



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 1Q80 / pdb_00001q80
BMRB ID : 4129
Title : Solution structure and dynamics of Nereis sarcoplasmic calcium binding protein
Authors : Rabah, G.; Popescu, R.; Cox, J.A.; Engelborghs, Y.; Craescu, C.T.
Deposited on : 2003-08-20

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<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

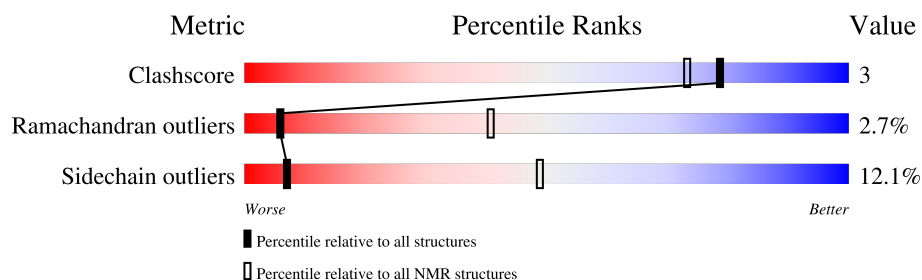
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 52%.

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	174	 68% 28% .

2 Ensemble composition and analysis

This entry contains 17 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:174 (174)	1.51	9

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2678 atoms, of which 1310 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sarcoplasmic calcium-binding protein.

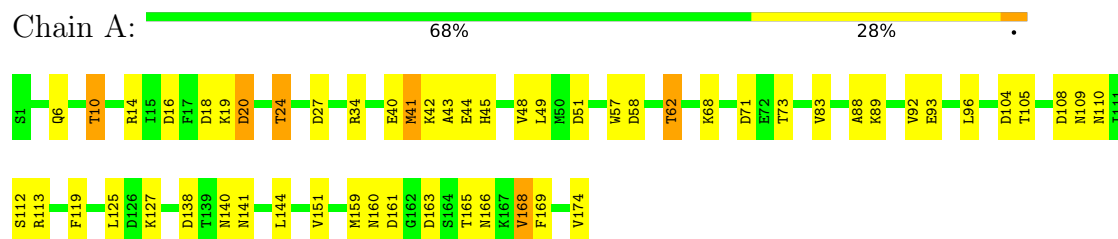
Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			2678	868	1310	218	272	10	

4 Residue-property plots [i](#)

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: Sarcoplasmic calcium-binding protein

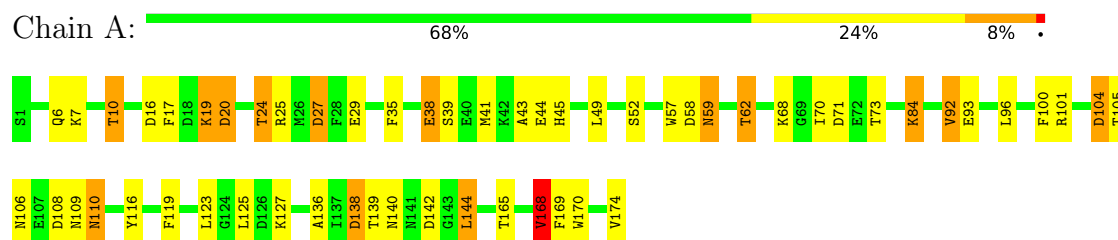


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

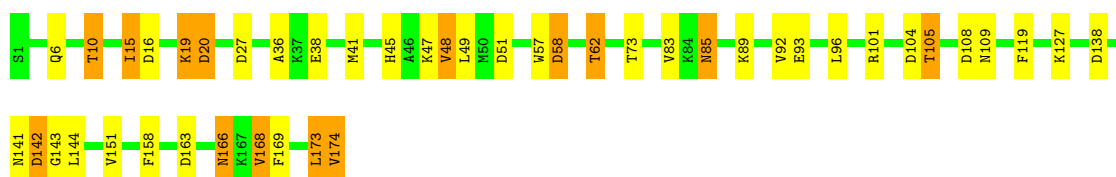
- Molecule 1: Sarcoplasmic calcium-binding protein



4.2.2 Score per residue for model 2

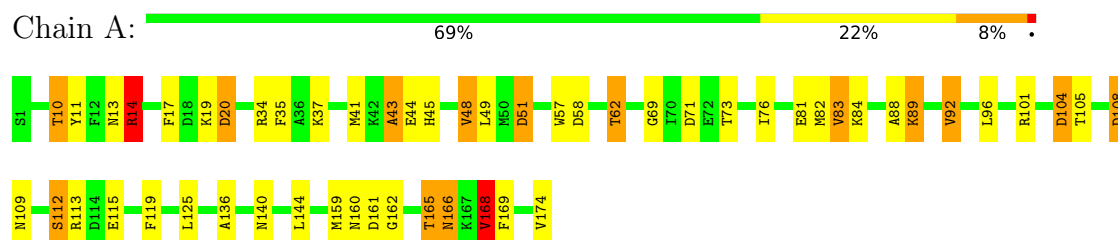
- Molecule 1: Sarcoplasmic calcium-binding protein





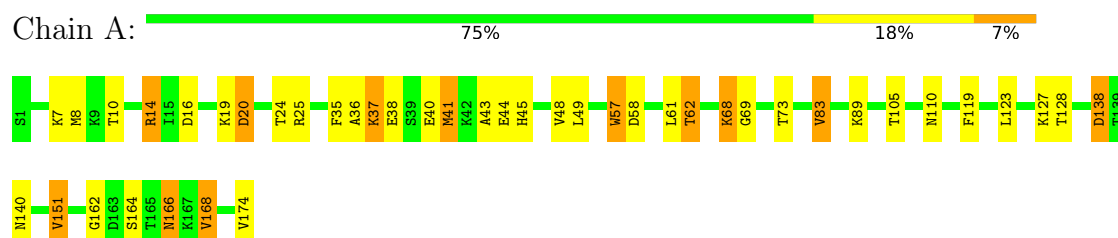
4.2.3 Score per residue for model 3

- Molecule 1: Sarcoplasmic calcium-binding protein



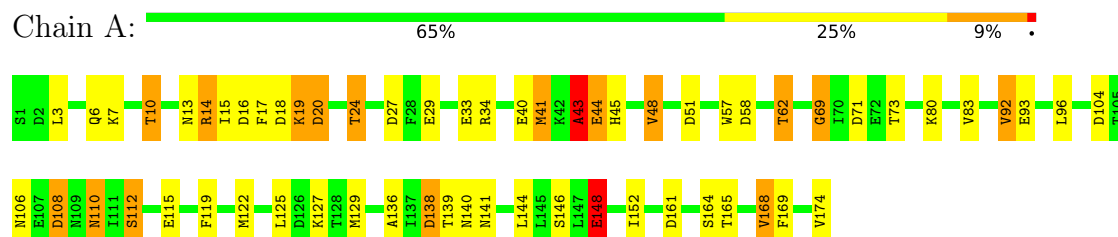
4.2.4 Score per residue for model 4

- Molecule 1: Sarcoplasmic calcium-binding protein



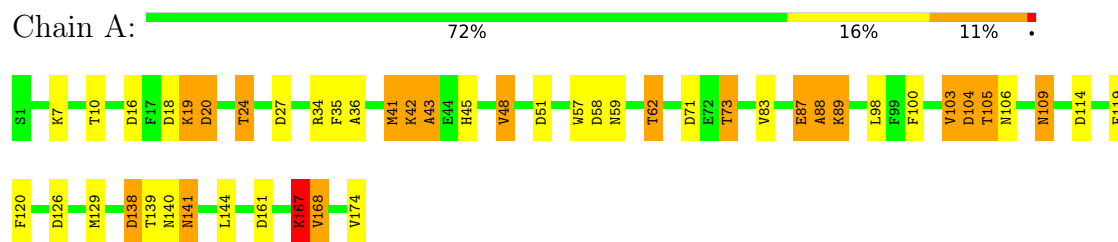
4.2.5 Score per residue for model 5

- Molecule 1: Sarcoplasmic calcium-binding protein



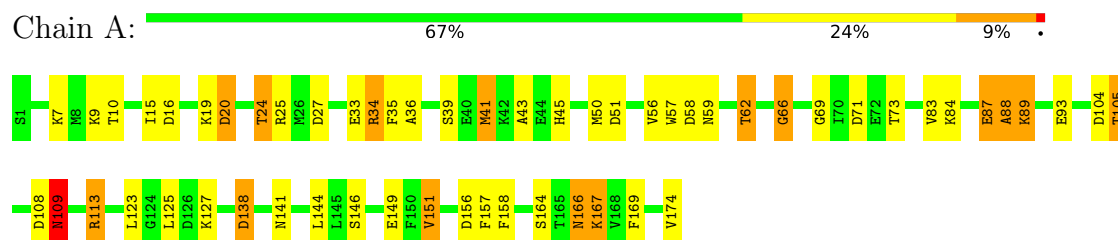
4.2.6 Score per residue for model 6

- Molecule 1: Sarcoplasmic calcium-binding protein



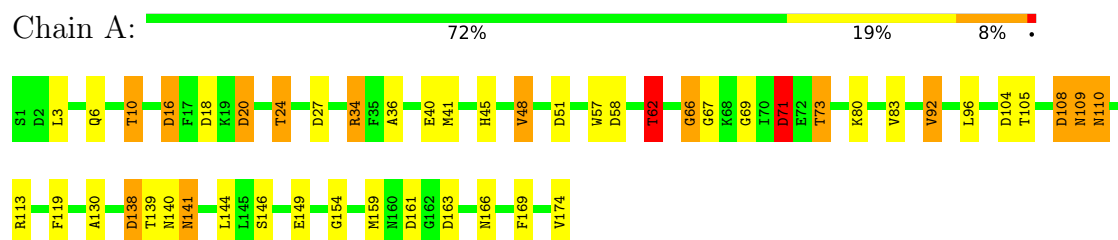
4.2.7 Score per residue for model 7

- Molecule 1: Sarcoplasmic calcium-binding protein



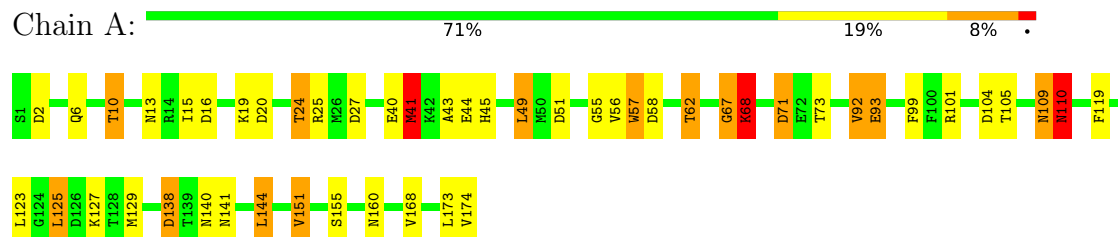
4.2.8 Score per residue for model 8

- Molecule 1: Sarcoplasmic calcium-binding protein



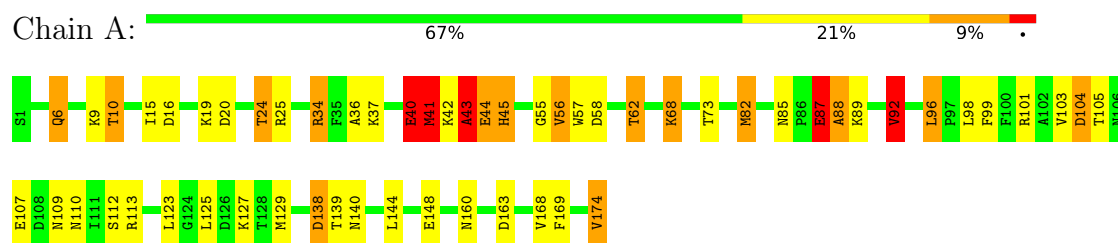
4.2.9 Score per residue for model 9 (medoid)

- Molecule 1: Sarcoplasmic calcium-binding protein



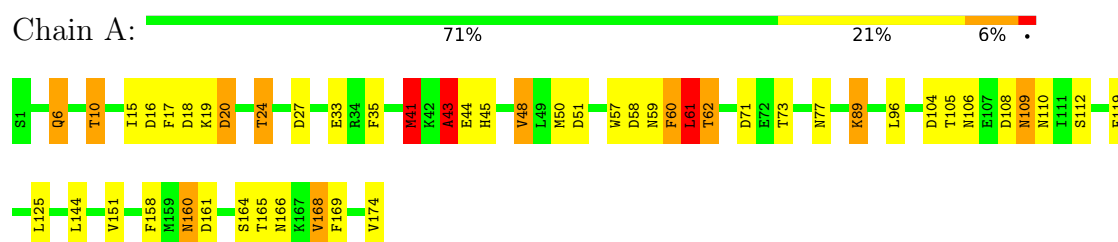
4.2.10 Score per residue for model 10

- Molecule 1: Sarcoplasmic calcium-binding protein



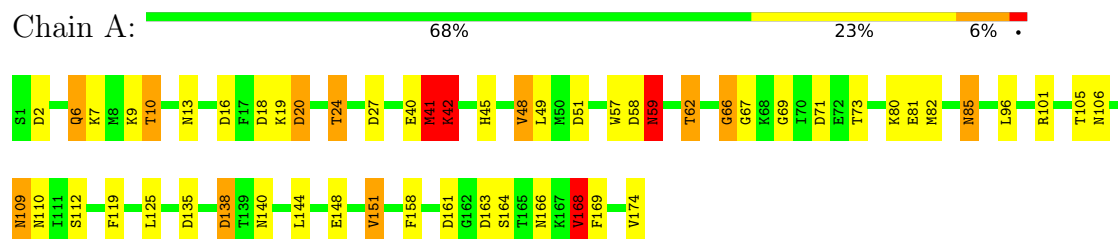
4.2.11 Score per residue for model 11

- Molecule 1: Sarcoplasmic calcium-binding protein



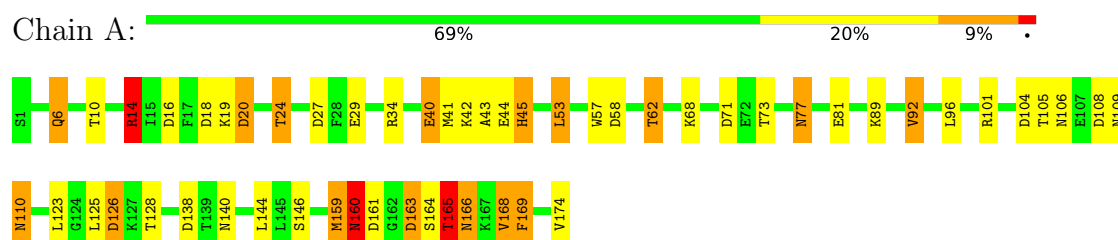
4.2.12 Score per residue for model 12

- Molecule 1: Sarcoplasmic calcium-binding protein



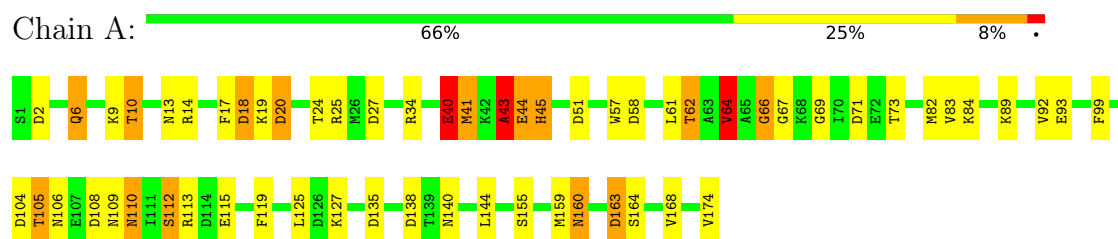
4.2.13 Score per residue for model 13

- Molecule 1: Sarcoplasmic calcium-binding protein



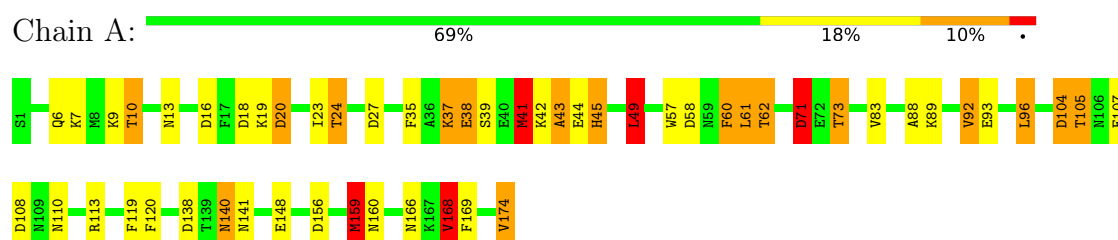
4.2.14 Score per residue for model 14

- Molecule 1: Sarcoplasmic calcium-binding protein



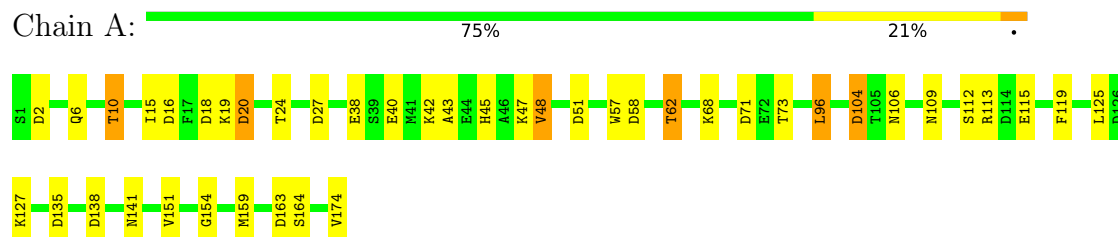
4.2.15 Score per residue for model 15

- Molecule 1: Sarcoplasmic calcium-binding protein



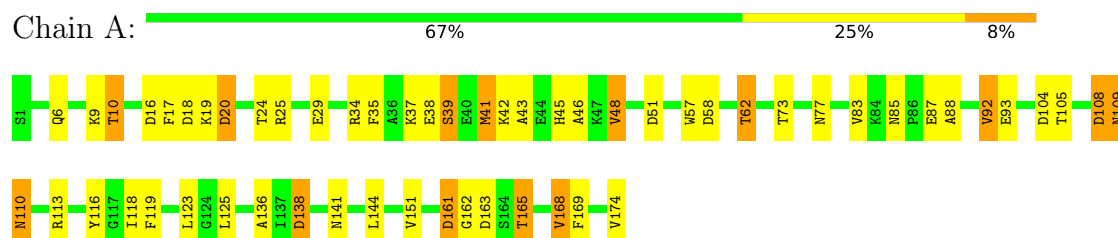
4.2.16 Score per residue for model 16

- Molecule 1: Sarcoplasmic calcium-binding protein



4.2.17 Score per residue for model 17

- Molecule 1: Sarcoplasmic calcium-binding protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *distance geometry, simulated annealing*.

Of the 17 calculated structures, 17 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
DGII	structure solution	2
Discover	structure solution	3
Discover	refinement	3

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	3
Total number of shifts	1210
Number of shifts mapped to atoms	1208
Number of unparsed shifts	0
Number of shifts with mapping errors	2
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	52%

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	1.97±0.02	10±3/1396 (0.7± 0.2%)	2.53±0.35	38±7/1880 (2.0± 0.4%)
All	All	1.97	166/23732 (0.7%)	2.56	650/31960 (2.0%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.1±2.5
All	All	0	86

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	168	VAL	CA-C	8.81	1.60	1.52	17	9
1	A	125	LEU	N-CA	7.23	1.50	1.46	12	1
1	A	174	VAL	C-OXT	7.10	1.37	1.23	17	17
1	A	83	VAL	CA-C	7.07	1.62	1.52	3	4
1	A	104	ASP	CA-C	6.90	1.62	1.52	10	4
1	A	163	ASP	CA-C	6.79	1.59	1.53	12	1
1	A	41	MET	C-N	-6.71	1.24	1.33	5	2
1	A	160	ASN	N-CA	6.53	1.54	1.46	13	2
1	A	167	LYS	N-CA	6.40	1.54	1.46	7	1
1	A	38	GLU	N-CA	6.35	1.54	1.46	4	2
1	A	96	LEU	CA-C	6.16	1.60	1.52	15	4
1	A	151	VAL	CA-C	6.16	1.60	1.52	11	3
1	A	167	LYS	CA-C	6.13	1.60	1.52	6	1
1	A	61	LEU	N-CA	6.12	1.54	1.46	11	2
1	A	43	ALA	C-N	-6.07	1.25	1.33	14	5
1	A	88	ALA	N-CA	5.93	1.53	1.46	7	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	15	ILE	N-CA	5.91	1.54	1.46	5	1
1	A	40	GLU	N-CA	5.91	1.53	1.46	10	1
1	A	45	HIS	N-CA	5.91	1.53	1.46	10	2
1	A	173	LEU	N-CA	5.90	1.53	1.46	2	1
1	A	169	PHE	N-CA	5.89	1.53	1.46	11	8
1	A	164	SER	N-CA	5.88	1.52	1.45	14	1
1	A	43	ALA	N-CA	5.81	1.53	1.46	6	1
1	A	41	MET	N-CA	5.80	1.53	1.46	13	3
1	A	109	ASN	CA-C	5.78	1.59	1.52	14	9
1	A	168	VAL	N-CA	5.76	1.53	1.46	6	1
1	A	42	LYS	N-CA	5.76	1.53	1.46	12	1
1	A	69	GLY	CA-C	5.70	1.57	1.52	7	2
1	A	84	LYS	N-CA	5.65	1.53	1.46	3	1
1	A	61	LEU	CA-C	5.65	1.60	1.52	11	1
1	A	40	GLU	C-N	-5.64	1.26	1.33	14	1
1	A	66	GLY	C-N	-5.61	1.25	1.33	7	3
1	A	160	ASN	CG-ND2	-5.56	1.21	1.33	11	2
1	A	7	LYS	CA-C	5.56	1.59	1.52	7	3
1	A	170	TRP	N-CA	5.54	1.51	1.46	1	1
1	A	68	LYS	N-CA	5.54	1.53	1.46	9	1
1	A	45	HIS	CG-CD2	5.53	1.42	1.35	16	3
1	A	6	GLN	CD-NE2	-5.52	1.21	1.33	13	2
1	A	166	ASN	CG-ND2	-5.51	1.21	1.33	4	1
1	A	87	GLU	C-N	-5.51	1.25	1.33	6	3
1	A	29	GLU	CA-C	5.50	1.59	1.52	17	3
1	A	168	VAL	C-N	-5.45	1.25	1.33	15	3
1	A	85	ASN	CG-ND2	-5.42	1.21	1.33	12	2
1	A	45	HIS	ND1-CE1	5.41	1.38	1.32	2	2
1	A	123	LEU	CA-C	5.41	1.60	1.52	17	3
1	A	67	GLY	C-N	-5.41	1.26	1.33	9	1
1	A	77	ASN	CG-ND2	-5.39	1.22	1.33	13	1
1	A	143	GLY	N-CA	5.39	1.53	1.45	2	1
1	A	59	ASN	CG-ND2	-5.33	1.22	1.33	1	2
1	A	159	MET	CA-C	5.31	1.59	1.52	13	2
1	A	110	ASN	CA-C	5.31	1.58	1.52	15	3
1	A	151	VAL	CA-CB	5.31	1.60	1.54	9	1
1	A	16	ASP	CA-C	5.30	1.59	1.53	17	4
1	A	160	ASN	C-N	-5.28	1.26	1.33	14	1
1	A	106	ASN	CA-C	5.26	1.59	1.52	11	1
1	A	69	GLY	N-CA	5.25	1.52	1.45	4	1
1	A	158	PHE	CA-C	5.24	1.59	1.52	12	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	64	VAL	CA-C	5.20	1.59	1.52	14	1
1	A	20	ASP	CA-C	5.20	1.59	1.52	5	1
1	A	67	GLY	N-CA	5.19	1.52	1.45	12	1
1	A	15	ILE	CA-C	5.18	1.59	1.52	11	4
1	A	152	ILE	CA-C	5.17	1.58	1.52	5	1
1	A	162	GLY	N-CA	5.13	1.52	1.45	17	1
1	A	92	VAL	CA-C	5.12	1.59	1.52	17	1
1	A	44	GLU	CA-C	5.10	1.59	1.52	14	1
1	A	76	ILE	CA-C	5.10	1.59	1.52	3	1
1	A	116	TYR	CA-C	5.09	1.59	1.52	17	2
1	A	93	GLU	CA-C	5.08	1.59	1.52	9	1
1	A	18	ASP	CA-C	5.06	1.59	1.52	14	1
1	A	84	LYS	CA-C	5.05	1.59	1.52	3	1
1	A	103	VAL	CA-C	5.03	1.60	1.52	10	1
1	A	8	MET	CA-C	5.02	1.59	1.52	4	1
1	A	44	GLU	C-N	-5.02	1.26	1.33	14	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	68	LYS	O-C-N	-54.35	61.55	122.96	10	3
1	A	41	MET	O-C-N	-53.88	61.83	123.25	15	6
1	A	64	VAL	O-C-N	-48.23	62.28	122.57	14	1
1	A	168	VAL	O-C-N	-48.13	81.53	121.96	2	8
1	A	43	ALA	O-C-N	-45.97	61.45	122.59	15	6
1	A	165	THR	O-C-N	-43.28	65.03	122.59	13	1
1	A	44	GLU	O-C-N	-41.45	78.19	122.12	14	2
1	A	59	ASN	OD1-CG-ND2	-40.04	82.56	122.60	12	2
1	A	6	GLN	OE1-CD-NE2	-39.82	82.78	122.60	11	2
1	A	60	PHE	O-C-N	-39.72	80.63	123.13	11	2
1	A	85	ASN	OD1-CG-ND2	-39.49	83.11	122.60	12	2
1	A	160	ASN	OD1-CG-ND2	-39.37	83.23	122.60	14	2
1	A	77	ASN	OD1-CG-ND2	-39.19	83.41	122.60	13	1
1	A	14	ARG	O-C-N	-38.93	68.74	122.46	5	1
1	A	166	ASN	OD1-CG-ND2	-38.64	83.96	122.60	4	1
1	A	40	GLU	O-C-N	-36.75	81.44	122.96	13	3
1	A	83	VAL	O-C-N	-36.55	71.68	122.12	3	1
1	A	167	LYS	O-C-N	-36.05	74.65	122.59	6	1
1	A	66	GLY	O-C-N	-33.74	77.48	122.35	12	4
1	A	166	ASN	O-C-N	-33.73	82.99	122.11	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	142	ASP	O-C-N	-32.48	78.07	121.92	2	1
1	A	161	ASP	O-C-N	-32.20	83.61	122.25	17	1
1	A	87	GLU	O-C-N	-32.01	86.38	122.55	7	3
1	A	159	MET	O-C-N	-31.49	80.71	122.59	13	2
1	A	67	GLY	O-C-N	-29.49	84.37	122.70	9	1
1	A	160	ASN	O-C-N	-29.32	88.41	123.01	14	1
1	A	125	LEU	O-C-N	-28.98	84.04	122.59	9	1
1	A	37	LYS	O-C-N	-28.61	83.78	121.83	4	2
1	A	163	ASP	O-C-N	-26.43	87.44	122.59	14	1
1	A	42	LYS	O-C-N	-24.67	89.81	122.38	6	1
1	A	41	MET	CA-C-O	-24.48	94.90	121.33	15	6
1	A	68	LYS	CA-C-O	-23.74	94.17	121.47	10	1
1	A	64	VAL	CA-C-O	-19.34	96.60	120.78	14	1
1	A	14	ARG	CA-C-O	-18.95	95.81	119.31	5	1
1	A	43	ALA	CA-C-O	-16.75	96.55	120.51	5	6
1	A	165	THR	CA-C-O	-15.79	97.93	120.51	13	1
1	A	83	VAL	CA-C-O	-14.67	101.83	119.58	3	1
1	A	51	ASP	CA-CB-CG	13.32	125.92	112.60	2	12
1	A	66	GLY	CA-C-O	-13.01	102.60	119.25	12	1
1	A	56	VAL	CA-CB-CG1	12.56	131.75	110.40	9	1
1	A	45	HIS	ND1-CE1-NE2	12.53	120.93	108.40	1	17
1	A	142	ASP	CA-C-O	-12.43	107.86	121.78	2	1
1	A	167	LYS	CA-C-O	-12.02	103.33	120.51	6	1
1	A	44	GLU	CA-C-O	-11.99	104.98	119.49	10	2
1	A	40	GLU	CA-C-O	-11.66	108.06	121.47	13	1
1	A	41	MET	CA-C-N	11.50	143.51	121.54	5	2
1	A	41	MET	C-N-CA	11.50	143.51	121.54	5	2
1	A	110	ASN	CA-CB-CG	11.39	123.99	112.60	9	7
1	A	109	ASN	CA-CB-CG	11.18	123.78	112.60	11	5
1	A	27	ASP	CA-CB-CG	10.97	123.57	112.60	6	13
1	A	56	VAL	N-CA-CB	-10.90	97.79	110.55	10	2
1	A	16	ASP	CA-CB-CG	10.65	123.25	112.60	7	14
1	A	141	ASN	CA-CB-CG	10.24	122.84	112.60	6	7
1	A	45	HIS	CE1-NE2-CD2	-10.12	98.88	109.00	6	17
1	A	10	THR	CA-CB-CG2	10.01	127.51	110.50	11	4
1	A	104	ASP	CA-CB-CG	9.99	122.59	112.60	13	15
1	A	161	ASP	CA-CB-CG	9.91	122.51	112.60	3	4
1	A	113	ARG	N-CA-CB	-9.88	95.21	109.94	17	2
1	A	160	ASN	CA-CB-CG	9.50	122.10	112.60	13	4
1	A	108	ASP	CA-CB-CG	9.29	121.89	112.60	17	11
1	A	99	PHE	CA-CB-CG	9.17	122.97	113.80	10	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	138	ASP	CA-CB-CG	9.12	121.72	112.60	12	13
1	A	13	ASN	CA-CB-CG	8.79	121.39	112.60	12	6
1	A	60	PHE	CA-C-O	-8.78	111.48	119.91	11	1
1	A	103	VAL	CA-CB-CG1	8.67	125.13	110.40	6	1
1	A	18	ASP	CA-CB-CG	8.66	121.26	112.60	5	9
1	A	166	ASN	CA-C-O	-8.61	111.76	120.80	7	1
1	A	166	ASN	CA-CB-CG	8.61	121.21	112.60	2	6
1	A	92	VAL	CA-CB-CG1	8.49	124.83	110.40	10	10
1	A	84	LYS	CA-CB-CG	8.45	130.99	114.10	1	1
1	A	49	LEU	N-CA-CB	8.33	122.49	110.16	15	6
1	A	156	ASP	CA-CB-CG	8.31	120.91	112.60	7	1
1	A	45	HIS	N-CA-C	8.30	120.32	111.28	15	6
1	A	143	GLY	N-CA-C	8.21	125.84	115.42	2	1
1	A	62	THR	N-CA-CB	-8.15	98.14	110.12	3	17
1	A	2	ASP	CA-CB-CG	8.11	120.71	112.60	14	3
1	A	10	THR	N-CA-CB	8.04	121.67	110.01	4	3
1	A	56	VAL	CB-CA-C	7.93	123.17	112.22	9	1
1	A	77	ASN	CA-CB-CG	7.93	120.53	112.60	17	2
1	A	45	HIS	CA-CB-CG	7.83	121.62	113.80	13	1
1	A	85	ASN	N-CA-CB	-7.81	99.13	110.14	10	2
1	A	55	GLY	CA-C-N	7.61	131.22	120.42	9	2
1	A	55	GLY	C-N-CA	7.61	131.22	120.42	9	2
1	A	168	VAL	CA-C-O	-7.60	116.02	122.63	2	2
1	A	87	GLU	CA-C-N	7.58	136.02	121.54	6	3
1	A	87	GLU	C-N-CA	7.58	136.02	121.54	6	3
1	A	128	THR	N-CA-CB	-7.57	98.19	110.14	4	1
1	A	58	ASP	CA-CB-CG	7.54	120.14	112.60	12	5
1	A	42	LYS	CA-C-N	7.49	135.84	121.54	6	1
1	A	42	LYS	C-N-CA	7.49	135.84	121.54	6	1
1	A	41	MET	N-CA-C	7.44	119.00	108.74	5	1
1	A	38	GLU	N-CA-C	7.43	122.11	112.89	17	2
1	A	125	LEU	CA-C-O	-7.35	110.00	120.51	9	1
1	A	71	ASP	CA-CB-CG	7.33	119.92	112.60	12	11
1	A	49	LEU	CB-CA-C	7.24	122.81	110.79	9	2
1	A	20	ASP	CA-CB-CG	7.23	119.83	112.60	10	17
1	A	158	PHE	CA-CB-CG	7.23	121.03	113.80	2	3
1	A	37	LYS	CA-C-O	-7.19	112.62	121.89	4	2
1	A	161	ASP	CA-C-O	-7.18	110.08	119.06	17	1
1	A	104	ASP	N-CA-CB	-7.18	98.36	110.49	10	8
1	A	69	GLY	N-CA-C	7.18	130.19	113.18	5	2
1	A	45	HIS	CB-CG-CD2	-7.09	121.98	131.20	14	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	169	PHE	CA-CB-CG	7.04	120.84	113.80	10	3
1	A	10	THR	OG1-CB-CG2	-7.03	95.24	109.30	11	1
1	A	140	ASN	CA-CB-CG	6.94	119.54	112.60	6	12
1	A	53	LEU	CB-CA-C	6.88	122.54	110.85	13	1
1	A	119	PHE	CA-CB-CG	6.79	120.59	113.80	6	14
1	A	35	PHE	CA-CB-CG	6.79	120.59	113.80	11	7
1	A	58	ASP	N-CA-C	6.78	119.25	111.11	10	17
1	A	44	GLU	N-CA-C	6.75	118.64	111.28	14	7
1	A	17	PHE	N-CA-C	6.59	118.12	111.07	17	3
1	A	40	GLU	CA-C-N	6.56	133.49	121.94	14	1
1	A	40	GLU	C-N-CA	6.56	133.49	121.94	14	1
1	A	169	PHE	N-CA-C	6.51	124.67	110.80	13	1
1	A	35	PHE	N-CA-CB	-6.49	100.66	110.07	6	2
1	A	10	THR	CB-CA-C	-6.49	100.69	110.88	4	3
1	A	23	ILE	N-CA-CB	-6.42	103.68	111.00	15	1
1	A	61	LEU	N-CA-C	6.42	124.46	110.80	11	1
1	A	105	THR	N-CA-C	6.37	119.91	111.75	14	5
1	A	106	ASN	CA-CB-CG	6.32	118.92	112.60	11	8
1	A	163	ASP	CA-CB-CG	6.31	118.91	112.60	13	1
1	A	45	HIS	CG-ND1-CE1	-6.30	98.59	109.30	1	17
1	A	89	LYS	N-CA-C	6.22	118.85	111.33	3	5
1	A	56	VAL	CA-CB-CG2	6.14	120.84	110.40	7	1
1	A	148	GLU	N-CA-CB	-6.14	101.11	110.01	15	2
1	A	83	VAL	N-CA-CB	-6.14	98.06	111.81	4	1
1	A	168	VAL	CA-CB-CG1	6.12	120.80	110.40	13	2
1	A	165	THR	N-CA-C	6.07	118.69	111.71	17	2
1	A	14	ARG	CB-CA-C	5.99	122.52	109.99	5	1
1	A	93	GLU	N-CA-CB	-5.98	101.28	110.20	17	2
1	A	9	LYS	N-CA-CB	-5.98	101.33	110.12	10	2
1	A	7	LYS	CB-CA-C	5.97	120.33	110.90	4	1
1	A	161	ASP	N-CA-C	5.97	119.39	111.75	13	1
1	A	14	ARG	CB-CG-CD	5.97	125.02	111.30	13	3
1	A	92	VAL	CB-CA-C	5.96	119.45	111.94	1	2
1	A	88	ALA	N-CA-C	5.93	120.38	113.20	17	3
1	A	148	GLU	CB-CA-C	5.92	120.17	110.88	5	2
1	A	151	VAL	CA-CB-CG1	5.91	120.45	110.40	9	3
1	A	141	ASN	N-CA-C	5.91	119.54	111.39	2	1
1	A	57	TRP	N-CA-C	-5.90	104.48	111.03	9	1
1	A	159	MET	CA-C-O	-5.87	112.12	120.51	15	2
1	A	82	MET	N-CA-C	5.86	117.66	111.28	10	3
1	A	164	SER	N-CA-CB	-5.80	102.06	110.36	7	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	LYS	N-CA-C	5.79	117.59	111.28	7	2
1	A	87	GLU	N-CA-C	5.78	118.53	111.82	17	1
1	A	106	ASN	OD1-CG-ND2	-5.78	116.82	122.60	5	1
1	A	6	GLN	CA-C-O	-5.74	113.37	119.97	14	2
1	A	120	PHE	CA-CB-CG	5.73	119.53	113.80	15	2
1	A	89	LYS	CA-CB-CG	5.71	125.51	114.10	6	2
1	A	66	GLY	CA-C-N	5.68	132.53	121.41	8	3
1	A	66	GLY	C-N-CA	5.68	132.53	121.41	8	3
1	A	36	ALA	N-CA-C	5.67	117.14	111.07	2	4
1	A	151	VAL	CB-CA-C	5.67	119.44	112.02	7	3
1	A	92	VAL	CA-CB-CG2	5.65	120.01	110.40	14	1
1	A	85	ASN	CB-CA-C	5.64	115.51	110.44	2	1
1	A	62	THR	CA-CB-CG2	5.60	120.03	110.50	15	2
1	A	142	ASP	CA-CB-CG	5.59	118.19	112.60	1	1
1	A	48	VAL	CA-CB-CG1	5.57	119.88	110.40	16	9
1	A	61	LEU	CA-C-N	5.57	128.00	120.38	15	3
1	A	61	LEU	C-N-CA	5.57	128.00	120.38	15	3
1	A	15	ILE	CA-C-O	-5.55	114.77	120.71	16	1
1	A	53	LEU	N-CA-CB	-5.54	101.95	110.16	13	1
1	A	24	THR	CA-CB-CG2	5.54	119.92	110.50	12	12
1	A	60	PHE	CA-C-N	5.53	132.10	121.54	15	1
1	A	60	PHE	C-N-CA	5.53	132.10	121.54	15	1
1	A	62	THR	N-CA-C	5.48	118.01	111.71	4	3
1	A	7	LYS	N-CA-CB	-5.46	101.94	109.91	5	1
1	A	46	ALA	N-CA-C	5.45	117.65	111.11	17	1
1	A	159	MET	N-CA-CB	-5.43	103.36	110.59	14	1
1	A	19	LYS	N-CA-C	5.42	119.18	112.24	13	4
1	A	148	GLU	CA-CB-CG	5.41	124.92	114.10	12	2
1	A	135	ASP	CA-CB-CG	5.39	117.99	112.60	12	3
1	A	61	LEU	N-CA-CB	-5.38	101.41	110.49	15	1
1	A	160	ASN	CB-CG-OD1	5.37	131.54	120.80	11	1
1	A	108	ASP	N-CA-CB	-5.36	103.77	110.90	1	1
1	A	27	ASP	N-CA-CB	-5.33	102.28	110.01	8	1
1	A	17	PHE	CA-CB-CG	5.33	119.13	113.80	1	1
1	A	57	TRP	CA-C-O	-5.32	115.42	120.90	4	1
1	A	159	MET	N-CA-C	5.32	119.82	113.23	8	3
1	A	6	GLN	CG-CD-OE1	5.31	131.41	120.80	13	2
1	A	77	ASN	CB-CG-OD1	5.31	131.41	120.80	13	1
1	A	162	GLY	N-CA-C	5.29	119.34	112.25	4	2
1	A	45	HIS	ND1-CG-CD2	5.22	111.33	106.10	15	1
1	A	130	ALA	CA-C-O	-5.21	114.13	119.08	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	100	PHE	N-CA-CB	-5.20	102.19	109.94	6	1
1	A	48	VAL	N-CA-C	5.19	115.81	110.36	5	1
1	A	69	GLY	CA-C-O	-5.19	116.84	121.41	7	1
1	A	126	ASP	CA-CB-CG	5.19	117.79	112.60	13	1
1	A	67	GLY	CA-C-O	-5.18	111.55	120.57	9	1
1	A	141	ASN	OD1-CG-ND2	-5.18	117.42	122.60	16	2
1	A	158	PHE	N-CA-C	5.17	118.06	111.69	7	1
1	A	59	ASN	CA-CB-CG	5.16	117.76	112.60	11	3
1	A	19	LYS	N-CA-CB	-5.15	104.76	113.15	1	1
1	A	173	LEU	N-CA-C	5.09	117.68	110.50	9	1
1	A	167	LYS	N-CA-C	5.09	121.64	110.80	7	1
1	A	139	THR	CA-CB-CG2	5.08	119.14	110.50	5	1
1	A	16	ASP	N-CA-CB	-5.04	102.53	110.49	13	1
1	A	70	ILE	CA-CB-CG1	5.03	118.94	110.40	1	1
1	A	71	ASP	N-CA-CB	-5.02	103.50	110.38	13	1
1	A	163	ASP	CA-C-N	5.00	131.85	122.74	14	1
1	A	163	ASP	C-N-CA	5.00	131.85	122.74	14	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	168	VAL	Mainchain	8
1	A	25	ARG	Sidechain	7
1	A	34	ARG	Sidechain	6
1	A	43	ALA	Mainchain	6
1	A	41	MET	Mainchain	6
1	A	14	ARG	Sidechain,Mainchain	4
1	A	66	GLY	Mainchain	4
1	A	68	LYS	Mainchain	3
1	A	87	GLU	Mainchain	3
1	A	40	GLU	Mainchain	3
1	A	59	ASN	Sidechain	2
1	A	85	ASN	Sidechain	2
1	A	37	LYS	Mainchain	2
1	A	166	ASN	Sidechain,Mainchain	2
1	A	113	ARG	Sidechain	2
1	A	44	GLU	Mainchain	2
1	A	6	GLN	Sidechain	2
1	A	60	PHE	Mainchain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	160	ASN	Sidechain,Mainchain	2
1	A	159	MET	Mainchain	2
1	A	45	HIS	Sidechain	2
1	A	100	PHE	Sidechain	1
1	A	142	ASP	Mainchain	1
1	A	83	VAL	Mainchain	1
1	A	42	LYS	Mainchain	1
1	A	167	LYS	Mainchain	1
1	A	157	PHE	Sidechain	1
1	A	67	GLY	Mainchain	1
1	A	125	LEU	Mainchain	1
1	A	77	ASN	Sidechain	1
1	A	165	THR	Mainchain	1
1	A	64	VAL	Mainchain	1
1	A	163	ASP	Mainchain	1
1	A	161	ASP	Mainchain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1368	1310	1310	7±2
All	All	23256	22270	22259	127

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ALA:HB2	1:A:165:THR:OG1	0.89	1.68	5	3
1:A:6:GLN:O	1:A:10:THR:OG1	0.81	1.97	14	11
1:A:41:MET:CB	1:A:105:THR:OG1	0.73	2.36	15	8
1:A:57:TRP:O	1:A:62:THR:OG1	0.68	2.11	7	17
1:A:41:MET:SD	1:A:105:THR:OG1	0.68	2.50	10	3
1:A:41:MET:HA	1:A:105:THR:OG1	0.66	1.90	11	7
1:A:41:MET:HB3	1:A:105:THR:OG1	0.65	1.91	17	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ALA:CB	1:A:165:THR:OG1	0.65	2.45	3	2
1:A:57:TRP:C	1:A:62:THR:HG1	0.61	2.03	3	5
1:A:41:MET:HB2	1:A:105:THR:OG1	0.58	1.98	1	3
1:A:110:ASN:CB	1:A:144:LEU:HD11	0.54	2.32	9	1
1:A:57:TRP:C	1:A:62:THR:OG1	0.53	2.51	4	11
1:A:41:MET:HA	1:A:105:THR:HG1	0.53	1.62	11	1
1:A:110:ASN:CB	1:A:144:LEU:HD12	0.53	2.34	5	8
1:A:71:ASP:OD1	1:A:73:THR:OG1	0.52	2.28	6	2
1:A:136:ALA:HB2	1:A:165:THR:HG1	0.52	1.65	5	1
1:A:41:MET:HE2	1:A:41:MET:O	0.52	2.05	17	1
1:A:7:LYS:HA	1:A:10:THR:OG1	0.51	2.04	15	2
1:A:136:ALA:HB1	1:A:165:THR:OG1	0.48	2.09	3	1
1:A:126:ASP:O	1:A:129:MET:SD	0.48	2.72	6	1
1:A:36:ALA:HA	1:A:41:MET:SD	0.48	2.49	4	1
1:A:49:LEU:H	1:A:49:LEU:HD23	0.47	1.69	15	1
1:A:56:VAL:CG2	1:A:98:LEU:HB3	0.47	2.39	10	1
1:A:96:LEU:HD21	1:A:154:GLY:HA3	0.47	1.85	16	1
1:A:41:MET:CA	1:A:105:THR:OG1	0.46	2.62	11	3
1:A:126:ASP:OD2	1:A:128:THR:OG1	0.46	2.33	13	1
1:A:36:ALA:O	1:A:41:MET:HE2	0.46	2.11	7	1
1:A:110:ASN:HB2	1:A:144:LEU:HD12	0.45	1.89	5	2
1:A:146:SER:OG	1:A:149:GLU:OE1	0.44	2.35	8	2
1:A:40:GLU:O	1:A:105:THR:OG1	0.44	2.27	8	2
1:A:41:MET:HG2	1:A:105:THR:OG1	0.44	2.11	4	1
1:A:14:ARG:HD3	1:A:125:LEU:HD11	0.43	1.89	3	1
1:A:112:SER:OG	1:A:115:GLU:OE1	0.43	2.36	16	4
1:A:96:LEU:HD23	1:A:151:VAL:HA	0.43	1.89	16	1
1:A:93:GLU:OE2	1:A:155:SER:OG	0.42	2.37	9	2
1:A:96:LEU:HD22	1:A:154:GLY:HA3	0.41	1.92	8	1
1:A:71:ASP:OD2	1:A:73:THR:OG1	0.41	2.33	15	1
1:A:39:SER:O	1:A:41:MET:HE3	0.41	2.14	7	1
1:A:146:SER:OG	1:A:148:GLU:OE1	0.41	2.37	5	1
1:A:10:THR:OG1	1:A:11:TYR:N	0.40	2.54	3	1
1:A:89:LYS:O	1:A:92:VAL:HG13	0.40	2.17	10	1
1:A:39:SER:HB3	1:A:41:MET:SD	0.40	2.57	17	1
1:A:110:ASN:HB2	1:A:144:LEU:HD11	0.40	1.93	9	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/174 (99%)	154±2 (90±1%)	13±3 (8±2%)	5±1 (3±1%)	6	41
All	All	2924/2958 (99%)	2624 (90%)	222 (8%)	78 (3%)	6	41

All 25 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	43	ALA	12
1	A	138	ASP	12
1	A	104	ASP	6
1	A	163	ASP	6
1	A	164	SER	6
1	A	109	ASN	5
1	A	69	GLY	4
1	A	44	GLU	3
1	A	88	ALA	3
1	A	165	THR	2
1	A	167	LYS	2
1	A	67	GLY	2
1	A	107	GLU	2
1	A	61	LEU	2
1	A	173	LEU	1
1	A	41	MET	1
1	A	105	THR	1
1	A	16	ASP	1
1	A	68	LYS	1
1	A	40	GLU	1
1	A	45	HIS	1
1	A	42	LYS	1
1	A	160	ASN	1
1	A	169	PHE	1
1	A	64	VAL	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	148/148 (100%)	130±3 (88±2%)	18±3 (12±2%)	7	49
All	All	2516/2516 (100%)	2211 (88%)	305 (12%)	7	49

All 77 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	73	THR	17
1	A	19	LYS	15
1	A	20	ASP	15
1	A	10	THR	14
1	A	24	THR	14
1	A	48	VAL	10
1	A	92	VAL	9
1	A	125	LEU	9
1	A	127	LYS	9
1	A	168	VAL	9
1	A	96	LEU	8
1	A	101	ARG	7
1	A	144	LEU	7
1	A	89	LYS	6
1	A	112	SER	6
1	A	83	VAL	6
1	A	34	ARG	6
1	A	42	LYS	6
1	A	151	VAL	5
1	A	113	ARG	5
1	A	40	GLU	5
1	A	109	ASN	5
1	A	38	GLU	4
1	A	93	GLU	4
1	A	139	THR	4
1	A	166	ASN	4
1	A	108	ASP	4
1	A	123	LEU	4
1	A	41	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	141	ASN	4
1	A	9	LYS	4
1	A	39	SER	3
1	A	68	LYS	3
1	A	174	VAL	3
1	A	37	LYS	3
1	A	81	GLU	3
1	A	33	GLU	3
1	A	80	LYS	3
1	A	129	MET	3
1	A	161	ASP	3
1	A	71	ASP	3
1	A	84	LYS	2
1	A	15	ILE	2
1	A	47	LYS	2
1	A	82	MET	2
1	A	14	ARG	2
1	A	3	LEU	2
1	A	148	GLU	2
1	A	50	MET	2
1	A	49	LEU	2
1	A	17	PHE	2
1	A	27	ASP	1
1	A	52	SER	1
1	A	58	ASP	1
1	A	51	ASP	1
1	A	44	GLU	1
1	A	122	MET	1
1	A	98	LEU	1
1	A	103	VAL	1
1	A	114	ASP	1
1	A	62	THR	1
1	A	110	ASN	1
1	A	87	GLU	1
1	A	61	LEU	1
1	A	2	ASP	1
1	A	6	GLN	1
1	A	59	ASN	1
1	A	29	GLU	1
1	A	45	HIS	1
1	A	53	LEU	1
1	A	146	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	160	ASN	1
1	A	18	ASP	1
1	A	140	ASN	1
1	A	156	ASP	1
1	A	159	MET	1
1	A	118	ILE	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 52% for the well-defined parts and 52% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1195
Number of shifts mapped to atoms	1195
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	165	2.68 ± 0.26	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 52%, i.e. 1195 atoms were assigned a chemical shift out of a possible 2303. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	511/873 (59%)	346/356 (97%)	0/348 (0%)	165/169 (98%)
Sidechain	582/1219 (48%)	571/789 (72%)	0/391 (0%)	11/39 (28%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	102/211 (48%)	99/105 (94%)	0/102 (0%)	3/4 (75%)
Overall	1195/2303 (52%)	1016/1250 (81%)	0/841 (0%)	179/212 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 52%, i.e. 1195 atoms were assigned a chemical shift out of a possible 2303. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	511/873 (59%)	346/356 (97%)	0/348 (0%)	165/169 (98%)
Sidechain	582/1219 (48%)	571/789 (72%)	0/391 (0%)	11/39 (28%)
Aromatic	102/211 (48%)	99/105 (94%)	0/102 (0%)	3/4 (75%)
Overall	1195/2303 (52%)	1016/1250 (81%)	0/841 (0%)	179/212 (84%)

7.1.4 Statistically unusual chemical shifts ⓘ

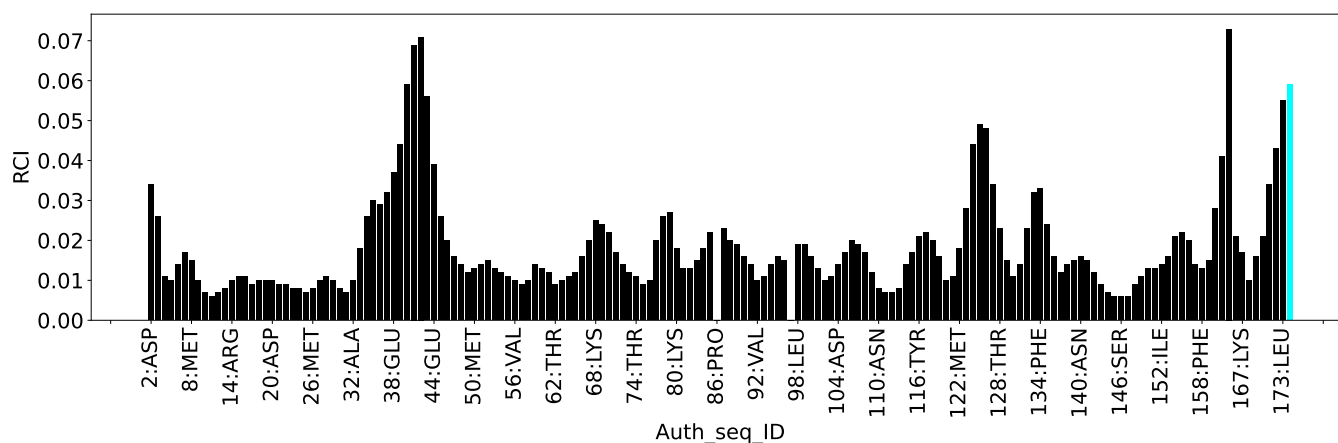
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	25	ARG	NE	115.80	76.53 – 92.65	19.4
1	A	14	ARG	NE	115.50	76.53 – 92.65	19.2
1	A	113	ARG	HG2	-0.06	0.26 – 2.87	-6.2
1	A	25	ARG	HB3	0.22	0.43 – 3.11	-5.8
1	A	154	GLY	HA3	1.81	2.08 – 5.71	-5.7

7.1.5 Random Coil Index (RCI) plots ⓘ

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping ⓘ

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	4
Number of shifts mapped to atoms	2
Number of unparsed shifts	0
Number of shifts with mapping errors	2
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 2 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	1	SER	H	9.54	0.01	1
2	A	1	SER	H3	1.84	0.01	1

7.2.2 Chemical shift referencing ⓘ

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 3 atoms were assigned a chemical shift out of a possible 2303. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	2/873 (0%)	2/356 (1%)	0/348 (0%)	0/169 (0%)
Sidechain	1/1219 (0%)	1/789 (0%)	0/391 (0%)	0/39 (0%)
Aromatic	0/211 (0%)	0/105 (0%)	0/102 (0%)	0/4 (0%)
Overall	3/2303 (0%)	3/1250 (0%)	0/841 (0%)	0/212 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 3 atoms were assigned a chemical shift out of a possible 2303. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	2/873 (0%)	2/356 (1%)	0/348 (0%)	0/169 (0%)
Sidechain	1/1219 (0%)	1/789 (0%)	0/391 (0%)	0/39 (0%)
Aromatic	0/211 (0%)	0/105 (0%)	0/102 (0%)	0/4 (0%)
Overall	3/2303 (0%)	3/1250 (0%)	0/841 (0%)	0/212 (0%)

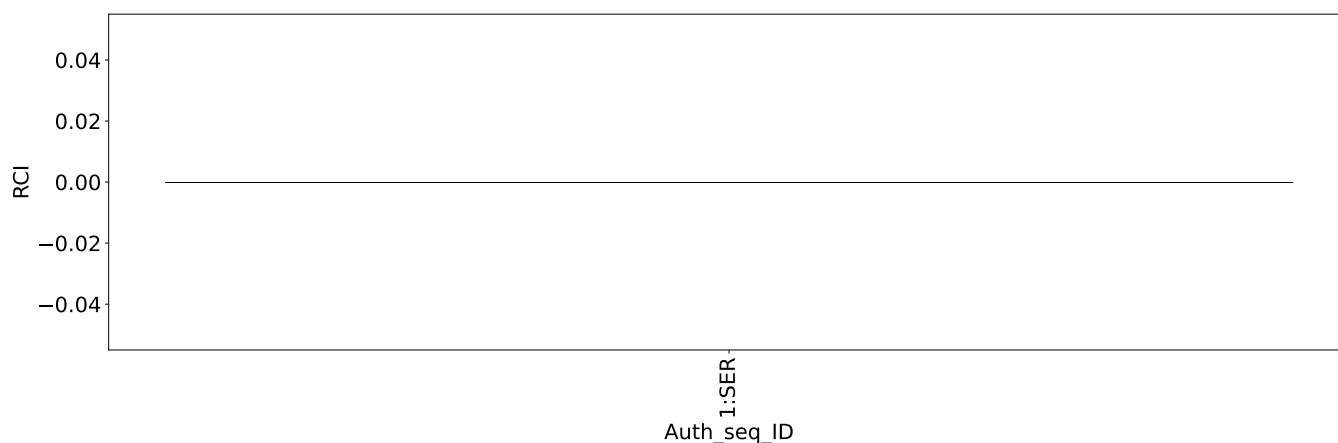
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	11
Number of shifts mapped to atoms	11
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.3.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 0%, i.e. 11 atoms were assigned a chemical shift out of a possible 2303. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	11/873 (1%)	11/356 (3%)	0/348 (0%)	0/169 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Sidechain	0/1219 (0%)	0/789 (0%)	0/391 (0%)	0/39 (0%)
Aromatic	0/211 (0%)	0/105 (0%)	0/102 (0%)	0/4 (0%)
Overall	11/2303 (0%)	11/1250 (1%)	0/841 (0%)	0/212 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 11 atoms were assigned a chemical shift out of a possible 2303. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	11/873 (1%)	11/356 (3%)	0/348 (0%)	0/169 (0%)
Sidechain	0/1219 (0%)	0/789 (0%)	0/391 (0%)	0/39 (0%)
Aromatic	0/211 (0%)	0/105 (0%)	0/102 (0%)	0/4 (0%)
Overall	11/2303 (0%)	11/1250 (1%)	0/841 (0%)	0/212 (0%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.3.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

