



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:21 pm BST

PDB ID : 2K2O
Title : Solution Structure of the inner DysF domain of human myoferlin
Authors : Patel, P.; Harris, R.; Keep, N.; Driscoll, P.
Deposited on : 2008-04-07

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

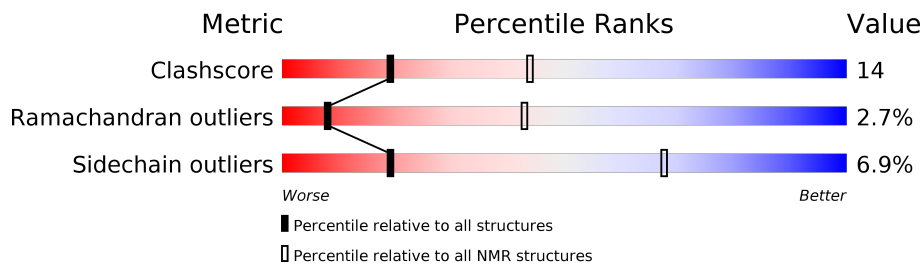
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	123	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:927-A:1033 (107)	0.54	7

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1932 atoms, of which 929 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Myoferlin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	123	1932	624	929	178	199	2	0

There are 5 discrepancies between the modelled and reference sequences:

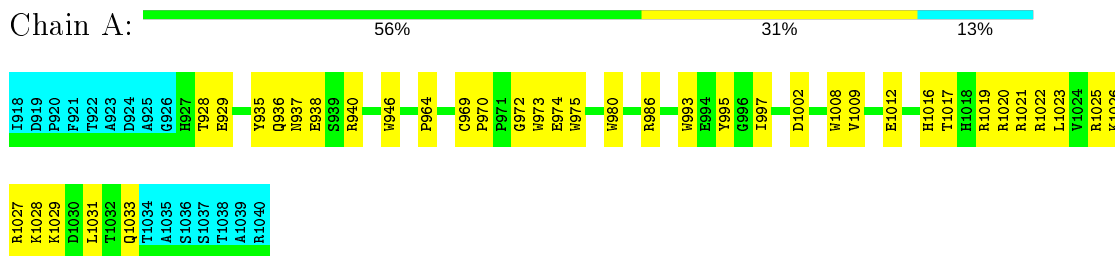
Chain	Residue	Modelled	Actual	Comment	Reference
A	918	ILE	-	expression tag	UNP Q9NZM1
A	919	ASP	-	expression tag	UNP Q9NZM1
A	920	PRO	-	expression tag	UNP Q9NZM1
A	921	PHE	-	expression tag	UNP Q9NZM1
A	922	THR	-	expression tag	UNP Q9NZM1

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Myoferlin

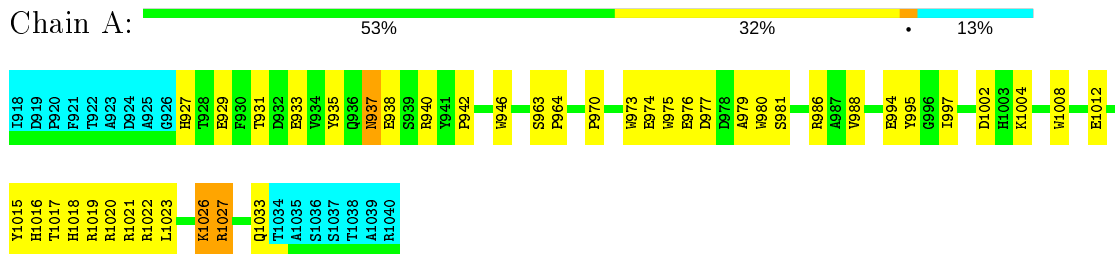


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Myoferlin



4.2.2 Score per residue for model 2

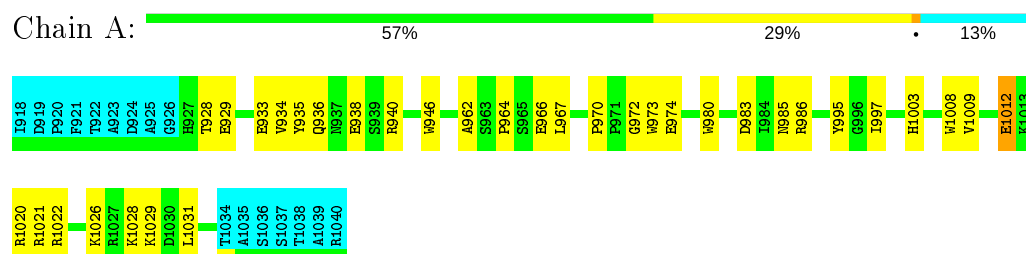
- Molecule 1: Myoferlin





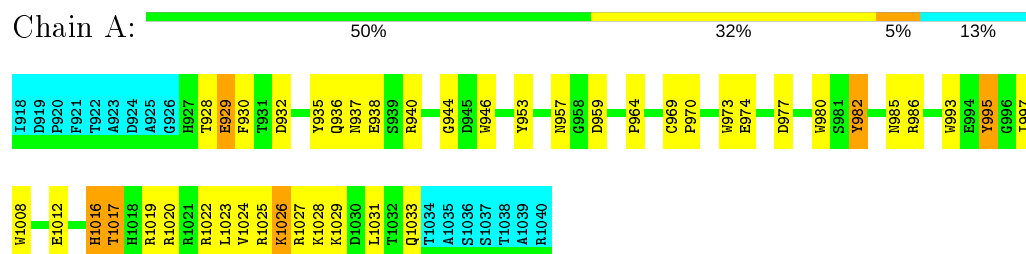
4.2.3 Score per residue for model 3

- Molecule 1: Myoferlin



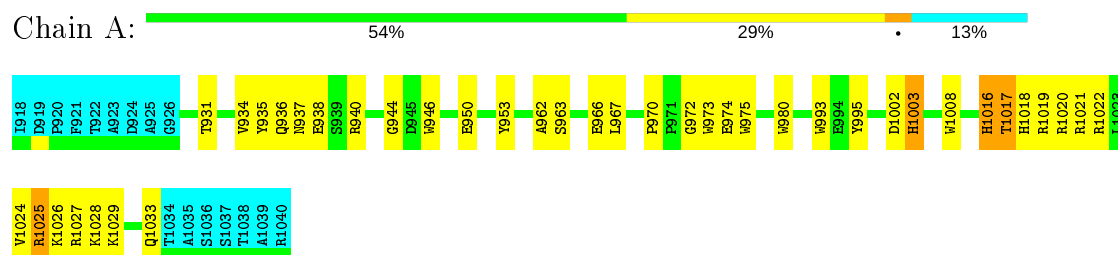
4.2.4 Score per residue for model 4

- Molecule 1: Myoferlin



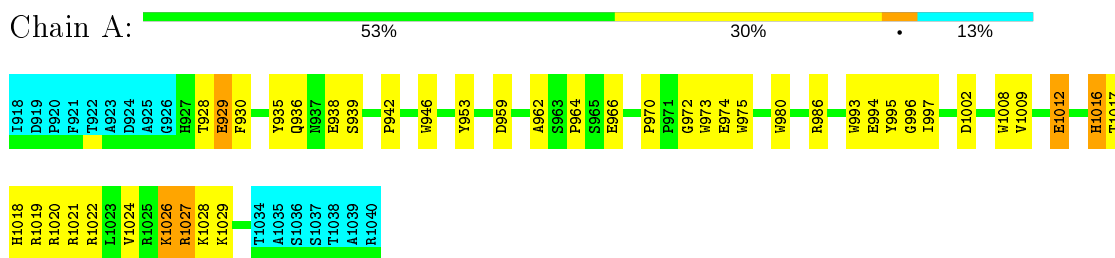
4.2.5 Score per residue for model 5

- Molecule 1: Myoferlin



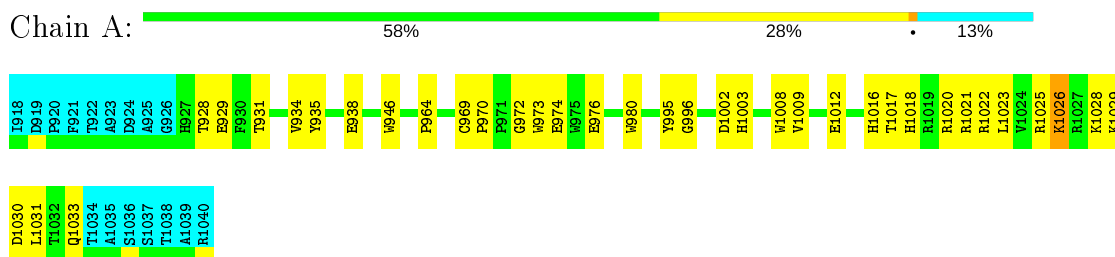
4.2.6 Score per residue for model 6

- Molecule 1: Myoferlin



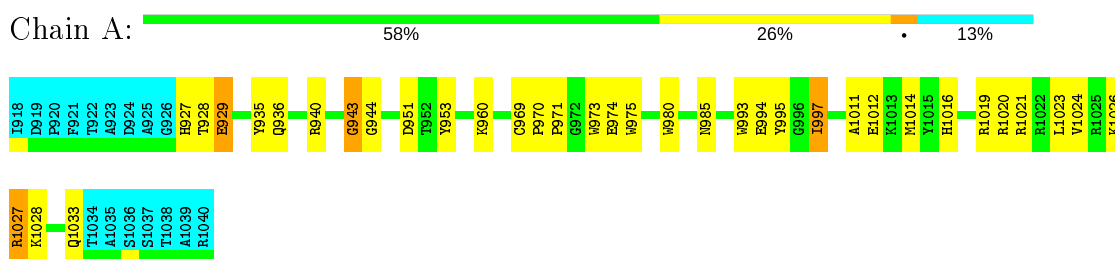
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Myoferlin



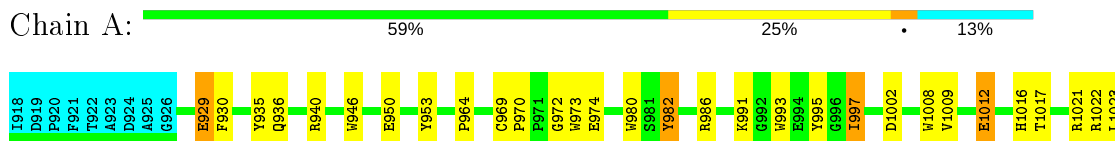
4.2.8 Score per residue for model 8

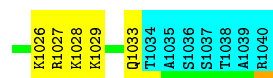
- Molecule 1: Myoferlin



4.2.9 Score per residue for model 9

- Molecule 1: Myoferlin

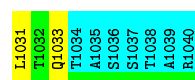
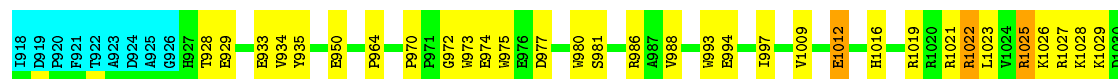




4.2.10 Score per residue for model 10

- Molecule 1: Myoferlin

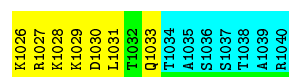
Chain A: 59% 25% 13%



4.2.11 Score per residue for model 11

- Molecule 1: Myoferlin

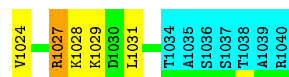
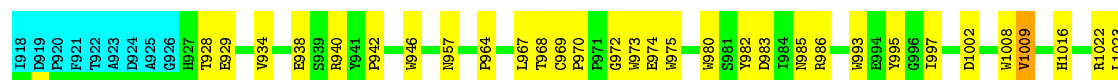
Chain A: 55% 28% 13%



4.2.12 Score per residue for model 12

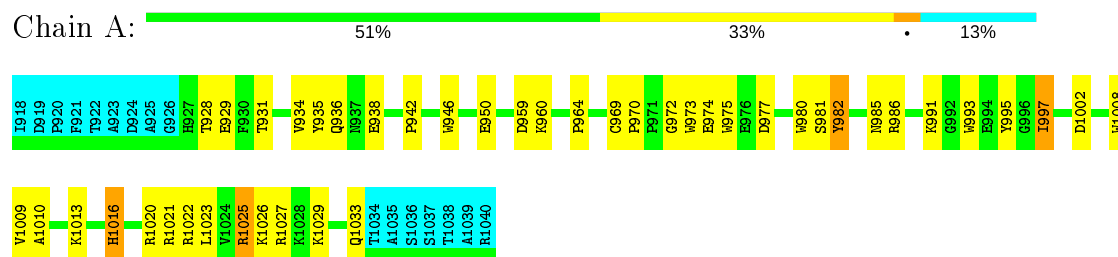
- Molecule 1: Myoferlin

Chain A: 58% 28% 13%



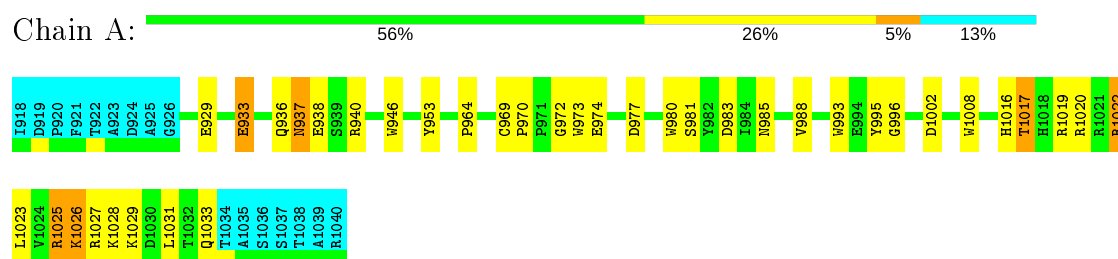
4.2.13 Score per residue for model 13

- Molecule 1: Myoferlin



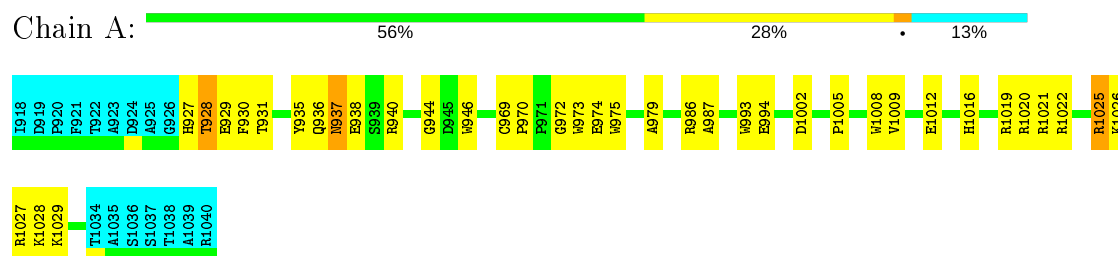
4.2.14 Score per residue for model 14

- Molecule 1: Myoferlin



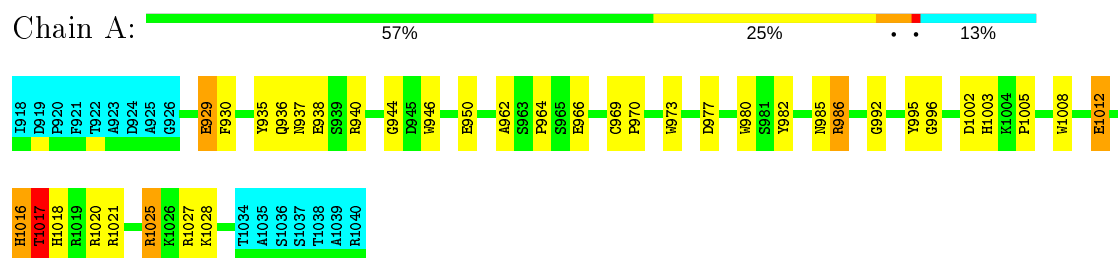
4.2.15 Score per residue for model 15

- Molecule 1: Myoferlin



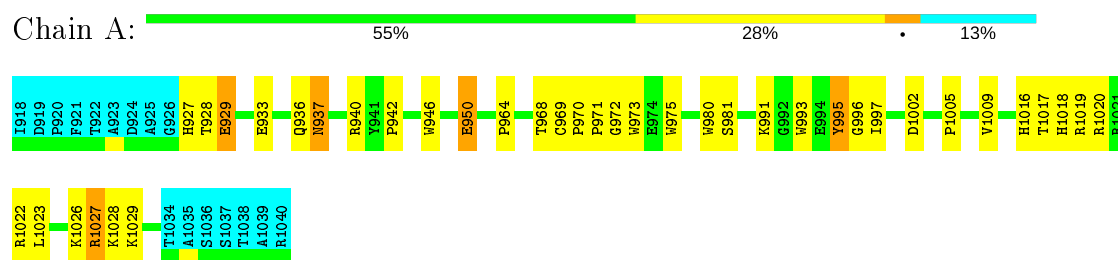
4.2.16 Score per residue for model 16

- Molecule 1: Myoferlin



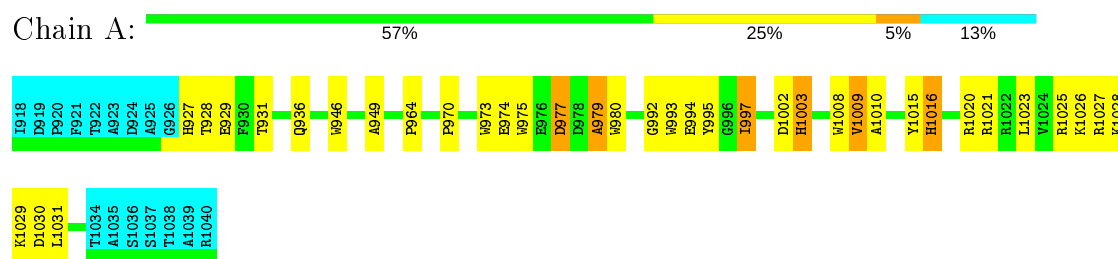
4.2.17 Score per residue for model 17

- Molecule 1: Myoferlin



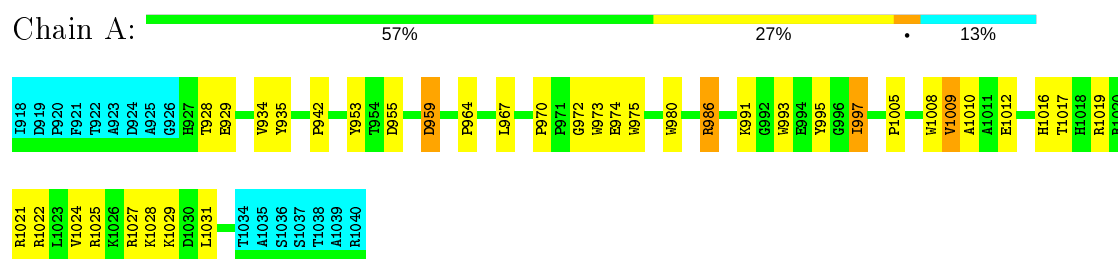
4.2.18 Score per residue for model 18

- Molecule 1: Myoferlin



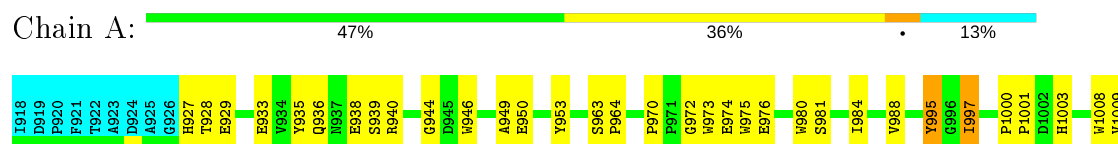
4.2.19 Score per residue for model 19

- Molecule 1: Myoferlin



4.2.20 Score per residue for model 20

- Molecule 1: Myoferlin



A1010	A1011	E1012	K1013	H1016	R1020	R1021	R1022	L1023	V1024	R1025	K1026	R1027	K1028	K1029	D1030	L1031	T1032	Q1033	T1034	A1035	S1036	S1037	T1038	A1039	R1040
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5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNSSOLVE	structure solution	1.2
CNSSOLVE	refinement	1.2

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1497
Number of shifts mapped to atoms	1497
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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	0.8±0.7
All	All	0	17

There are no bond-length outliers.

There are no bond-angle outliers.

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	1027	ARG	Sidechain	8
1	A	1022	ARG	Sidechain	5
1	A	986	ARG	Sidechain	3
1	A	1021	ARG	Sidechain	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	892	825	821	24±4
All	All	17840	16500	16420	486

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:937:ASN:HB3	1:A:1020:ARG:HB3	0.85	1.45	1	2
1:A:937:ASN:HB3	1:A:1020:ARG:HG2	0.81	1.53	11	2
1:A:974:GLU:HB3	1:A:1033:GLN:HE22	0.80	1.35	13	1
1:A:972:GLY:HA2	1:A:1033:GLN:HB3	0.74	1.57	14	2
1:A:997:ILE:HB	1:A:1016:HIS:HD2	0.73	1.41	10	1
1:A:995:TYR:HA	1:A:1016:HIS:NE2	0.72	2.00	14	10
1:A:933:GLU:HB2	1:A:1022:ARG:HG3	0.71	1.63	20	6
1:A:974:GLU:HB2	1:A:1033:GLN:HE21	0.71	1.46	4	2
1:A:988:VAL:HG12	1:A:994:GLU:HG2	0.70	1.63	10	2
1:A:929:GLU:HA	1:A:1028:LYS:HA	0.68	1.65	16	5
1:A:1025:ARG:HA	1:A:1025:ARG:NE	0.68	2.02	13	4
1:A:977:ASP:HB3	1:A:1025:ARG:NH1	0.67	2.05	16	3
1:A:981:SER:O	1:A:1023:LEU:HA	0.67	1.90	20	7
1:A:993:TRP:HB3	1:A:1019:ARG:HD2	0.66	1.66	15	3
1:A:997:ILE:O	1:A:1005:PRO:HA	0.66	1.90	17	1
1:A:995:TYR:O	1:A:1008:TRP:HA	0.65	1.92	13	14
1:A:1025:ARG:NE	1:A:1025:ARG:HA	0.64	2.06	11	1
1:A:995:TYR:HB3	1:A:1011:ALA:HA	0.64	1.67	20	1
1:A:936:GLN:O	1:A:1020:ARG:HA	0.63	1.94	5	13
1:A:930:PHE:O	1:A:1027:ARG:HG2	0.63	1.93	4	6
1:A:1009:VAL:HG12	1:A:1010:ALA:H	0.62	1.53	19	3
1:A:994:GLU:HG3	1:A:1008:TRP:CE3	0.60	2.31	15	4
1:A:1028:LYS:HG2	1:A:1030:ASP:H	0.60	1.54	7	1
1:A:1012:GLU:HA	1:A:1016:HIS:CE1	0.60	2.32	11	12
1:A:994:GLU:HG2	1:A:1020:ARG:O	0.59	1.97	6	2
1:A:964:PRO:HB3	1:A:980:TRP:CG	0.59	2.32	19	16
1:A:935:TYR:HA	1:A:1021:ARG:O	0.59	1.98	5	15
1:A:1005:PRO:HB2	1:A:1008:TRP:CZ2	0.59	2.32	4	4
1:A:997:ILE:HB	1:A:1016:HIS:CD2	0.59	2.31	10	1
1:A:993:TRP:CE3	1:A:1019:ARG:HG2	0.58	2.32	4	7
1:A:972:GLY:O	1:A:1029:LYS:HG3	0.58	1.99	6	11
1:A:974:GLU:HB3	1:A:1033:GLN:NE2	0.58	2.13	13	1
1:A:997:ILE:HD12	1:A:1015:TYR:HE1	0.57	1.59	18	1
1:A:977:ASP:OD1	1:A:1026:LYS:HB3	0.57	2.00	4	5
1:A:976:GLU:HB2	1:A:1028:LYS:HD2	0.56	1.77	20	1
1:A:975:TRP:CZ3	1:A:1027:ARG:HB3	0.56	2.35	20	10
1:A:969:CYS:HB2	1:A:973:TRP:O	0.56	1.99	11	11
1:A:940:ARG:HG2	1:A:946:TRP:CZ3	0.56	2.34	15	3
1:A:993:TRP:HB3	1:A:1019:ARG:CD	0.56	2.31	19	1
1:A:939:SER:OG	1:A:949:ALA:HA	0.56	2.00	20	1
1:A:939:SER:HB3	1:A:1018:HIS:CD2	0.56	2.36	6	1
1:A:995:TYR:HB3	1:A:1009:VAL:H	0.56	1.61	13	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:940:ARG:O	1:A:1017:THR:HA	0.56	2.00	5	4
1:A:974:GLU:HB3	1:A:1028:LYS:O	0.55	2.01	19	11
1:A:975:TRP:CE3	1:A:1025:ARG:HG2	0.55	2.37	15	2
1:A:946:TRP:CZ2	1:A:1019:ARG:HG2	0.55	2.37	15	1
1:A:995:TYR:HB2	1:A:1016:HIS:CG	0.55	2.35	20	1
1:A:1026:LYS:HE2	1:A:1028:LYS:HE3	0.55	1.79	2	1
1:A:946:TRP:CH2	1:A:1016:HIS:HB3	0.54	2.38	4	8
1:A:929:GLU:HB3	1:A:1028:LYS:HB3	0.54	1.79	8	2
1:A:964:PRO:HB3	1:A:980:TRP:CD1	0.53	2.38	4	12
1:A:934:VAL:O	1:A:1022:ARG:HA	0.53	2.04	12	6
1:A:997:ILE:HG22	1:A:1016:HIS:HA	0.53	1.79	20	1
1:A:951:ASP:HB3	1:A:960:LYS:HD3	0.53	1.79	8	1
1:A:935:TYR:O	1:A:953:TYR:HA	0.52	2.05	5	6
1:A:986:ARG:HD2	1:A:1022:ARG:NH1	0.52	2.19	19	3
1:A:929:GLU:HB3	1:A:1028:LYS:HD3	0.52	1.81	2	1
1:A:996:GLY:O	1:A:1018:HIS:HB2	0.52	2.04	6	2
1:A:975:TRP:CE3	1:A:1027:ARG:HB3	0.52	2.40	8	6
1:A:996:GLY:HA3	1:A:1008:TRP:CZ3	0.52	2.40	14	3
1:A:993:TRP:CE3	1:A:1019:ARG:HB3	0.52	2.40	15	1
1:A:970:PRO:HD2	1:A:973:TRP:HB2	0.52	1.82	9	20
1:A:937:ASN:CB	1:A:1020:ARG:HG2	0.51	2.33	11	1
1:A:957:ASN:HD21	1:A:959:ASP:HB2	0.51	1.65	4	1
1:A:985:ASN:C	1:A:986:ARG:HD2	0.51	2.26	4	5
1:A:940:ARG:HD2	1:A:944:GLY:O	0.51	2.05	15	7
1:A:980:TRP:HA	1:A:1024:VAL:O	0.51	2.06	6	6
1:A:993:TRP:CG	1:A:1019:ARG:HD3	0.51	2.41	17	1
1:A:1029:LYS:C	1:A:1031:LEU:H	0.50	2.09	10	8
1:A:1026:LYS:HD2	1:A:1027:ARG:N	0.50	2.21	4	3
1:A:993:TRP:CD2	1:A:1019:ARG:HD3	0.50	2.41	17	1
1:A:997:ILE:HG23	1:A:1016:HIS:CD2	0.50	2.42	8	1
1:A:935:TYR:CD2	1:A:1020:ARG:HD3	0.50	2.42	13	1
1:A:929:GLU:CB	1:A:1028:LYS:HB3	0.49	2.37	17	2
1:A:993:TRP:HE3	1:A:1019:ARG:HG2	0.49	1.67	4	1
1:A:997:ILE:HA	1:A:1016:HIS:HA	0.49	1.83	8	1
1:A:980:TRP:HB3	1:A:1023:LEU:HB3	0.49	1.83	12	7
1:A:938:GLU:HB3	1:A:946:TRP:HB3	0.49	1.84	7	13
1:A:955:ASP:HB3	1:A:959:ASP:HB3	0.49	1.84	19	1
1:A:997:ILE:HG22	1:A:1016:HIS:CD2	0.49	2.42	19	3
1:A:995:TYR:CE2	1:A:1009:VAL:HB	0.49	2.42	20	1
1:A:977:ASP:HB3	1:A:1025:ARG:NE	0.49	2.23	13	2
1:A:982:TYR:HA	1:A:1022:ARG:O	0.48	2.08	4	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:943:GLY:HA2	1:A:1014:MET:SD	0.48	2.48	8	1
1:A:994:GLU:O	1:A:1019:ARG:HG3	0.48	2.08	8	1
1:A:936:GLN:HG2	1:A:953:TYR:CE1	0.48	2.44	9	1
1:A:995:TYR:CE1	1:A:1013:LYS:HD3	0.48	2.43	2	1
1:A:932:ASP:HB2	1:A:1027:ARG:HD2	0.48	1.85	4	1
1:A:974:GLU:HB2	1:A:1033:GLN:NE2	0.48	2.23	10	4
1:A:995:TYR:CD2	1:A:1016:HIS:HE1	0.48	2.27	16	1
1:A:982:TYR:CD2	1:A:991:LYS:HA	0.47	2.44	13	1
1:A:993:TRP:HB3	1:A:1019:ARG:HD3	0.47	1.85	19	1
1:A:983:ASP:OD2	1:A:986:ARG:HD3	0.47	2.10	3	2
1:A:995:TYR:HA	1:A:1016:HIS:CE1	0.47	2.44	12	2
1:A:1008:TRP:CZ3	1:A:1020:ARG:HG2	0.47	2.44	2	5
1:A:946:TRP:CE2	1:A:1019:ARG:HG2	0.47	2.44	15	1
1:A:995:TYR:CE1	1:A:997:ILE:HB	0.47	2.44	4	1
1:A:995:TYR:HD2	1:A:1009:VAL:HB	0.47	1.70	17	1
1:A:995:TYR:HB3	1:A:1009:VAL:N	0.47	2.24	6	3
1:A:974:GLU:HB2	1:A:1033:GLN:HE22	0.46	1.69	1	2
1:A:931:THR:HA	1:A:1026:LYS:HA	0.46	1.85	18	7
1:A:991:LYS:HB2	1:A:993:TRP:CD1	0.46	2.45	13	4
1:A:940:ARG:HH21	1:A:1016:HIS:HB2	0.46	1.70	16	1
1:A:1029:LYS:O	1:A:1030:ASP:HB3	0.46	2.11	7	1
1:A:936:GLN:OE1	1:A:1023:LEU:HD21	0.46	2.11	8	1
1:A:976:GLU:HG2	1:A:1028:LYS:HB3	0.45	1.86	7	1
1:A:975:TRP:CZ3	1:A:1027:ARG:HD2	0.45	2.45	8	1
1:A:928:THR:HB	1:A:1029:LYS:HB2	0.45	1.87	15	1
1:A:933:GLU:HA	1:A:1023:LEU:O	0.45	2.12	2	1
1:A:997:ILE:HD12	1:A:1015:TYR:HB3	0.45	1.88	1	1
1:A:962:ALA:HB1	1:A:966:GLU:HB2	0.45	1.88	3	4
1:A:1013:LYS:O	1:A:1016:HIS:HB2	0.45	2.12	13	1
1:A:1029:LYS:O	1:A:1033:GLN:HG2	0.45	2.11	5	1
1:A:980:TRP:CD2	1:A:1025:ARG:HB2	0.45	2.47	20	5
1:A:936:GLN:HB3	1:A:953:TYR:CE2	0.45	2.47	14	1
1:A:995:TYR:CD2	1:A:1011:ALA:HA	0.45	2.47	8	1
1:A:1025:ARG:HA	1:A:1025:ARG:HE	0.45	1.72	10	3
1:A:1005:PRO:HG2	1:A:1018:HIS:HB2	0.44	1.87	16	1
1:A:995:TYR:CD2	1:A:1009:VAL:HB	0.44	2.48	17	1
1:A:974:GLU:HB2	1:A:1033:GLN:CD	0.44	2.33	5	1
1:A:970:PRO:HG2	1:A:973:TRP:HB2	0.44	1.90	19	5
1:A:972:GLY:O	1:A:1029:LYS:HA	0.44	2.12	9	1
1:A:1029:LYS:O	1:A:1033:GLN:HB2	0.44	2.12	7	1
1:A:993:TRP:CE3	1:A:1019:ARG:HD2	0.43	2.48	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:972:GLY:O	1:A:1029:LYS:HG2	0.43	2.12	15	1
1:A:927:HIS:HB2	1:A:929:GLU:OE1	0.43	2.14	2	1
1:A:977:ASP:HB3	1:A:1025:ARG:CZ	0.43	2.44	10	3
1:A:995:TYR:HE1	1:A:997:ILE:HB	0.43	1.71	4	1
1:A:970:PRO:CG	1:A:973:TRP:HB2	0.43	2.44	19	4
1:A:997:ILE:HG22	1:A:1016:HIS:HD2	0.43	1.74	19	1
1:A:940:ARG:HG2	1:A:946:TRP:CE3	0.43	2.49	12	3
1:A:950:GLU:CD	1:A:950:GLU:H	0.42	2.18	17	1
1:A:937:ASN:HA	1:A:1019:ARG:O	0.42	2.14	5	2
1:A:986:ARG:HG2	1:A:987:ALA:H	0.42	1.73	15	1
1:A:957:ASN:ND2	1:A:959:ASP:HB2	0.42	2.29	4	1
1:A:995:TYR:HB2	1:A:1016:HIS:CD2	0.42	2.50	20	1
1:A:929:GLU:HG3	1:A:1026:LYS:CE	0.42	2.45	6	1
1:A:929:GLU:HG3	1:A:1026:LYS:HE2	0.42	1.92	6	1
1:A:940:ARG:HB3	1:A:946:TRP:HA	0.42	1.91	1	2
1:A:937:ASN:OD1	1:A:1020:ARG:HB3	0.41	2.14	4	1
1:A:984:ILE:HA	1:A:988:VAL:HG21	0.41	1.91	20	1
1:A:993:TRP:CD2	1:A:1019:ARG:HD2	0.41	2.50	6	1
1:A:976:GLU:HG2	1:A:1026:LYS:HE2	0.41	1.90	1	1
1:A:962:ALA:HB1	1:A:966:GLU:CB	0.41	2.46	5	1
1:A:983:ASP:O	1:A:988:VAL:HG21	0.41	2.14	14	1
1:A:1013:LYS:O	1:A:1016:HIS:ND1	0.41	2.53	20	1
1:A:995:TYR:HB3	1:A:1009:VAL:HB	0.41	1.92	7	1
1:A:993:TRP:HA	1:A:1021:ARG:HB3	0.41	1.92	8	2
1:A:974:GLU:HB2	1:A:1033:GLN:OE1	0.41	2.15	14	1
1:A:973:TRP:CZ3	1:A:1029:LYS:HG3	0.41	2.50	15	1
1:A:1009:VAL:HG12	1:A:1010:ALA:N	0.41	2.29	19	1
1:A:1016:HIS:CD2	1:A:1019:ARG:HB3	0.41	2.51	1	1
1:A:969:CYS:HB3	1:A:975:TRP:NE1	0.41	2.31	17	1
1:A:986:ARG:HD3	1:A:1022:ARG:NH1	0.40	2.31	6	1
1:A:934:VAL:HG22	1:A:935:TYR:H	0.40	1.75	10	1
1:A:972:GLY:CA	1:A:1033:GLN:HB3	0.40	2.40	14	1
1:A:1000:PRO:HA	1:A:1001:PRO:HA	0.40	1.67	20	1
1:A:967:LEU:HD13	1:A:980:TRP:CH2	0.40	2.51	3	2
1:A:979:ALA:C	1:A:1025:ARG:HD3	0.40	2.37	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	107/123 (87%)	91±3 (85±2%)	13±3 (12±3%)	3±2 (3±1%)	8	43
All	All	2140/2460 (87%)	1816 (85%)	266 (12%)	58 (3%)	8	43

All 19 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	1002	ASP	14
1	A	942	PRO	6
1	A	1009	VAL	5
1	A	1003	HIS	5
1	A	950	GLU	4
1	A	979	ALA	3
1	A	959	ASP	3
1	A	1031	LEU	3
1	A	1030	ASP	3
1	A	1017	THR	2
1	A	992	GLY	2
1	A	943	GLY	1
1	A	1010	ALA	1
1	A	949	ALA	1
1	A	993	TRP	1
1	A	1012	GLU	1
1	A	1016	HIS	1
1	A	963	SER	1
1	A	927	HIS	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	93/104 (89%)	87±1 (93±1%)	6±1 (7±1%)	19	68
All	All	1860/2080 (89%)	1732 (93%)	128 (7%)	19	68

All 27 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	929	GLU	19
1	A	928	THR	13
1	A	1026	LYS	11
1	A	1017	THR	11
1	A	997	ILE	11
1	A	1012	GLU	7
1	A	1025	ARG	7
1	A	937	ASN	6
1	A	1016	HIS	6
1	A	950	GLU	4
1	A	982	TYR	4
1	A	995	TYR	4
1	A	927	HIS	3
1	A	1003	HIS	3
1	A	1018	HIS	3
1	A	963	SER	2
1	A	967	LEU	2
1	A	985	ASN	2
1	A	968	THR	2
1	A	1004	LYS	1
1	A	986	ARG	1
1	A	1033	GLN	1
1	A	960	LYS	1
1	A	1014	MET	1
1	A	957	ASN	1
1	A	933	GLU	1
1	A	977	ASP	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 carbohydrates 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	1497
Number of shifts mapped to atoms	1497
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	19

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	123	0.18 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	116	-0.43 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	121	0.44 ± 0.19	None needed (< 0.5 ppm)
^{15}N	113	0.04 ± 0.43	None needed (< 0.5 ppm)

7.1.3 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 90%, i.e. 1234 atoms were assigned a chemical shift out of a possible 1371. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	517/519 (100%)	206/206 (100%)	212/214 (99%)	99/99 (100%)
Sidechain	573/691 (83%)	364/411 (89%)	197/242 (81%)	12/38 (32%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	144/161 (89%)	72/81 (89%)	66/66 (100%)	6/14 (43%)
Overall	1234/1371 (90%)	642/698 (92%)	475/522 (91%)	117/151 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1376 atoms were assigned a chemical shift out of a possible 1531. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	593/597 (99%)	236/237 (100%)	244/246 (99%)	113/114 (99%)
Sidechain	631/764 (83%)	399/453 (88%)	219/270 (81%)	13/41 (32%)
Aromatic	152/170 (89%)	76/86 (88%)	70/70 (100%)	6/14 (43%)
Overall	1376/1531 (90%)	711/776 (92%)	533/586 (91%)	132/169 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	1025	ARG	HD2	-0.49	4.27 – 1.97	-15.7
1	A	1019	ARG	HD2	0.13	4.27 – 1.97	-13.0
1	A	940	ARG	HD2	0.31	4.27 – 1.97	-12.2
1	A	1025	ARG	HD3	0.10	4.36 – 1.86	-12.0
1	A	1021	ARG	HD2	0.43	4.27 – 1.97	-11.7
1	A	1019	ARG	HD3	0.43	4.36 – 1.86	-10.7
1	A	1025	ARG	HB3	-0.49	3.17 – 0.37	-8.1
1	A	1025	ARG	HB2	-0.31	3.15 – 0.45	-7.8
1	A	1029	LYS	HB2	0.01	3.03 – 0.53	-7.1
1	A	1013	LYS	HB2	0.07	3.03 – 0.53	-6.8
1	A	1019	ARG	HG2	-0.10	2.92 – 0.22	-6.2
1	A	1021	ARG	HD3	1.68	4.36 – 1.86	-5.7
1	A	1019	ARG	HG3	-0.10	3.00 – 0.10	-5.7
1	A	964	PRO	HB2	0.13	3.82 – 0.32	-5.5
1	A	940	ARG	HG2	0.08	2.92 – 0.22	-5.5
1	A	1020	ARG	HD2	1.86	4.27 – 1.97	-5.5
1	A	1012	GLU	HB2	0.94	3.08 – 0.98	-5.2
1	A	1027	ARG	HD2	1.93	4.27 – 1.97	-5.2
1	A	1005	PRO	HB2	0.30	3.82 – 0.32	-5.0

7.1.5 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.

Random coil index (RCI) for chain A:

