Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 02:47 PM EST

PDB ID	:	2HA1
Title	:	Complex of the first and second type III domains of human Fibronectin in solution
Authors	:	Vakonakis, I.; Campbell, I.D.
Deposited on	:	2006-06-12

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

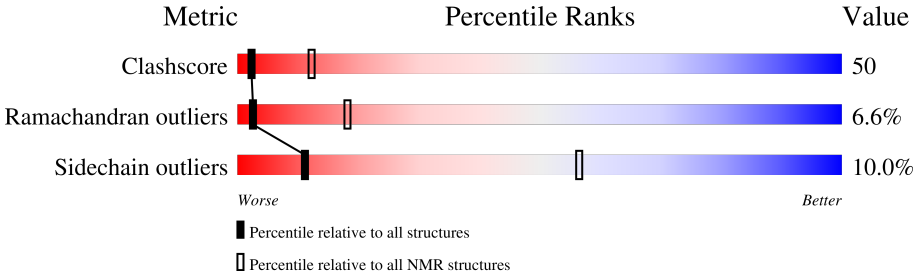
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	201	35% 39% 9% 16%

2 Ensemble composition and analysis (i)

This entry contains 39 models. Model 18 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:93 (93)	0.04	18
2	A:126-A:201 (76)	0.02	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 7 clusters and 2 single-model clusters were found.

Cluster number	Models
1	4, 6, 7, 9, 10, 11, 14, 15, 16, 17, 18, 20, 29, 34, 35, 37, 38
2	2, 5, 13, 36, 39
3	1, 8, 24, 26, 33
4	21, 27, 30, 32
5	12, 23
6	22, 28
7	3, 31
Single-model clusters	19; 25

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3081 atoms, of which 1518 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	201	3081	987	1518	255	321	0

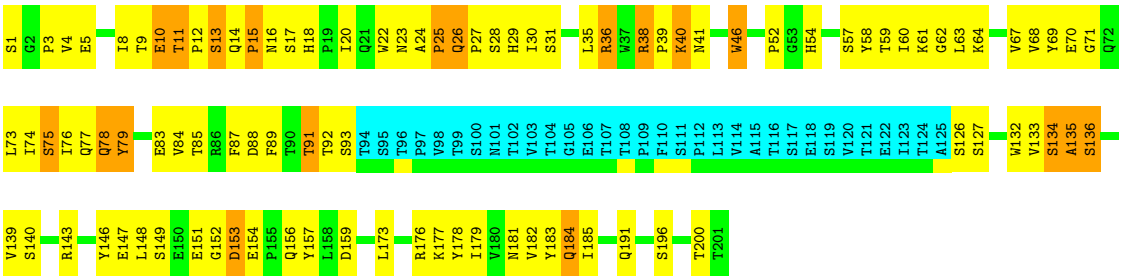
4 Residue-property plots (i)

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: Fibronectin

Chain A: 35% 39% 9% 16%



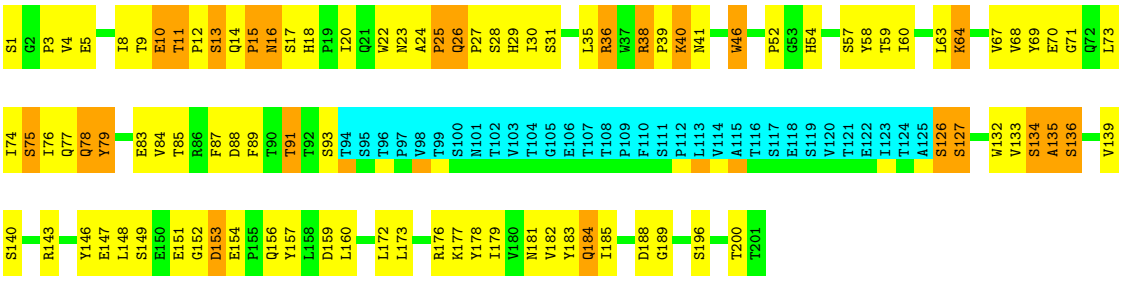
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Fibronectin

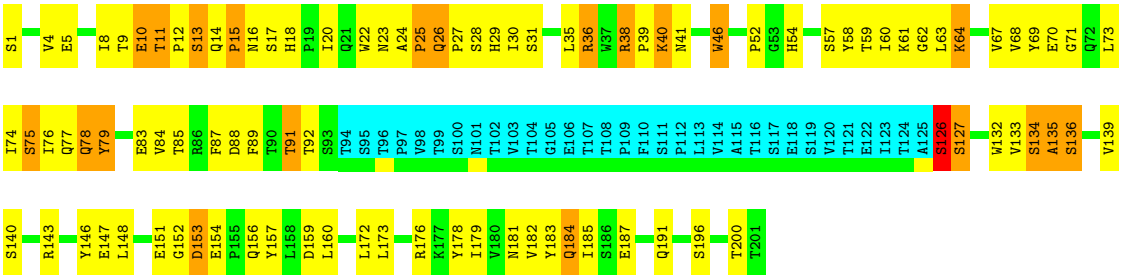
Chain A: 35% 37% 11% 16%



4.2.2 Score per residue for model 2

- Molecule 1: Fibronectin

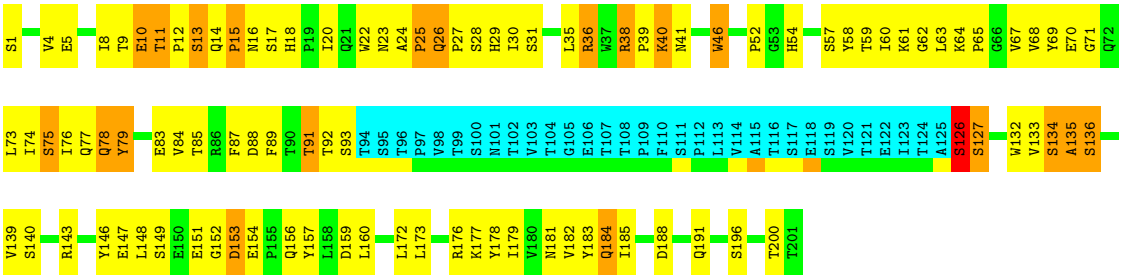
Chain A: 36% 37% 10% 16%



4.2.3 Score per residue for model 3

- Molecule 1: Fibronectin

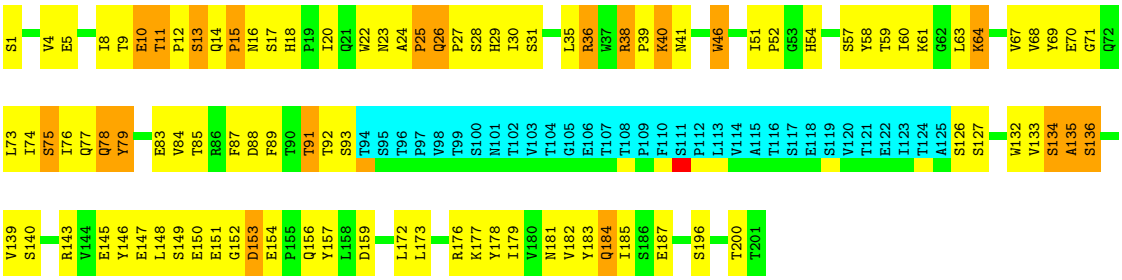
Chain A: 34% 40% 10% 16%



4.2.4 Score per residue for model 4

- Molecule 1: Fibronectin

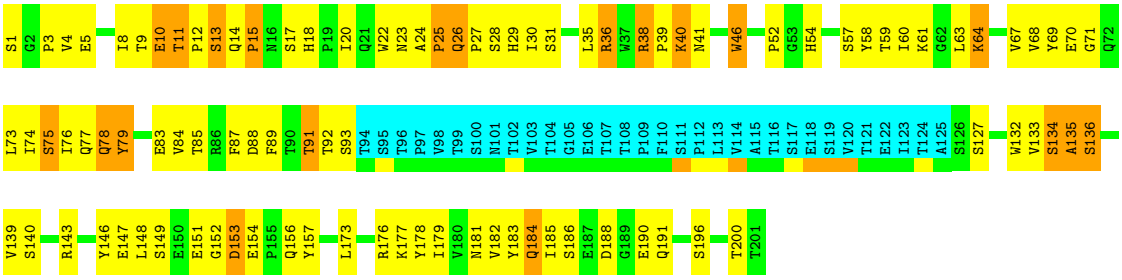
Chain A: 34% 40% 10% 16%



4.2.5 Score per residue for model 5

- Molecule 1: Fibronectin

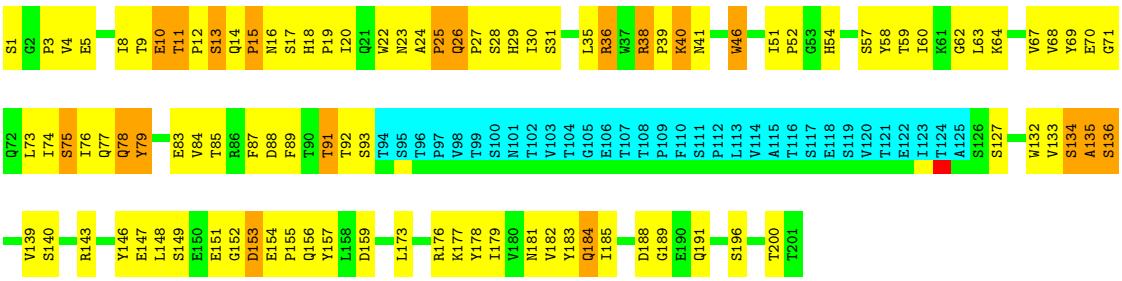
Chain A: 36% 38% 10% 16%



4.2.6 Score per residue for model 6

- Molecule 1: Fibronectin

Chain A: 34% 41% 9% 16%



4.2.7 Score per residue for model 7

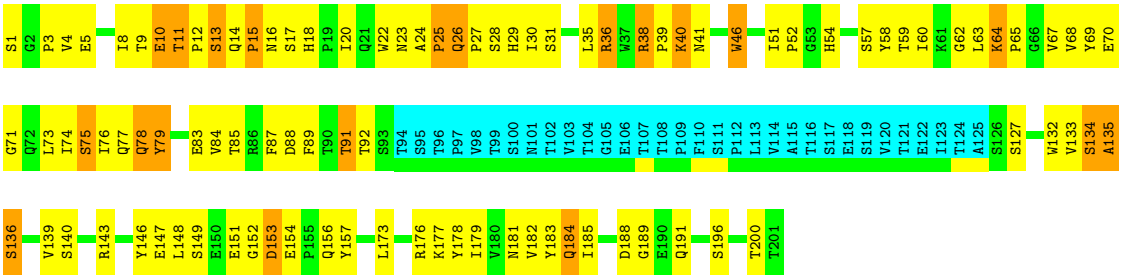
- Molecule 1: Fibronectin

Chain A: 33% 40% 10% 16%

4.2.8 Score per residue for model 8

- Molecule 1: Fibronectin

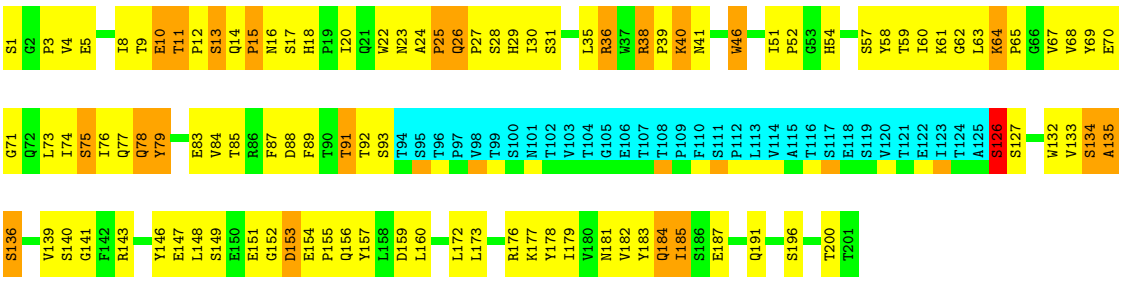
Chain A: 35% 39% 10% 16%



4.2.9 Score per residue for model 9

- Molecule 1: Fibronectin

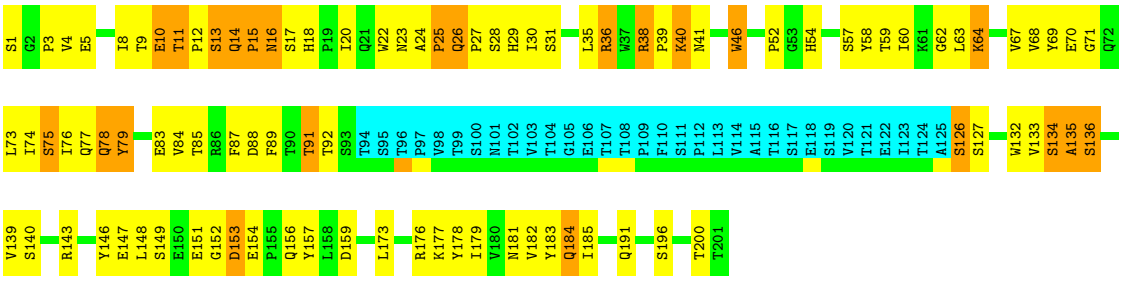
Chain A: 32% 41% 10% 16%



4.2.10 Score per residue for model 10

- Molecule 1: Fibronectin

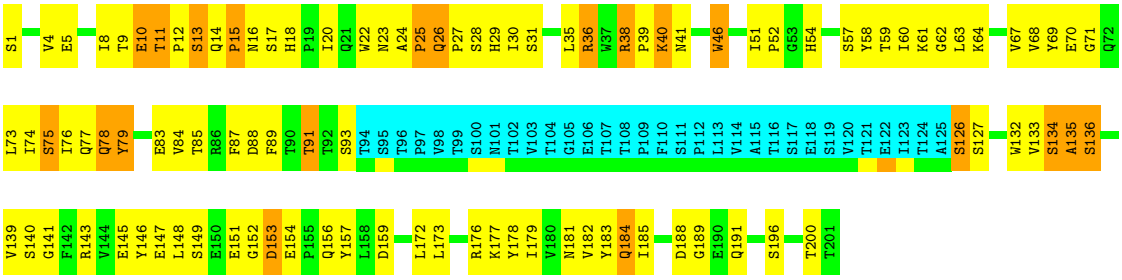
Chain A: 36% 36% 11% 16%



4.2.11 Score per residue for model 11

- Molecule 1: Fibronectin

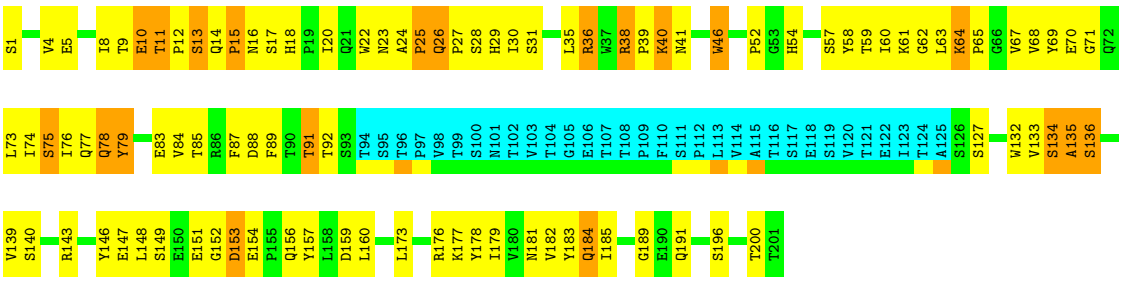
Chain A: 33% 41% 10% 16%



4.2.12 Score per residue for model 12

- Molecule 1: Fibronectin

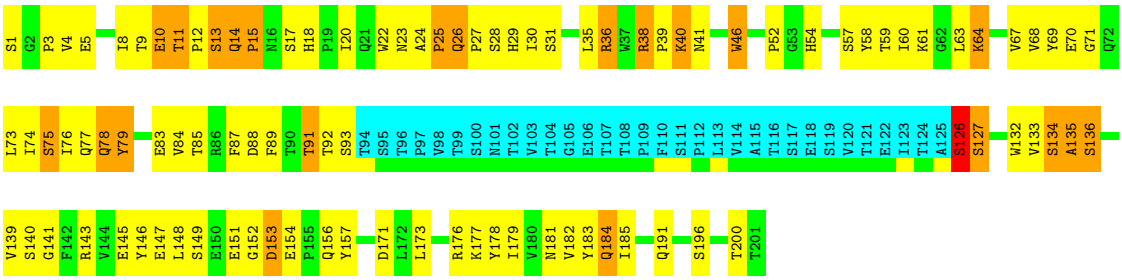
Chain A: 35% 39% 10% 16%



4.2.13 Score per residue for model 13

- Molecule 1: Fibronectin

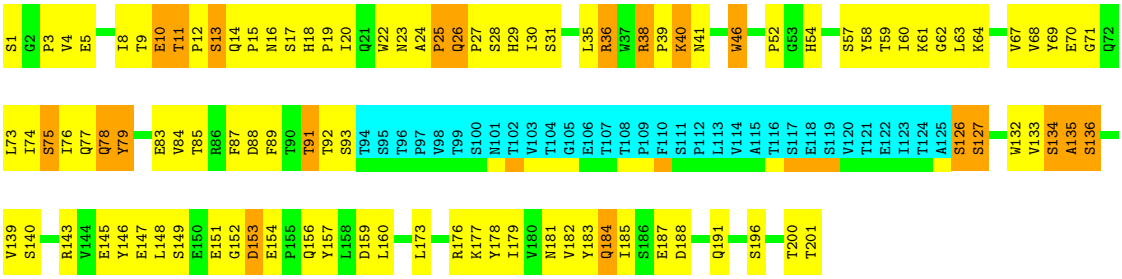
Chain A: 35% 37% 11% 16%



4.2.14 Score per residue for model 14

- Molecule 1: Fibronectin

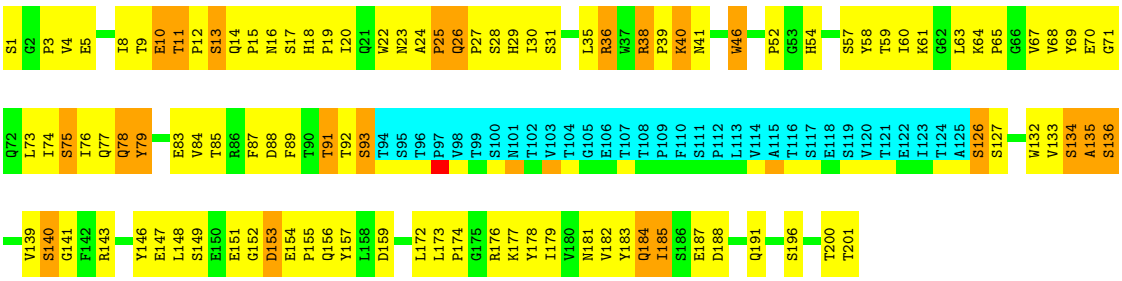
Chain A: 32% 42% 10% 16%



4.2.15 Score per residue for model 15

- Molecule 1: Fibronectin

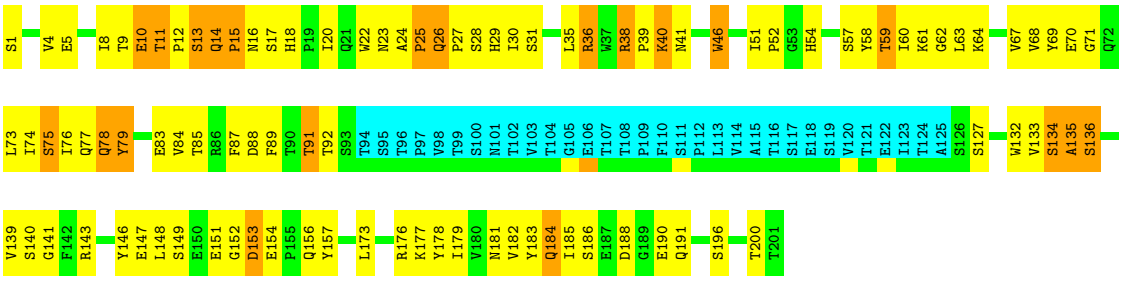
Chain A: 31% 42% 11% 16%



4.2.16 Score per residue for model 16

- Molecule 1: Fibronectin

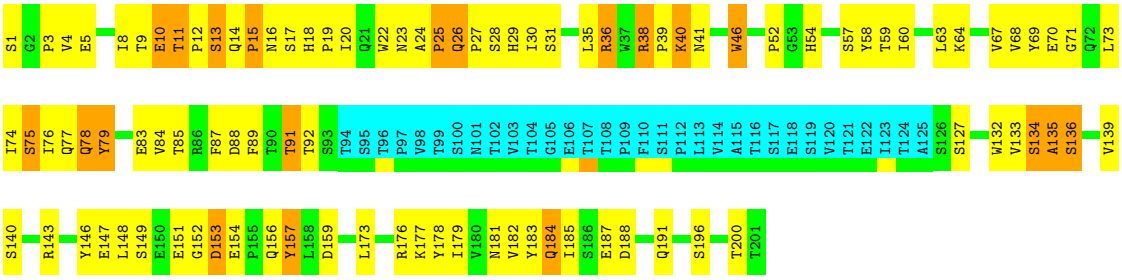
Chain A: 35% 39% 10% 16%



4.2.17 Score per residue for model 17

- Molecule 1: Fibronectin

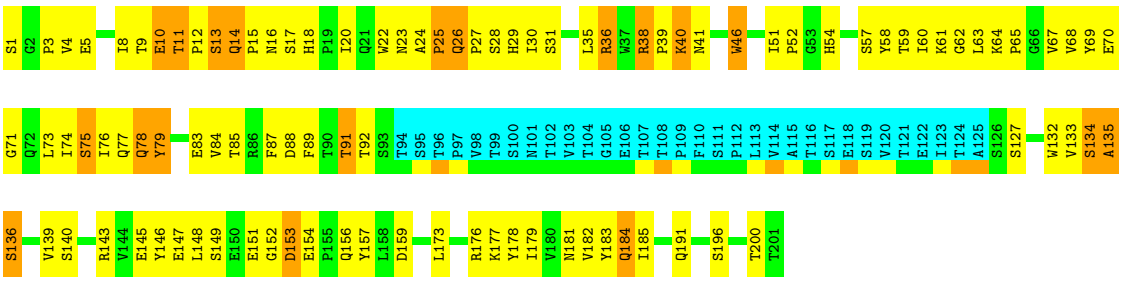
Chain A: 36% 38% 10% 16%



4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Fibronectin

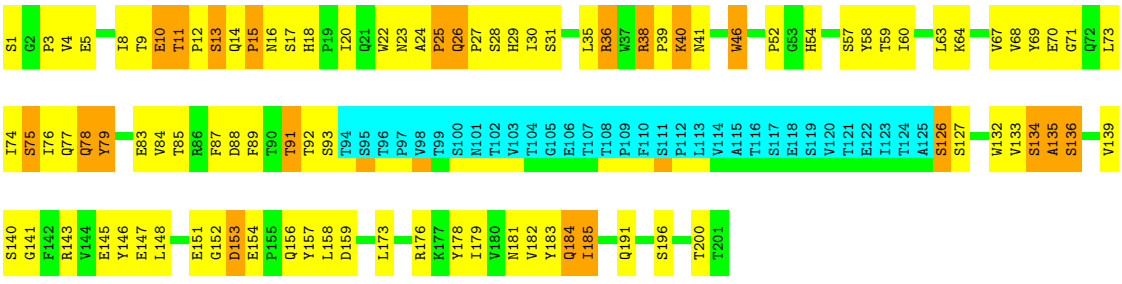
Chain A: 35% 40% 9% 16%



4.2.19 Score per residue for model 19

- Molecule 1: Fibronectin

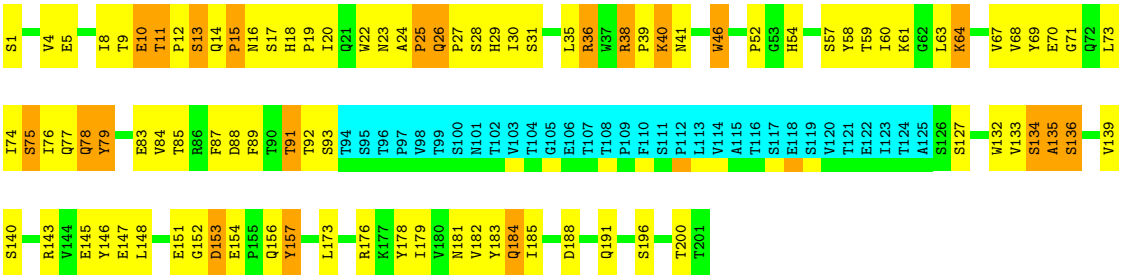
Chain A: 36% 38% 10% 16%



4.2.20 Score per residue for model 20

- Molecule 1: Fibronectin

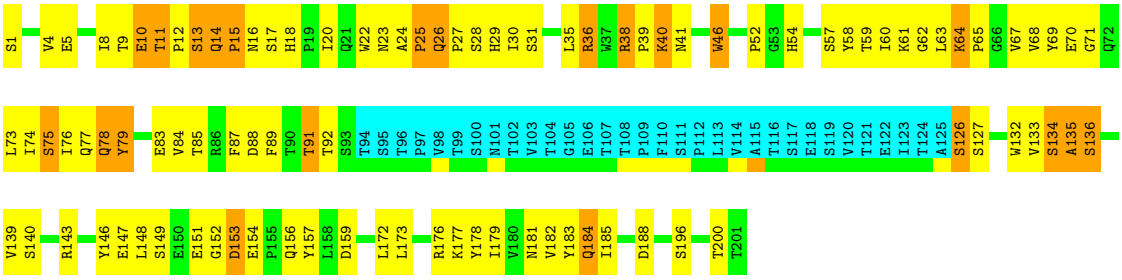
Chain A: 37% 37% 10% 16%



4.2.21 Score per residue for model 21

- Molecule 1: Fibronectin

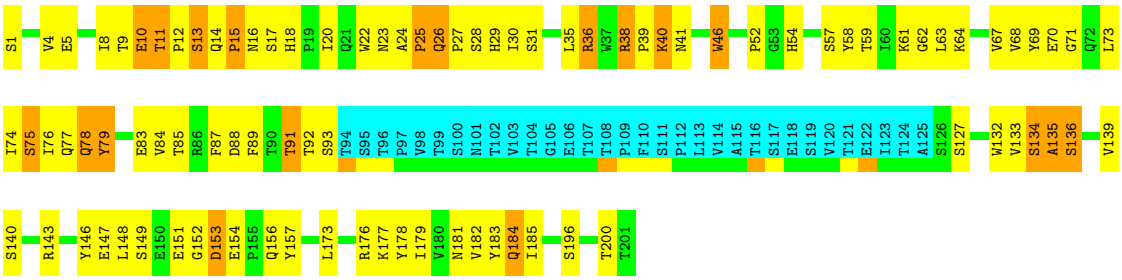
Chain A: 35% 38% 11% 16%



4.2.22 Score per residue for model 22

- Molecule 1: Fibronectin

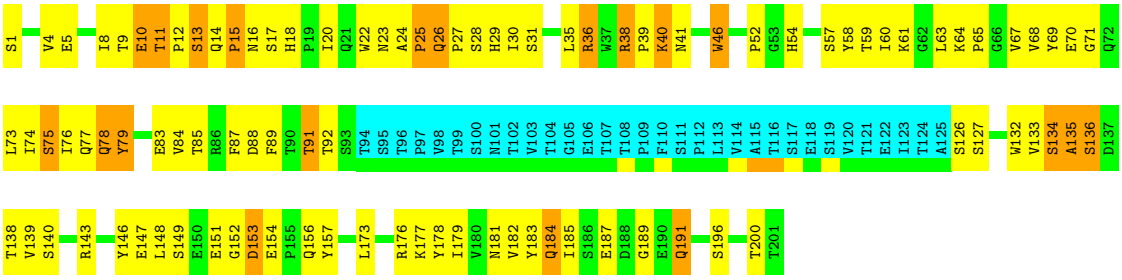
Chain A: 38% 37% 9% 16%



4.2.23 Score per residue for model 23

- Molecule 1: Fibronectin

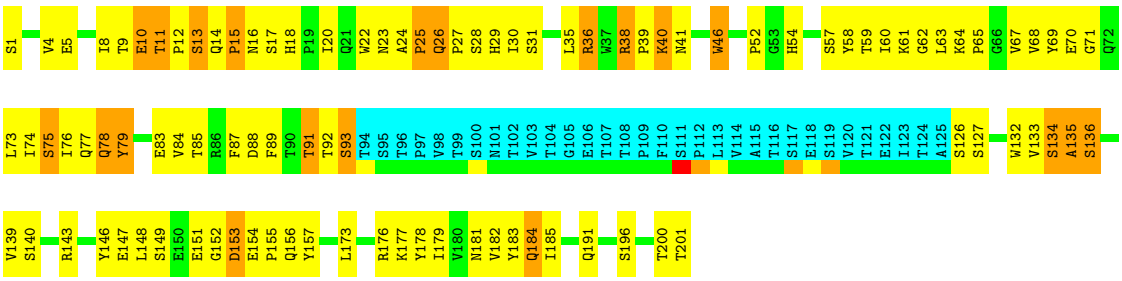
Chain A: 35% 39% 10% 16%



4.2.24 Score per residue for model 24

- Molecule 1: Fibronectin

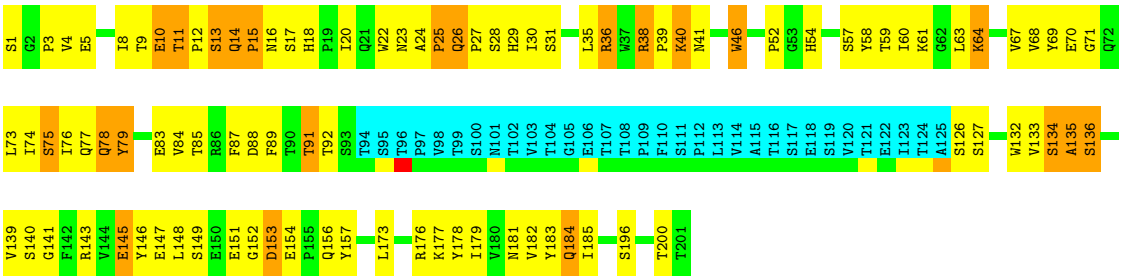
Chain A: 35% 39% 10% 16%



4.2.25 Score per residue for model 25

- Molecule 1: Fibronectin

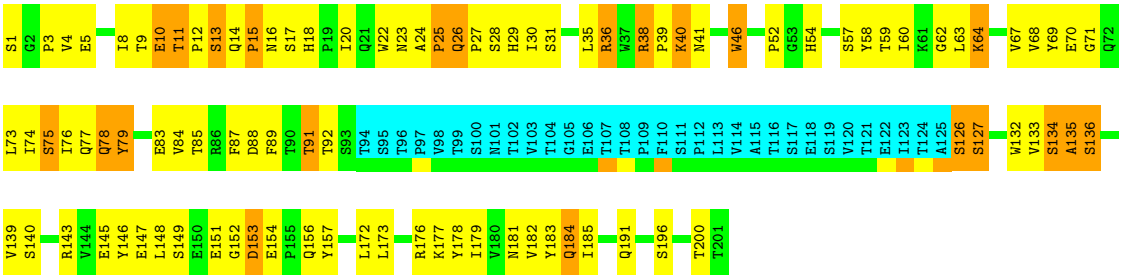
Chain A: 36% 37% 11% 16%



4.2.26 Score per residue for model 26

- Molecule 1: Fibronectin

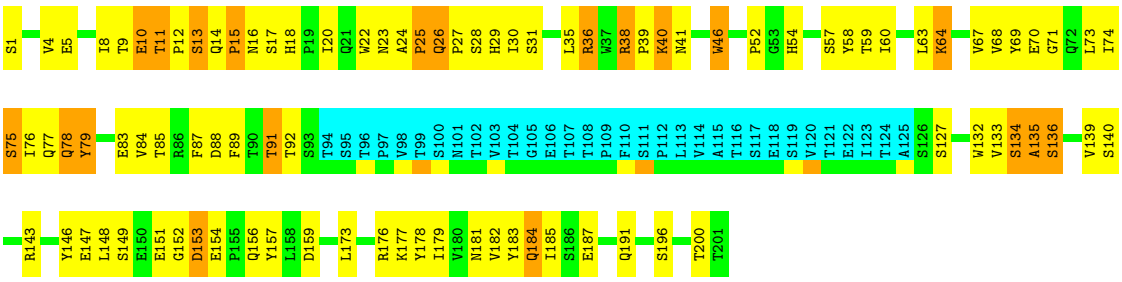
Chain A: 36% 37% 11% 16%



4.2.27 Score per residue for model 27

- Molecule 1: Fibronectin

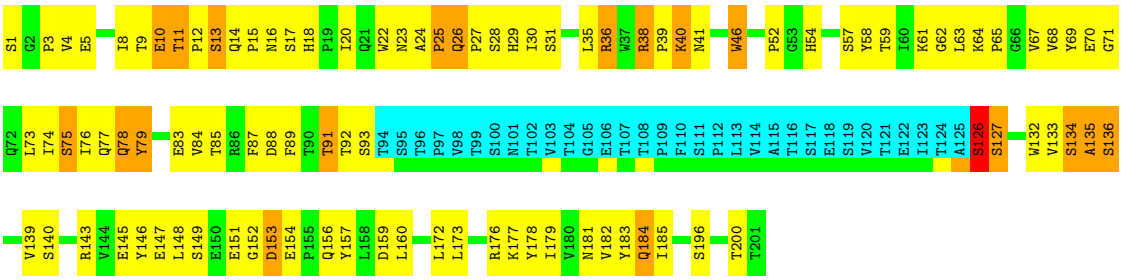
Chain A: 37% 37% 10% 16%



4.2.28 Score per residue for model 28

- Molecule 1: Fibronectin

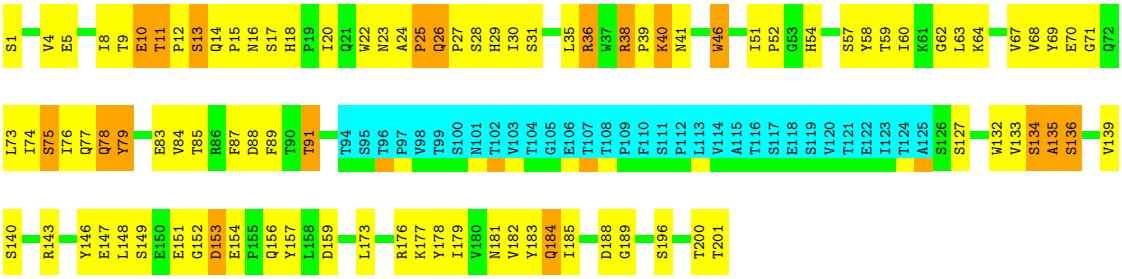
Chain A: 34% 40% 9% 16%



4.2.29 Score per residue for model 29

- Molecule 1: Fibronectin

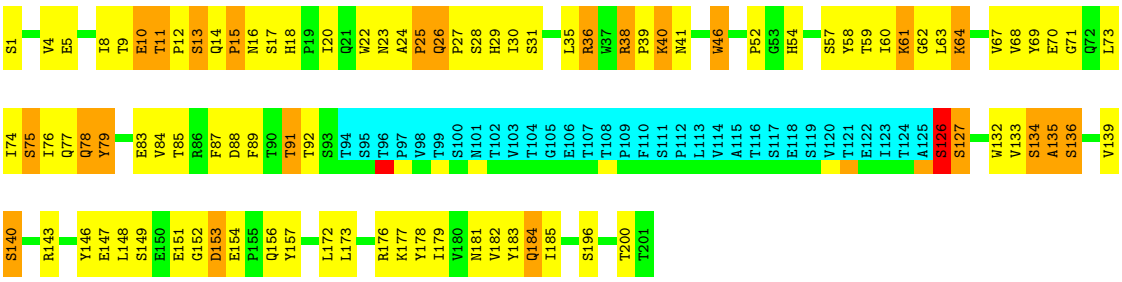
Chain A: 36% 39% 9% 16%



4.2.30 Score per residue for model 30

- Molecule 1: Fibronectin

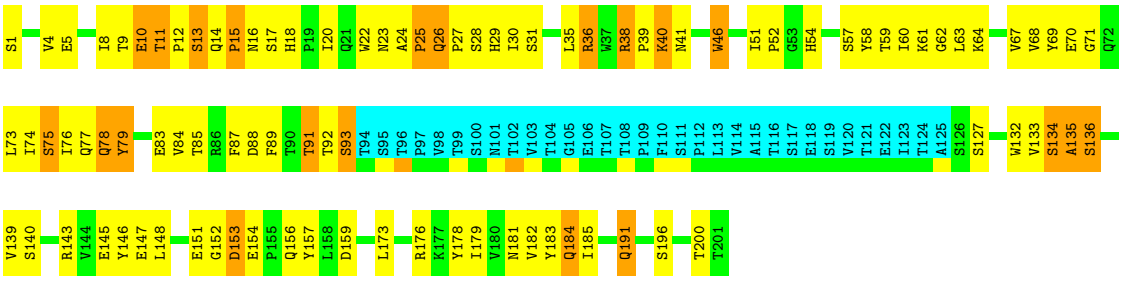
Chain A: 37% 35% 11% 16%



4.2.31 Score per residue for model 31

- Molecule 1: Fibronectin

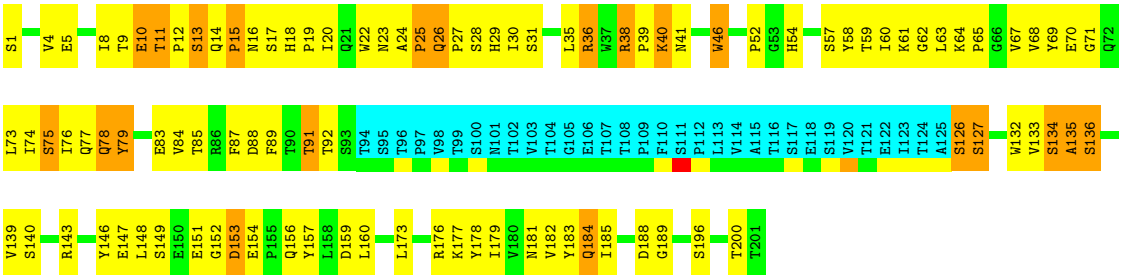
Chain A: 36% 37% 10% 16%



4.2.32 Score per residue for model 32

- Molecule 1: Fibronectin

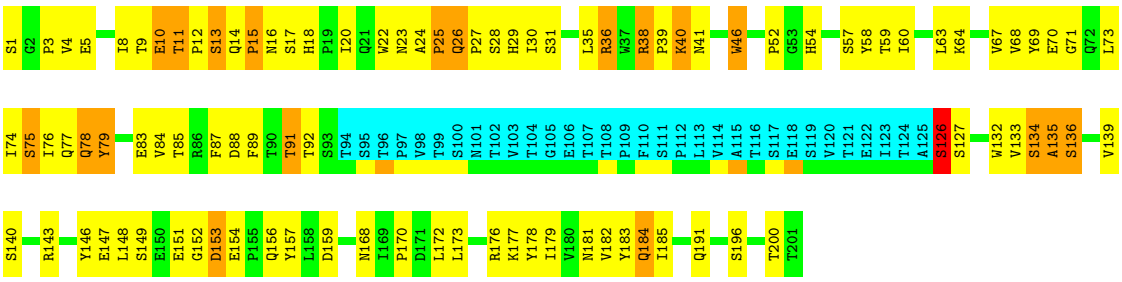
Chain A: 34% 39% 10% 16%



4.2.33 Score per residue for model 33

- Molecule 1: Fibronectin

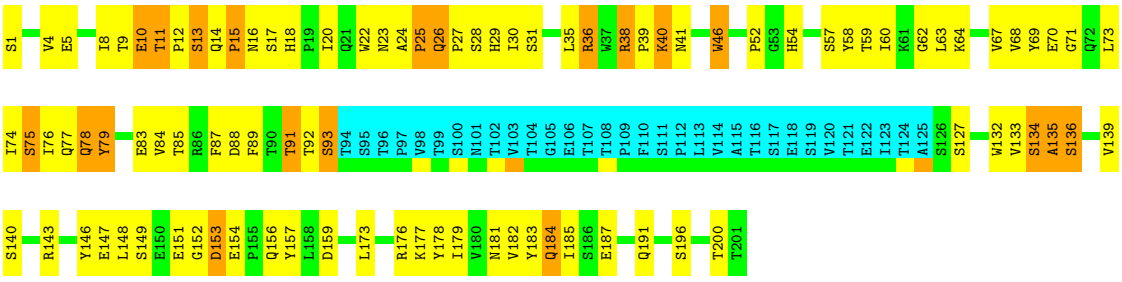
Chain A: 35% 39% 9% 16%



4.2.34 Score per residue for model 34

- Molecule 1: Fibronectin

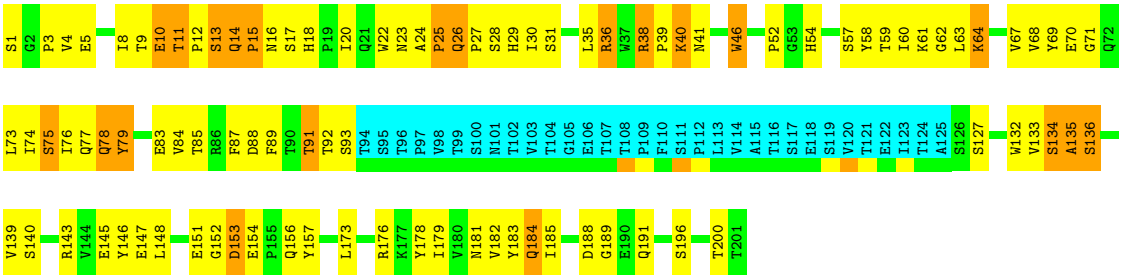
Chain A: 36% 38% 10% 16%



4.2.35 Score per residue for model 35

- Molecule 1: Fibronectin

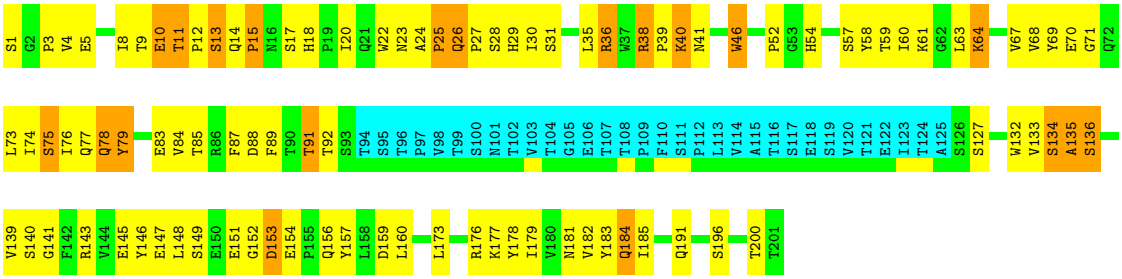
Chain A: 36% 38% 10% 16%



4.2.36 Score per residue for model 36

- Molecule 1: Fibronectin

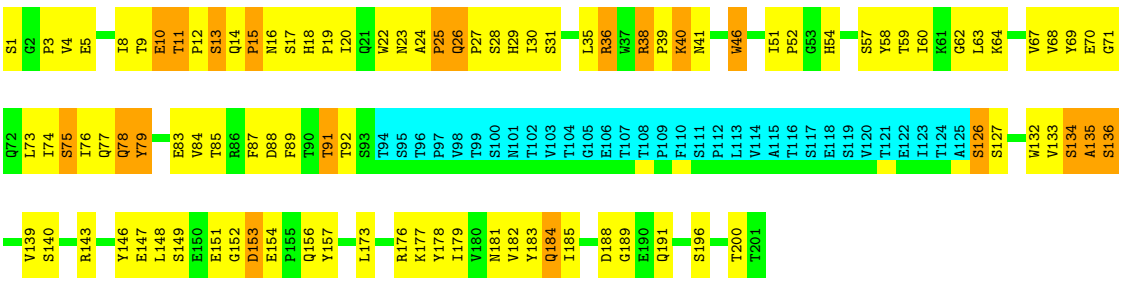
Chain A: 36% 38% 10% 16%



4.2.37 Score per residue for model 37

- Molecule 1: Fibronectin

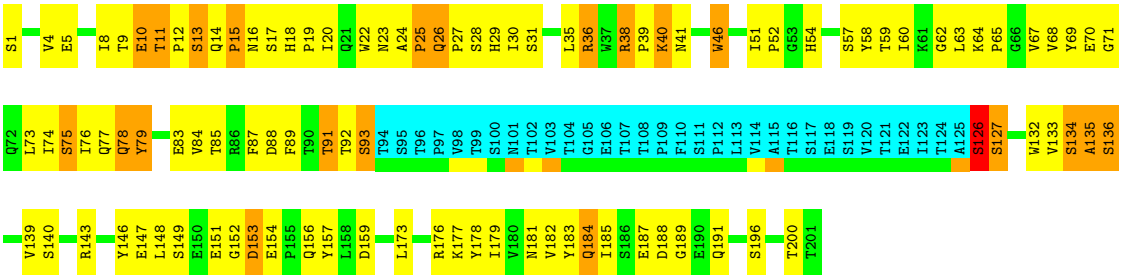
Chain A: 35% 39% 10% 16%



4.2.38 Score per residue for model 38

- Molecule 1: Fibronectin

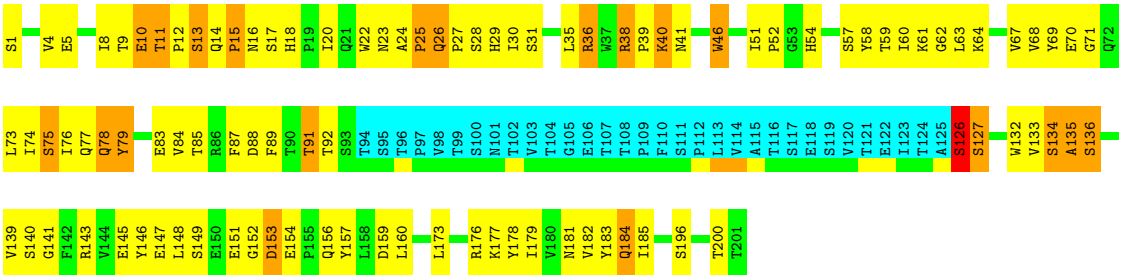
Chain A: 33% 40% 10% 16%



4.2.39 Score per residue for model 39

- Molecule 1: Fibronectin

Chain A: 35% 39% 10% 16%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Rigid body docking with torsional flexibility at the interfacial amino acid sidechains.*

Of the 100 calculated structures, 39 were deposited, based on the following criterion: *Structures forming a single cluster after imposing a 50% lowest energy cutoff.*

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

Software name	Classification	Version
XPLOR-NIH	structure solution	2.12
XPLOR-NIH	refinement	2.12

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1338	1298	1294	131±6
All	All	52182	50622	50466	5126

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:GLU:CD	1:A:176:ARG:HH21	1.41	1.19	21	39
1:A:153:ASP:OD1	1:A:154:GLU:CD	1.34	1.64	29	39
1:A:151:GLU:CD	1:A:176:ARG:NH2	1.23	1.92	31	39
1:A:153:ASP:OD1	1:A:154:GLU:OE1	1.19	1.61	26	39
1:A:134:SER:O	1:A:136:SER:N	1.18	1.77	7	39
1:A:151:GLU:OE1	1:A:176:ARG:NH2	1.12	1.82	35	39
1:A:151:GLU:OE2	1:A:176:ARG:NH2	1.12	1.83	19	39
1:A:152:GLY:O	1:A:153:ASP:O	1.10	1.69	25	39
1:A:143:ARG:NE	1:A:185:ILE:HD11	1.08	1.62	31	1
1:A:61:LYS:HZ3	1:A:140:SER:CB	0.94	1.74	23	1
1:A:59:THR:HG21	1:A:187:GLU:O	0.91	1.65	27	3
1:A:141:GLY:O	1:A:185:ILE:HG22	0.91	1.65	25	2
1:A:148:LEU:HD13	1:A:151:GLU:OE1	0.90	1.67	36	39
1:A:148:LEU:HD21	1:A:178:TYR:CZ	0.89	2.03	12	39

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ASN:ND2	1:A:157:TYR:CD1	0.89	2.41	17	4
1:A:14:GLN:HE22	1:A:91:THR:HG23	0.88	1.26	18	1
1:A:153:ASP:OD1	1:A:154:GLU:N	0.86	2.08	28	39
1:A:65:PRO:HB3	1:A:93:SER:O	0.85	1.70	24	1
1:A:143:ARG:NH2	1:A:183:TYR:CD2	0.84	2.46	28	5
1:A:61:LYS:NZ	1:A:141:GLY:N	0.84	2.25	11	4
1:A:143:ARG:NH2	1:A:157:TYR:CE1	0.83	2.46	25	1
1:A:154:GLU:OE1	1:A:154:GLU:N	0.83	2.12	3	39
1:A:143:ARG:NH2	1:A:157:TYR:CD1	0.82	2.47	25	1
1:A:29:HIS:CE1	1:A:77:GLN:NE2	0.82	2.48	6	39
1:A:134:SER:C	1:A:136:SER:H	0.82	1.77	31	39
1:A:16:ASN:ND2	1:A:157:TYR:CE2	0.81	2.48	22	2
1:A:14:GLN:NE2	1:A:91:THR:HG23	0.81	1.91	18	1
1:A:76:ILE:N	1:A:76:ILE:HD12	0.81	1.91	19	39
1:A:148:LEU:CD1	1:A:151:GLU:OE1	0.81	2.29	2	39
1:A:143:ARG:NH1	1:A:191:GLN:HE22	0.79	1.74	35	1
1:A:61:LYS:HZ2	1:A:140:SER:C	0.79	1.81	39	3
1:A:143:ARG:NH2	1:A:191:GLN:NE2	0.79	2.31	16	4
1:A:143:ARG:NE	1:A:191:GLN:NE2	0.79	2.31	34	7
1:A:143:ARG:NE	1:A:191:GLN:HE22	0.78	1.75	10	6
1:A:143:ARG:NE	1:A:185:ILE:CD1	0.78	2.46	31	1
1:A:143:ARG:HE	1:A:191:GLN:NE2	0.78	1.75	34	6
1:A:64:LYS:O	1:A:67:VAL:HG12	0.78	1.79	19	39
1:A:143:ARG:NH2	1:A:191:GLN:HE22	0.78	1.76	16	2
1:A:16:ASN:HD21	1:A:157:TYR:HB2	0.78	1.38	17	2
1:A:16:ASN:ND2	1:A:62:GLY:H	0.77	1.77	39	4
1:A:153:ASP:OD1	1:A:154:GLU:OE2	0.77	2.03	4	39
1:A:143:ARG:NH2	1:A:145:GLU:OE2	0.76	2.17	4	1
1:A:16:ASN:ND2	1:A:157:TYR:CD2	0.76	2.54	15	5
1:A:59:THR:OG1	1:A:189:GLY:N	0.76	2.18	6	7
1:A:143:ARG:HH21	1:A:159:ASP:N	0.76	1.78	19	1
1:A:20:ILE:HD11	1:A:35:LEU:HD13	0.76	1.58	14	39
1:A:16:ASN:ND2	1:A:143:ARG:CD	0.76	2.49	17	2
1:A:143:ARG:NE	1:A:145:GLU:OE2	0.75	2.18	4	1
1:A:61:LYS:NZ	1:A:140:SER:OG	0.75	2.18	23	4
1:A:16:ASN:HD21	1:A:157:TYR:CB	0.75	1.94	29	2
1:A:154:GLU:CD	1:A:154:GLU:H	0.75	1.85	25	39
1:A:61:LYS:NZ	1:A:140:SER:O	0.75	2.19	4	5
1:A:133:VAL:O	1:A:135:ALA:N	0.74	2.20	31	39
1:A:16:ASN:CG	1:A:157:TYR:CD1	0.74	2.60	27	5
1:A:59:THR:OG1	1:A:188:ASP:C	0.74	2.25	29	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:GLY:O	1:A:191:GLN:NE2	0.74	2.21	23	1
1:A:17:SER:OG	1:A:61:LYS:NZ	0.74	2.20	30	1
1:A:14:GLN:HB2	1:A:17:SER:O	0.73	1.82	18	26
1:A:16:ASN:ND2	1:A:157:TYR:CG	0.73	2.57	17	3
1:A:61:LYS:HZ1	1:A:141:GLY:N	0.73	1.81	11	1
1:A:143:ARG:CD	1:A:185:ILE:HD11	0.73	2.13	31	1
1:A:143:ARG:NH2	1:A:191:GLN:OE1	0.73	2.21	13	11
1:A:68:VAL:HG23	1:A:89:PHE:O	0.73	1.84	22	39
1:A:58:TYR:CE2	1:A:59:THR:O	0.73	2.42	37	39
1:A:143:ARG:HH22	1:A:191:GLN:NE2	0.73	1.82	17	2
1:A:143:ARG:HH21	1:A:191:GLN:NE2	0.72	1.80	16	2
1:A:16:ASN:OD1	1:A:157:TYR:CD1	0.72	2.42	27	3
1:A:14:GLN:H	1:A:14:GLN:CD	0.72	1.87	18	1
1:A:143:ARG:NH1	1:A:157:TYR:CE1	0.72	2.57	36	5
1:A:143:ARG:HH12	1:A:191:GLN:NE2	0.72	1.83	27	2
1:A:61:LYS:NZ	1:A:140:SER:CB	0.72	2.53	23	2
1:A:143:ARG:HE	1:A:191:GLN:HE22	0.71	1.27	10	2
1:A:15:PRO:HG2	1:A:143:ARG:NE	0.71	2.00	39	5
1:A:16:ASN:ND2	1:A:159:ASP:OD1	0.71	2.24	11	2
1:A:16:ASN:OD1	1:A:159:ASP:OD2	0.71	2.07	11	1
1:A:61:LYS:NZ	1:A:140:SER:C	0.71	2.43	13	5
1:A:14:GLN:CD	1:A:14:GLN:N	0.71	2.42	18	1
1:A:14:GLN:O	1:A:92:THR:O	0.71	2.08	30	34
1:A:59:THR:OG1	1:A:187:GLU:O	0.71	2.08	2	5
1:A:16:ASN:OD1	1:A:157:TYR:CD2	0.71	2.44	29	5
1:A:16:ASN:CG	1:A:157:TYR:CD2	0.70	2.65	26	8
1:A:157:TYR:N	1:A:157:TYR:CD1	0.70	2.57	20	1
1:A:16:ASN:OD1	1:A:63:LEU:N	0.70	2.24	18	12
1:A:143:ARG:NH2	1:A:183:TYR:CE2	0.70	2.60	26	2
1:A:15:PRO:CG	1:A:143:ARG:NH1	0.70	2.55	35	9
1:A:39:PRO:O	1:A:41:ASN:N	0.70	2.25	23	39
1:A:143:ARG:NH1	1:A:191:GLN:OE1	0.69	2.25	3	4
1:A:14:GLN:N	1:A:14:GLN:CD	0.69	2.44	16	3
1:A:16:ASN:CG	1:A:157:TYR:CE1	0.69	2.65	37	5
1:A:8:ILE:HG22	1:A:11:THR:OG1	0.69	1.88	13	39
1:A:153:ASP:CG	1:A:154:GLU:H	0.69	1.91	31	39
1:A:16:ASN:CG	1:A:157:TYR:CE2	0.69	2.66	26	8
1:A:16:ASN:OD1	1:A:157:TYR:CE2	0.69	2.45	29	5
1:A:16:ASN:ND2	1:A:63:LEU:N	0.69	2.41	22	1
1:A:16:ASN:C	1:A:16:ASN:ND2	0.69	2.46	1	1
1:A:40:LYS:O	1:A:41:ASN:ND2	0.69	2.26	12	39

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:ASN:ND2	1:A:159:ASP:CG	0.69	2.46	11	2
1:A:173:LEU:HB2	1:A:178:TYR:OH	0.68	1.88	25	39
1:A:13:SER:O	1:A:14:GLN:NE2	0.68	2.26	6	6
1:A:24:ALA:HB1	1:A:25:PRO:HD2	0.68	1.66	34	39
1:A:16:ASN:OD1	1:A:157:TYR:CG	0.68	2.46	29	3
1:A:143:ARG:HH21	1:A:191:GLN:HE22	0.68	1.24	16	2
1:A:16:ASN:OD1	1:A:157:TYR:CE1	0.68	2.47	27	6
1:A:14:GLN:NE2	1:A:191:GLN:OE1	0.68	2.27	10	3
1:A:46:TRP:CD1	1:A:46:TRP:N	0.68	2.62	2	39
1:A:16:ASN:ND2	1:A:63:LEU:O	0.68	2.25	22	1
1:A:61:LYS:HZ2	1:A:141:GLY:N	0.68	1.85	39	1
1:A:76:ILE:N	1:A:76:ILE:CD1	0.68	2.57	36	39
1:A:143:ARG:NH1	1:A:191:GLN:NE2	0.68	2.41	35	1
1:A:16:ASN:OD1	1:A:17:SER:N	0.67	2.27	33	4
1:A:16:ASN:OD1	1:A:63:LEU:O	0.67	2.12	2	7
1:A:16:ASN:ND2	1:A:159:ASP:OD2	0.67	2.28	2	3
1:A:188:ASP:OD1	1:A:190:GLU:N	0.67	2.26	5	2
1:A:16:ASN:OD1	1:A:157:TYR:CZ	0.67	2.48	29	2
1:A:148:LEU:CD2	1:A:178:TYR:CZ	0.67	2.78	25	39
1:A:61:LYS:HZ1	1:A:141:GLY:CA	0.67	2.01	11	1
1:A:16:ASN:OD1	1:A:143:ARG:CD	0.67	2.43	15	1
1:A:61:LYS:CD	1:A:185:ILE:HD12	0.67	2.19	9	1
1:A:58:TYR:CG	1:A:59:THR:N	0.67	2.63	1	39
1:A:65:PRO:CD	1:A:157:TYR:CE1	0.67	2.78	12	6
1:A:143:ARG:NH1	1:A:157:TYR:CD1	0.66	2.62	13	5
1:A:16:ASN:OD1	1:A:143:ARG:NH1	0.66	2.27	32	1
1:A:61:LYS:HD2	1:A:185:ILE:HG21	0.66	1.66	28	1
1:A:16:ASN:ND2	1:A:17:SER:N	0.66	2.43	7	2
1:A:16:ASN:HD21	1:A:62:GLY:H	0.66	1.33	11	1
1:A:58:TYR:CD2	1:A:59:THR:N	0.66	2.64	19	39
1:A:14:GLN:OE1	1:A:191:GLN:NE2	0.66	2.29	2	1
1:A:16:ASN:HD22	1:A:17:SER:N	0.66	1.88	1	2
1:A:136:SER:O	1:A:139:VAL:HG12	0.66	1.91	32	39
1:A:143:ARG:CZ	1:A:191:GLN:HE22	0.66	2.04	10	2
1:A:61:LYS:HZ3	1:A:140:SER:C	0.65	1.94	11	2
1:A:143:ARG:NH2	1:A:191:GLN:CD	0.65	2.49	17	4
1:A:67:VAL:CG1	1:A:69:TYR:CE2	0.65	2.80	3	39
1:A:153:ASP:CG	1:A:154:GLU:N	0.65	2.50	29	39
1:A:15:PRO:CG	1:A:143:ARG:CZ	0.65	2.74	4	16
1:A:61:LYS:NZ	1:A:142:PHE:N	0.65	2.45	7	1
1:A:12:PRO:O	1:A:13:SER:CB	0.64	2.45	23	39

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:PRO:O	1:A:29:HIS:N	0.64	2.30	20	39
1:A:141:GLY:C	1:A:185:ILE:HG22	0.64	2.11	16	2
1:A:157:TYR:CD1	1:A:157:TYR:C	0.64	2.70	17	5
1:A:64:LYS:N	1:A:69:TYR:OH	0.64	2.26	37	39
1:A:143:ARG:CZ	1:A:191:GLN:OE1	0.64	2.45	35	3
1:A:126:SER:OG	1:A:172:LEU:O	0.63	2.15	4	12
1:A:77:GLN:O	1:A:79:TYR:N	0.63	2.32	22	39
1:A:61:LYS:NZ	1:A:141:GLY:CA	0.63	2.60	11	4
1:A:143:ARG:NH1	1:A:157:TYR:CB	0.63	2.61	30	3
1:A:59:THR:CG2	1:A:187:GLU:O	0.63	2.46	17	4
1:A:16:ASN:CB	1:A:143:ARG:NH1	0.63	2.62	39	2
1:A:61:LYS:CG	1:A:62:GLY:N	0.62	2.62	14	6
1:A:15:PRO:HG2	1:A:143:ARG:NH1	0.62	2.10	35	10
1:A:16:ASN:OD1	1:A:16:ASN:C	0.62	2.38	33	3
1:A:14:GLN:HE22	1:A:191:GLN:CD	0.62	1.98	2	1
1:A:143:ARG:HH22	1:A:191:GLN:CD	0.61	1.97	31	3
1:A:16:ASN:HD21	1:A:62:GLY:C	0.61	1.99	22	1
1:A:61:LYS:NZ	1:A:141:GLY:C	0.61	2.52	7	1
1:A:14:GLN:N	1:A:14:GLN:NE2	0.61	2.49	21	3
1:A:61:LYS:NZ	1:A:185:ILE:HD13	0.61	2.10	32	1
1:A:152:GLY:C	1:A:153:ASP:O	0.61	2.39	24	39
1:A:16:ASN:HB3	1:A:143:ARG:NH1	0.61	2.10	39	3
1:A:143:ARG:CZ	1:A:191:GLN:NE2	0.61	2.64	16	3
1:A:143:ARG:HH22	1:A:191:GLN:CG	0.61	2.08	31	1
1:A:140:SER:N	1:A:185:ILE:O	0.61	2.31	33	39
1:A:159:ASP:OD1	1:A:160:LEU:N	0.60	2.34	39	10
1:A:134:SER:C	1:A:136:SER:N	0.60	2.44	23	19
1:A:143:ARG:NH2	1:A:191:GLN:CG	0.60	2.64	31	1
1:A:17:SER:OG	1:A:61:LYS:CE	0.60	2.49	30	1
1:A:15:PRO:CG	1:A:143:ARG:NE	0.60	2.64	39	3
1:A:61:LYS:NZ	1:A:185:ILE:CD1	0.60	2.65	21	1
1:A:4:VAL:N	1:A:85:THR:OG1	0.60	2.35	28	39
1:A:75:SER:C	1:A:76:ILE:HD12	0.60	2.17	28	39
1:A:13:SER:C	1:A:14:GLN:NE2	0.59	2.55	21	8
1:A:14:GLN:OE1	1:A:191:GLN:OE1	0.59	2.20	10	1
1:A:186:SER:OG	1:A:188:ASP:OD1	0.59	2.19	5	2
1:A:16:ASN:ND2	1:A:16:ASN:C	0.59	2.56	7	1
1:A:8:ILE:CG2	1:A:11:THR:OG1	0.59	2.51	16	39
1:A:138:THR:O	1:A:187:GLU:CD	0.59	2.41	23	1
1:A:15:PRO:HD2	1:A:143:ARG:NH1	0.59	2.13	11	2
1:A:15:PRO:N	1:A:93:SER:OG	0.59	2.36	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:ILE:HG12	1:A:84:VAL:HG23	0.58	1.76	4	39
1:A:15:PRO:HG2	1:A:143:ARG:CZ	0.58	2.28	4	10
1:A:18:HIS:CE1	1:A:89:PHE:CD2	0.58	2.91	39	39
1:A:191:GLN:N	1:A:191:GLN:CD	0.58	2.56	23	1
1:A:145:GLU:CD	1:A:145:GLU:C	0.58	2.61	25	1
1:A:16:ASN:ND2	1:A:159:ASP:CB	0.58	2.66	2	1
1:A:14:GLN:HE21	1:A:17:SER:C	0.58	2.00	31	2
1:A:88:ASP:OD1	1:A:88:ASP:O	0.58	2.22	4	39
1:A:143:ARG:CZ	1:A:145:GLU:OE2	0.58	2.51	4	1
1:A:12:PRO:O	1:A:13:SER:OG	0.57	2.22	19	39
1:A:148:LEU:CD2	1:A:178:TYR:CE2	0.57	2.88	5	39
1:A:16:ASN:HD22	1:A:143:ARG:CD	0.57	2.13	17	3
1:A:14:GLN:NE2	1:A:91:THR:CG2	0.57	2.65	18	1
1:A:143:ARG:CZ	1:A:157:TYR:HB3	0.57	2.29	39	2
1:A:16:ASN:CB	1:A:143:ARG:CZ	0.57	2.83	29	1
1:A:16:ASN:HD22	1:A:61:LYS:NZ	0.57	1.98	21	1
1:A:188:ASP:OD1	1:A:188:ASP:C	0.57	2.44	5	2
1:A:17:SER:OG	1:A:185:ILE:HD13	0.56	2.00	5	1
1:A:19:PRO:HB3	1:A:188:ASP:O	0.56	2.00	15	7
1:A:61:LYS:HD3	1:A:185:ILE:HG21	0.56	1.75	24	2
1:A:154:GLU:CD	1:A:154:GLU:N	0.56	2.58	15	19
1:A:61:LYS:HG2	1:A:62:GLY:N	0.56	2.16	21	7
1:A:15:PRO:CG	1:A:143:ARG:NH2	0.56	2.68	16	2
1:A:143:ARG:NH2	1:A:157:TYR:CB	0.56	2.68	39	2
1:A:16:ASN:ND2	1:A:157:TYR:CB	0.56	2.67	29	2
1:A:143:ARG:HE	1:A:185:ILE:CG1	0.56	2.12	31	1
1:A:14:GLN:CG	1:A:17:SER:O	0.56	2.54	16	3
1:A:152:GLY:O	1:A:153:ASP:C	0.56	2.44	19	38
1:A:141:GLY:N	1:A:185:ILE:HG12	0.56	2.16	19	3
1:A:1:SER:C	1:A:83:GLU:OE1	0.55	2.45	7	39
1:A:13:SER:C	1:A:14:GLN:OE1	0.55	2.45	23	5
1:A:13:SER:O	1:A:14:GLN:OE1	0.55	2.25	30	3
1:A:16:ASN:ND2	1:A:157:TYR:CE1	0.55	2.71	30	1
1:A:16:ASN:HB3	1:A:61:LYS:HZ2	0.55	1.61	30	1
1:A:185:ILE:HD12	1:A:185:ILE:N	0.55	2.17	32	1
1:A:185:ILE:O	1:A:185:ILE:CG1	0.55	2.53	15	3
1:A:16:ASN:ND2	1:A:62:GLY:C	0.55	2.60	22	1
1:A:16:ASN:ND2	1:A:62:GLY:N	0.55	2.52	39	1
1:A:20:ILE:HD11	1:A:35:LEU:CD1	0.55	2.32	3	39
1:A:146:TYR:CZ	1:A:156:GLN:HB2	0.55	2.37	23	39
1:A:159:ASP:O	1:A:159:ASP:OD1	0.55	2.25	33	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:GLN:OE1	1:A:191:GLN:CD	0.55	2.45	2	1
1:A:15:PRO:HD2	1:A:143:ARG:HH12	0.54	1.62	11	1
1:A:16:ASN:CG	1:A:159:ASP:OD2	0.54	2.46	21	2
1:A:65:PRO:HD3	1:A:157:TYR:CE1	0.54	2.38	15	6
1:A:61:LYS:HD3	1:A:185:ILE:HD13	0.54	1.80	25	1
1:A:143:ARG:NH2	1:A:157:TYR:HB3	0.54	2.17	2	3
1:A:141:GLY:HA3	1:A:185:ILE:HD11	0.54	1.80	9	1
1:A:159:ASP:OD1	1:A:159:ASP:C	0.54	2.45	39	5
1:A:92:THR:O	1:A:93:SER:CB	0.54	2.55	24	3
1:A:61:LYS:CD	1:A:185:ILE:HD13	0.54	2.32	25	2
1:A:16:ASN:CB	1:A:61:LYS:HZ2	0.54	2.15	30	1
1:A:14:GLN:CB	1:A:17:SER:O	0.54	2.56	37	39
1:A:143:ARG:NH1	1:A:185:ILE:HD11	0.54	2.18	23	1
1:A:138:THR:O	1:A:187:GLU:OE2	0.53	2.26	23	1
1:A:27:PRO:C	1:A:29:HIS:H	0.53	2.07	34	39
1:A:61:LYS:CE	1:A:140:SER:OG	0.53	2.57	5	1
1:A:145:GLU:OE2	1:A:157:TYR:OH	0.53	2.21	35	5
1:A:143:ARG:NH2	1:A:157:TYR:HB2	0.53	2.18	39	1
1:A:67:VAL:HG13	1:A:69:TYR:CE2	0.53	2.39	30	39
1:A:14:GLN:CD	1:A:191:GLN:OE1	0.53	2.47	10	1
1:A:16:ASN:ND2	1:A:61:LYS:HZ1	0.53	2.02	21	1
1:A:61:LYS:HZ2	1:A:185:ILE:CD1	0.53	2.16	21	1
1:A:143:ARG:HH21	1:A:158:LEU:C	0.53	2.06	19	1
1:A:4:VAL:HG12	1:A:5:GLU:N	0.53	2.19	20	39
1:A:16:ASN:ND2	1:A:143:ARG:HD2	0.53	2.19	27	4
1:A:64:LYS:O	1:A:67:VAL:CG1	0.52	2.57	8	39
1:A:10:GLU:O	1:A:10:GLU:HG2	0.52	2.05	31	3
1:A:16:ASN:OD1	1:A:62:GLY:CA	0.52	2.57	37	7
1:A:93:SER:OG	1:A:157:TYR:CE2	0.52	2.58	5	2
1:A:145:GLU:CD	1:A:157:TYR:CE2	0.52	2.83	11	5
1:A:14:GLN:CG	1:A:191:GLN:HE22	0.52	2.17	27	1
1:A:15:PRO:CB	1:A:157:TYR:CZ	0.52	2.92	35	1
1:A:15:PRO:CB	1:A:143:ARG:NH2	0.52	2.73	30	3
1:A:143:ARG:NH1	1:A:159:ASP:HB2	0.52	2.19	29	1
1:A:24:ALA:HB1	1:A:25:PRO:CD	0.52	2.35	36	39
1:A:93:SER:OG	1:A:157:TYR:OH	0.52	2.28	35	4
1:A:92:THR:O	1:A:93:SER:OG	0.52	2.23	20	1
1:A:14:GLN:HG3	1:A:191:GLN:NE2	0.52	2.20	11	3
1:A:14:GLN:CD	1:A:191:GLN:HE21	0.52	2.08	31	1
1:A:65:PRO:CG	1:A:157:TYR:CE1	0.52	2.93	12	2
1:A:9:THR:O	1:A:11:THR:N	0.51	2.44	4	39

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LYS:HE2	1:A:185:ILE:HG21	0.51	1.82	13	3
1:A:16:ASN:CG	1:A:157:TYR:CG	0.51	2.84	29	2
1:A:92:THR:OG1	1:A:93:SER:N	0.51	2.43	20	2
1:A:143:ARG:HH11	1:A:191:GLN:HE22	0.51	1.46	35	1
1:A:16:ASN:ND2	1:A:159:ASP:HB2	0.51	2.21	2	3
1:A:1:SER:N	1:A:83:GLU:OE1	0.51	2.39	11	39
1:A:93:SER:OG	1:A:157:TYR:CZ	0.51	2.64	5	2
1:A:140:SER:OG	1:A:187:GLU:OE1	0.51	2.28	9	1
1:A:15:PRO:HG3	1:A:143:ARG:CZ	0.51	2.35	25	8
1:A:22:TRP:CZ3	1:A:58:TYR:N	0.51	2.79	3	39
1:A:143:ARG:NH1	1:A:157:TYR:HB2	0.51	2.21	30	3
1:A:185:ILE:HD12	1:A:191:GLN:OE1	0.50	2.06	23	1
1:A:61:LYS:NZ	1:A:141:GLY:HA3	0.50	2.21	11	1
1:A:126:SER:CB	1:A:201:THR:HB	0.50	2.37	24	2
1:A:145:GLU:C	1:A:145:GLU:OE1	0.50	2.49	25	1
1:A:143:ARG:HE	1:A:185:ILE:CD1	0.50	2.17	31	1
1:A:16:ASN:OD1	1:A:62:GLY:N	0.50	2.38	35	1
1:A:145:GLU:CD	1:A:156:GLN:O	0.50	2.50	26	3
1:A:4:VAL:HG12	1:A:5:GLU:H	0.50	1.67	23	39
1:A:143:ARG:HH21	1:A:191:GLN:CD	0.50	2.08	16	2
1:A:67:VAL:HG11	1:A:69:TYR:CZ	0.50	2.42	9	39
1:A:16:ASN:C	1:A:61:LYS:HZ2	0.50	2.10	30	1
1:A:126:SER:OG	1:A:127:SER:N	0.50	2.45	32	1
1:A:38:ARG:NE	1:A:70:GLU:OE2	0.49	2.45	35	39
1:A:187:GLU:CD	1:A:187:GLU:H	0.49	2.10	7	1
1:A:14:GLN:NE2	1:A:17:SER:C	0.49	2.66	15	2
1:A:16:ASN:OD1	1:A:62:GLY:C	0.49	2.50	37	11
1:A:16:ASN:ND2	1:A:143:ARG:HD3	0.49	2.21	17	1
1:A:15:PRO:CD	1:A:143:ARG:NH1	0.49	2.75	35	2
1:A:15:PRO:HB3	1:A:157:TYR:CZ	0.49	2.42	35	3
1:A:141:GLY:N	1:A:185:ILE:CG2	0.49	2.75	25	2
1:A:16:ASN:CG	1:A:159:ASP:OD1	0.49	2.51	11	1
1:A:126:SER:HB2	1:A:201:THR:HB	0.49	1.83	15	2
1:A:59:THR:HG23	1:A:189:GLY:CA	0.49	2.38	32	1
1:A:181:ASN:HB3	1:A:183:TYR:CZ	0.49	2.43	39	39
1:A:14:GLN:NE2	1:A:17:SER:CB	0.49	2.75	15	2
1:A:143:ARG:NH2	1:A:159:ASP:OD2	0.49	2.45	29	1
1:A:26:GLN:N	1:A:27:PRO:CD	0.48	2.76	19	39
1:A:14:GLN:NE2	1:A:191:GLN:CD	0.48	2.65	2	1
1:A:141:GLY:CA	1:A:185:ILE:CD1	0.48	2.91	9	1
1:A:16:ASN:HD21	1:A:62:GLY:CA	0.48	2.20	22	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:TRP:CH2	1:A:57:SER:C	0.48	2.87	12	39
1:A:61:LYS:CD	1:A:185:ILE:CD1	0.48	2.91	9	1
1:A:16:ASN:HB2	1:A:143:ARG:NH2	0.48	2.23	39	1
1:A:52:PRO:HB2	1:A:54:HIS:CE1	0.48	2.44	13	39
1:A:68:VAL:CG2	1:A:89:PHE:O	0.48	2.61	28	39
1:A:146:TYR:HA	1:A:179:ILE:O	0.48	2.09	7	39
1:A:61:LYS:NZ	1:A:185:ILE:HD12	0.48	2.24	21	1
1:A:15:PRO:CG	1:A:143:ARG:HE	0.48	2.21	39	1
1:A:88:ASP:OD1	1:A:88:ASP:C	0.48	2.52	6	39
1:A:29:HIS:CE1	1:A:77:GLN:HE22	0.48	2.26	26	39
1:A:132:TRP:CD2	1:A:182:VAL:HG11	0.48	2.44	1	39
1:A:16:ASN:HD22	1:A:159:ASP:CB	0.48	2.21	2	1
1:A:16:ASN:ND2	1:A:157:TYR:HB2	0.48	2.24	20	2
1:A:13:SER:H	1:A:14:GLN:HE22	0.48	1.50	36	2
1:A:15:PRO:HB2	1:A:143:ARG:NH2	0.48	2.23	8	5
1:A:61:LYS:HE3	1:A:185:ILE:HG21	0.48	1.86	5	1
1:A:16:ASN:OD1	1:A:159:ASP:CG	0.48	2.52	7	1
1:A:181:ASN:OD1	1:A:196:SER:CB	0.47	2.62	20	39
1:A:141:GLY:H	1:A:185:ILE:HG12	0.47	1.67	9	3
1:A:16:ASN:CG	1:A:143:ARG:NH1	0.47	2.67	32	1
1:A:69:TYR:HB2	1:A:89:PHE:CZ	0.47	2.44	19	39
1:A:4:VAL:CG1	1:A:23:ASN:O	0.47	2.62	22	39
1:A:61:LYS:CE	1:A:185:ILE:HG13	0.47	2.39	2	1
1:A:61:LYS:HZ2	1:A:141:GLY:HA3	0.47	1.69	7	1
1:A:16:ASN:HD22	1:A:159:ASP:CG	0.47	2.13	19	2
1:A:16:ASN:HB2	1:A:143:ARG:CZ	0.47	2.38	29	1
1:A:4:VAL:HG12	1:A:23:ASN:O	0.47	2.10	34	39
1:A:46:TRP:N	1:A:46:TRP:HD1	0.47	2.08	37	39
1:A:67:VAL:CG1	1:A:69:TYR:CZ	0.47	2.98	3	39
1:A:148:LEU:HD21	1:A:178:TYR:CE2	0.47	2.43	7	14
1:A:136:SER:HB2	1:A:184:GLN:NE2	0.47	2.25	10	39
1:A:59:THR:OG1	1:A:61:LYS:NZ	0.47	2.47	5	1
1:A:141:GLY:CA	1:A:185:ILE:HD11	0.47	2.39	9	1
1:A:14:GLN:NE2	1:A:17:SER:HB2	0.47	2.25	15	1
1:A:65:PRO:HD3	1:A:157:TYR:CZ	0.47	2.44	15	2
1:A:145:GLU:O	1:A:145:GLU:CG	0.47	2.62	25	1
1:A:14:GLN:HE22	1:A:19:PRO:CD	0.47	2.23	32	1
1:A:16:ASN:HD21	1:A:62:GLY:N	0.47	2.07	39	2
1:A:16:ASN:HB2	1:A:157:TYR:CD1	0.46	2.45	37	3
1:A:13:SER:C	1:A:14:GLN:CD	0.46	2.73	6	4
1:A:185:ILE:O	1:A:185:ILE:HG23	0.46	2.10	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:THR:OG1	1:A:189:GLY:CA	0.46	2.63	35	1
1:A:15:PRO:HG2	1:A:143:ARG:CD	0.46	2.40	5	2
1:A:16:ASN:CG	1:A:159:ASP:CG	0.46	2.73	11	1
1:A:15:PRO:CA	1:A:93:SER:OG	0.46	2.63	20	1
1:A:9:THR:O	1:A:10:GLU:C	0.46	2.54	1	39
1:A:14:GLN:C	1:A:92:THR:O	0.46	2.53	30	7
1:A:16:ASN:HB3	1:A:61:LYS:NZ	0.46	2.26	30	1
1:A:27:PRO:C	1:A:29:HIS:N	0.46	2.70	32	39
1:A:16:ASN:ND2	1:A:61:LYS:NZ	0.46	2.62	21	1
1:A:1:SER:O	1:A:83:GLU:OE1	0.46	2.34	31	39
1:A:16:ASN:CB	1:A:61:LYS:NZ	0.46	2.78	30	1
1:A:61:LYS:NZ	1:A:185:ILE:HB	0.46	2.26	13	3
1:A:14:GLN:CG	1:A:191:GLN:NE2	0.46	2.78	20	2
1:A:22:TRP:CB	1:A:73:LEU:HD22	0.45	2.42	11	39
1:A:36:ARG:CZ	1:A:46:TRP:CH2	0.45	3.00	1	39
1:A:181:ASN:OD1	1:A:196:SER:OG	0.45	2.30	29	39
1:A:143:ARG:NH2	1:A:191:GLN:HB3	0.45	2.26	31	1
1:A:36:ARG:HB2	1:A:46:TRP:CZ3	0.45	2.47	22	39
1:A:61:LYS:HD3	1:A:62:GLY:H	0.45	1.70	30	1
1:A:9:THR:C	1:A:11:THR:N	0.45	2.70	39	39
1:A:14:GLN:HB3	1:A:17:SER:O	0.45	2.10	26	31
1:A:61:LYS:HZ2	1:A:141:GLY:CA	0.45	2.23	7	1
1:A:14:GLN:HE21	1:A:191:GLN:HE21	0.45	1.54	9	1
1:A:145:GLU:HG2	1:A:157:TYR:CD2	0.45	2.45	20	1
1:A:15:PRO:HG3	1:A:143:ARG:NH1	0.45	2.27	34	2
1:A:5:GLU:O	1:A:23:ASN:N	0.45	2.42	39	34
1:A:9:THR:CB	1:A:10:GLU:OE1	0.45	2.64	26	1
1:A:62:GLY:H	1:A:143:ARG:HH22	0.45	1.54	29	1
1:A:65:PRO:HG3	1:A:157:TYR:CE1	0.45	2.47	12	1
1:A:16:ASN:OD1	1:A:159:ASP:OD1	0.45	2.34	7	1
1:A:22:TRP:CZ3	1:A:35:LEU:HD11	0.45	2.47	28	39
1:A:16:ASN:OD1	1:A:143:ARG:HD2	0.45	2.11	15	1
1:A:16:ASN:HB2	1:A:157:TYR:CG	0.45	2.47	28	1
1:A:15:PRO:HB2	1:A:143:ARG:CZ	0.45	2.42	32	1
1:A:40:LYS:O	1:A:41:ASN:CG	0.44	2.56	12	39
1:A:146:TYR:CE2	1:A:156:GLN:OE1	0.44	2.71	24	39
1:A:16:ASN:HB2	1:A:157:TYR:CD2	0.44	2.48	26	4
1:A:16:ASN:HD22	1:A:143:ARG:CG	0.44	2.25	17	1
1:A:143:ARG:NH1	1:A:157:TYR:HB3	0.44	2.27	30	1
1:A:62:GLY:N	1:A:159:ASP:OD2	0.44	2.51	34	1
1:A:16:ASN:HD21	1:A:159:ASP:HB2	0.44	1.73	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:GLY:O	1:A:185:ILE:HG12	0.44	2.13	9	1
1:A:13:SER:O	1:A:14:GLN:CD	0.44	2.55	23	3
1:A:18:HIS:CB	1:A:63:LEU:CD1	0.44	2.96	7	39
1:A:16:ASN:OD1	1:A:62:GLY:HA2	0.44	2.12	11	1
1:A:16:ASN:CB	1:A:157:TYR:CD2	0.44	3.01	26	2
1:A:143:ARG:HH12	1:A:157:TYR:CB	0.44	2.24	30	1
1:A:93:SER:HB2	1:A:157:TYR:CE1	0.44	2.48	31	1
1:A:61:LYS:HZ3	1:A:141:GLY:N	0.44	2.07	13	1
1:A:141:GLY:N	1:A:185:ILE:CG1	0.44	2.80	9	1
1:A:16:ASN:ND2	1:A:159:ASP:HB3	0.44	2.28	18	1
1:A:143:ARG:HG2	1:A:159:ASP:OD1	0.44	2.13	31	1
1:A:77:GLN:O	1:A:78:GLN:C	0.43	2.57	22	39
1:A:143:ARG:NH1	1:A:191:GLN:CD	0.43	2.71	35	1
1:A:16:ASN:ND2	1:A:16:ASN:N	0.43	2.66	15	1
1:A:143:ARG:NH2	1:A:191:GLN:CB	0.43	2.81	17	1
1:A:136:SER:O	1:A:139:VAL:CG1	0.43	2.66	29	39
1:A:16:ASN:HB3	1:A:157:TYR:CD2	0.43	2.49	4	1
1:A:17:SER:OG	1:A:191:GLN:NE2	0.43	2.51	8	1
1:A:61:LYS:HD3	1:A:185:ILE:HD12	0.43	1.91	9	1
1:A:15:PRO:HB2	1:A:143:ARG:HH21	0.43	1.74	39	3
1:A:30:ILE:HD13	1:A:75:SER:CB	0.43	2.44	39	39
1:A:61:LYS:HZ1	1:A:140:SER:CB	0.43	2.26	36	2
1:A:15:PRO:CG	1:A:191:GLN:HE22	0.43	2.27	19	1
1:A:64:LYS:NZ	1:A:157:TYR:OH	0.43	2.42	33	1
1:A:15:PRO:HB3	1:A:93:SER:CB	0.43	2.44	38	1
1:A:38:ARG:CB	1:A:46:TRP:HB3	0.43	2.44	31	39
1:A:59:THR:HG23	1:A:189:GLY:HA3	0.43	1.91	32	2
1:A:143:ARG:NE	1:A:191:GLN:OE1	0.43	2.51	24	1
1:A:14:GLN:HG2	1:A:191:GLN:NE2	0.43	2.28	31	1
1:A:143:ARG:HH22	1:A:191:GLN:HG2	0.43	1.74	31	1
1:A:145:GLU:CD	1:A:157:TYR:CE1	0.42	2.92	13	3
1:A:16:ASN:HB3	1:A:143:ARG:CZ	0.42	2.44	19	2
1:A:143:ARG:HH12	1:A:191:GLN:CD	0.42	2.17	20	1
1:A:143:ARG:NE	1:A:185:ILE:CG1	0.42	2.81	31	1
1:A:143:ARG:CZ	1:A:157:TYR:CB	0.42	2.98	4	1
1:A:65:PRO:HG3	1:A:157:TYR:CD1	0.42	2.49	23	1
1:A:16:ASN:HD22	1:A:159:ASP:HB2	0.42	1.74	14	1
1:A:14:GLN:CD	1:A:191:GLN:NE2	0.42	2.72	31	1
1:A:143:ARG:NH2	1:A:191:GLN:HG2	0.42	2.30	31	1
1:A:26:GLN:CB	1:A:27:PRO:HD3	0.42	2.45	11	39
1:A:16:ASN:HD21	1:A:62:GLY:HA2	0.42	1.74	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:PRO:HB2	1:A:157:TYR:CD1	0.42	2.49	35	1
1:A:132:TRP:CE2	1:A:182:VAL:HG11	0.42	2.50	19	39
1:A:16:ASN:CB	1:A:143:ARG:HH12	0.42	2.25	39	1
1:A:14:GLN:O	1:A:91:THR:HG22	0.42	2.15	29	39
1:A:65:PRO:HD3	1:A:157:TYR:CD1	0.42	2.50	3	1
1:A:61:LYS:HZ3	1:A:141:GLY:CA	0.41	2.28	13	1
1:A:15:PRO:HG3	1:A:191:GLN:HE22	0.41	1.75	19	1
1:A:16:ASN:HD22	1:A:61:LYS:HZ1	0.41	1.57	21	1
1:A:16:ASN:ND2	1:A:157:TYR:CZ	0.41	2.88	22	1
1:A:59:THR:OG1	1:A:189:GLY:HA2	0.41	2.14	37	1
1:A:157:TYR:CD1	1:A:157:TYR:O	0.41	2.72	29	1
1:A:60:ILE:CG2	1:A:63:LEU:HD21	0.41	2.46	20	37
1:A:71:GLY:HA3	1:A:87:PHE:CZ	0.41	2.51	34	39
1:A:185:ILE:CD1	1:A:191:GLN:OE1	0.41	2.68	23	1
1:A:15:PRO:CB	1:A:157:TYR:CE1	0.41	3.02	35	1
1:A:16:ASN:HB2	1:A:157:TYR:CE2	0.41	2.50	2	1
1:A:61:LYS:HE3	1:A:185:ILE:CD1	0.41	2.45	12	1
1:A:61:LYS:HB3	1:A:185:ILE:CD1	0.41	2.46	16	1
1:A:67:VAL:HG11	1:A:69:TYR:OH	0.41	2.16	7	39
1:A:149:SER:OG	1:A:177:LYS:HB3	0.41	2.16	24	34
1:A:141:GLY:HA3	1:A:185:ILE:CD1	0.41	2.46	9	1
1:A:15:PRO:CD	1:A:143:ARG:NH2	0.41	2.83	10	1
1:A:16:ASN:OD1	1:A:157:TYR:CB	0.41	2.68	25	1
1:A:16:ASN:OD1	1:A:157:TYR:HB2	0.41	2.15	25	1
1:A:63:LEU:O	1:A:157:TYR:CZ	0.41	2.74	26	1
1:A:145:GLU:O	1:A:145:GLU:HG3	0.41	2.16	25	1
1:A:143:ARG:CZ	1:A:157:TYR:HB2	0.41	2.45	2	1
1:A:51:ILE:N	1:A:51:ILE:HD12	0.41	2.31	38	11
1:A:16:ASN:HB2	1:A:143:ARG:NH1	0.41	2.29	39	1
1:A:16:ASN:HB2	1:A:157:TYR:CE1	0.41	2.50	1	1
1:A:185:ILE:O	1:A:185:ILE:HG12	0.41	2.16	9	1
1:A:14:GLN:NE2	1:A:17:SER:O	0.41	2.51	15	1
1:A:59:THR:OG1	1:A:188:ASP:CA	0.41	2.69	15	1
1:A:159:ASP:OD1	1:A:159:ASP:N	0.41	2.53	18	1
1:A:61:LYS:HE2	1:A:185:ILE:CD1	0.40	2.47	30	1
1:A:16:ASN:HD22	1:A:143:ARG:HG3	0.40	1.75	17	1
1:A:145:GLU:CD	1:A:145:GLU:O	0.40	2.60	25	1
1:A:61:LYS:HZ2	1:A:141:GLY:C	0.40	2.20	7	1
1:A:61:LYS:HE2	1:A:185:ILE:CG2	0.40	2.47	13	1
1:A:145:GLU:OE1	1:A:146:TYR:N	0.40	2.54	25	1
1:A:51:ILE:HD12	1:A:51:ILE:N	0.40	2.31	31	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:168:ASN:O	1:A:170:PRO:HD3	0.40	2.17	33	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	167/201 (83%)	143±1 (86±0%)	13±1 (8±0%)	11±1 (7±0%)	2	18
All	All	6513/7839 (83%)	5581 (86%)	499 (8%)	433 (7%)	2	18

All 13 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	10	GLU	39
1	A	13	SER	39
1	A	15	PRO	39
1	A	25	PRO	39
1	A	28	SER	39
1	A	40	LYS	39
1	A	78	GLN	39
1	A	134	SER	39
1	A	135	ALA	39
1	A	153	ASP	39
1	A	3	PRO	20
1	A	126	SER	19
1	A	93	SER	4

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	154/183 (84%)	139±1 (90±1%)	15±1 (10±1%)	11	56
All	All	6006/7137 (84%)	5404 (90%)	602 (10%)	11	56

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	11	THR	39
1	A	26	GLN	39
1	A	31	SER	39
1	A	36	ARG	39
1	A	38	ARG	39
1	A	46	TRP	39
1	A	75	SER	39
1	A	79	TYR	39
1	A	91	THR	39
1	A	127	SER	39
1	A	136	SER	39
1	A	147	GLU	39
1	A	184	GLN	39
1	A	200	THR	39
1	A	64	LYS	17
1	A	126	SER	14
1	A	14	GLN	7
1	A	16	ASN	3
1	A	191	GLN	3
1	A	185	ILE	3
1	A	140	SER	2
1	A	157	TYR	2
1	A	187	GLU	1
1	A	59	THR	1
1	A	145	GLU	1
1	A	61	LYS	1
1	A	93	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (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)

No chemical shift data were provided