Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1Q38
Title	:	Anastellin
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Deposited on	:	2003-07-28

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:

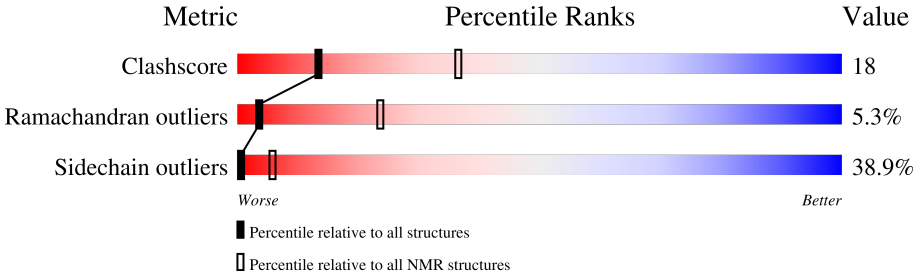
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	89	22% 40% 7% 30%

2 Ensemble composition and analysis (i)

This entry contains 35 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:11-A:72 (62)	0.67	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 6 clusters and 12 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1419 atoms, of which 699 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1419	451	699	140	128	1	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	cloning artifact	UNP P02751
A	2	ARG	-	cloning artifact	UNP P02751
A	3	GLY	-	cloning artifact	UNP P02751
A	4	SER	-	cloning artifact	UNP P02751
A	80	GLY	-	cloning artifact	UNP P02751
A	81	SER	-	cloning artifact	UNP P02751
A	82	ARG	-	cloning artifact	UNP P02751
A	83	SER	-	cloning artifact	UNP P02751
A	84	HIS	-	cloning artifact	UNP P02751
A	85	HIS	-	cloning artifact	UNP P02751
A	86	HIS	-	cloning artifact	UNP P02751
A	87	HIS	-	cloning artifact	UNP P02751
A	88	HIS	-	cloning artifact	UNP P02751
A	89	HIS	-	cloning artifact	UNP P02751

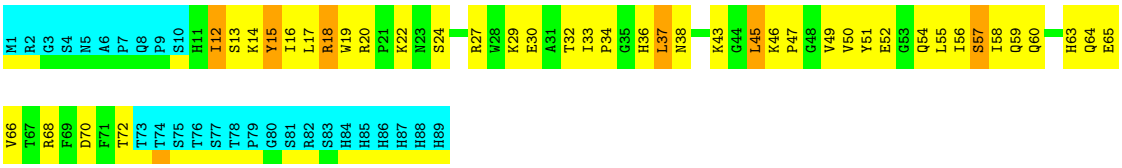
4 Residue-property plots (i)

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: 22% 40% 7% 30%



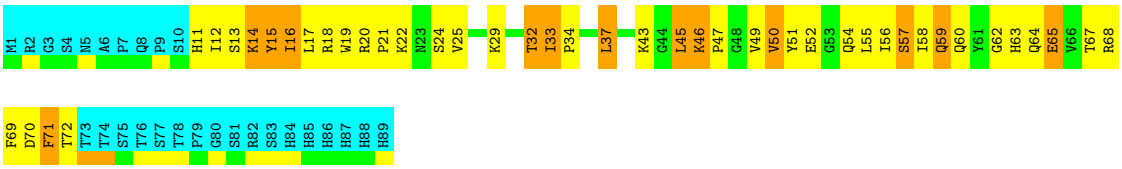
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Fibronectin

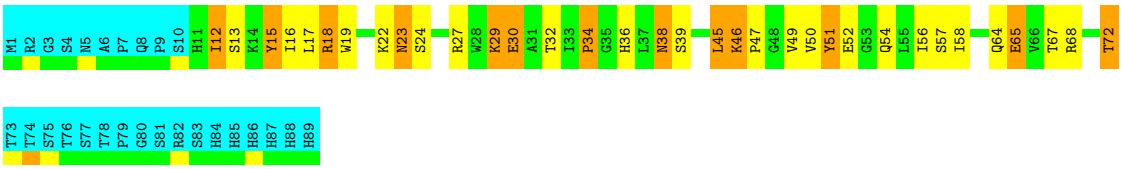
Chain A: 20% 35% 15% 30%



4.2.2 Score per residue for model 2

• Molecule 1: Fibronectin

Chain A: 31% 24% 15% 30%



4.2.3 Score per residue for model 3

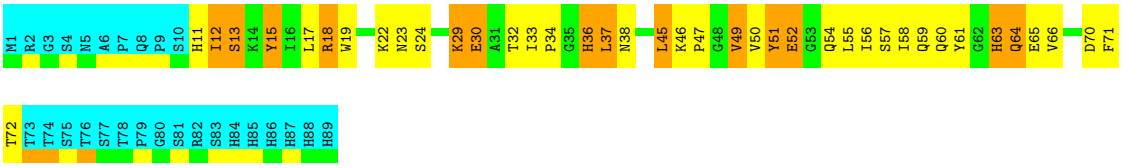
- Molecule 1: Fibronectin

Chain A: 31% 25% 13% 30%

4.2.4 Score per residue for model 4

- Molecule 1: Fibronectin

Chain A: 25% 29% 16% 30%



4.2.5 Score per residue for model 5

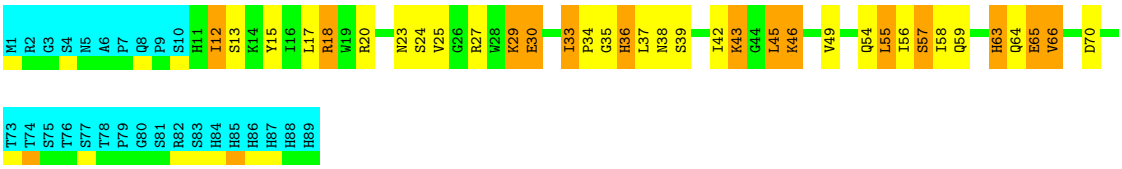
- Molecule 1: Fibronectin

Chain A: 37% 24% 9% 30%

4.2.6 Score per residue for model 6

- Molecule 1: Fibronectin

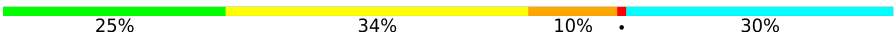
Chain A: 30% 24% 16% 30%

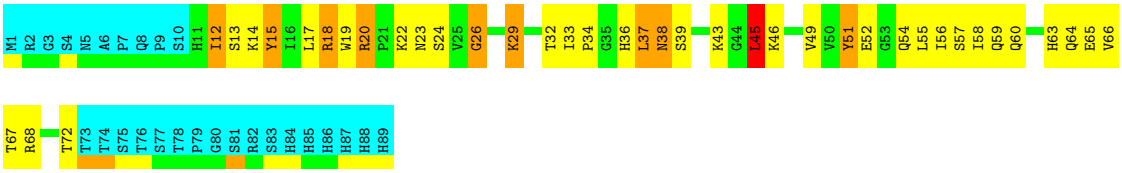


4.2.7 Score per residue for model 7

- Molecule 1: Fibronectin

Chain A:

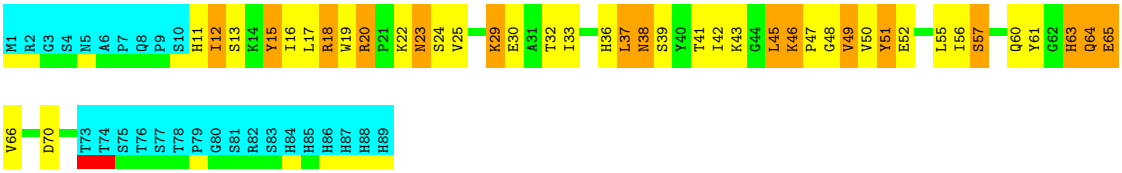




4.2.8 Score per residue for model 8

- Molecule 1: Fibronectin

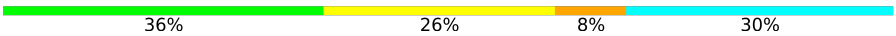
Chain A:

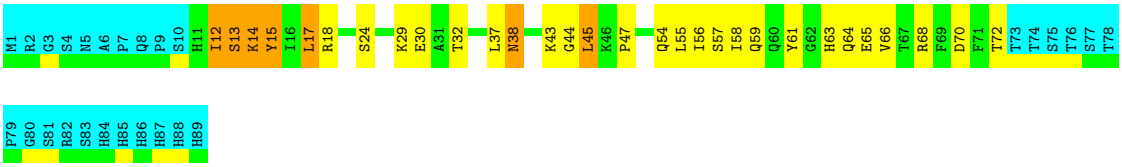


4.2.9 Score per residue for model 9

- Molecule 1: Fibronectin

Chain A:

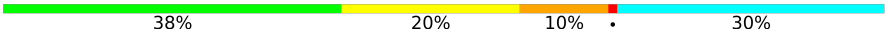


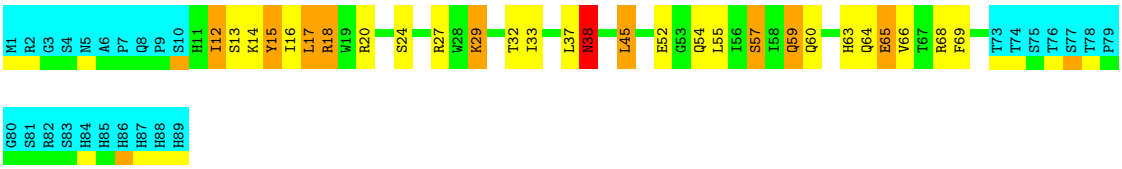


4.2.10 Score per residue for model 10

- Molecule 1: Fibronectin

Chain A:

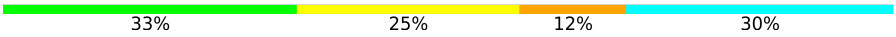




4.2.11 Score per residue for model 11

- Molecule 1: Fibronectin

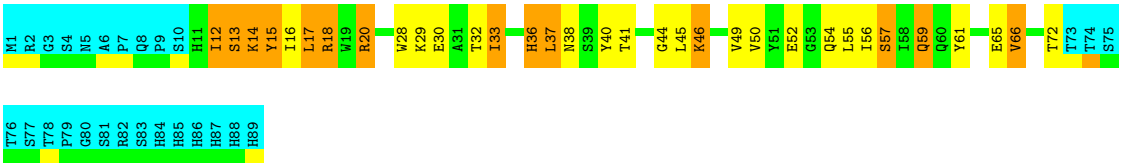
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: Fibronectin

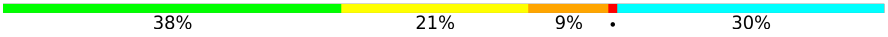
Chain A:

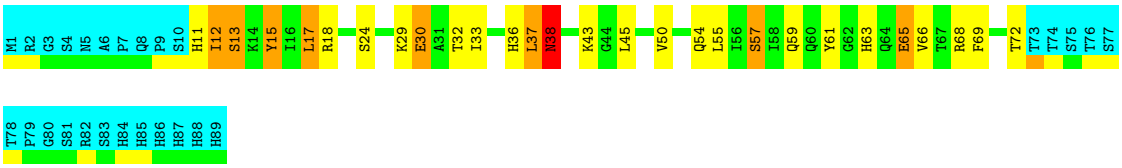


4.2.13 Score per residue for model 13

- Molecule 1: Fibronectin

Chain A:

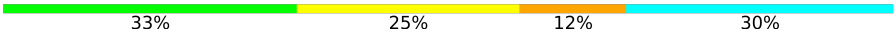


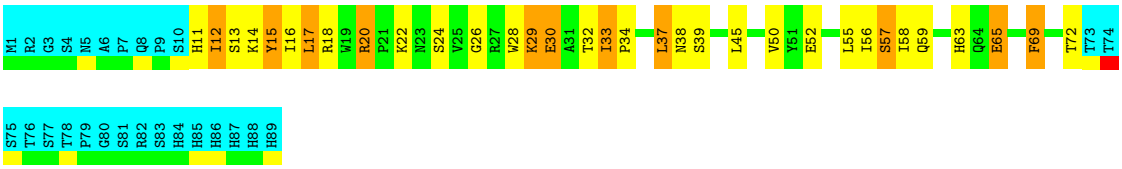


4.2.14 Score per residue for model 14

- Molecule 1: Fibronectin

Chain A:

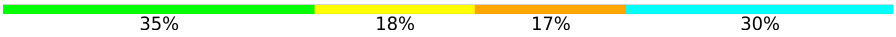


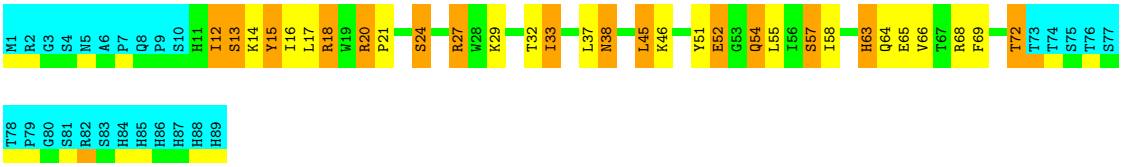


4.2.15 Score per residue for model 15

- Molecule 1: Fibronectin

Chain A:

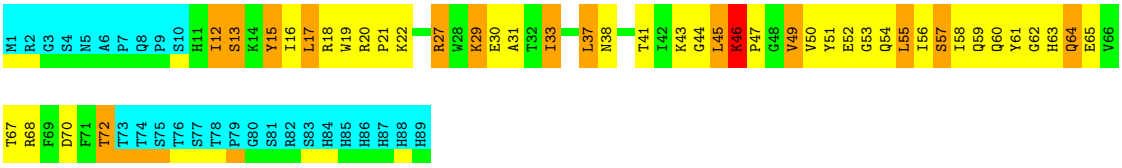




4.2.16 Score per residue for model 16

- Molecule 1: Fibronectin

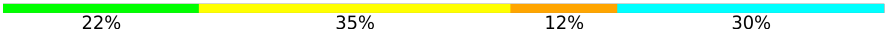
Chain A:

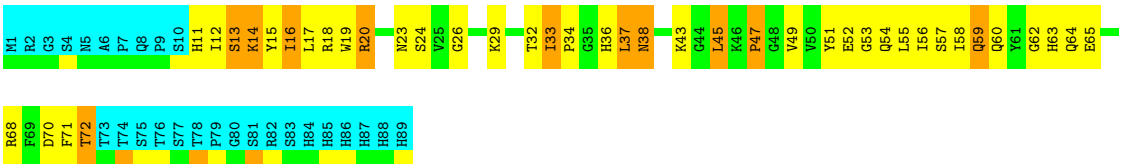


4.2.17 Score per residue for model 17

- Molecule 1: Fibronectin

Chain A:

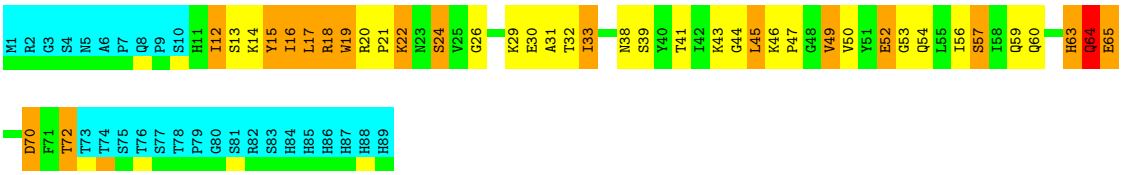




4.2.18 Score per residue for model 18

- Molecule 1: Fibronectin

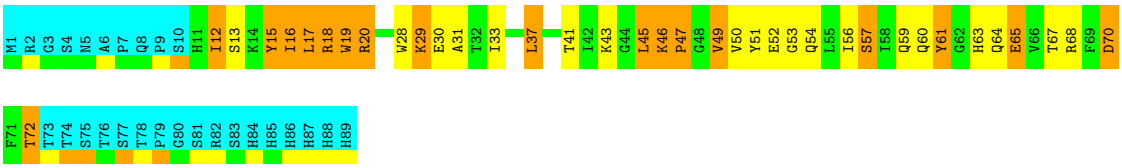
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Fibronectin

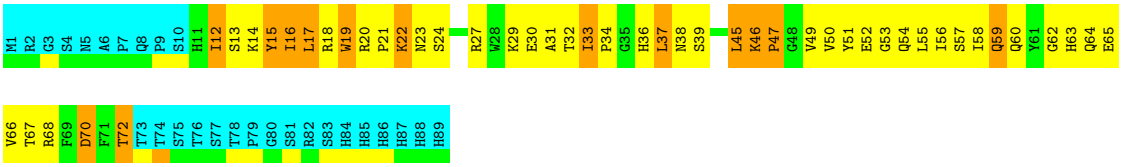
Chain A: 28% 21% 20% 30%



4.2.20 Score per residue for model 20

- Molecule 1: Fibronectin

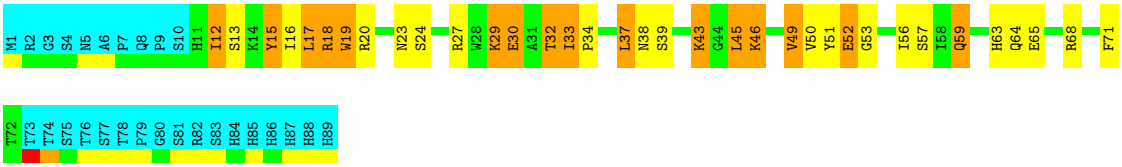
Chain A: 16% 38% 16% 30%



4.2.21 Score per residue for model 21

- Molecule 1: Fibronectin

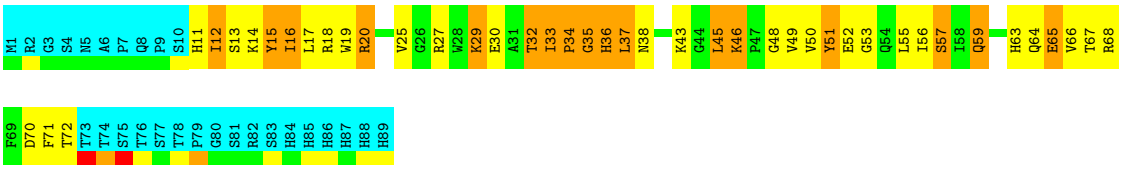
Chain A: 30% 21% 18% 30%



4.2.22 Score per residue for model 22

- Molecule 1: Fibronectin

Chain A: 21% 29% 19% 30%



4.2.23 Score per residue for model 23

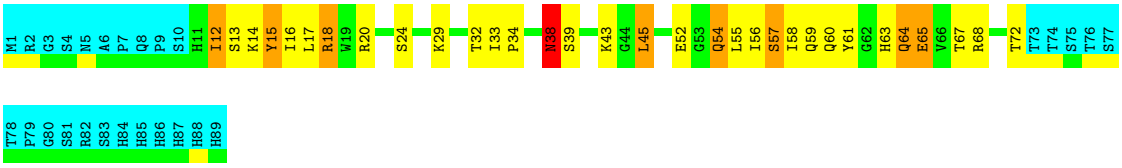
- Molecule 1: Fibronectin

Chain A: 31% 34% • 30%

4.2.24 Score per residue for model 24

- Molecule 1: Fibronectin

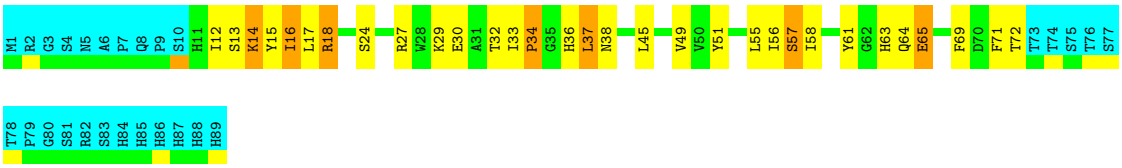
Chain A: 34% 26% 9% • 30%



4.2.25 Score per residue for model 25

- Molecule 1: Fibronectin

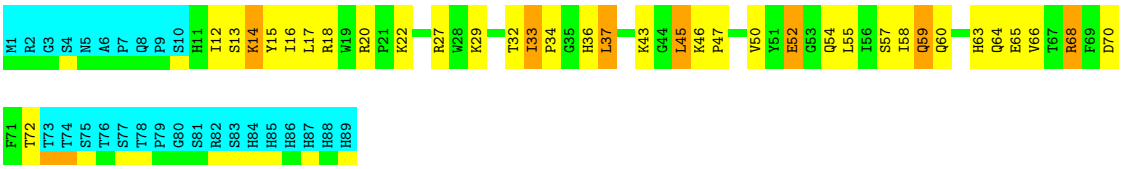
Chain A: 35% 27% 8% 30%



4.2.26 Score per residue for model 26

- Molecule 1: Fibronectin

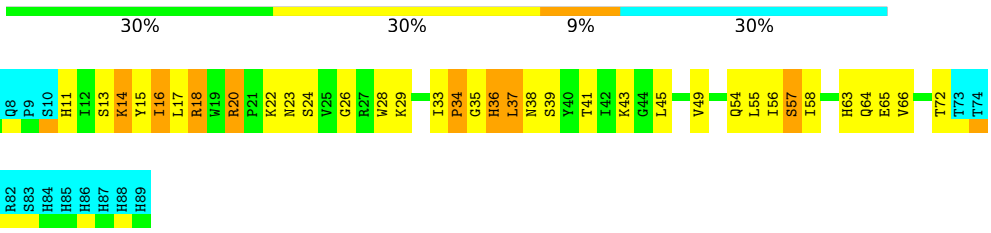
Chain A: 30% 31% 8% 30%



4.2.27 Score per residue for model 27

- Molecule 1: Fibronectin

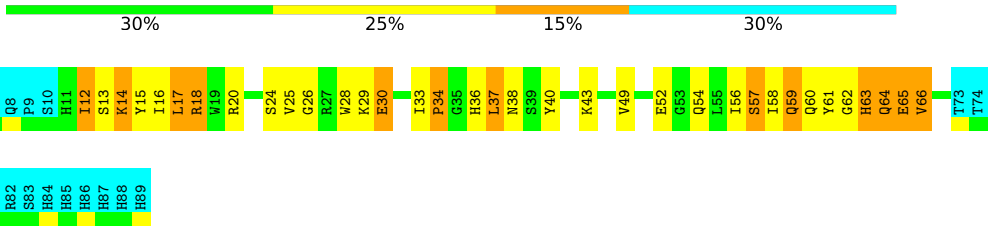
Chain A:



4.2.28 Score per residue for model 28

- Molecule 1: Fibronectin

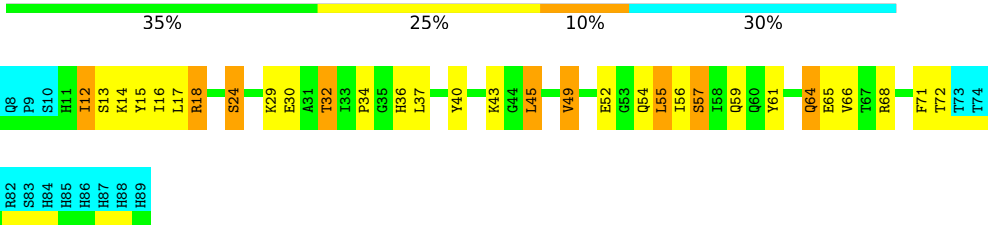
Chain A:



4.2.29 Score per residue for model 29

- Molecule 1: Fibronectin

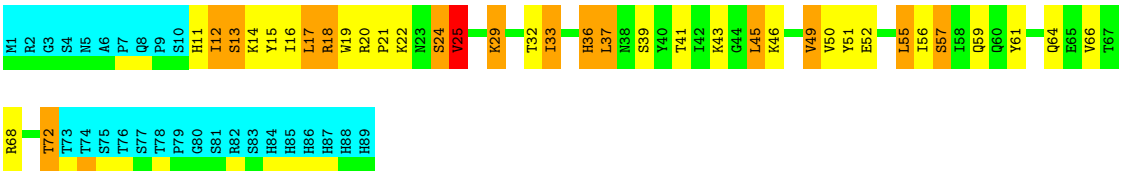
Chain A:



4.2.30 Score per residue for model 30

- Molecule 1: Fibronectin

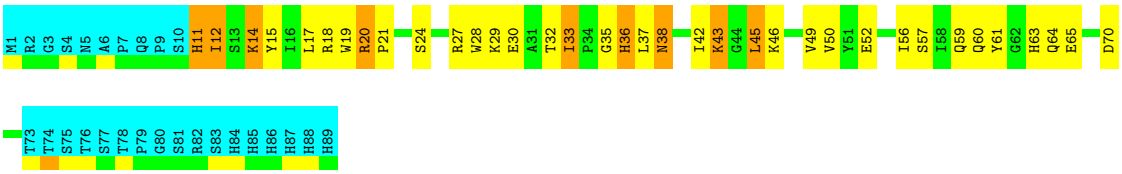
Chain A:



4.2.31 Score per residue for model 31

- Molecule 1: Fibronectin

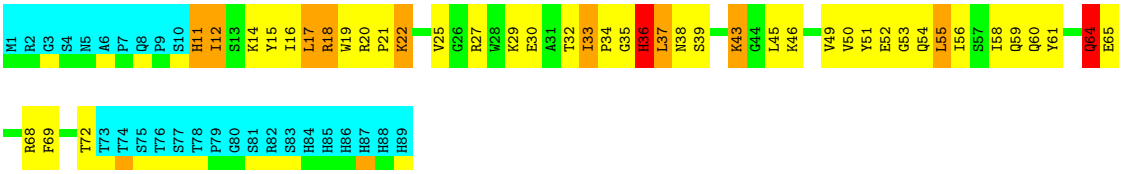
Chain A: 29% 30% 10% 30%



4.2.32 Score per residue for model 32

- Molecule 1: Fibronectin

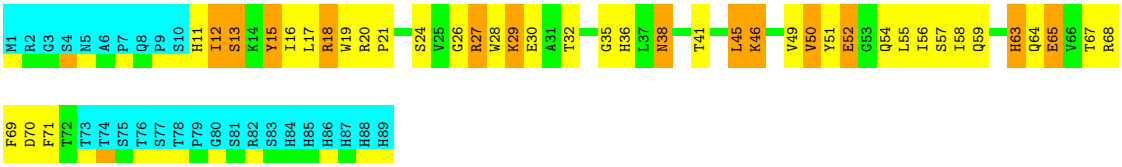
Chain A: 21% 36% 10% • 30%



4.2.33 Score per residue for model 33

- Molecule 1: Fibronectin

Chain A: 24% 31% 15% 30%



4.2.34 Score per residue for model 34

- Molecule 1: Fibronectin

Chain A: 24% 33% 12% • 30%

M1 R2 G3 S4 N5 A6 P7 Q8 P9 S10 H11 T12 S13 K14 Y15 I16 L17 R18 W19 R20 P21 K22 N23 S24 R27 W28 K29 E30 A31 T32 I33 L37 N38 L45 K46 P47 G48 V49 V50 Y51 E52 G53 Q54 L55 I56 S57 I58 Q59 Q60 Y61 Q64 E65 V66 T67 R68 F69

D70 F71 T72 T73 T74 S75 T76 S77 T78 P79 G80 S81 R82 S83 H84 H85 H86 H87 H88 H89

4.2.35 Score per residue for model 35

- Molecule 1: Fibronectin

Chain A: 25% 26% 19% 30%

M1 R2 G3 S4 N5 A6 P7 Q8 P9 S10 S13 K14 Y15 I16 L17 R18 W19 R20 P21 K22 N23 S24 K29 T32 I33 P34 G35 H36 L37 N38 S39 I42 K43 G44 L45 K46 P47 G48 V49 V50 Y51 E52 L55 I56 S57 I58 Q59 Q60 H63 Q64 E65 V66 F69

T72 T73 T74 S75 T76 S77 T78 P79 G80 S81 R82 S83 H84 H85 H86 H87 H88 H89

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Aria protocol*.

Of the 100 calculated structures, 35 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
CNS	structure solution	1.0
ARIA	structure solution	1.0
ARIA	refinement	1.0

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	514	516	516	19±7
All	All	17990	18060	18060	653

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG23	1:A:72:THR:HG22	0.88	1.45	30	1
1:A:15:TYR:CZ	1:A:55:LEU:HD13	0.82	2.10	6	1
1:A:50:VAL:HG23	1:A:72:THR:HG23	0.81	1.53	35	2
1:A:33:ILE:HG22	1:A:37:LEU:HD11	0.81	1.50	17	4
1:A:52:GLU:HA	1:A:70:ASP:HA	0.80	1.53	17	5
1:A:37:LEU:HD13	1:A:37:LEU:H	0.75	1.41	25	3
1:A:45:LEU:HD22	1:A:72:THR:HA	0.75	1.59	19	1
1:A:59:GLN:HB2	1:A:64:GLN:HG2	0.74	1.59	35	5
1:A:12:ILE:HD13	1:A:57:SER:HB3	0.71	1.62	20	12
1:A:59:GLN:HG2	1:A:64:GLN:HB2	0.70	1.63	34	1
1:A:18:ARG:HA	1:A:29:LYS:O	0.70	1.85	18	35
1:A:45:LEU:HD12	1:A:45:LEU:N	0.69	2.00	16	3
1:A:17:LEU:HD12	1:A:55:LEU:HD13	0.68	1.65	9	4
1:A:58:ILE:HG23	1:A:62:GLY:HA2	0.67	1.65	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:GLN:HB2	1:A:64:GLN:HB2	0.66	1.68	30	1
1:A:37:LEU:HG	1:A:39:SER:HB2	0.66	1.66	35	1
1:A:14:LYS:HA	1:A:34:PRO:HA	0.66	1.68	32	10
1:A:37:LEU:H	1:A:37:LEU:HD22	0.66	1.51	32	7
1:A:46:LYS:O	1:A:49:VAL:HG23	0.65	1.91	21	4
1:A:42:ILE:HG22	1:A:45:LEU:HD11	0.65	1.67	3	1
1:A:12:ILE:HG13	1:A:13:SER:N	0.65	2.06	22	27
1:A:21:PRO:HA	1:A:51:TYR:HA	0.64	1.67	20	2
1:A:15:TYR:HB2	1:A:33:ILE:O	0.64	1.92	31	13
1:A:59:GLN:HB3	1:A:64:GLN:NE2	0.64	2.08	34	1
1:A:46:LYS:O	1:A:49:VAL:HG12	0.64	1.92	1	3
1:A:45:LEU:HD13	1:A:45:LEU:N	0.63	2.09	17	2
1:A:57:SER:HB2	1:A:65:GLU:H	0.63	1.54	34	2
1:A:15:TYR:HB3	1:A:33:ILE:O	0.63	1.93	6	1
1:A:45:LEU:HD23	1:A:51:TYR:HB2	0.62	1.69	19	2
1:A:45:LEU:HD22	1:A:45:LEU:H	0.62	1.54	6	4
1:A:17:LEU:HD12	1:A:55:LEU:HD21	0.62	1.71	12	1
1:A:43:LYS:H	1:A:43:LYS:HD2	0.62	1.55	21	1
1:A:33:ILE:HG22	1:A:37:LEU:HD12	0.62	1.72	34	1
1:A:19:TRP:HA	1:A:52:GLU:O	0.62	1.95	30	8
1:A:22:LYS:HG3	1:A:52:GLU:HB2	0.62	1.71	34	2
1:A:58:ILE:HG12	1:A:63:HIS:HB3	0.61	1.73	4	1
1:A:50:VAL:HA	1:A:72:THR:HB	0.61	1.71	20	2
1:A:33:ILE:HG22	1:A:37:LEU:HD23	0.61	1.73	14	1
1:A:57:SER:O	1:A:64:GLN:HB2	0.60	1.96	19	8
1:A:55:LEU:O	1:A:66:VAL:HA	0.60	1.96	10	12
1:A:43:LYS:HD2	1:A:43:LYS:N	0.60	2.11	21	1
1:A:12:ILE:HG21	1:A:57:SER:OG	0.60	1.96	6	3
1:A:12:ILE:HD11	1:A:57:SER:HB3	0.60	1.72	34	1
1:A:18:ARG:HD3	1:A:56:ILE:HD13	0.60	1.74	8	2
1:A:58:ILE:HA	1:A:63:HIS:HA	0.60	1.72	4	8
1:A:19:TRP:HB2	1:A:52:GLU:O	0.60	1.96	20	11
1:A:59:GLN:HE21	1:A:64:GLN:NE2	0.60	1.94	34	1
1:A:35:GLY:O	1:A:37:LEU:HD23	0.59	1.98	35	1
1:A:37:LEU:H	1:A:37:LEU:HD13	0.58	1.57	4	5
1:A:15:TYR:CE1	1:A:55:LEU:HD13	0.58	2.34	6	1
1:A:57:SER:O	1:A:64:GLN:HB3	0.58	1.99	20	2
1:A:33:ILE:HG22	1:A:37:LEU:HD21	0.58	1.76	1	2
1:A:45:LEU:HD23	1:A:51:TYR:CD1	0.58	2.33	33	1
1:A:17:LEU:HD22	1:A:42:ILE:HD13	0.58	1.75	35	1
1:A:14:LYS:HE3	1:A:58:ILE:HD13	0.58	1.75	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:58:ILE:HG23	1:A:62:GLY:O	0.58	1.98	20	1
1:A:59:GLN:HB2	1:A:64:GLN:CD	0.57	2.18	19	3
1:A:57:SER:HB2	1:A:64:GLN:HB3	0.57	1.74	34	1
1:A:17:LEU:HD12	1:A:55:LEU:HG	0.57	1.75	32	2
1:A:43:LYS:H	1:A:43:LYS:HE2	0.57	1.59	7	1
1:A:33:ILE:CG2	1:A:39:SER:HB3	0.57	2.30	35	1
1:A:15:TYR:OH	1:A:55:LEU:HD22	0.57	2.00	6	1
1:A:37:LEU:HD13	1:A:37:LEU:N	0.57	2.15	32	8
1:A:11:HIS:HB3	1:A:35:GLY:HA3	0.57	1.77	5	1
1:A:19:TRP:HB2	1:A:53:GLY:HA2	0.57	1.75	21	6
1:A:56:ILE:HA	1:A:65:GLU:O	0.56	1.99	1	16
1:A:59:GLN:HG3	1:A:63:HIS:HB2	0.56	1.75	10	2
1:A:23:ASN:HB2	1:A:49:VAL:HG23	0.56	1.76	27	1
1:A:50:VAL:HG23	1:A:72:THR:CG2	0.56	2.28	35	2
1:A:54:GLN:HG3	1:A:66:VAL:HG23	0.56	1.77	15	2
1:A:22:LYS:HG2	1:A:52:GLU:HB2	0.56	1.76	35	1
1:A:15:TYR:O	1:A:32:THR:HA	0.56	2.01	14	25
1:A:21:PRO:HG3	1:A:51:TYR:CE2	0.56	2.36	30	5
1:A:12:ILE:HG21	1:A:15:TYR:CE1	0.56	2.36	31	1
1:A:16:ILE:O	1:A:55:LEU:HD23	0.56	2.01	12	4
1:A:12:ILE:HD13	1:A:57:SER:OG	0.56	2.00	28	2
1:A:17:LEU:HD21	1:A:42:ILE:HD11	0.55	1.78	8	1
1:A:16:ILE:HG21	1:A:18:ARG:HH11	0.55	1.60	12	1
1:A:34:PRO:HB2	1:A:37:LEU:HB3	0.55	1.76	17	1
1:A:12:ILE:HD11	1:A:59:GLN:HG2	0.55	1.78	29	1
1:A:51:TYR:HB2	1:A:71:PHE:HB3	0.55	1.79	33	3
1:A:33:ILE:HD12	1:A:38:ASN:O	0.55	2.02	32	1
1:A:37:LEU:CG	1:A:39:SER:HB2	0.55	2.32	35	1
1:A:46:LYS:HD3	1:A:49:VAL:HG23	0.55	1.79	6	1
1:A:19:TRP:CB	1:A:53:GLY:HA2	0.55	2.32	16	6
1:A:37:LEU:HD13	1:A:38:ASN:N	0.54	2.17	17	3
1:A:45:LEU:HB3	1:A:51:TYR:HD1	0.54	1.61	20	1
1:A:54:GLN:HE21	1:A:68:ARG:HG2	0.54	1.62	24	1
1:A:16:ILE:HD13	1:A:58:ILE:HG13	0.54	1.79	2	1
1:A:15:TYR:CD1	1:A:55:LEU:HD12	0.54	2.38	16	1
1:A:49:VAL:O	1:A:72:THR:HB	0.54	2.01	16	1
1:A:56:ILE:HD13	1:A:66:VAL:HB	0.53	1.78	4	1
1:A:58:ILE:HA	1:A:64:GLN:HB3	0.53	1.79	20	1
1:A:17:LEU:O	1:A:30:GLU:HA	0.53	2.02	6	10
1:A:37:LEU:HD13	1:A:38:ASN:HD22	0.53	1.63	13	1
1:A:59:GLN:HB2	1:A:64:GLN:NE2	0.53	2.19	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:TYR:CE1	1:A:55:LEU:HG	0.53	2.39	3	2
1:A:37:LEU:HD22	1:A:37:LEU:N	0.53	2.18	20	3
1:A:59:GLN:HB2	1:A:64:GLN:CG	0.53	2.33	31	3
1:A:15:TYR:HE1	1:A:57:SER:HG	0.53	1.45	23	1
1:A:22:LYS:HB3	1:A:50:VAL:HG13	0.52	1.80	18	2
1:A:12:ILE:HD12	1:A:59:GLN:HG3	0.52	1.81	28	1
1:A:15:TYR:HB3	1:A:33:ILE:HD12	0.52	1.80	12	1
1:A:16:ILE:HD13	1:A:58:ILE:HD12	0.52	1.81	15	1
1:A:37:LEU:O	1:A:38:ASN:HB3	0.52	2.05	34	1
1:A:50:VAL:CG2	1:A:72:THR:HG23	0.52	2.31	35	1
1:A:15:TYR:CD1	1:A:55:LEU:HD22	0.52	2.39	1	5
1:A:33:ILE:O	1:A:35:GLY:N	0.52	2.43	6	1
1:A:37:LEU:HD23	1:A:37:LEU:H	0.52	1.64	16	1
1:A:45:LEU:HB3	1:A:51:TYR:CD1	0.52	2.40	17	2
1:A:33:ILE:CB	1:A:37:LEU:HD23	0.51	2.35	32	1
1:A:47:PRO:HA	1:A:72:THR:OG1	0.51	2.05	16	1
1:A:11:HIS:HB2	1:A:35:GLY:HA3	0.51	1.81	22	2
1:A:20:ARG:HB3	1:A:28:TRP:HA	0.51	1.83	23	4
1:A:45:LEU:CD2	1:A:51:TYR:HB2	0.51	2.35	16	1
1:A:16:ILE:O	1:A:55:LEU:HA	0.51	2.06	20	3
1:A:37:LEU:HD22	1:A:38:ASN:HB3	0.51	1.81	17	3
1:A:12:ILE:HG21	1:A:15:TYR:CD1	0.51	2.40	31	1
1:A:24:SER:O	1:A:25:VAL:HG22	0.51	2.06	30	1
1:A:38:ASN:HD22	1:A:39:SER:H	0.51	1.48	24	2
1:A:45:LEU:HD12	1:A:72:THR:HA	0.50	1.82	15	1
1:A:17:LEU:HG	1:A:55:LEU:HD22	0.50	1.83	30	1
1:A:37:LEU:O	1:A:38:ASN:CB	0.50	2.59	34	1
1:A:57:SER:N	1:A:65:GLU:O	0.50	2.44	26	6
1:A:14:LYS:HD2	1:A:16:ILE:HD11	0.50	1.83	12	1
1:A:57:SER:OG	1:A:65:GLU:HB3	0.50	2.07	14	4
1:A:50:VAL:HG22	1:A:71:PHE:O	0.50	2.06	34	3
1:A:57:SER:HB3	1:A:65:GLU:CB	0.50	2.37	8	2
1:A:50:VAL:HA	1:A:72:THR:HG22	0.50	1.83	12	3
1:A:44:GLY:H	1:A:45:LEU:HD12	0.50	1.66	16	1
1:A:63:HIS:C	1:A:64:GLN:HG2	0.50	2.27	8	1
1:A:37:LEU:CD1	1:A:39:SER:HB2	0.50	2.37	35	1
1:A:46:LYS:HD3	1:A:49:VAL:HG11	0.49	1.83	12	1
1:A:37:LEU:HD23	1:A:38:ASN:OD1	0.49	2.06	7	1
1:A:16:ILE:O	1:A:55:LEU:HD12	0.49	2.08	14	3
1:A:45:LEU:N	1:A:45:LEU:CD1	0.49	2.73	16	2
1:A:15:TYR:HE1	1:A:56:ILE:N	0.49	2.06	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:HG22	1:A:72:THR:HG21	0.49	1.83	12	2
1:A:16:ILE:HG22	1:A:56:ILE:H	0.49	1.68	18	2
1:A:33:ILE:HG21	1:A:40:TYR:CD2	0.49	2.42	28	1
1:A:56:ILE:HG13	1:A:66:VAL:HB	0.49	1.84	35	1
1:A:15:TYR:CE2	1:A:17:LEU:HB2	0.49	2.43	6	1
1:A:18:ARG:O	1:A:54:GLN:N	0.49	2.46	19	5
1:A:38:ASN:ND2	1:A:39:SER:H	0.49	2.06	32	1
1:A:15:TYR:CE1	1:A:55:LEU:HD22	0.49	2.43	8	1
1:A:14:LYS:HD2	1:A:58:ILE:HD12	0.49	1.84	9	1
1:A:18:ARG:HH11	1:A:30:GLU:HG2	0.49	1.67	14	1
1:A:57:SER:O	1:A:65:GLU:N	0.49	2.44	20	1
1:A:16:ILE:HG13	1:A:58:ILE:HD12	0.49	1.84	24	1
1:A:17:LEU:HD13	1:A:55:LEU:HD13	0.48	1.83	3	1
1:A:34:PRO:O	1:A:37:LEU:HD12	0.48	2.08	17	1
1:A:22:LYS:HB3	1:A:50:VAL:HG12	0.48	1.85	1	1
1:A:20:ARG:O	1:A:52:GLU:HG2	0.48	2.08	8	3
1:A:16:ILE:HG22	1:A:56:ILE:HB	0.48	1.85	27	1
1:A:18:ARG:O	1:A:53:GLY:HA2	0.48	2.08	32	2
1:A:30:GLU:O	1:A:30:GLU:HG2	0.48	2.09	16	1
1:A:56:ILE:CG1	1:A:66:VAL:HB	0.48	2.39	28	2
1:A:16:ILE:HG21	1:A:18:ARG:HD2	0.48	1.86	20	2
1:A:14:LYS:HB2	1:A:32:THR:CG2	0.48	2.38	31	1
1:A:33:ILE:HB	1:A:37:LEU:HD23	0.48	1.85	32	1
1:A:16:ILE:HG23	1:A:18:ARG:HG2	0.47	1.86	18	1
1:A:12:ILE:HG22	1:A:35:GLY:N	0.47	2.25	32	1
1:A:56:ILE:HG23	1:A:65:GLU:O	0.47	2.10	19	3
1:A:59:GLN:HB2	1:A:64:GLN:OE1	0.47	2.08	1	1
1:A:57:SER:HB2	1:A:65:GLU:N	0.47	2.25	35	2
1:A:54:GLN:HA	1:A:67:THR:O	0.47	2.10	33	1
1:A:14:LYS:HB2	1:A:32:THR:HG22	0.47	1.86	35	2
1:A:52:GLU:HA	1:A:70:ASP:CA	0.47	2.40	16	2
1:A:54:GLN:NE2	1:A:56:ILE:HD11	0.47	2.25	17	1
1:A:45:LEU:HD12	1:A:51:TYR:CE1	0.47	2.44	30	1
1:A:42:ILE:O	1:A:45:LEU:HD11	0.47	2.09	8	1
1:A:12:ILE:HD11	1:A:58:ILE:C	0.47	2.30	28	2
1:A:20:ARG:NH1	1:A:25:VAL:HG23	0.47	2.25	28	1
1:A:23:ASN:HB2	1:A:50:VAL:HB	0.47	1.86	2	1
1:A:16:ILE:CG2	1:A:56:ILE:HB	0.47	2.39	20	2
1:A:42:ILE:O	1:A:43:LYS:C	0.47	2.54	31	2
1:A:52:GLU:HB2	1:A:70:ASP:HB3	0.47	1.87	20	1
1:A:57:SER:HB3	1:A:65:GLU:HB3	0.46	1.87	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ILE:HG13	1:A:66:VAL:HG22	0.46	1.86	9	1
1:A:15:TYR:OH	1:A:55:LEU:HA	0.46	2.09	6	1
1:A:12:ILE:HD12	1:A:59:GLN:HG2	0.46	1.87	4	1
1:A:37:LEU:N	1:A:37:LEU:HD22	0.46	2.26	7	1
1:A:52:GLU:O	1:A:52:GLU:HG3	0.46	2.09	15	4
1:A:37:LEU:HD13	1:A:38:ASN:ND2	0.46	2.25	13	1
1:A:35:GLY:O	1:A:36:HIS:C	0.46	2.54	35	2
1:A:45:LEU:H	1:A:45:LEU:HD22	0.46	1.71	31	2
1:A:37:LEU:N	1:A:37:LEU:HD12	0.46	2.26	19	1
1:A:54:GLN:HE21	1:A:56:ILE:HD11	0.46	1.70	34	1
1:A:37:LEU:H	1:A:37:LEU:CD1	0.46	2.18	25	1
1:A:15:TYR:HE2	1:A:17:LEU:HB2	0.46	1.70	6	1
1:A:45:LEU:HD22	1:A:51:TYR:CE1	0.46	2.46	15	1
1:A:56:ILE:HD12	1:A:56:ILE:N	0.46	2.26	29	2
1:A:18:ARG:NE	1:A:56:ILE:HD13	0.45	2.25	7	1
1:A:45:LEU:HD22	1:A:51:TYR:HB2	0.45	1.88	20	1
1:A:34:PRO:HB2	1:A:37:LEU:HD12	0.45	1.87	25	1
1:A:50:VAL:HG22	1:A:70:ASP:HB2	0.45	1.88	16	1
1:A:61:TYR:CD1	1:A:61:TYR:N	0.45	2.85	19	1
1:A:54:GLN:CB	1:A:68:ARG:HA	0.45	2.42	32	1
1:A:12:ILE:HD11	1:A:64:GLN:HG3	0.45	1.89	1	1
1:A:37:LEU:HD22	1:A:37:LEU:C	0.44	2.33	28	1
1:A:58:ILE:HG23	1:A:63:HIS:H	0.44	1.72	28	1
1:A:53:GLY:O	1:A:69:PHE:O	0.44	2.35	32	1
1:A:14:LYS:HB2	1:A:32:THR:HG23	0.44	1.88	31	1
1:A:45:LEU:HD22	1:A:45:LEU:N	0.44	2.24	6	2
1:A:17:LEU:CB	1:A:31:ALA:HB3	0.44	2.42	20	2
1:A:50:VAL:HG23	1:A:71:PHE:O	0.44	2.12	21	1
1:A:51:TYR:HB2	1:A:71:PHE:CB	0.44	2.42	1	1
1:A:56:ILE:HG23	1:A:66:VAL:HG22	0.44	1.88	30	1
1:A:59:GLN:HB3	1:A:64:GLN:CD	0.44	2.32	34	1
1:A:12:ILE:HG21	1:A:15:TYR:CD2	0.44	2.47	10	3
1:A:21:PRO:HB2	1:A:24:SER:O	0.44	2.13	15	2
1:A:71:PHE:C	1:A:71:PHE:CD1	0.44	2.90	17	1
1:A:45:LEU:HD11	1:A:71:PHE:CE2	0.44	2.47	29	1
1:A:54:GLN:NE2	1:A:68:ARG:HG2	0.44	2.27	24	1
1:A:21:PRO:HA	1:A:50:VAL:O	0.44	2.11	32	2
1:A:15:TYR:HB2	1:A:33:ILE:HG13	0.44	1.89	32	1
1:A:59:GLN:H	1:A:64:GLN:HB2	0.44	1.72	20	1
1:A:45:LEU:HB3	1:A:51:TYR:CE2	0.44	2.47	25	1
1:A:20:ARG:HG2	1:A:28:TRP:CE2	0.43	2.48	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LEU:HB3	1:A:31:ALA:HB3	0.43	1.90	20	3
1:A:59:GLN:NE2	1:A:60:GLN:HG2	0.43	2.27	26	1
1:A:17:LEU:HG	1:A:19:TRP:CE3	0.43	2.48	7	3
1:A:13:SER:HB2	1:A:59:GLN:HA	0.43	1.89	12	2
1:A:45:LEU:HD12	1:A:51:TYR:CG	0.43	2.48	17	2
1:A:55:LEU:HB2	1:A:69:PHE:CE2	0.43	2.48	14	1
1:A:45:LEU:H	1:A:45:LEU:HD12	0.43	1.73	19	1
1:A:20:ARG:HD3	1:A:28:TRP:CE2	0.43	2.48	28	1
1:A:34:PRO:HB2	1:A:37:LEU:CD2	0.43	2.42	35	1
1:A:20:ARG:HG3	1:A:26:GLY:HA2	0.43	1.90	7	1
1:A:45:LEU:O	1:A:46:LYS:HB3	0.43	2.12	16	1
1:A:59:GLN:HB2	1:A:64:GLN:HE21	0.43	1.74	20	1
1:A:12:ILE:HD13	1:A:57:SER:CB	0.43	2.44	14	2
1:A:21:PRO:HG2	1:A:24:SER:O	0.43	2.14	18	1
1:A:44:GLY:C	1:A:45:LEU:HD12	0.43	2.33	18	1
1:A:20:ARG:N	1:A:20:ARG:CD	0.43	2.82	19	1
1:A:21:PRO:HG3	1:A:51:TYR:CE1	0.43	2.48	32	2
1:A:46:LYS:NZ	1:A:49:VAL:HG11	0.43	2.29	11	1
1:A:46:LYS:HB2	1:A:47:PRO:HD2	0.43	1.89	16	2
1:A:45:LEU:HG	1:A:72:THR:HA	0.43	1.89	11	1
1:A:37:LEU:CD1	1:A:37:LEU:N	0.43	2.82	21	1
1:A:37:LEU:HG	1:A:38:ASN:OD1	0.42	2.14	10	1
1:A:33:ILE:HG22	1:A:37:LEU:CD1	0.42	2.44	21	2
1:A:68:ARG:HE	1:A:68:ARG:H	0.42	1.57	26	1
1:A:18:ARG:HG3	1:A:56:ILE:HD12	0.42	1.91	14	1
1:A:12:ILE:HG13	1:A:13:SER:H	0.42	1.74	12	1
1:A:50:VAL:HA	1:A:72:THR:HG23	0.42	1.90	35	1
1:A:57:SER:O	1:A:63:HIS:HA	0.42	2.13	8	1
1:A:37:LEU:HD23	1:A:38:ASN:H	0.42	1.75	10	1
1:A:51:TYR:HB2	1:A:71:PHE:O	0.42	2.14	25	1
1:A:24:SER:HB2	1:A:49:VAL:CG1	0.42	2.45	29	1
1:A:32:THR:C	1:A:33:ILE:HG13	0.42	2.35	15	1
1:A:24:SER:HB2	1:A:49:VAL:HG11	0.42	1.91	30	1
1:A:59:GLN:NE2	1:A:61:TYR:HB2	0.42	2.28	13	1
1:A:59:GLN:HG2	1:A:60:GLN:H	0.42	1.73	32	1
1:A:27:ARG:HG2	1:A:28:TRP:N	0.42	2.30	33	1
1:A:17:LEU:HD13	1:A:55:LEU:CD2	0.42	2.44	7	1
1:A:20:ARG:HH12	1:A:25:VAL:HG23	0.42	1.73	8	1
1:A:37:LEU:HG	1:A:38:ASN:N	0.42	2.30	14	1
1:A:51:TYR:N	1:A:71:PHE:O	0.42	2.52	22	2
1:A:12:ILE:HG22	1:A:35:GLY:CA	0.42	2.45	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ASN:HD22	1:A:50:VAL:HG12	0.41	1.74	4	1
1:A:18:ARG:HG3	1:A:54:GLN:HB2	0.41	1.91	7	1
1:A:45:LEU:HD12	1:A:51:TYR:CE2	0.41	2.51	21	1
1:A:61:TYR:HB2	1:A:64:GLN:HE22	0.41	1.75	29	2
1:A:36:HIS:HB3	1:A:37:LEU:HD13	0.41	1.92	32	1
1:A:46:LYS:O	1:A:46:LYS:HG2	0.41	2.15	21	1
1:A:33:ILE:HG22	1:A:39:SER:HB3	0.41	1.93	35	1
1:A:17:LEU:CD1	1:A:55:LEU:HD13	0.41	2.46	3	1
1:A:46:LYS:HG2	1:A:49:VAL:HG23	0.41	1.91	18	1
1:A:45:LEU:O	1:A:46:LYS:CB	0.41	2.67	16	1
1:A:37:LEU:HD13	1:A:38:ASN:OD1	0.41	2.15	22	1
1:A:59:GLN:NE2	1:A:60:GLN:H	0.41	2.14	35	1
1:A:51:TYR:HB2	1:A:71:PHE:CD1	0.41	2.50	34	1
1:A:37:LEU:HD13	1:A:38:ASN:H	0.41	1.76	28	1
1:A:16:ILE:HG22	1:A:18:ARG:HD2	0.41	1.93	8	1
1:A:23:ASN:HB2	1:A:50:VAL:CG1	0.41	2.46	8	1
1:A:37:LEU:HD12	1:A:37:LEU:N	0.41	2.30	13	1
1:A:20:ARG:HG3	1:A:28:TRP:CD2	0.41	2.51	19	1
1:A:32:THR:C	1:A:33:ILE:HD13	0.41	2.36	22	1
1:A:14:LYS:HD2	1:A:58:ILE:HB	0.41	1.93	25	1
1:A:54:GLN:HB3	1:A:68:ARG:HA	0.41	1.93	32	1
1:A:59:GLN:HB2	1:A:61:TYR:CD1	0.41	2.50	34	1
1:A:33:ILE:HG22	1:A:37:LEU:CD2	0.40	2.46	12	1
1:A:37:LEU:HG	1:A:38:ASN:HD22	0.40	1.75	15	1
1:A:15:TYR:OH	1:A:55:LEU:HB3	0.40	2.16	7	1
1:A:20:ARG:HB2	1:A:27:ARG:O	0.40	2.16	15	1
1:A:46:LYS:HG2	1:A:47:PRO:HD2	0.40	1.92	26	1
1:A:34:PRO:C	1:A:36:HIS:N	0.40	2.74	2	1
1:A:60:GLN:HG3	1:A:61:TYR:N	0.40	2.30	16	1
1:A:45:LEU:HD12	1:A:51:TYR:CD1	0.40	2.51	17	1
1:A:46:LYS:CG	1:A:49:VAL:HG23	0.40	2.47	18	1
1:A:37:LEU:HD22	1:A:38:ASN:N	0.40	2.30	25	1
1:A:45:LEU:N	1:A:45:LEU:HD13	0.40	2.32	9	1
1:A:20:ARG:HB2	1:A:28:TRP:HA	0.40	1.93	31	1
1:A:56:ILE:HG13	1:A:66:VAL:HG13	0.40	1.94	34	1
1:A:43:LYS:HE2	1:A:43:LYS:N	0.40	2.31	7	1
1:A:20:ARG:CD	1:A:20:ARG:N	0.40	2.85	17	1
1:A:16:ILE:CG2	1:A:18:ARG:HD3	0.40	2.47	25	1
1:A:22:LYS:HB2	1:A:50:VAL:CG1	0.40	2.46	32	1
1:A:22:LYS:HD2	1:A:52:GLU:HB2	0.40	1.94	32	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	62/89 (70%)	52±2 (84±4%)	6±2 (10±3%)	3±2 (5±2%)	3 23
All	All	2170/3115 (70%)	1831 (84%)	225 (10%)	114 (5%)	3 23

All 18 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	38	ASN	14
1	A	34	PRO	13
1	A	63	HIS	12
1	A	36	HIS	12
1	A	64	GLN	10
1	A	26	GLY	9
1	A	11	HIS	7
1	A	47	PRO	7
1	A	35	GLY	5
1	A	45	LEU	5
1	A	25	VAL	4
1	A	44	GLY	4
1	A	43	LYS	3
1	A	27	ARG	3
1	A	48	GLY	2
1	A	62	GLY	2
1	A	46	LYS	1
1	A	22	LYS	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	55/79 (70%)	34±3 (61±5%)	21±3 (39±5%)	0 6
All	All	1925/2765 (70%)	1177 (61%)	748 (39%)	0 6

All 48 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	17	LEU	28
1	A	20	ARG	28
1	A	37	LEU	28
1	A	12	ILE	28
1	A	24	SER	27
1	A	33	ILE	27
1	A	57	SER	27
1	A	15	TYR	25
1	A	45	LEU	25
1	A	59	GLN	23
1	A	18	ARG	22
1	A	14	LYS	21
1	A	72	THR	21
1	A	38	ASN	21
1	A	46	LYS	20
1	A	43	LYS	19
1	A	68	ARG	18
1	A	30	GLU	18
1	A	16	ILE	17
1	A	29	LYS	17
1	A	13	SER	17
1	A	65	GLU	16
1	A	36	HIS	16
1	A	49	VAL	16
1	A	54	GLN	15
1	A	22	LYS	15
1	A	64	GLN	15
1	A	60	GLN	14
1	A	70	ASP	14
1	A	27	ARG	13
1	A	39	SER	12
1	A	66	VAL	11
1	A	52	GLU	11
1	A	61	TYR	11
1	A	63	HIS	11
1	A	67	THR	10

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Mol	Chain	Res	Type	Models (Total)
1	A	69	PHE	9
1	A	55	LEU	9
1	A	32	THR	8
1	A	23	ASN	8
1	A	41	THR	8
1	A	51	TYR	7
1	A	11	HIS	6
1	A	50	VAL	5
1	A	19	TRP	4
1	A	71	PHE	3
1	A	40	TYR	2
1	A	25	VAL	2

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