.61	103.19	113.80	15	3
1	A	81	ARG	N-CA-CB	-10.33	95.30	110.49	19	6
1	A	53	GLY	N-CA-C	10.29	133.34	112.34	8	2
1	A	68	ARG	NE-CZ-NH1	-9.61	111.89	121.50	5	3
1	A	11	HIS	CA-CB-CG	-9.12	104.68	113.80	18	8
1	A	107	ILE	N-CA-C	-9.06	102.50	110.74	14	1
1	A	109	TYR	N-CA-C	-9.04	100.37	111.40	19	2
1	A	106	GLY	N-CA-C	9.01	134.54	113.18	12	1
1	A	121	VAL	N-CA-CB	-8.96	102.02	112.32	2	12
1	A	100	THR	OG1-CB-CG2	-8.90	91.49	109.30	4	16
1	A	71	ASN	OD1-CG-ND2	-8.64	113.96	122.60	5	17
1	A	18	ASN	N-CA-C	-8.57	101.06	112.72	20	8
1	A	35	ASP	CA-CB-CG	-8.51	104.09	112.60	13	3
1	A	58	ARG	NE-CZ-NH2	-8.42	111.62	119.20	10	1
1	A	92	ASP	CA-CB-CG	8.40	121.00	112.60	15	2
1	A	48	TRP	N-CA-C	8.27	128.42	110.80	15	6
1	A	62	ALA	N-CA-C	-8.25	103.74	113.88	4	5
1	A	119	GLN	OE1-CD-NE2	-8.17	114.43	122.60	1	10
1	A	19	ASN	OD1-CG-ND2	-8.09	114.51	122.60	16	13
1	A	105	ASN	OD1-CG-ND2	-8.00	114.60	122.60	3	13
1	A	121	VAL	N-CA-C	7.90	118.17	108.53	2	6
1	A	27	VAL	O-C-N	7.83	127.80	121.85	8	5
1	A	20	TRP	CB-CG-CD1	-7.78	115.22	126.90	6	8
1	A	58	ARG	NH1-CZ-NH2	7.78	129.42	119.30	10	2
1	A	94	ASP	CA-CB-CG	-7.77	104.83	112.60	8	4
1	A	21	ASP	CA-CB-CG	-7.63	104.97	112.60	19	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	88	ASN	OD1-CG-ND2	-7.59	115.01	122.60	7	18
1	A	83	VAL	N-CA-C	7.59	118.34	111.81	2	2
1	A	30	TYR	N-CA-C	7.59	126.96	110.80	10	8
1	A	2	GLN	OE1-CD-NE2	-7.53	115.07	122.60	20	9
1	A	81	ARG	NH1-CZ-NH2	7.51	129.06	119.30	16	3
1	A	115	ASN	OD1-CG-ND2	-7.37	115.23	122.60	3	9
1	A	81	ARG	CB-CA-C	7.37	122.12	110.19	16	2
1	A	99	PHE	N-CA-C	7.33	119.27	111.28	17	5
1	A	117	ASN	CA-CB-CG	-7.30	105.30	112.60	18	4
1	A	46	TYR	N-CA-C	7.29	121.16	109.79	7	2
1	A	99	PHE	CA-CB-CG	-7.29	106.51	113.80	4	4
1	A	21	ASP	N-CA-CB	-7.28	98.19	110.49	17	4
1	A	18	ASN	OD1-CG-ND2	-7.27	115.33	122.60	7	12
1	A	84	ASP	N-CA-C	7.25	121.12	110.17	11	4
1	A	5	ASP	CA-CB-CG	-7.24	105.36	112.60	11	4
1	A	4	ASN	OD1-CG-ND2	-7.22	115.38	122.60	10	17
1	A	83	VAL	N-CA-CB	-7.17	105.76	111.64	15	1
1	A	9	THR	OG1-CB-CG2	-7.12	95.06	109.30	18	6
1	A	77	GLN	OE1-CD-NE2	-7.07	115.53	122.60	16	15
1	A	48	TRP	CB-CG-CD1	-7.06	116.31	126.90	6	4
1	A	17	GLN	OE1-CD-NE2	-7.06	115.54	122.60	19	10
1	A	122	ASP	CA-CB-CG	-7.03	105.57	112.60	8	1
1	A	49	THR	CA-CB-OG1	-7.03	99.06	109.60	16	1
1	A	44	SER	N-CA-C	-6.97	103.12	111.69	2	1
1	A	48	TRP	CG-CD1-NE1	-6.95	101.17	110.20	20	14
1	A	111	GLN	OE1-CD-NE2	-6.93	115.67	122.60	19	15
1	A	25	PRO	N-CA-C	-6.93	98.19	112.47	17	1
1	A	81	ARG	N-CA-C	6.93	120.78	108.24	19	4
1	A	29	ALA	N-CA-C	6.87	121.50	109.96	13	9
1	A	48	TRP	CG-CD2-CE3	6.83	140.73	133.90	6	4
1	A	110	GLN	OE1-CD-NE2	-6.71	115.89	122.60	3	12
1	A	75	GLY	N-CA-C	-6.69	105.84	115.27	1	8
1	A	85	GLN	OE1-CD-NE2	-6.68	115.92	122.60	12	11
1	A	92	ASP	N-CA-C	6.68	119.91	108.02	13	1
1	A	35	ASP	O-C-N	6.66	129.57	122.38	11	1
1	A	60	GLN	OE1-CD-NE2	-6.65	115.95	122.60	20	19
1	A	20	TRP	NE1-CE2-CZ2	6.65	140.07	130.10	19	9
1	A	27	VAL	CB-CA-C	-6.65	106.06	111.71	9	4
1	A	95	TRP	CA-CB-CG	-6.58	101.09	113.60	1	1
1	A	42	TRP	NE1-CE2-CZ2	6.58	139.97	130.10	13	7
1	A	92	ASP	N-CA-CB	-6.58	100.84	110.84	13	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	SER	N-CA-C	-6.57	102.76	111.24	5	1
1	A	7	ARG	NE-CZ-NH1	-6.56	114.94	121.50	5	4
1	A	36	ALA	N-CA-C	6.56	124.77	110.80	11	1
1	A	19	ASN	CA-CB-CG	-6.48	106.12	112.60	14	3
1	A	63	CYS	N-CA-CB	-6.48	101.45	110.65	12	1
1	A	95	TRP	CG-CD1-NE1	-6.47	101.79	110.20	18	18
1	A	20	TRP	CG-CD1-NE1	-6.45	101.82	110.20	17	6
1	A	34	TRP	N-CA-CB	-6.44	102.33	110.90	14	5
1	A	17	GLN	N-CA-C	-6.40	104.22	111.07	19	1
1	A	81	ARG	CD-NE-CZ	-6.39	115.46	124.40	19	1
1	A	115	ASN	CA-CB-CG	-6.38	106.22	112.60	6	2
1	A	104	THR	OG1-CB-CG2	-6.33	96.65	109.30	9	2
1	A	34	TRP	NE1-CE2-CZ2	6.32	139.58	130.10	8	18
1	A	20	TRP	CB-CG-CD2	6.28	135.59	126.80	6	3
1	A	14	ARG	NE-CZ-NH1	-6.28	115.22	121.50	10	4
1	A	117	ASN	OD1-CG-ND2	-6.24	116.36	122.60	12	5
1	A	48	TRP	CA-CB-CG	-6.19	101.84	113.60	5	1
1	A	84	ASP	N-CA-CB	-6.18	99.52	110.14	7	7
1	A	79	THR	OG1-CB-CG2	-6.16	96.97	109.30	10	3
1	A	63	CYS	N-CA-C	-6.12	106.48	112.97	12	2
1	A	113	HIS	CA-CB-CG	-6.12	107.68	113.80	6	1
1	A	97	THR	OG1-CB-CG2	-6.11	97.09	109.30	11	4
1	A	58	ARG	NE-CZ-NH1	-6.09	115.41	121.50	16	1
1	A	45	LYS	N-CA-C	6.09	117.71	111.14	3	1
1	A	48	TRP	NE1-CE2-CZ2	6.07	139.21	130.10	4	2
1	A	103	ASP	CA-CB-CG	-6.07	106.53	112.60	14	1
1	A	107	ILE	CA-C-O	6.07	128.37	120.78	12	1
1	A	58	ARG	N-CA-CB	-6.06	101.99	111.56	19	3
1	A	34	TRP	CG-CD1-NE1	-6.05	102.33	110.20	6	20
1	A	113	HIS	CE1-NE2-CD2	-6.05	102.95	109.00	18	13
1	A	102	ILE	CA-C-O	6.04	126.49	119.36	8	1
1	A	20	TRP	CA-CB-CG	6.03	125.05	113.60	1	3
1	A	51	PHE	N-CA-C	-5.98	97.40	107.99	5	2
1	A	104	THR	CA-CB-OG1	-5.97	100.64	109.60	11	1
1	A	82	ILE	N-CA-CB	-5.96	106.32	112.28	2	1
1	A	35	ASP	CA-C-O	-5.94	114.18	120.71	11	1
1	A	42	TRP	CG-CD1-NE1	-5.93	102.49	110.20	9	19
1	A	37	SER	CA-CB-OG	-5.93	99.24	111.10	16	1
1	A	84	ASP	CA-CB-CG	5.89	118.49	112.60	7	1
1	A	19	ASN	N-CA-CB	-5.86	103.11	111.84	12	1
1	A	105	ASN	CB-CG-ND2	5.85	125.17	116.40	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	96	ASP	N-CA-CB	-5.81	103.31	111.62	17	1
1	A	97	THR	CA-CB-OG1	-5.79	100.91	109.60	9	1
1	A	35	ASP	CB-CA-C	-5.79	101.63	112.00	11	1
1	A	41	SER	CA-CB-OG	-5.78	99.54	111.10	10	4
1	A	71	ASN	CB-CG-ND2	5.77	125.06	116.40	5	2
1	A	103	ASP	N-CA-C	5.75	117.83	109.71	10	1
1	A	95	TRP	NE1-CE2-CZ2	5.75	138.72	130.10	19	11
1	A	94	ASP	N-CA-CB	-5.75	100.78	110.49	9	2
1	A	34	TRP	CG-CD2-CE3	-5.72	128.18	133.90	2	1
1	A	68	ARG	N-CA-C	-5.72	99.86	108.96	13	2
1	A	118	TYR	N-CA-C	5.70	118.06	109.23	16	1
1	A	71	ASN	N-CA-C	5.70	121.57	108.93	9	1
1	A	79	THR	CA-CB-OG1	-5.69	101.07	109.60	3	2
1	A	9	THR	N-CA-C	-5.68	101.51	109.69	6	1
1	A	44	SER	CA-CB-OG	-5.68	99.75	111.10	8	1
1	A	78	ILE	N-CA-CB	-5.66	104.59	112.52	13	5
1	A	35	ASP	CA-C-N	5.66	132.35	121.54	11	1
1	A	35	ASP	C-N-CA	5.66	132.35	121.54	11	1
1	A	43	ARG	NE-CZ-NH1	-5.66	115.84	121.50	19	1
1	A	9	THR	CA-CB-OG1	-5.63	101.15	109.60	17	1
1	A	18	ASN	CA-CB-CG	5.62	118.22	112.60	2	1
1	A	49	THR	OG1-CB-CG2	-5.61	98.08	109.30	16	2
1	A	111	GLN	N-CA-C	-5.58	104.69	112.45	7	3
1	A	20	TRP	NE1-CE2-CD2	-5.55	100.18	107.40	8	2
1	A	19	ASN	N-CA-C	-5.55	104.25	111.74	2	1
1	A	50	ALA	N-CA-C	-5.51	99.53	108.52	16	1
1	A	86	CYS	N-CA-CB	-5.50	102.84	110.65	4	1
1	A	113	HIS	CB-CG-ND1	5.48	130.93	122.70	19	1
1	A	52	CYS	N-CA-C	-5.48	99.13	110.80	20	3
1	A	71	ASN	CA-CB-CG	-5.48	107.12	112.60	2	4
1	A	68	ARG	NH1-CZ-NH2	5.46	126.39	119.30	5	2
1	A	93	LEU	N-CA-C	-5.42	103.15	110.68	4	1
1	A	49	THR	N-CA-C	5.41	118.39	109.85	6	1
1	A	42	TRP	CA-C-O	-5.39	115.34	121.00	19	1
1	A	124	ARG	N-CA-CB	-5.37	103.94	111.62	16	1
1	A	20	TRP	CG-CD2-CE3	-5.37	128.53	133.90	15	2
1	A	60	GLN	N-CA-C	-5.37	105.83	112.38	7	1
1	A	124	ARG	N-CA-C	5.37	117.73	111.02	17	1
1	A	110	GLN	N-CA-CB	-5.35	104.36	110.35	17	1
1	A	59	GLY	N-CA-C	-5.31	104.58	113.02	7	1
1	A	119	GLN	CG-CD-NE2	5.29	124.33	116.40	1	4

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	CYS	N-CA-CB	-5.26	102.68	111.20	19	1
1	A	12	TYR	N-CA-C	5.26	117.24	108.99	20	2
1	A	7	ARG	NH1-CZ-NH2	5.24	126.11	119.30	4	2
1	A	107	ILE	N-CA-CB	-5.23	102.60	111.23	12	1
1	A	27	VAL	CA-C-O	5.22	127.30	120.78	7	1
1	A	5	ASP	N-CA-CB	-5.21	103.78	111.71	14	3
1	A	124	ARG	NE-CZ-NH1	-5.21	116.29	121.50	17	1
1	A	38	LYS	N-CA-C	5.21	115.98	109.57	11	1
1	A	7	ARG	N-CA-C	5.20	117.70	109.96	9	2
1	A	124	ARG	NH1-CZ-NH2	5.20	126.06	119.30	11	1
1	A	33	THR	OG1-CB-CG2	-5.16	98.97	109.30	17	1
1	A	14	ARG	NE-CZ-NH2	-5.16	114.56	119.20	13	1
1	A	27	VAL	N-CA-C	5.12	120.00	109.34	17	1
1	A	18	ASN	CB-CG-ND2	5.11	124.07	116.40	2	1
1	A	11	HIS	CE1-NE2-CD2	-5.11	103.89	109.00	15	4
1	A	86	CYS	N-CA-C	5.08	118.36	112.97	4	1
1	A	20	TRP	N-CA-C	-5.08	99.97	110.80	14	1
1	A	33	THR	CA-CB-OG1	-5.08	101.98	109.60	2	1
1	A	48	TRP	N-CA-CB	-5.08	103.46	111.23	7	1
1	A	102	ILE	CA-CB-CG2	-5.07	101.88	110.50	9	1
1	A	88	ASN	CA-CB-CG	5.07	117.67	112.60	6	1
1	A	49	THR	N-CA-CB	5.07	119.42	111.56	5	1
1	A	35	ASP	N-CA-C	5.07	119.42	112.68	7	1
1	A	120	PHE	CA-CB-CG	-5.07	108.73	113.80	3	1
1	A	88	ASN	CB-CG-ND2	5.06	123.99	116.40	7	1
1	A	96	ASP	N-CA-C	-5.06	107.39	113.21	16	1
1	A	4	ASN	CA-CB-CG	-5.05	107.55	112.60	10	1
1	A	122	ASP	N-CA-CB	-5.04	102.39	110.46	8	1
1	A	113	HIS	CB-CG-CD2	-5.04	124.65	131.20	19	1
1	A	42	TRP	CG-CD2-CE3	-5.02	128.88	133.90	13	1
1	A	95	TRP	CD1-NE1-CE2	5.02	117.93	108.90	18	1
1	A	113	HIS	N-CA-C	5.01	117.42	109.50	5	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	124	ARG	Sidechain	20
1	A	7	ARG	Sidechain	19
1	A	58	ARG	Sidechain	19

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	81	ARG	Sidechain	19
1	A	14	ARG	Sidechain	18
1	A	43	ARG	Sidechain	18
1	A	68	ARG	Sidechain	18
1	A	53	GLY	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	968	895	895	34±9
All	All	19360	17900	17900	683

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:CYS:SG	1:A:81:ARG:NH1	0.84	2.50	3	1
1:A:47:GLY:C	1:A:48:TRP:CD1	0.82	2.57	5	3
1:A:48:TRP:CD1	1:A:48:TRP:N	0.77	2.49	5	6
1:A:22:LEU:CD2	1:A:48:TRP:CH2	0.77	2.68	10	4
1:A:48:TRP:H	1:A:81:ARG:CB	0.77	1.92	19	3
1:A:20:TRP:CZ3	1:A:48:TRP:NE1	0.74	2.55	7	5
1:A:48:TRP:O	1:A:48:TRP:CD1	0.70	2.44	19	5
1:A:66:CYS:SG	1:A:81:ARG:NH2	0.69	2.66	10	2
1:A:20:TRP:CE3	1:A:48:TRP:CE2	0.69	2.81	6	6
1:A:22:LEU:HD11	1:A:48:TRP:CZ3	0.67	2.25	11	5
1:A:81:ARG:CD	1:A:81:ARG:N	0.67	2.58	15	2
1:A:20:TRP:CE3	1:A:48:TRP:CZ2	0.66	2.82	12	10
1:A:48:TRP:H	1:A:81:ARG:CG	0.66	2.03	5	1
1:A:20:TRP:HB3	1:A:48:TRP:CZ2	0.66	2.26	6	6
1:A:48:TRP:CE3	1:A:93:LEU:HD21	0.66	2.26	12	2
1:A:20:TRP:HB3	1:A:48:TRP:CH2	0.66	2.25	5	5
1:A:22:LEU:CD2	1:A:48:TRP:CZ2	0.64	2.81	15	2
1:A:20:TRP:CZ3	1:A:48:TRP:CZ2	0.63	2.86	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:ASP:O	1:A:23:GLY:N	0.63	2.31	17	3
1:A:11:HIS:NE2	1:A:13:TYR:CE1	0.63	2.66	7	1
1:A:20:TRP:CH2	1:A:48:TRP:CE2	0.63	2.85	15	1
1:A:96:ASP:O	1:A:101:LYS:NZ	0.63	2.32	6	3
1:A:49:THR:HG21	1:A:80:ALA:HB1	0.63	1.71	19	1
1:A:31:CYS:SG	1:A:83:VAL:HG22	0.62	2.33	15	2
1:A:81:ARG:NH1	1:A:123:CYS:SG	0.61	2.73	3	3
1:A:22:LEU:HD21	1:A:48:TRP:CH2	0.61	2.31	8	7
1:A:11:HIS:CD2	1:A:13:TYR:CD1	0.61	2.89	7	1
1:A:47:GLY:N	1:A:81:ARG:NE	0.61	2.49	15	1
1:A:20:TRP:O	1:A:22:LEU:N	0.60	2.34	17	7
1:A:13:TYR:CD1	1:A:13:TYR:O	0.60	2.55	7	1
1:A:22:LEU:HD21	1:A:48:TRP:CE3	0.60	2.32	18	1
1:A:107:ILE:CD1	1:A:107:ILE:H	0.60	2.09	12	3
1:A:1:GLU:N	1:A:55:ALA:O	0.59	2.34	15	3
1:A:48:TRP:N	1:A:81:ARG:CB	0.59	2.66	9	3
1:A:22:LEU:HD21	1:A:48:TRP:CZ3	0.59	2.33	18	2
1:A:20:TRP:CD2	1:A:48:TRP:CZ2	0.59	2.91	16	6
1:A:95:TRP:O	1:A:96:ASP:C	0.58	2.46	5	4
1:A:48:TRP:H	1:A:81:ARG:HB2	0.58	1.58	19	1
1:A:48:TRP:H	1:A:81:ARG:C	0.58	2.07	16	2
1:A:86:CYS:SG	1:A:89:GLY:N	0.57	2.77	16	1
1:A:47:GLY:CA	1:A:81:ARG:HG3	0.57	2.29	5	1
1:A:68:ARG:NH2	1:A:79:THR:OG1	0.56	2.38	10	1
1:A:48:TRP:HB3	1:A:81:ARG:CZ	0.56	2.30	14	1
1:A:14:ARG:N	1:A:15:PRO:CD	0.56	2.68	15	1
1:A:46:TYR:CG	1:A:66:CYS:SG	0.56	2.99	9	2
1:A:48:TRP:N	1:A:81:ARG:CG	0.56	2.69	5	1
1:A:105:ASN:H	1:A:105:ASN:ND2	0.56	1.98	14	1
1:A:35:ASP:CG	1:A:43:ARG:NH2	0.56	2.63	17	1
1:A:20:TRP:CZ3	1:A:94:ASP:HB2	0.56	2.35	13	2
1:A:20:TRP:CH2	1:A:43:ARG:O	0.56	2.59	3	1
1:A:20:TRP:CH2	1:A:48:TRP:CZ2	0.56	2.94	15	1
1:A:13:TYR:CD1	1:A:13:TYR:N	0.56	2.74	12	2
1:A:66:CYS:SG	1:A:81:ARG:HA	0.56	2.40	20	1
1:A:35:ASP:O	1:A:43:ARG:NH1	0.56	2.38	4	2
1:A:20:TRP:CZ3	1:A:48:TRP:CD1	0.55	2.95	8	1
1:A:58:ARG:HG2	1:A:59:GLY:N	0.55	2.16	15	1
1:A:47:GLY:N	1:A:81:ARG:HB3	0.55	2.16	9	1
1:A:48:TRP:CZ2	1:A:93:LEU:HG	0.55	2.36	10	1
1:A:107:ILE:HD12	1:A:107:ILE:H	0.55	1.62	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:TRP:CE3	1:A:93:LEU:HD11	0.55	2.36	12	1
1:A:11:HIS:CD2	1:A:12:TYR:H	0.55	2.20	18	2
1:A:47:GLY:N	1:A:81:ARG:HG3	0.54	2.17	5	1
1:A:22:LEU:HD22	1:A:48:TRP:CH2	0.54	2.36	10	1
1:A:48:TRP:O	1:A:49:THR:HG23	0.54	2.02	19	1
1:A:95:TRP:O	1:A:95:TRP:CG	0.54	2.60	17	5
1:A:19:ASN:O	1:A:19:ASN:ND2	0.54	2.41	16	1
1:A:94:ASP:CG	1:A:95:TRP:N	0.54	2.65	11	1
1:A:48:TRP:H	1:A:81:ARG:NE	0.54	2.00	5	1
1:A:49:THR:CG2	1:A:81:ARG:C	0.54	2.81	15	1
1:A:18:ASN:C	1:A:20:TRP:N	0.54	2.64	19	2
1:A:13:TYR:O	1:A:14:ARG:CB	0.54	2.56	7	1
1:A:20:TRP:CG	1:A:48:TRP:CZ2	0.54	2.96	4	7
1:A:11:HIS:CG	1:A:12:TYR:H	0.54	2.20	18	4
1:A:49:THR:CG2	1:A:80:ALA:HB1	0.54	2.32	5	2
1:A:48:TRP:O	1:A:93:LEU:CD2	0.54	2.56	10	1
1:A:48:TRP:CE2	1:A:93:LEU:HG	0.53	2.38	10	1
1:A:47:GLY:CA	1:A:81:ARG:HE	0.53	2.17	15	1
1:A:48:TRP:O	1:A:93:LEU:HD23	0.53	2.02	10	2
1:A:48:TRP:HB3	1:A:81:ARG:NH2	0.53	2.18	14	3
1:A:66:CYS:SG	1:A:81:ARG:HG2	0.53	2.43	4	1
1:A:15:PRO:O	1:A:17:GLN:N	0.53	2.42	5	3
1:A:13:TYR:O	1:A:13:TYR:CG	0.53	2.62	7	1
1:A:18:ASN:N	1:A:21:ASP:HB2	0.53	2.18	17	1
1:A:48:TRP:H	1:A:81:ARG:CD	0.53	2.17	5	1
1:A:22:LEU:HD11	1:A:48:TRP:CH2	0.53	2.38	12	3
1:A:11:HIS:CG	1:A:12:TYR:N	0.53	2.77	13	4
1:A:81:ARG:NE	1:A:81:ARG:H	0.53	2.01	15	1
1:A:22:LEU:CD2	1:A:48:TRP:CZ3	0.52	2.92	18	2
1:A:13:TYR:N	1:A:13:TYR:CD1	0.52	2.77	20	1
1:A:80:ALA:HA	1:A:81:ARG:CZ	0.52	2.34	15	1
1:A:99:PHE:O	1:A:101:LYS:N	0.52	2.43	8	3
1:A:107:ILE:H	1:A:107:ILE:HD12	0.52	1.64	12	3
1:A:48:TRP:N	1:A:81:ARG:HB2	0.52	2.19	19	2
1:A:117:ASN:ND2	1:A:117:ASN:N	0.52	2.57	4	2
1:A:48:TRP:CE3	1:A:93:LEU:CB	0.52	2.92	6	2
1:A:38:LYS:O	1:A:43:ARG:CZ	0.52	2.58	16	3
1:A:51:PHE:CG	1:A:51:PHE:O	0.52	2.62	11	1
1:A:51:PHE:CE2	1:A:56:GLY:HA3	0.52	2.40	15	1
1:A:48:TRP:NE1	1:A:93:LEU:HD22	0.52	2.19	17	1
1:A:35:ASP:C	1:A:43:ARG:NH1	0.51	2.68	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:TYR:O	1:A:14:ARG:HB2	0.51	2.04	7	2
1:A:105:ASN:ND2	1:A:106:GLY:H	0.51	2.03	14	1
1:A:49:THR:N	1:A:81:ARG:O	0.51	2.44	4	3
1:A:68:ARG:NH1	1:A:77:GLN:OE1	0.51	2.43	10	2
1:A:3:ALA:HB3	1:A:118:TYR:CZ	0.51	2.41	11	6
1:A:86:CYS:SG	1:A:89:GLY:CA	0.51	2.99	16	1
1:A:107:ILE:H	1:A:107:ILE:CD1	0.51	2.19	4	1
1:A:81:ARG:N	1:A:81:ARG:HD3	0.51	2.21	8	2
1:A:40:LEU:O	1:A:41:SER:C	0.51	2.53	12	8
1:A:103:ASP:O	1:A:104:THR:C	0.51	2.53	11	2
1:A:51:PHE:O	1:A:51:PHE:CD1	0.50	2.64	1	1
1:A:7:ARG:O	1:A:7:ARG:CG	0.50	2.59	5	1
1:A:19:ASN:OD1	1:A:43:ARG:NH1	0.50	2.44	1	2
1:A:100:THR:OG1	1:A:101:LYS:NZ	0.50	2.44	10	1
1:A:18:ASN:H	1:A:21:ASP:HB2	0.50	1.65	17	1
1:A:51:PHE:CE2	1:A:53:GLY:HA2	0.50	2.42	8	1
1:A:56:GLY:CA	1:A:120:PHE:CZ	0.50	2.94	15	2
1:A:31:CYS:SG	1:A:63:CYS:O	0.50	2.69	1	1
1:A:45:LYS:HE3	1:A:125:ASP:CG	0.50	2.31	9	1
1:A:36:ALA:O	1:A:43:ARG:NH2	0.50	2.45	1	2
1:A:10:TYR:CD1	1:A:10:TYR:O	0.50	2.64	3	1
1:A:107:ILE:O	1:A:109:TYR:N	0.50	2.45	11	1
1:A:46:TYR:O	1:A:47:GLY:C	0.50	2.54	2	2
1:A:76:ALA:HB2	1:A:103:ASP:HB2	0.50	1.83	4	1
1:A:72:PRO:HG2	1:A:117:ASN:ND2	0.50	2.22	6	3
1:A:76:ALA:CB	1:A:103:ASP:HB2	0.50	2.36	4	1
1:A:20:TRP:CD1	1:A:43:ARG:HD2	0.50	2.42	13	1
1:A:95:TRP:CE3	1:A:96:ASP:HB3	0.50	2.42	18	2
1:A:31:CYS:O	1:A:32:ALA:C	0.49	2.55	17	5
1:A:46:TYR:HB3	1:A:66:CYS:SG	0.49	2.47	9	2
1:A:22:LEU:HD23	1:A:48:TRP:CZ2	0.49	2.42	15	1
1:A:46:TYR:CA	1:A:81:ARG:HG2	0.49	2.37	19	1
1:A:59:GLY:O	1:A:60:GLN:C	0.49	2.55	3	5
1:A:15:PRO:HG3	1:A:48:TRP:CE3	0.49	2.42	8	1
1:A:72:PRO:HD3	1:A:117:ASN:ND2	0.49	2.22	13	1
1:A:15:PRO:HA	1:A:21:ASP:N	0.49	2.23	15	1
1:A:46:TYR:O	1:A:81:ARG:NH2	0.49	2.46	1	1
1:A:86:CYS:SG	1:A:86:CYS:O	0.49	2.69	2	1
1:A:88:ASN:OD1	1:A:89:GLY:N	0.49	2.46	15	1
1:A:112:GLY:O	1:A:113:HIS:C	0.49	2.55	17	1
1:A:84:ASP:CG	1:A:85:GLN:H	0.49	2.14	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLY:O	1:A:81:ARG:N	0.49	2.45	2	3
1:A:94:ASP:O	1:A:96:ASP:N	0.49	2.46	15	1
1:A:35:ASP:CB	1:A:43:ARG:HH21	0.49	2.21	17	1
1:A:10:TYR:C	1:A:10:TYR:CD1	0.49	2.90	2	1
1:A:20:TRP:C	1:A:22:LEU:N	0.49	2.67	3	2
1:A:48:TRP:O	1:A:92:ASP:HA	0.49	2.08	7	4
1:A:20:TRP:CZ3	1:A:43:ARG:O	0.49	2.65	8	1
1:A:48:TRP:O	1:A:93:LEU:HD22	0.49	2.07	13	2
1:A:48:TRP:CG	1:A:48:TRP:O	0.49	2.65	4	2
1:A:48:TRP:CE3	1:A:93:LEU:HB3	0.49	2.43	6	1
1:A:20:TRP:CD1	1:A:20:TRP:N	0.49	2.81	8	1
1:A:107:ILE:C	1:A:109:TYR:H	0.49	2.16	10	2
1:A:53:GLY:O	1:A:58:ARG:NH2	0.49	2.45	19	1
1:A:94:ASP:O	1:A:95:TRP:C	0.49	2.56	2	2
1:A:48:TRP:O	1:A:48:TRP:CG	0.48	2.66	13	2
1:A:48:TRP:NE1	1:A:93:LEU:CD2	0.48	2.76	13	2
1:A:96:ASP:O	1:A:101:LYS:HE2	0.48	2.08	9	1
1:A:96:ASP:O	1:A:101:LYS:CE	0.48	2.61	8	2
1:A:5:ASP:CG	1:A:115:ASN:HD21	0.48	2.17	18	1
1:A:94:ASP:O	1:A:95:TRP:CB	0.48	2.61	4	1
1:A:48:TRP:O	1:A:49:THR:CG2	0.48	2.61	19	1
1:A:97:THR:OG1	1:A:98:VAL:N	0.48	2.47	1	7
1:A:59:GLY:O	1:A:61:ALA:N	0.48	2.47	5	1
1:A:30:TYR:CZ	1:A:61:ALA:HB2	0.48	2.43	7	1
1:A:5:ASP:C	1:A:115:ASN:ND2	0.48	2.72	9	1
1:A:3:ALA:HB3	1:A:118:TYR:CE1	0.48	2.44	14	4
1:A:18:ASN:O	1:A:19:ASN:C	0.48	2.56	4	2
1:A:11:HIS:CE1	1:A:88:ASN:OD1	0.48	2.67	12	1
1:A:105:ASN:HD22	1:A:106:GLY:N	0.48	2.06	19	1
1:A:86:CYS:O	1:A:87:ALA:C	0.48	2.57	2	2
1:A:62:ALA:C	1:A:64:GLY:H	0.48	2.17	18	3
1:A:13:TYR:C	1:A:14:ARG:HD3	0.48	2.34	2	1
1:A:42:TRP:HE1	1:A:125:ASP:CG	0.48	2.16	2	2
1:A:20:TRP:CZ3	1:A:48:TRP:CE2	0.48	3.01	15	2
1:A:58:ARG:HH11	1:A:82:ILE:CD1	0.48	2.21	13	1
1:A:25:PRO:HD2	1:A:27:VAL:HG23	0.48	1.86	17	1
1:A:85:GLN:HG2	1:A:86:CYS:N	0.48	2.24	20	1
1:A:81:ARG:HH11	1:A:81:ARG:HB2	0.48	1.67	8	1
1:A:58:ARG:NH1	1:A:120:PHE:CG	0.47	2.82	1	1
1:A:58:ARG:NH1	1:A:59:GLY:O	0.47	2.46	12	1
1:A:76:ALA:HB2	1:A:103:ASP:CB	0.47	2.38	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLY:H	1:A:81:ARG:HA	0.47	1.69	9	1
1:A:85:GLN:HG2	1:A:86:CYS:SG	0.47	2.49	15	1
1:A:38:LYS:O	1:A:43:ARG:NH1	0.47	2.48	2	1
1:A:47:GLY:O	1:A:48:TRP:CB	0.47	2.62	4	2
1:A:94:ASP:OD1	1:A:94:ASP:N	0.47	2.47	20	1
1:A:96:ASP:O	1:A:101:LYS:HE3	0.47	2.09	4	1
1:A:97:THR:O	1:A:101:LYS:NZ	0.47	2.44	14	1
1:A:118:TYR:CD1	1:A:118:TYR:C	0.47	2.92	9	3
1:A:114:LEU:HG	1:A:115:ASN:N	0.47	2.24	5	1
1:A:20:TRP:CE3	1:A:48:TRP:CD2	0.47	3.02	6	1
1:A:59:GLY:C	1:A:61:ALA:N	0.47	2.71	7	1
1:A:48:TRP:H	1:A:81:ARG:CA	0.47	2.21	16	1
1:A:18:ASN:H	1:A:21:ASP:CB	0.47	2.21	17	1
1:A:40:LEU:H	1:A:40:LEU:CD2	0.47	2.23	17	1
1:A:95:TRP:O	1:A:95:TRP:CD1	0.47	2.68	17	1
1:A:107:ILE:C	1:A:109:TYR:N	0.47	2.73	12	2
1:A:51:PHE:CD2	1:A:84:ASP:O	0.47	2.67	1	2
1:A:22:LEU:HD21	1:A:48:TRP:CZ2	0.47	2.44	8	2
1:A:65:LYS:NZ	1:A:122:ASP:OD1	0.47	2.47	9	1
1:A:92:ASP:N	1:A:92:ASP:OD1	0.47	2.48	20	1
1:A:93:LEU:CD2	1:A:93:LEU:N	0.47	2.77	10	1
1:A:35:ASP:O	1:A:36:ALA:C	0.46	2.57	4	2
1:A:47:GLY:O	1:A:48:TRP:HB3	0.46	2.10	4	1
1:A:95:TRP:C	1:A:97:THR:H	0.46	2.17	16	1
1:A:60:GLN:O	1:A:62:ALA:N	0.46	2.48	12	1
1:A:122:ASP:OD2	1:A:124:ARG:NH1	0.46	2.48	13	1
1:A:16:ALA:O	1:A:19:ASN:N	0.46	2.49	11	4
1:A:81:ARG:HH11	1:A:81:ARG:CA	0.46	2.23	4	1
1:A:48:TRP:CE3	1:A:93:LEU:HB2	0.46	2.45	15	2
1:A:96:ASP:HA	1:A:100:THR:CG2	0.46	2.40	10	1
1:A:2:GLN:HG2	1:A:119:GLN:NE2	0.46	2.26	20	1
1:A:49:THR:HG23	1:A:82:ILE:HA	0.46	1.87	15	1
1:A:118:TYR:C	1:A:119:GLN:CD	0.46	2.84	14	3
1:A:36:ALA:C	1:A:43:ARG:HH12	0.46	2.19	13	1
1:A:10:TYR:CD1	1:A:10:TYR:N	0.46	2.84	17	1
1:A:49:THR:OG1	1:A:81:ARG:N	0.46	2.49	19	1
1:A:48:TRP:N	1:A:81:ARG:HG3	0.46	2.25	5	1
1:A:46:TYR:C	1:A:81:ARG:HB3	0.46	2.35	16	2
1:A:107:ILE:HD12	1:A:107:ILE:N	0.46	2.25	9	1
1:A:15:PRO:HB3	1:A:22:LEU:CB	0.46	2.41	15	1
1:A:15:PRO:C	1:A:17:GLN:N	0.46	2.73	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:106:GLY:C	1:A:108:GLY:H	0.46	2.19	11	1
1:A:46:TYR:HA	1:A:81:ARG:CG	0.46	2.41	16	1
1:A:20:TRP:HB2	1:A:48:TRP:CZ2	0.46	2.45	19	1
1:A:48:TRP:O	1:A:93:LEU:N	0.46	2.48	6	2
1:A:45:LYS:O	1:A:81:ARG:NE	0.46	2.48	9	1
1:A:96:ASP:CB	1:A:99:PHE:HB3	0.46	2.41	15	1
1:A:9:THR:OG1	1:A:10:TYR:N	0.46	2.49	10	2
1:A:81:ARG:CD	1:A:81:ARG:H	0.45	2.23	5	1
1:A:11:HIS:NE2	1:A:13:TYR:CD1	0.45	2.84	7	1
1:A:10:TYR:HA	1:A:12:TYR:CE1	0.45	2.46	8	1
1:A:48:TRP:NE1	1:A:93:LEU:HD23	0.45	2.26	13	1
1:A:24:ALA:O	1:A:25:PRO:C	0.45	2.59	19	2
1:A:21:ASP:C	1:A:23:GLY:N	0.45	2.74	8	2
1:A:19:ASN:ND2	1:A:43:ARG:HH22	0.45	2.09	8	1
1:A:48:TRP:CH2	1:A:93:LEU:CD1	0.45	2.99	10	1
1:A:35:ASP:CG	1:A:43:ARG:HH21	0.45	2.18	17	1
1:A:62:ALA:O	1:A:64:GLY:N	0.45	2.50	20	2
1:A:2:GLN:CD	1:A:2:GLN:C	0.45	2.85	1	1
1:A:21:ASP:O	1:A:22:LEU:C	0.45	2.60	5	2
1:A:53:GLY:N	1:A:54:PRO:CD	0.45	2.80	7	3
1:A:96:ASP:HB3	1:A:99:PHE:HB3	0.45	1.87	12	2
1:A:42:TRP:CZ3	1:A:81:ARG:NE	0.45	2.85	17	1
1:A:58:ARG:NH2	1:A:120:PHE:CZ	0.45	2.85	4	1
1:A:118:TYR:C	1:A:119:GLN:NE2	0.45	2.74	10	2
1:A:48:TRP:O	1:A:93:LEU:HD13	0.45	2.11	11	1
1:A:15:PRO:HB3	1:A:22:LEU:CA	0.45	2.41	15	1
1:A:80:ALA:C	1:A:81:ARG:HD3	0.45	2.36	15	1
1:A:47:GLY:O	1:A:81:ARG:HB2	0.45	2.12	1	1
1:A:19:ASN:O	1:A:20:TRP:HB2	0.45	2.12	16	4
1:A:20:TRP:CE3	1:A:48:TRP:HZ2	0.45	2.30	2	2
1:A:47:GLY:C	1:A:48:TRP:CG	0.45	2.95	5	1
1:A:58:ARG:O	1:A:59:GLY:C	0.45	2.60	5	1
1:A:91:LEU:O	1:A:92:ASP:C	0.45	2.60	7	2
1:A:12:TYR:CD1	1:A:12:TYR:N	0.45	2.85	6	2
1:A:17:GLN:C	1:A:19:ASN:H	0.45	2.19	20	1
1:A:11:HIS:CD2	1:A:11:HIS:C	0.45	2.95	12	1
1:A:38:LYS:HB2	1:A:43:ARG:NE	0.45	2.26	17	1
1:A:94:ASP:HB3	1:A:97:THR:CG2	0.44	2.41	16	1
1:A:71:ASN:HD22	1:A:102:ILE:CD1	0.44	2.24	4	1
1:A:21:ASP:C	1:A:23:GLY:H	0.44	2.20	7	2
1:A:20:TRP:CE3	1:A:48:TRP:NE1	0.44	2.86	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:LYS:O	1:A:43:ARG:NE	0.44	2.50	8	1
1:A:48:TRP:O	1:A:81:ARG:NH2	0.44	2.50	15	1
1:A:58:ARG:HG3	1:A:62:ALA:HB2	0.44	1.90	1	1
1:A:90:GLY:O	1:A:91:LEU:C	0.44	2.60	11	2
1:A:9:THR:OG1	1:A:90:GLY:N	0.44	2.50	18	1
1:A:51:PHE:O	1:A:85:GLN:NE2	0.44	2.50	8	1
1:A:105:ASN:HD22	1:A:105:ASN:N	0.44	2.11	14	1
1:A:51:PHE:CD1	1:A:58:ARG:CZ	0.44	3.00	7	1
1:A:49:THR:OG1	1:A:81:ARG:C	0.44	2.61	19	1
1:A:88:ASN:OD1	1:A:88:ASN:N	0.44	2.51	1	1
1:A:46:TYR:CG	1:A:81:ARG:NH2	0.44	2.86	10	1
1:A:108:GLY:O	1:A:109:TYR:C	0.44	2.61	9	4
1:A:115:ASN:C	1:A:115:ASN:OD1	0.44	2.60	4	1
1:A:44:SER:OG	1:A:45:LYS:N	0.44	2.50	19	2
1:A:108:GLY:O	1:A:112:GLY:N	0.44	2.51	14	1
1:A:93:LEU:H	1:A:93:LEU:HD23	0.44	1.73	18	1
1:A:51:PHE:HB3	1:A:82:ILE:CG2	0.44	2.43	1	1
1:A:20:TRP:C	1:A:22:LEU:H	0.44	2.21	3	1
1:A:20:TRP:HB2	1:A:43:ARG:NH1	0.44	2.28	7	2
1:A:58:ARG:C	1:A:62:ALA:HB2	0.44	2.37	8	2
1:A:96:ASP:HA	1:A:100:THR:HG23	0.44	1.89	11	2
1:A:22:LEU:CD2	1:A:48:TRP:CE2	0.44	3.01	15	1
1:A:46:TYR:HB3	1:A:81:ARG:HB3	0.43	1.90	5	1
1:A:96:ASP:C	1:A:98:VAL:N	0.43	2.76	5	1
1:A:121:VAL:HG13	1:A:122:ASP:N	0.43	2.29	2	2
1:A:37:SER:O	1:A:43:ARG:NH2	0.43	2.51	5	1
1:A:16:ALA:HA	1:A:20:TRP:N	0.43	2.29	17	1
1:A:10:TYR:HB3	1:A:12:TYR:CE2	0.43	2.48	8	1
1:A:83:VAL:CG1	1:A:84:ASP:N	0.43	2.82	9	1
1:A:105:ASN:ND2	1:A:105:ASN:N	0.43	2.63	14	1
1:A:11:HIS:C	1:A:12:TYR:CD1	0.43	2.97	18	1
1:A:111:GLN:O	1:A:113:HIS:N	0.43	2.51	18	1
1:A:51:PHE:O	1:A:51:PHE:CG	0.43	2.72	4	1
1:A:14:ARG:N	1:A:15:PRO:HD2	0.43	2.28	15	1
1:A:20:TRP:CG	1:A:48:TRP:HZ2	0.43	2.31	20	2
1:A:91:LEU:HD23	1:A:91:LEU:N	0.43	2.28	3	1
1:A:58:ARG:HG3	1:A:62:ALA:CB	0.43	2.43	5	1
1:A:122:ASP:CG	1:A:124:ARG:HG3	0.43	2.38	11	1
1:A:114:LEU:HD23	1:A:114:LEU:H	0.43	1.74	18	1
1:A:13:TYR:CZ	1:A:14:ARG:NH2	0.43	2.84	2	1
1:A:48:TRP:CE2	1:A:93:LEU:HD22	0.43	2.49	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:THR:O	1:A:101:LYS:HG3	0.43	2.13	17	1
1:A:113:HIS:ND1	1:A:113:HIS:C	0.43	2.75	2	1
1:A:106:GLY:O	1:A:108:GLY:N	0.43	2.52	17	2
1:A:44:SER:O	1:A:45:LYS:C	0.43	2.61	5	3
1:A:45:LYS:O	1:A:46:TYR:CD1	0.43	2.71	9	1
1:A:105:ASN:H	1:A:105:ASN:HD22	0.43	1.56	14	1
1:A:21:ASP:O	1:A:24:ALA:N	0.43	2.52	16	1
1:A:94:ASP:HB3	1:A:97:THR:HG23	0.43	1.89	20	1
1:A:39:PRO:O	1:A:40:LEU:C	0.43	2.62	3	2
1:A:22:LEU:HD11	1:A:48:TRP:CZ2	0.43	2.49	8	1
1:A:46:TYR:CE2	1:A:79:THR:HB	0.43	2.48	13	1
1:A:48:TRP:O	1:A:92:ASP:HB3	0.43	2.14	15	1
1:A:18:ASN:O	1:A:20:TRP:N	0.43	2.51	19	2
1:A:51:PHE:O	1:A:52:CYS:SG	0.43	2.77	11	1
1:A:19:ASN:O	1:A:21:ASP:N	0.43	2.52	1	2
1:A:38:LYS:O	1:A:43:ARG:CD	0.43	2.67	3	1
1:A:1:GLU:OE1	1:A:1:GLU:N	0.43	2.48	5	1
1:A:48:TRP:H	1:A:98:VAL:CG2	0.43	2.27	8	1
1:A:107:ILE:CD1	1:A:107:ILE:N	0.43	2.82	9	1
1:A:20:TRP:NE1	1:A:43:ARG:CB	0.43	2.82	17	1
1:A:31:CYS:HB2	1:A:83:VAL:HG23	0.42	1.90	3	2
1:A:109:TYR:C	1:A:109:TYR:CD1	0.42	2.96	9	1
1:A:22:LEU:CB	1:A:32:ALA:HB2	0.42	2.44	11	1
1:A:13:TYR:CD2	1:A:14:ARG:N	0.42	2.87	12	1
1:A:3:ALA:HB2	1:A:55:ALA:HB2	0.42	1.91	18	1
1:A:71:ASN:O	1:A:72:PRO:C	0.42	2.62	1	3
1:A:9:THR:HG22	1:A:113:HIS:HB3	0.42	1.90	15	1
1:A:35:ASP:OD1	1:A:43:ARG:NH2	0.42	2.52	17	1
1:A:106:GLY:HA3	1:A:114:LEU:HD22	0.42	1.89	4	1
1:A:61:ALA:O	1:A:65:LYS:NZ	0.42	2.53	10	1
1:A:93:LEU:HD22	1:A:93:LEU:H	0.42	1.74	12	1
1:A:123:CYS:O	1:A:124:ARG:C	0.42	2.62	18	2
1:A:48:TRP:CD1	1:A:93:LEU:HD22	0.42	2.49	2	1
1:A:14:ARG:NH1	1:A:48:TRP:CH2	0.42	2.87	7	1
1:A:81:ARG:HB2	1:A:81:ARG:NH1	0.42	2.29	11	2
1:A:112:GLY:C	1:A:113:HIS:ND1	0.42	2.78	12	1
1:A:48:TRP:CE3	1:A:83:VAL:HG11	0.42	2.49	13	1
1:A:38:LYS:O	1:A:43:ARG:HD3	0.42	2.15	3	1
1:A:49:THR:CG2	1:A:98:VAL:HG21	0.42	2.44	3	1
1:A:99:PHE:O	1:A:100:THR:C	0.42	2.61	14	2
1:A:105:ASN:HD22	1:A:105:ASN:C	0.42	2.23	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ARG:N	1:A:81:ARG:NE	0.42	2.67	15	1
1:A:3:ALA:CB	1:A:118:TYR:CZ	0.42	3.03	16	1
1:A:48:TRP:CD1	1:A:93:LEU:HB3	0.42	2.50	19	1
1:A:98:VAL:O	1:A:99:PHE:C	0.42	2.63	1	1
1:A:12:TYR:CD1	1:A:92:ASP:O	0.42	2.72	8	1
1:A:90:GLY:O	1:A:91:LEU:CB	0.42	2.68	13	2
1:A:19:ASN:HD21	1:A:43:ARG:NH1	0.42	2.11	16	1
1:A:92:ASP:C	1:A:93:LEU:HD12	0.42	2.40	17	1
1:A:37:SER:OG	1:A:38:LYS:N	0.42	2.53	2	1
1:A:16:ALA:N	1:A:20:TRP:HB3	0.42	2.30	1	1
1:A:49:THR:HG23	1:A:81:ARG:O	0.42	2.15	5	1
1:A:46:TYR:CE2	1:A:123:CYS:SG	0.42	3.13	12	1
1:A:14:ARG:HH12	1:A:17:GLN:CD	0.42	2.23	17	1
1:A:106:GLY:O	1:A:107:ILE:C	0.42	2.63	17	2
1:A:48:TRP:CZ3	1:A:93:LEU:HD11	0.42	2.50	18	1
1:A:81:ARG:HH11	1:A:81:ARG:CB	0.41	2.27	4	1
1:A:47:GLY:O	1:A:93:LEU:HD22	0.41	2.15	5	1
1:A:54:PRO:O	1:A:58:ARG:NH2	0.41	2.53	10	1
1:A:77:GLN:N	1:A:77:GLN:CD	0.41	2.78	13	1
1:A:88:ASN:CG	1:A:89:GLY:H	0.41	2.23	14	1
1:A:20:TRP:CH2	1:A:48:TRP:NE1	0.41	2.88	15	1
1:A:93:LEU:HD23	1:A:93:LEU:N	0.41	2.30	18	1
1:A:81:ARG:N	1:A:81:ARG:CD	0.41	2.83	8	1
1:A:99:PHE:C	1:A:101:LYS:H	0.41	2.23	9	1
1:A:92:ASP:C	1:A:94:ASP:H	0.41	2.23	11	1
1:A:20:TRP:CB	1:A:48:TRP:CH2	0.41	3.03	16	1
1:A:10:TYR:OH	1:A:111:GLN:N	0.41	2.52	17	1
1:A:4:ASN:O	1:A:6:VAL:HG23	0.41	2.15	4	1
1:A:117:ASN:N	1:A:117:ASN:HD22	0.41	2.13	4	1
1:A:48:TRP:HA	1:A:93:LEU:HD13	0.41	1.92	5	1
1:A:15:PRO:C	1:A:17:GLN:H	0.41	2.23	6	1
1:A:81:ARG:HD3	1:A:81:ARG:H	0.41	1.73	8	1
1:A:35:ASP:OD1	1:A:38:LYS:NZ	0.41	2.53	13	1
1:A:15:PRO:CG	1:A:48:TRP:CH2	0.41	3.04	15	1
1:A:58:ARG:O	1:A:62:ALA:CB	0.41	2.68	17	1
1:A:47:GLY:O	1:A:81:ARG:NH2	0.41	2.52	20	1
1:A:116:VAL:C	1:A:117:ASN:ND2	0.41	2.78	4	1
1:A:105:ASN:ND2	1:A:105:ASN:O	0.41	2.53	11	1
1:A:58:ARG:NH1	1:A:82:ILE:CD1	0.41	2.83	13	1
1:A:70:THR:OG1	1:A:77:GLN:HB3	0.41	2.14	17	1
1:A:2:GLN:NE2	1:A:2:GLN:O	0.41	2.53	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ASP:C	1:A:43:ARG:HH12	0.41	2.23	4	1
1:A:10:TYR:OH	1:A:109:TYR:HA	0.41	2.14	11	1
1:A:94:ASP:C	1:A:96:ASP:N	0.41	2.79	15	1
1:A:20:TRP:CG	1:A:48:TRP:CH2	0.41	3.08	16	1
1:A:29:ALA:O	1:A:30:TYR:C	0.41	2.63	3	2
1:A:18:ASN:O	1:A:19:ASN:CB	0.41	2.68	5	1
1:A:11:HIS:O	1:A:95:TRP:CD1	0.41	2.74	9	1
1:A:13:TYR:HB2	1:A:94:ASP:O	0.41	2.16	9	1
1:A:31:CYS:C	1:A:33:THR:N	0.41	2.78	13	1
1:A:59:GLY:H	1:A:62:ALA:HB2	0.41	1.75	4	1
1:A:15:PRO:HB3	1:A:48:TRP:CH2	0.41	2.51	7	1
1:A:58:ARG:HG2	1:A:62:ALA:CB	0.41	2.45	7	1
1:A:51:PHE:C	1:A:52:CYS:SG	0.41	3.04	11	1
1:A:77:GLN:NE2	1:A:78:ILE:N	0.41	2.69	15	1
1:A:118:TYR:CD1	1:A:118:TYR:O	0.41	2.73	11	1
1:A:95:TRP:CE3	1:A:95:TRP:O	0.41	2.74	15	1
1:A:8:ALA:O	1:A:113:HIS:HA	0.41	2.16	2	1
1:A:72:PRO:CD	1:A:117:ASN:ND2	0.41	2.84	4	1
1:A:7:ARG:HB2	1:A:113:HIS:CE1	0.41	2.51	5	1
1:A:13:TYR:O	1:A:14:ARG:HD3	0.41	2.16	5	1
1:A:15:PRO:C	1:A:20:TRP:CD1	0.41	2.99	8	1
1:A:31:CYS:SG	1:A:83:VAL:HG13	0.41	2.56	11	1
1:A:96:ASP:O	1:A:97:THR:C	0.41	2.62	12	1
1:A:47:GLY:O	1:A:81:ARG:CB	0.41	2.68	18	1
1:A:42:TRP:CH2	1:A:81:ARG:NE	0.41	2.89	1	1
1:A:60:GLN:C	1:A:62:ALA:H	0.41	2.24	8	2
1:A:58:ARG:CD	1:A:58:ARG:C	0.41	2.94	10	1
1:A:58:ARG:NH1	1:A:58:ARG:O	0.41	2.54	14	1
1:A:31:CYS:O	1:A:33:THR:N	0.41	2.54	15	1
1:A:92:ASP:O	1:A:93:LEU:HD12	0.41	2.15	17	1
1:A:88:ASN:CG	1:A:89:GLY:N	0.41	2.79	18	1
1:A:105:ASN:OD1	1:A:106:GLY:N	0.41	2.54	20	1
1:A:51:PHE:CD1	1:A:52:CYS:N	0.40	2.89	2	1
1:A:1:GLU:N	1:A:1:GLU:CD	0.40	2.80	6	1
1:A:106:GLY:C	1:A:108:GLY:N	0.40	2.79	11	1
1:A:96:ASP:O	1:A:98:VAL:N	0.40	2.55	15	1
1:A:48:TRP:N	1:A:81:ARG:HB3	0.40	2.31	16	1
1:A:99:PHE:CD1	1:A:99:PHE:O	0.40	2.74	17	1
1:A:47:GLY:C	1:A:81:ARG:NH2	0.40	2.80	15	1
1:A:46:TYR:CD1	1:A:66:CYS:SG	0.40	3.14	16	1
1:A:76:ALA:CB	1:A:103:ASP:CB	0.40	3.00	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ASP:C	1:A:37:SER:N	0.40	2.79	5	1
1:A:46:TYR:HA	1:A:81:ARG:HG2	0.40	1.91	9	2
1:A:72:PRO:CD	1:A:117:ASN:HD22	0.40	2.29	10	1
1:A:20:TRP:O	1:A:21:ASP:C	0.40	2.64	11	1
1:A:49:THR:HB	1:A:91:LEU:O	0.40	2.16	20	1
1:A:56:GLY:HA3	1:A:120:PHE:CZ	0.40	2.52	14	1
1:A:118:TYR:O	1:A:119:GLN:NE2	0.40	2.55	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	123/125 (98%)	80±3 (65±3%)	31±5 (25±4%)	12±3 (10±2%)	1	9
All	All	2460/2500 (98%)	1595 (65%)	616 (25%)	249 (10%)	1	9

All 53 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	15	PRO	15
1	A	28	SER	13
1	A	21	ASP	12
1	A	20	TRP	11
1	A	99	PHE	11
1	A	95	TRP	9
1	A	107	ILE	9
1	A	41	SER	8
1	A	30	TYR	7
1	A	63	CYS	7
1	A	14	ARG	7
1	A	16	ALA	6
1	A	22	LEU	6
1	A	100	THR	6
1	A	104	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	61	ALA	5
1	A	97	THR	5
1	A	106	GLY	5
1	A	83	VAL	5
1	A	108	GLY	5
1	A	19	ASN	5
1	A	60	GLN	5
1	A	91	LEU	5
1	A	39	PRO	4
1	A	87	ALA	4
1	A	96	ASP	4
1	A	48	TRP	4
1	A	64	GLY	4
1	A	56	GLY	4
1	A	92	ASP	4
1	A	73	ALA	3
1	A	110	GLN	3
1	A	25	PRO	3
1	A	26	ALA	3
1	A	59	GLY	3
1	A	54	PRO	3
1	A	47	GLY	3
1	A	109	TYR	3
1	A	36	ALA	3
1	A	72	PRO	2
1	A	33	THR	2
1	A	53	GLY	2
1	A	24	ALA	2
1	A	112	GLY	2
1	A	57	PRO	2
1	A	82	ILE	2
1	A	93	LEU	1
1	A	38	LYS	1
1	A	90	GLY	1
1	A	102	ILE	1
1	A	103	ASP	1
1	A	32	ALA	1
1	A	111	GLN	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	97/97 (100%)	82±2 (85±2%)	15±2 (15±2%)	5	42
All	All	1940/1940 (100%)	1649 (85%)	291 (15%)	5	42

All 60 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	30	TYR	20
1	A	100	THR	20
1	A	113	HIS	20
1	A	121	VAL	20
1	A	119	GLN	16
1	A	67	LEU	15
1	A	58	ARG	15
1	A	46	TYR	13
1	A	86	CYS	10
1	A	13	TYR	7
1	A	14	ARG	7
1	A	40	LEU	7
1	A	92	ASP	7
1	A	77	GLN	6
1	A	105	ASN	6
1	A	81	ARG	6
1	A	78	ILE	5
1	A	104	THR	5
1	A	12	TYR	5
1	A	4	ASN	5
1	A	91	LEU	4
1	A	22	LEU	4
1	A	48	TRP	4
1	A	93	LEU	4
1	A	31	CYS	3
1	A	18	ASN	3
1	A	51	PHE	3
1	A	45	LYS	3
1	A	124	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	52	CYS	3
1	A	97	THR	3
1	A	122	ASP	2
1	A	10	TYR	2
1	A	35	ASP	2
1	A	38	LYS	2
1	A	1	GLU	2
1	A	49	THR	2
1	A	19	ASN	2
1	A	7	ARG	2
1	A	83	VAL	2
1	A	94	ASP	2
1	A	103	ASP	1
1	A	116	VAL	1
1	A	88	ASN	1
1	A	115	ASN	1
1	A	65	LYS	1
1	A	43	ARG	1
1	A	11	HIS	1
1	A	17	GLN	1
1	A	84	ASP	1
1	A	101	LYS	1
1	A	107	ILE	1
1	A	9	THR	1
1	A	63	CYS	1
1	A	21	ASP	1
1	A	111	GLN	1
1	A	96	ASP	1
1	A	70	THR	1
1	A	2	GLN	1
1	A	99	PHE	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 [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 [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided