



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 08:35 pm BST

PDB ID : 1SM7
Title : Solution structure of the recombinant pronapin precursor, BnIb.
Authors : Pantoja-Uceda, D.; Palomares, O.; Bruix, M.; Villalba, M.; Rodriguez, R.; Rico, M.; Santoro, J.
Deposited on : 2004-03-08

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

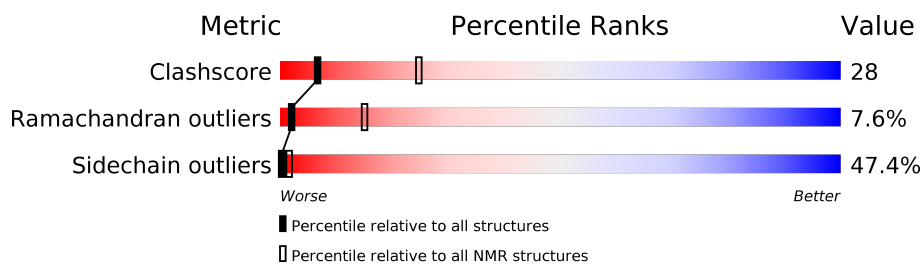
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	109	

2 Ensemble composition and analysis

This entry contains 19 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4-A:24, A:43-A:71, A:81-A:109 (79)	0.50	1

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 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 6, 7, 8, 12, 13, 14, 15, 16, 19
2	1, 3, 4, 9
3	11, 17, 18
Single-model clusters	5; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1725 atoms, of which 849 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called recombinant Ib pronapin.

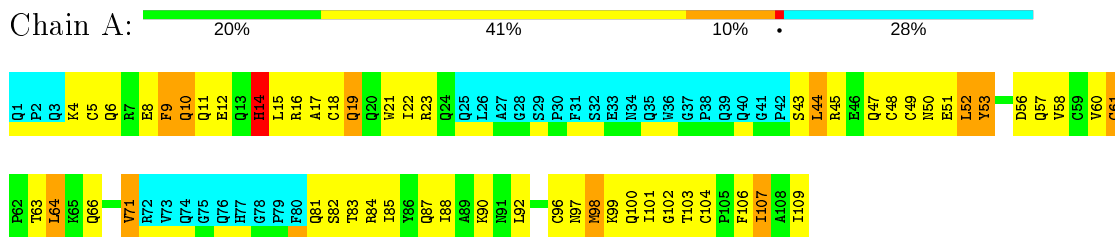
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	109	1725	541	849	165	161	9	0

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: recombinant Ib pronapin

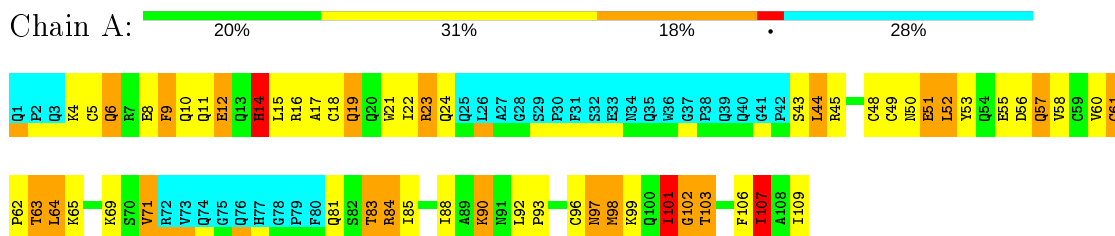


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

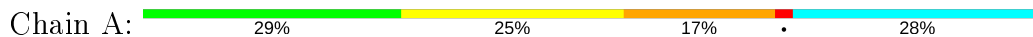
4.2.1 Score per residue for model 1 (medoid)

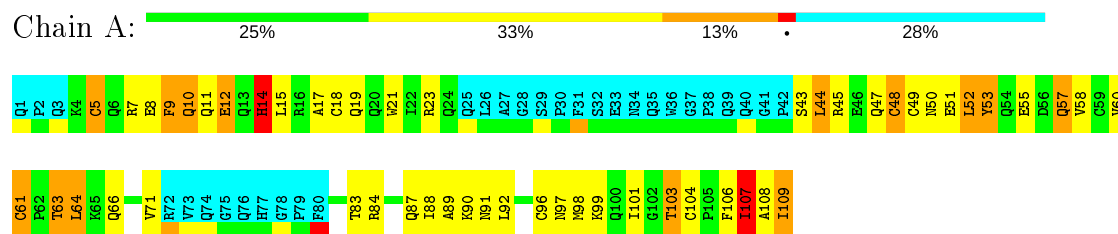
- Molecule 1: recombinant Ib pronapin



4.2.2 Score per residue for model 2

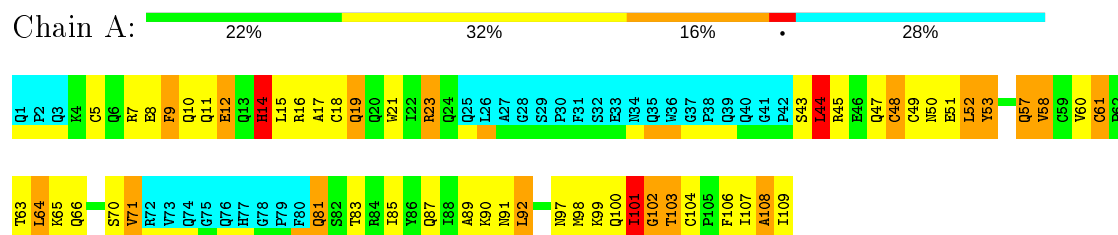
- Molecule 1: recombinant Ib pronapin





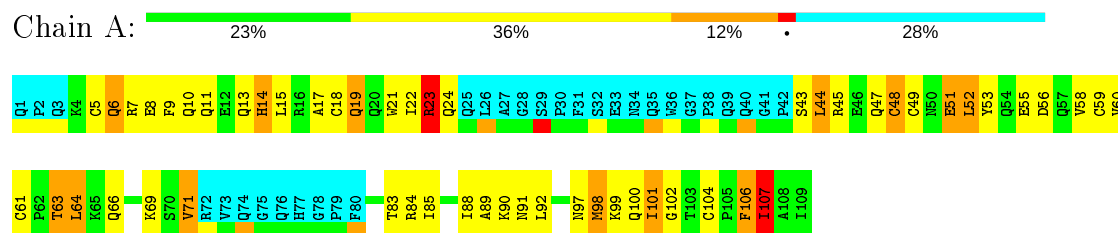
4.2.7 Score per residue for model 7

- Molecule 1: recombinant Ib pronapin



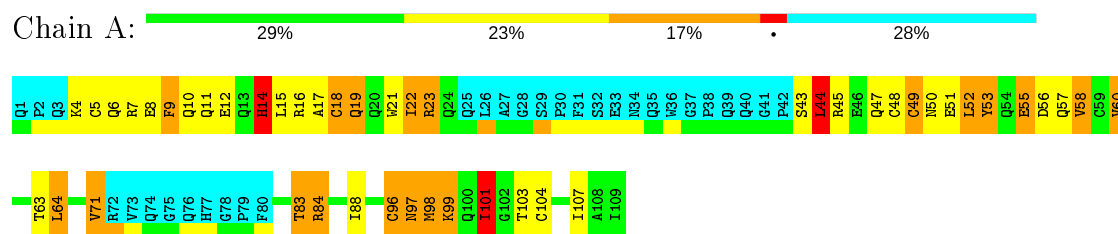
4.2.8 Score per residue for model 8

- Molecule 1: recombinant Ib pronapin



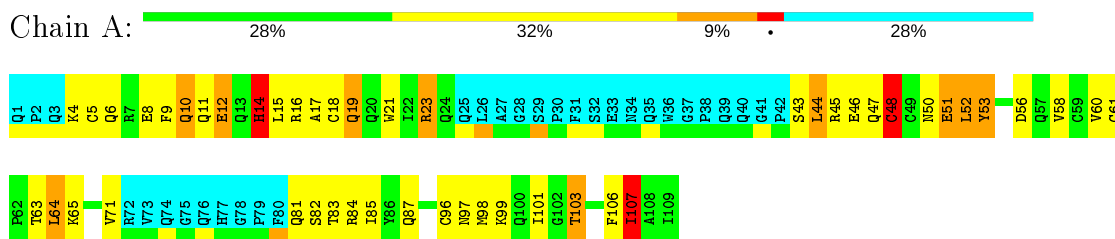
4.2.9 Score per residue for model 9

- Molecule 1: recombinant Ib pronapin



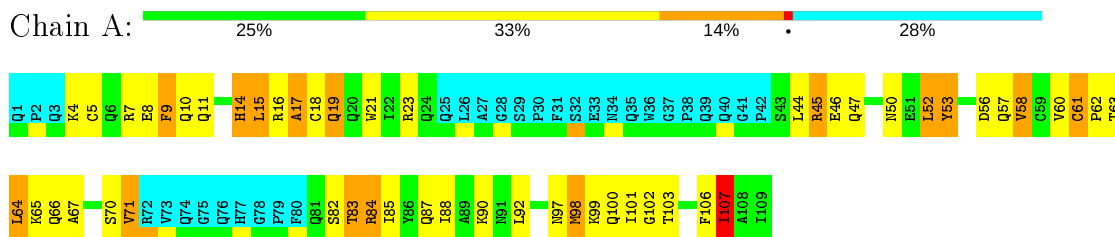
4.2.10 Score per residue for model 10

- Molecule 1: recombinant Ib pronapin



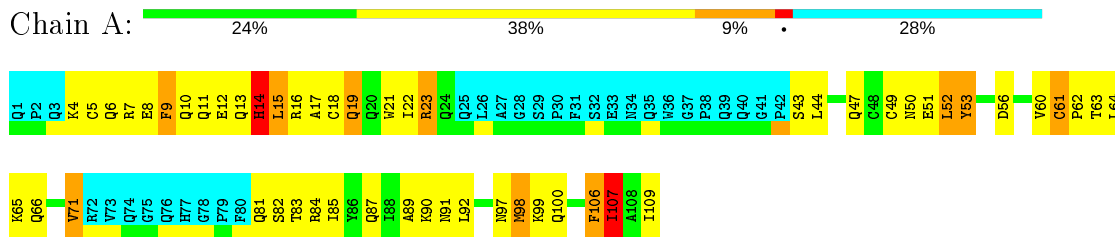
4.2.11 Score per residue for model 11

- Molecule 1: recombinant Ib pronapin



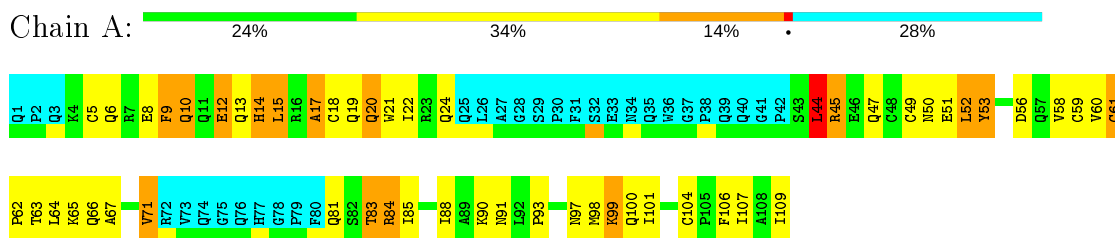
4.2.12 Score per residue for model 12

- Molecule 1: recombinant Ib pronapin



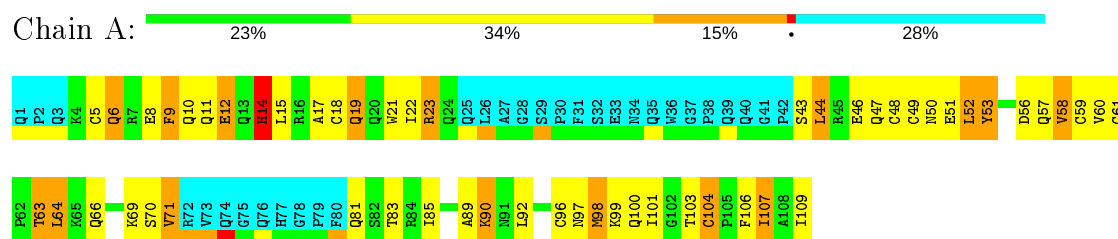
4.2.13 Score per residue for model 13

- Molecule 1: recombinant Ib pronapin



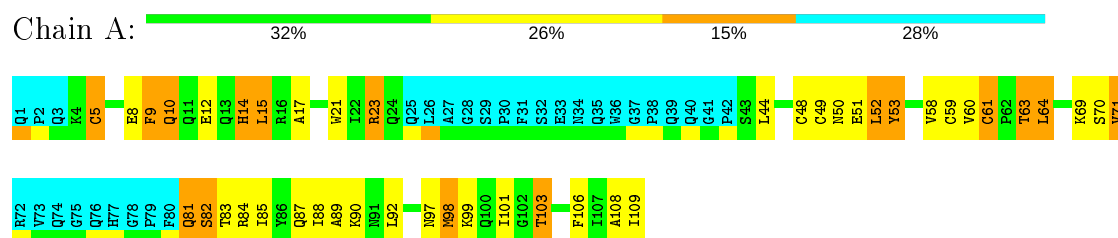
4.2.14 Score per residue for model 14

- Molecule 1: recombinant Ib pronapin



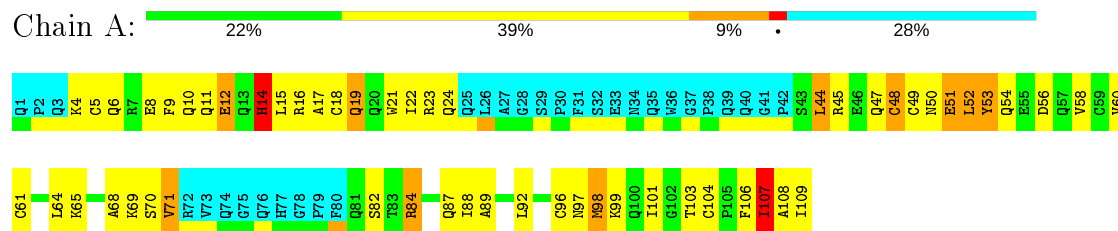
4.2.15 Score per residue for model 15

- Molecule 1: recombinant Ib pronapin



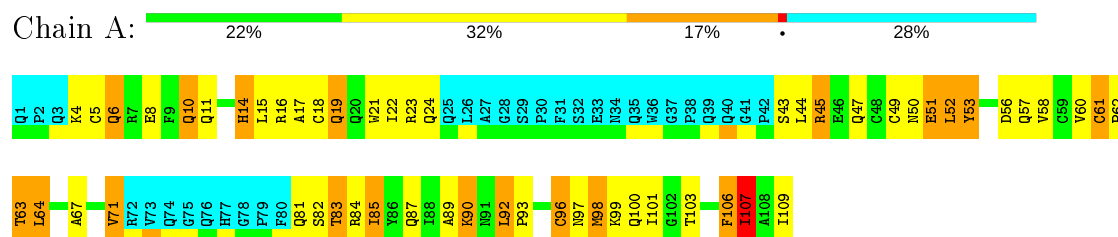
4.2.16 Score per residue for model 16

- Molecule 1: recombinant Ib pronapin



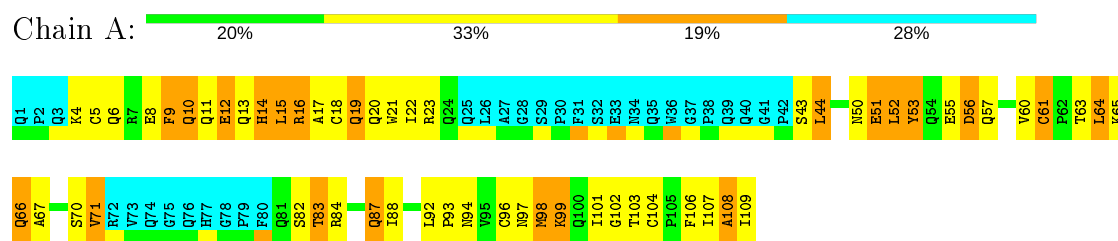
4.2.17 Score per residue for model 17

- Molecule 1: recombinant Ib pronapin



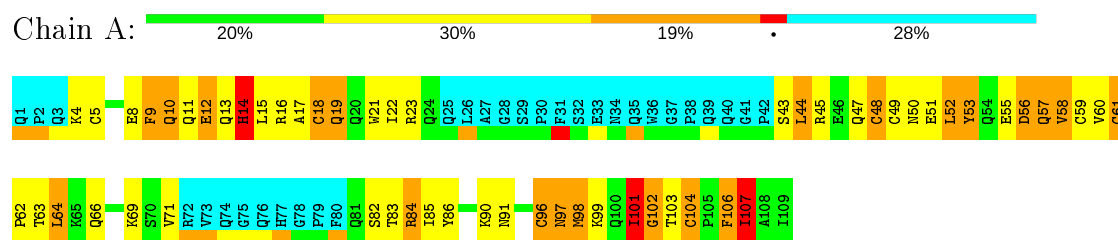
4.2.18 Score per residue for model 18

- Molecule 1: recombinant Ib pronapin



4.2.19 Score per residue for model 19

- Molecule 1: recombinant Ib pronapin



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 50 calculated structures, 19 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
DIANA	structure solution	1.5
DIANA	refinement	1.5

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	643	637	636	36±9
All	All	12217	12103	12084	676

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD23	1:A:64:LEU:HD12	0.96	1.35	4	5
1:A:22:ILE:HG21	1:A:85:ILE:HG23	0.87	1.46	3	1
1:A:52:LEU:HD23	1:A:64:LEU:CD1	0.85	2.01	1	15
1:A:52:LEU:HD13	1:A:53:TYR:N	0.83	1.87	1	18
1:A:17:ALA:HA	1:A:44:LEU:HD23	0.82	1.52	17	5
1:A:15:LEU:HD12	1:A:18:CYS:SG	0.81	2.15	18	4
1:A:17:ALA:HB1	1:A:44:LEU:CD2	0.80	2.06	9	3
1:A:71:VAL:HG11	1:A:85:ILE:HD12	0.80	1.54	13	7
1:A:23:ARG:HD3	1:A:71:VAL:HG22	0.80	1.53	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ALA:HB1	1:A:44:LEU:HD23	0.77	1.55	14	11
1:A:52:LEU:HD23	1:A:64:LEU:HD11	0.76	1.57	14	9
1:A:17:ALA:HB3	1:A:51:GLU:OE1	0.75	1.80	5	5
1:A:19:GLN:HB2	1:A:71:VAL:HG23	0.75	1.57	19	11
1:A:9:PHE:CG	1:A:63:THR:HG22	0.75	2.16	14	5
1:A:19:GLN:NE2	1:A:71:VAL:HG23	0.74	1.98	17	3
1:A:71:VAL:CG1	1:A:85:ILE:HD12	0.74	2.13	5	12
1:A:22:ILE:HD12	1:A:71:VAL:HG21	0.73	1.60	14	3
1:A:14:HIS:C	1:A:15:LEU:HD23	0.73	2.04	9	14
1:A:90:LYS:HD3	1:A:107:ILE:HG22	0.72	1.61	17	2
1:A:17:ALA:HB3	1:A:51:GLU:OE2	0.72	1.85	1	3
1:A:21:TRP:HB3	1:A:44:LEU:HD22	0.71	1.62	19	7
1:A:52:LEU:HD21	1:A:98:MET:CG	0.71	2.16	19	12
1:A:89:ALA:HA	1:A:92:LEU:HD12	0.71	1.62	14	9
1:A:90:LYS:HB2	1:A:107:ILE:HG22	0.70	1.63	3	1
1:A:90:LYS:HE3	1:A:109:ILE:OXT	0.70	1.87	14	1
1:A:84:ARG:NE	1:A:88:ILE:HD11	0.69	2.01	1	1
1:A:6:GLN:HG2	1:A:63:THR:HG23	0.69	1.64	1	2
1:A:52:LEU:HD21	1:A:98:MET:HG3	0.69	1.65	19	12
1:A:52:LEU:HD22	1:A:60:VAL:HG22	0.69	1.63	3	11
1:A:21:TRP:CH2	1:A:88:ILE:HG22	0.69	2.23	13	5
1:A:52:LEU:CD2	1:A:60:VAL:HG22	0.67	2.20	3	17
1:A:19:GLN:HB3	1:A:67:ALA:HB1	0.67	1.65	13	1
1:A:19:GLN:HG3	1:A:67:ALA:HB1	0.67	1.65	11	1
1:A:23:ARG:CD	1:A:71:VAL:HG22	0.66	2.20	2	2
1:A:21:TRP:HB3	1:A:44:LEU:HD13	0.66	1.67	9	1
1:A:106:PHE:O	1:A:107:ILE:HG23	0.66	1.89	7	12
1:A:52:LEU:HD13	1:A:52:LEU:C	0.66	2.09	19	7
1:A:19:GLN:CB	1:A:71:VAL:HG23	0.66	2.20	7	10
1:A:21:TRP:HE1	1:A:92:LEU:HD11	0.66	1.51	11	7
1:A:9:PHE:CD2	1:A:63:THR:HG22	0.65	2.25	15	3
1:A:52:LEU:C	1:A:52:LEU:HD13	0.65	2.12	1	8
1:A:90:LYS:HG2	1:A:107:ILE:HG22	0.65	1.67	4	1
1:A:6:GLN:HA	1:A:63:THR:HG23	0.63	1.70	2	5
1:A:15:LEU:HD13	1:A:51:GLU:OE2	0.63	1.93	18	1
1:A:9:PHE:CE2	1:A:15:LEU:HD23	0.63	2.29	15	5
1:A:14:HIS:O	1:A:15:LEU:HD23	0.62	1.94	19	7
1:A:90:LYS:CD	1:A:107:ILE:HG22	0.62	2.25	12	2
1:A:22:ILE:HG22	1:A:23:ARG:NH1	0.61	2.10	12	1
1:A:19:GLN:O	1:A:71:VAL:HG23	0.61	1.95	16	2
1:A:17:ALA:HB1	1:A:44:LEU:HD21	0.61	1.73	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLN:CG	1:A:67:ALA:HB1	0.61	2.25	11	2
1:A:48:CYS:O	1:A:52:LEU:HD12	0.61	1.94	8	7
1:A:21:TRP:HH2	1:A:88:ILE:HG22	0.60	1.56	18	3
1:A:90:LYS:CB	1:A:106:PHE:CZ	0.60	2.85	1	1
1:A:52:LEU:HD21	1:A:60:VAL:HG22	0.59	1.74	10	4
1:A:20:GLN:NE2	1:A:44:LEU:HD21	0.59	2.11	13	1
1:A:107:ILE:HG23	1:A:109:ILE:H	0.59	1.57	16	1
1:A:87:GLN:HG3	1:A:109:ILE:HG22	0.59	1.75	18	2
1:A:84:ARG:O	1:A:88:ILE:HD12	0.58	1.98	16	1
1:A:19:GLN:HG2	1:A:67:ALA:HB1	0.58	1.73	18	2
1:A:106:PHE:CD1	1:A:109:ILE:HD11	0.58	2.34	15	1
1:A:90:LYS:CG	1:A:107:ILE:HG22	0.58	2.28	1	2
1:A:17:ALA:HB3	1:A:51:GLU:CD	0.58	2.19	13	2
1:A:83:THR:HG22	1:A:84:ARG:N	0.57	2.14	18	6
1:A:60:VAL:HG21	1:A:98:MET:O	0.57	2.00	12	6
1:A:49:CYS:HA	1:A:52:LEU:HD12	0.57	1.77	13	4
1:A:87:GLN:HG2	1:A:109:ILE:HD11	0.56	1.77	12	1
1:A:106:PHE:CE2	1:A:109:ILE:HD11	0.56	2.34	18	1
1:A:21:TRP:NE1	1:A:92:LEU:HD11	0.56	2.15	11	1
1:A:109:ILE:HD12	1:A:109:ILE:OXT	0.56	2.01	1	1
1:A:19:GLN:CA	1:A:71:VAL:HG23	0.56	2.31	9	5
1:A:14:HIS:CD2	1:A:14:HIS:N	0.55	2.75	19	8
1:A:53:TYR:CE1	1:A:57:GLN:NE2	0.55	2.74	19	3
1:A:52:LEU:HD22	1:A:52:LEU:O	0.55	2.01	19	7
1:A:21:TRP:NE1	1:A:92:LEU:HD21	0.55	2.16	17	1
1:A:9:PHE:CD2	1:A:15:LEU:HD23	0.55	2.37	18	4
1:A:17:ALA:CB	1:A:44:LEU:HD23	0.55	2.31	5	9
1:A:87:GLN:HG2	1:A:109:ILE:OXT	0.55	2.02	6	1
1:A:21:TRP:CZ3	1:A:45:ARG:NH2	0.54	2.75	1	2
1:A:101:ILE:HD12	1:A:101:ILE:C	0.54	2.23	1	1
1:A:71:VAL:HG11	1:A:85:ILE:HG23	0.54	1.78	14	4
1:A:71:VAL:HG11	1:A:85:ILE:HG21	0.54	1.79	3	1
1:A:53:TYR:CE2	1:A:98:MET:HA	0.54	2.37	18	9
1:A:19:GLN:HE21	1:A:71:VAL:HG23	0.54	1.60	17	2
1:A:93:PRO:HG2	1:A:107:ILE:HG21	0.54	1.80	13	1
1:A:14:HIS:N	1:A:14:HIS:CD2	0.53	2.76	1	11
1:A:61:CYS:SG	1:A:104:CYS:N	0.53	2.81	6	2
1:A:22:ILE:HD11	1:A:92:LEU:HD11	0.53	1.80	16	1
1:A:90:LYS:HG3	1:A:107:ILE:HG22	0.53	1.80	1	1
1:A:60:VAL:HG11	1:A:99:LYS:CB	0.53	2.34	9	1
1:A:53:TYR:CE2	1:A:98:MET:CB	0.52	2.92	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:GLN:HA	1:A:71:VAL:HG23	0.52	1.82	9	3
1:A:52:LEU:HD22	1:A:52:LEU:C	0.52	2.24	12	2
1:A:21:TRP:CB	1:A:44:LEU:HD13	0.52	2.34	9	2
1:A:99:LYS:CG	1:A:101:ILE:HG23	0.52	2.35	9	1
1:A:10:GLN:HA	1:A:14:HIS:CD2	0.52	2.40	1	17
1:A:21:TRP:CZ3	1:A:45:ARG:CZ	0.52	2.93	11	2
1:A:52:LEU:O	1:A:52:LEU:HD22	0.51	2.05	7	7
1:A:108:ALA:C	1:A:109:ILE:HD12	0.51	2.25	16	1
1:A:52:LEU:HD21	1:A:98:MET:SD	0.51	2.45	19	7
1:A:22:ILE:HG23	1:A:88:ILE:CG2	0.51	2.35	9	1
1:A:19:GLN:OE1	1:A:64:LEU:HD23	0.51	2.05	10	1
1:A:60:VAL:HG13	1:A:98:MET:HG3	0.51	1.83	18	5
1:A:52:LEU:HD11	1:A:98:MET:SD	0.51	2.46	6	3
1:A:61:CYS:SG	1:A:62:PRO:HA	0.51	2.47	19	5
1:A:9:PHE:CZ	1:A:63:THR:O	0.51	2.64	19	2
1:A:99:LYS:HG3	1:A:103:THR:HG22	0.50	1.83	10	1
1:A:9:PHE:C	1:A:9:PHE:CD1	0.50	2.84	1	3
1:A:9:PHE:CD1	1:A:66:GLN:NE2	0.50	2.80	18	1
1:A:53:TYR:CE1	1:A:57:GLN:OE1	0.50	2.65	7	3
1:A:22:ILE:HG23	1:A:88:ILE:HG21	0.50	1.84	9	1
1:A:107:ILE:O	1:A:108:ALA:HB2	0.50	2.07	18	3
1:A:90:LYS:HD2	1:A:107:ILE:HG22	0.50	1.82	12	1
1:A:22:ILE:HB	1:A:71:VAL:HG21	0.50	1.82	18	1
1:A:9:PHE:CD2	1:A:55:GLU:OE1	0.49	2.65	9	1
1:A:104:CYS:O	1:A:104:CYS:SG	0.49	2.70	2	4
1:A:82:SER:O	1:A:86:TYR:CD1	0.49	2.65	19	1
1:A:93:PRO:HA	1:A:98:MET:SD	0.49	2.46	4	1
1:A:17:ALA:O	1:A:44:LEU:HD22	0.49	2.08	13	2
1:A:59:CYS:HA	1:A:63:THR:HG21	0.49	1.84	14	4
1:A:21:TRP:CH2	1:A:88:ILE:CG2	0.48	2.97	9	3
1:A:21:TRP:CE2	1:A:22:ILE:CG1	0.48	2.96	18	3
1:A:106:PHE:O	1:A:106:PHE:CG	0.48	2.67	7	1
1:A:51:GLU:HG3	1:A:51:GLU:O	0.48	2.08	16	1
1:A:68:ALA:O	1:A:71:VAL:HG12	0.48	2.08	16	2
1:A:9:PHE:CD1	1:A:9:PHE:C	0.48	2.86	19	4
1:A:89:ALA:CA	1:A:92:LEU:HD12	0.48	2.39	16	3
1:A:15:LEU:HD22	1:A:51:GLU:O	0.48	2.09	16	2
1:A:101:ILE:HG23	1:A:102:GLY:H	0.48	1.69	1	3
1:A:96:CYS:O	1:A:97:ASN:C	0.47	2.52	4	5
1:A:98:MET:N	1:A:98:MET:SD	0.47	2.87	4	1
1:A:52:LEU:C	1:A:52:LEU:HD22	0.47	2.29	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:CYS:HA	1:A:21:TRP:CD1	0.47	2.44	19	2
1:A:44:LEU:H	1:A:44:LEU:HD12	0.47	1.70	11	2
1:A:61:CYS:O	1:A:103:THR:HG21	0.46	2.09	1	5
1:A:21:TRP:CZ3	1:A:88:ILE:CG2	0.46	2.98	9	1
1:A:60:VAL:CG1	1:A:99:LYS:HB2	0.46	2.41	9	1
1:A:71:VAL:HG13	1:A:85:ILE:HD12	0.46	1.88	2	1
1:A:5:CYS:SG	1:A:63:THR:HG21	0.46	2.51	6	1
1:A:92:LEU:N	1:A:93:PRO:CD	0.45	2.80	1	1
1:A:106:PHE:CD1	1:A:106:PHE:C	0.45	2.89	19	1
1:A:101:ILE:HG23	1:A:102:GLY:N	0.45	2.27	18	1
1:A:103:THR:HG23	1:A:104:CYS:N	0.45	2.26	19	2
1:A:21:TRP:CD1	1:A:44:LEU:HD22	0.45	2.46	10	1
1:A:55:GLU:O	1:A:56:ASP:CB	0.45	2.64	19	4
1:A:60:VAL:CG1	1:A:98:MET:HG3	0.45	2.41	19	5
1:A:99:LYS:HG2	1:A:101:ILE:HG23	0.45	1.89	9	1
1:A:90:LYS:HB3	1:A:106:PHE:CZ	0.45	2.46	1	1
1:A:90:LYS:HA	1:A:106:PHE:CZ	0.45	2.46	17	1
1:A:106:PHE:CD1	1:A:107:ILE:N	0.45	2.85	19	2
1:A:17:ALA:CA	1:A:44:LEU:HD23	0.44	2.42	1	2
1:A:61:CYS:CB	1:A:62:PRO:HA	0.44	2.41	17	2
1:A:14:HIS:CD2	1:A:14:HIS:H	0.44	2.29	5	2
1:A:17:ALA:CB	1:A:44:LEU:HD21	0.44	2.41	9	2
1:A:94:ASN:OD1	1:A:107:ILE:HD13	0.44	2.13	18	1
1:A:57:GLN:NE2	1:A:57:GLN:N	0.44	2.65	19	1
1:A:5:CYS:HB2	1:A:58:VAL:HG12	0.44	1.89	15	1
1:A:14:HIS:H	1:A:14:HIS:CD2	0.44	2.29	4	3
1:A:53:TYR:CE2	1:A:98:MET:HB3	0.44	2.47	7	2
1:A:57:GLN:HE21	1:A:57:GLN:N	0.44	2.10	6	1
1:A:19:GLN:NE2	1:A:71:VAL:CG2	0.44	2.80	18	2
1:A:104:CYS:SG	1:A:104:CYS:O	0.44	2.76	19	1
1:A:21:TRP:CE2	1:A:22:ILE:HG13	0.44	2.47	1	1
1:A:83:THR:CG2	1:A:84:ARG:N	0.43	2.81	1	6
1:A:19:GLN:CB	1:A:67:ALA:HB1	0.43	2.41	13	1
1:A:53:TYR:CE1	1:A:57:GLN:CD	0.43	2.91	19	1
1:A:52:LEU:CD2	1:A:64:LEU:HD12	0.43	2.26	4	1
1:A:98:MET:O	1:A:99:LYS:C	0.43	2.56	9	1
1:A:61:CYS:HB3	1:A:103:THR:HG22	0.43	1.90	18	1
1:A:9:PHE:CD2	1:A:63:THR:HB	0.43	2.48	11	1
1:A:21:TRP:CZ2	1:A:22:ILE:HG12	0.43	2.49	18	1
1:A:22:ILE:HG21	1:A:71:VAL:HG11	0.43	1.90	18	1
1:A:106:PHE:C	1:A:107:ILE:CG1	0.43	2.87	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LYS:HB3	1:A:106:PHE:CE1	0.43	2.48	14	1
1:A:93:PRO:CB	1:A:98:MET:CE	0.43	2.96	4	1
1:A:15:LEU:HD13	1:A:52:LEU:HB2	0.43	1.91	10	2
1:A:21:TRP:HA	1:A:44:LEU:HD13	0.43	1.91	13	2
1:A:9:PHE:CD1	1:A:10:GLN:N	0.43	2.87	18	1
1:A:9:PHE:CG	1:A:63:THR:HB	0.42	2.49	12	1
1:A:23:ARG:NH1	1:A:85:ILE:CD1	0.42	2.82	12	1
1:A:9:PHE:CE2	1:A:15:LEU:CD2	0.42	3.01	11	1
1:A:9:PHE:HZ	1:A:67:ALA:HB2	0.42	1.74	11	2
1:A:60:VAL:CG1	1:A:99:LYS:CB	0.42	2.97	9	1
1:A:71:VAL:HG11	1:A:85:ILE:CG2	0.42	2.45	19	2
1:A:106:PHE:O	1:A:109:ILE:HG23	0.42	2.15	3	2
1:A:106:PHE:CG	1:A:106:PHE:O	0.42	2.72	4	1
1:A:56:ASP:O	1:A:60:VAL:HG23	0.42	2.14	17	3
1:A:62:PRO:O	1:A:65:LYS:CB	0.42	2.68	13	1
1:A:57:GLN:OE1	1:A:101:ILE:CG2	0.42	2.68	1	1
1:A:53:TYR:CZ	1:A:98:MET:HA	0.42	2.49	18	4
1:A:90:LYS:NZ	1:A:91:ASN:ND2	0.42	2.68	7	1
1:A:92:LEU:CB	1:A:93:PRO:HD3	0.42	2.44	17	2
1:A:17:ALA:HA	1:A:44:LEU:CD2	0.42	2.45	1	2
1:A:45:ARG:O	1:A:49:CYS:SG	0.42	2.77	1	1
1:A:90:LYS:HB3	1:A:106:PHE:CE2	0.42	2.49	1	1
1:A:106:PHE:C	1:A:106:PHE:CD1	0.42	2.93	8	1
1:A:17:ALA:CA	1:A:44:LEU:HD21	0.41	2.45	6	1
1:A:106:PHE:CD2	1:A:109:ILE:HD11	0.41	2.50	18	1
1:A:21:TRP:N	1:A:44:LEU:HD22	0.41	2.29	18	1
1:A:106:PHE:O	1:A:106:PHE:CD2	0.41	2.73	18	1
1:A:62:PRO:HA	1:A:104:CYS:SG	0.41	2.55	19	1
1:A:18:CYS:N	1:A:48:CYS:HB2	0.41	2.31	4	1
1:A:96:CYS:O	1:A:98:MET:SD	0.41	2.78	17	2
1:A:84:ARG:NE	1:A:88:ILE:CD1	0.41	2.80	1	1
1:A:87:GLN:CG	1:A:109:ILE:HG22	0.41	2.43	18	1
1:A:60:VAL:HA	1:A:64:LEU:HD12	0.41	1.92	3	1
1:A:55:GLU:HB3	1:A:59:CYS:CB	0.41	2.46	8	1
1:A:19:GLN:HA	1:A:71:VAL:CG2	0.41	2.46	14	3
1:A:15:LEU:HD21	1:A:55:GLU:OE2	0.41	2.15	5	1
1:A:61:CYS:O	1:A:103:THR:CG2	0.41	2.69	1	1
1:A:93:PRO:CA	1:A:98:MET:SD	0.41	3.09	4	1
1:A:16:ARG:O	1:A:20:GLN:CG	0.41	2.69	18	1
1:A:21:TRP:CE2	1:A:22:ILE:HG12	0.41	2.51	18	1
1:A:55:GLU:O	1:A:59:CYS:SG	0.41	2.79	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:TRP:CH2	1:A:45:ARG:NH2	0.41	2.88	13	1
1:A:60:VAL:CG1	1:A:60:VAL:O	0.41	2.69	19	1
1:A:106:PHE:HD1	1:A:109:ILE:HD11	0.41	1.73	15	1
1:A:86:TYR:O	1:A:109:ILE:HD11	0.40	2.16	3	1
1:A:89:ALA:CB	1:A:92:LEU:HD12	0.40	2.45	7	1
1:A:15:LEU:HD23	1:A:15:LEU:N	0.40	2.31	7	1
1:A:99:LYS:O	1:A:99:LYS:HG2	0.40	2.16	18	1
1:A:90:LYS:O	1:A:107:ILE:CG2	0.40	2.70	19	1
1:A:21:TRP:CE3	1:A:45:ARG:NH2	0.40	2.89	5	1
1:A:15:LEU:HD13	1:A:51:GLU:HG3	0.40	1.91	13	1
1:A:93:PRO:HG3	1:A:104:CYS:SG	0.40	2.57	5	1

5.2 Torsion angles [i](#)

5.2.1 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	78/109 (72%)	55±2 (70±3%)	18±3 (22±4%)	6±1 (8±2%)	2	15
All	All	1482/2071 (72%)	1036 (70%)	333 (22%)	113 (8%)	2	15

All 17 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	97	ASN	18
1	A	14	HIS	16
1	A	12	GLU	15
1	A	107	ILE	12
1	A	56	ASP	9
1	A	101	ILE	8
1	A	102	GLY	6
1	A	81	GLN	5
1	A	108	ALA	5
1	A	17	ALA	4
1	A	83	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	44	LEU	3
1	A	13	GLN	2
1	A	82	SER	2
1	A	104	CYS	2
1	A	99	LYS	2
1	A	61	CYS	1

5.2.2 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	73/97 (75%)	38±4 (53±6%)	35±4 (47±6%)	0 1
All	All	1387/1843 (75%)	730 (53%)	657 (47%)	0 1

All 62 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	52	LEU	19
1	A	8	GLU	19
1	A	5	CYS	19
1	A	64	LEU	18
1	A	61	CYS	18
1	A	53	TYR	17
1	A	19	GLN	17
1	A	50	ASN	17
1	A	9	PHE	17
1	A	99	LYS	16
1	A	11	GLN	16
1	A	71	VAL	16
1	A	58	VAL	16
1	A	98	MET	16
1	A	51	GLU	16
1	A	101	ILE	15
1	A	23	ARG	15
1	A	48	CYS	14
1	A	14	HIS	14

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Mol	Chain	Res	Type	Models (Total)
1	A	47	GLN	14
1	A	18	CYS	14
1	A	84	ARG	14
1	A	63	THR	14
1	A	44	LEU	13
1	A	107	ILE	13
1	A	12	GLU	13
1	A	10	GLN	13
1	A	4	LYS	13
1	A	43	SER	13
1	A	83	THR	12
1	A	16	ARG	11
1	A	66	GLN	11
1	A	103	THR	11
1	A	6	GLN	11
1	A	45	ARG	11
1	A	100	GLN	10
1	A	49	CYS	10
1	A	90	LYS	10
1	A	69	LYS	8
1	A	65	LYS	8
1	A	87	GLN	8
1	A	82	SER	8
1	A	7	ARG	8
1	A	96	CYS	8
1	A	91	ASN	6
1	A	106	PHE	6
1	A	70	SER	6
1	A	57	GLN	5
1	A	104	CYS	5
1	A	15	LEU	5
1	A	24	GLN	5
1	A	13	GLN	4
1	A	109	ILE	4
1	A	46	GLU	3
1	A	81	GLN	3
1	A	22	ILE	3
1	A	55	GLU	2
1	A	92	LEU	2
1	A	20	GLN	1
1	A	54	GLN	1
1	A	85	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	60	VAL	1

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

No chemical shift data were provided