Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:31 PM BST

PDB ID	:	1E9T
Title	:	HIGH RESOLUTION SOLUTION STRUCTURE OF HUMAN INTESTINAL TREFOIL FACTOR
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Deposited on	:	2000-10-26

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

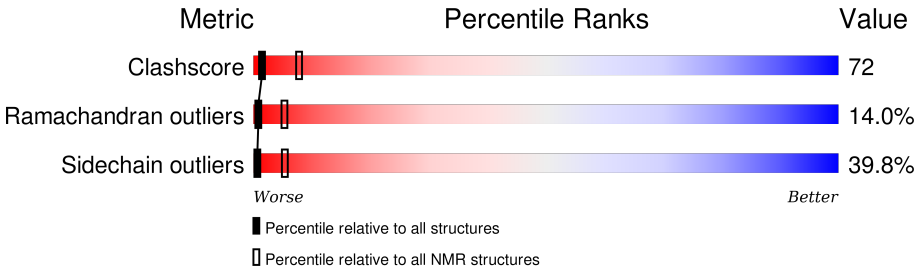
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 is 47%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	59	10% 46% 19% 25%

2 Ensemble composition and analysis

This entry contains 85 models. Model 4 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:10-A:53 (44)	0.12	4

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 3 single-model clusters were found.

Cluster number	Models
1	4, 6, 7, 9, 10, 14, 16, 18, 19, 21, 22, 23, 24, 25, 26, 27, 30, 32, 33, 34, 35, 37, 42, 44, 45, 47, 49, 50, 53, 54, 59, 60, 64, 65, 72, 73
2	36, 43, 46, 48, 51, 52, 55, 63, 67, 68, 69, 70, 74, 75, 76, 78, 84, 85
3	1, 2, 3, 5, 8, 11, 12, 13, 15, 31, 38, 39, 41, 62
4	20, 29, 40, 57, 61, 71
5	56, 58, 66, 80
6	17, 28
7	79, 82
Single-model clusters	77; 81; 83

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 878 atoms, of which 421 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTESTINAL TREFOIL FACTOR.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	59	878	285	421	79	86	7	0

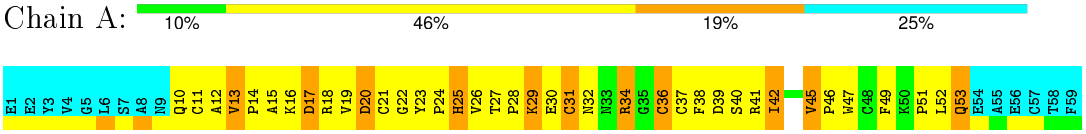
4 Residue-property plots

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: INTESTINAL TREFOIL FACTOR

Chain A:



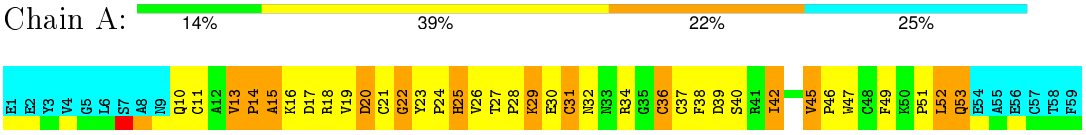
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: INTESTINAL TREFOIL FACTOR

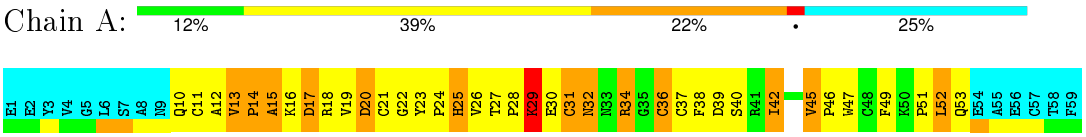
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: INTESTINAL TREFOIL FACTOR

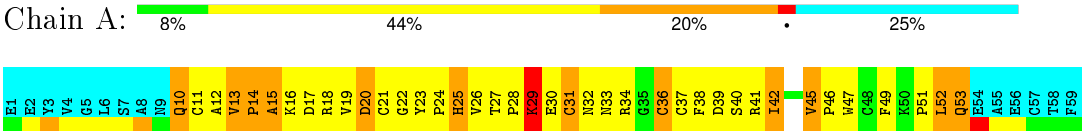
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: INTESTINAL TREFOIL FACTOR

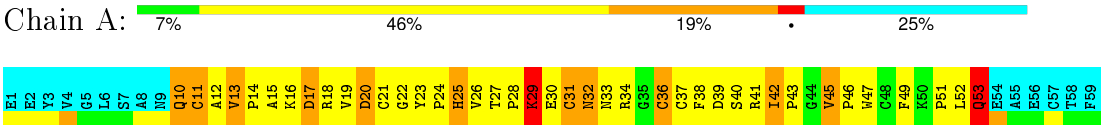
Chain A:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: INTESTINAL TREFOIL FACTOR

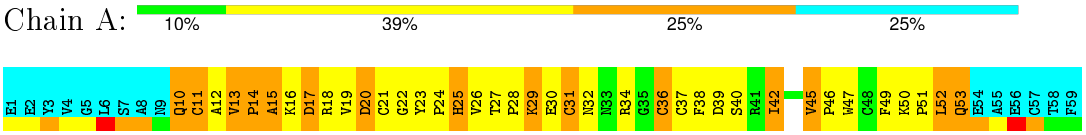
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: INTESTINAL TREFOIL FACTOR

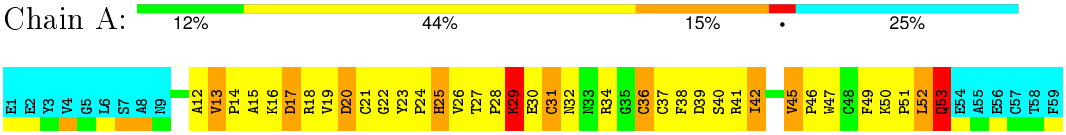
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: INTESTINAL TREFOIL FACTOR

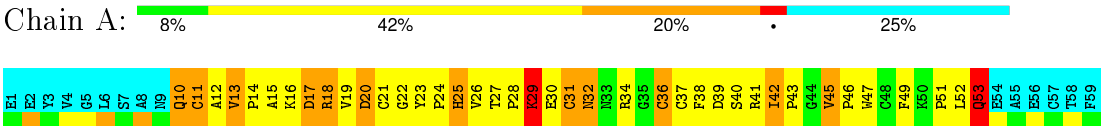
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: INTESTINAL TREFOIL FACTOR

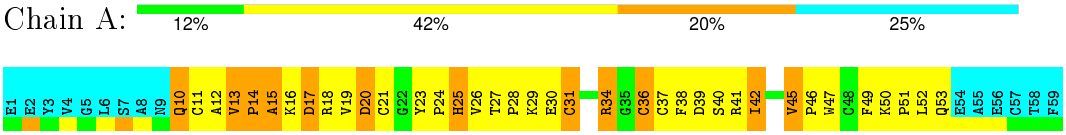
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:



4.2.9 Score per residue for model 9

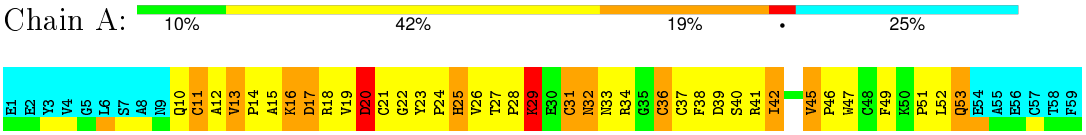
• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:

4.2.10 Score per residue for model 10

• Molecule 1: INTESTINAL TREFOIL FACTOR

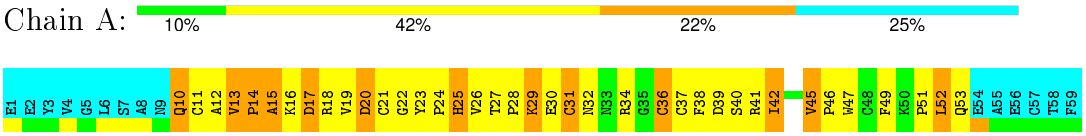
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: INTESTINAL TREFOIL FACTOR

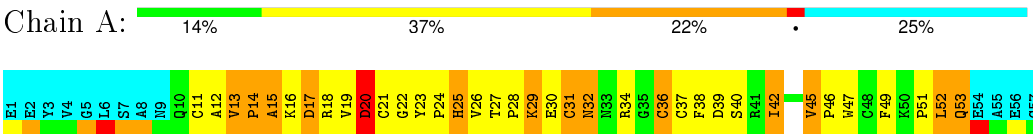
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: INTESTINAL TREFOIL FACTOR

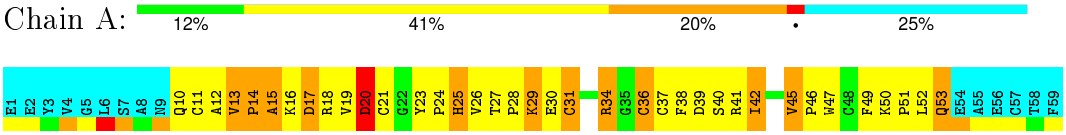
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: INTESTINAL TREFOIL FACTOR

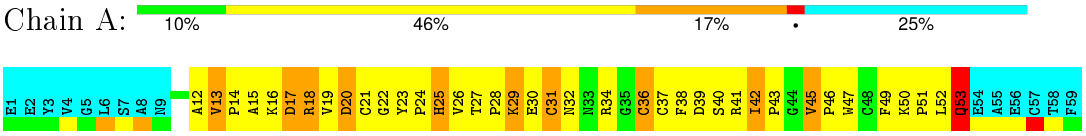
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: INTESTINAL TREFOIL FACTOR

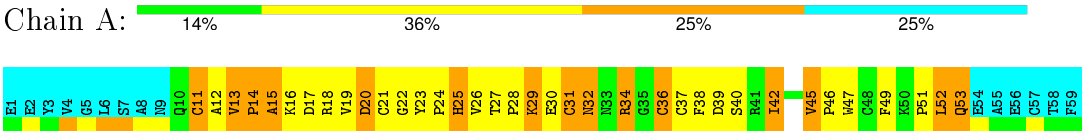
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: INTESTINAL TREFOIL FACTOR

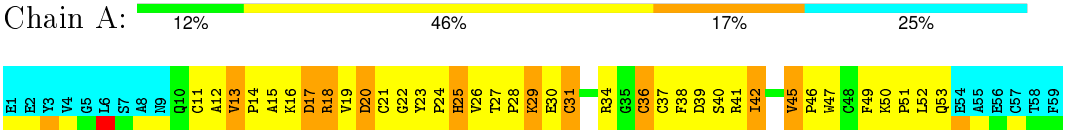
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: INTESTINAL TREFOIL FACTOR

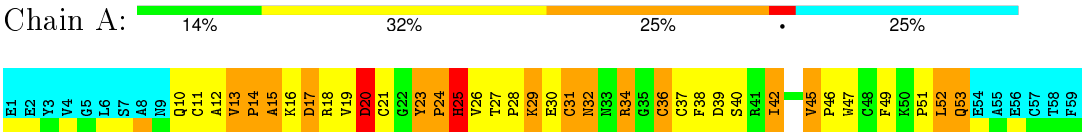
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:



4.2.18 Score per residue for model 18

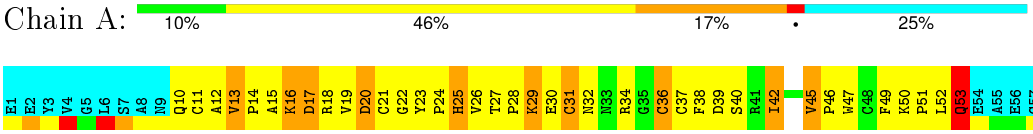
• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:

4.2.19 Score per residue for model 19

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:



4.2.20 Score per residue for model 20

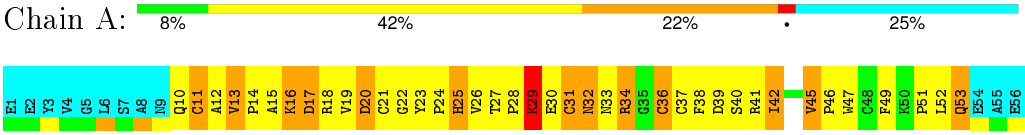
• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:

4.2.21 Score per residue for model 21

• Molecule 1: INTESTINAL TREFOIL FACTOR

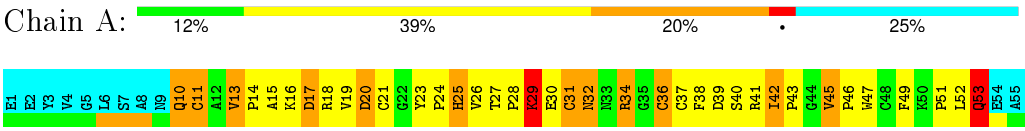
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: INTESTINAL TREFOIL FACTOR

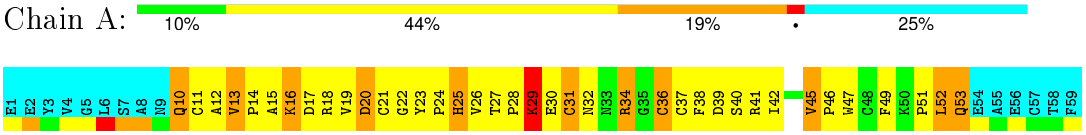
Chain A:



4.2.23 Score per residue for model 23

• Molecule 1: INTESTINAL TREFOIL FACTOR

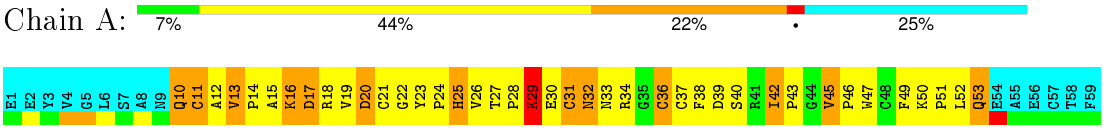
Chain A:



4.2.24 Score per residue for model 24

• Molecule 1: INTESTINAL TREFOIL FACTOR

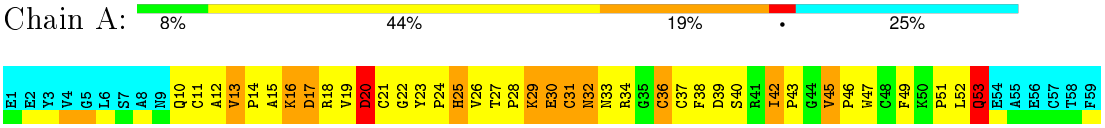
Chain A:



4.2.25 Score per residue for model 25

• Molecule 1: INTESTINAL TREFOIL FACTOR

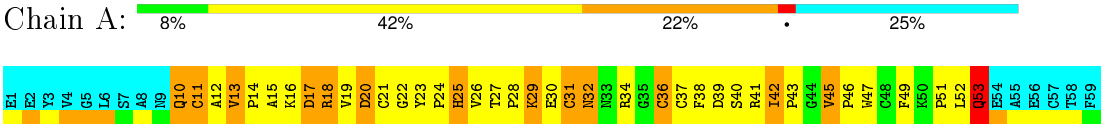
Chain A:



4.2.26 Score per residue for model 26

• Molecule 1: INTESTINAL TREFOIL FACTOR

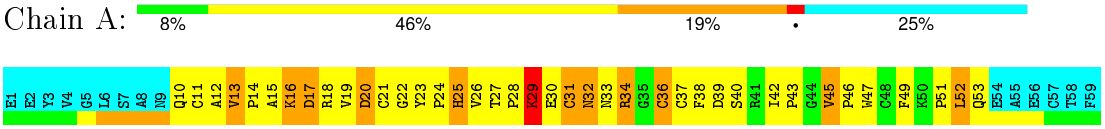
Chain A:



4.2.27 Score per residue for model 27

• Molecule 1: INTESTINAL TREFOIL FACTOR

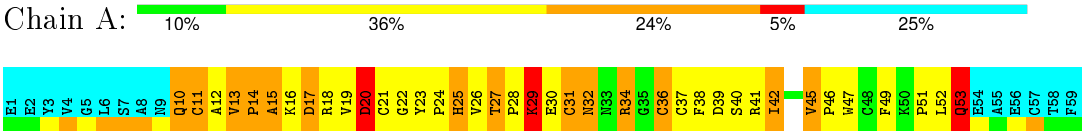
Chain A:



4.2.28 Score per residue for model 28

• Molecule 1: INTESTINAL TREFOIL FACTOR

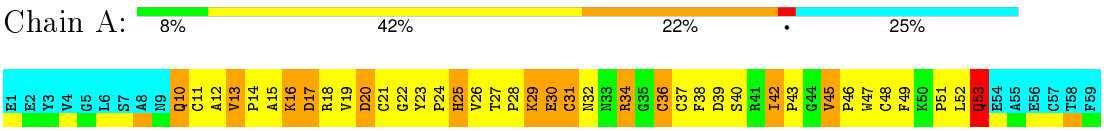
Chain A:



4.2.29 Score per residue for model 29

• Molecule 1: INTESTINAL TREFOIL FACTOR

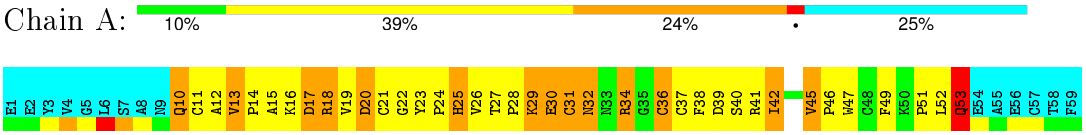
Chain A:



4.2.30 Score per residue for model 30

• Molecule 1: INTESTINAL TREFOIL FACTOR

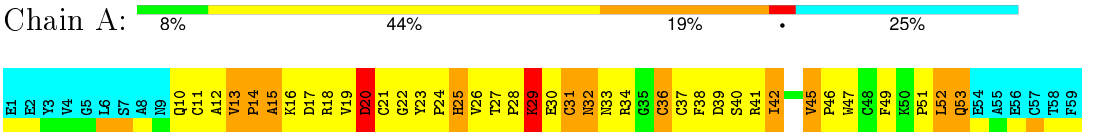
Chain A:



4.2.31 Score per residue for model 31

• Molecule 1: INTESTINAL TREFOIL FACTOR

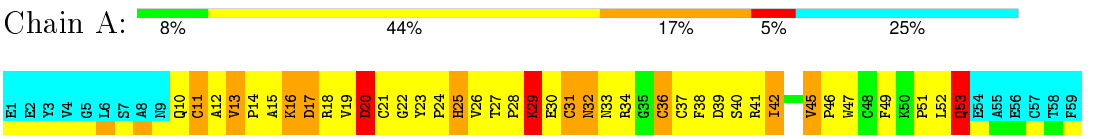
Chain A:



4.2.32 Score per residue for model 32

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:



4.2.33 Score per residue for model 33

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 7% 51% 14% 25%

4.2.34 Score per residue for model 34

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 5% 47% 22% 25%

4.2.35 Score per residue for model 35

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 7% 47% 19% 25%

4.2.36 Score per residue for model 36

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 8% 39% 24% 25%

4.2.37 Score per residue for model 37

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 10% 46% 17% 25%

4.2.38 Score per residue for model 38

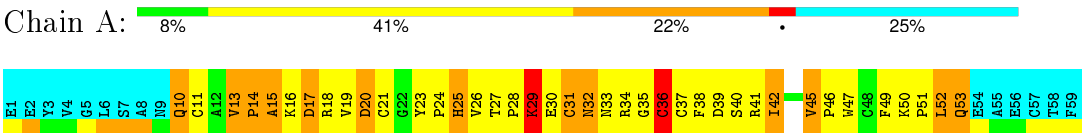
• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:

4.2.39 Score per residue for model 39

• Molecule 1: INTESTINAL TREFOIL FACTOR

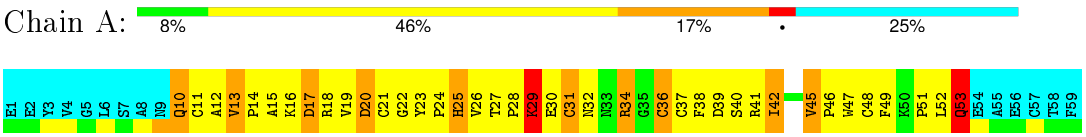
Chain A:



4.2.40 Score per residue for model 40

• Molecule 1: INTESTINAL TREFOIL FACTOR

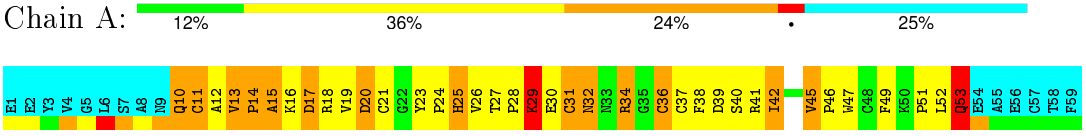
Chain A:



4.2.41 Score per residue for model 41

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:



4.2.42 Score per residue for model 42

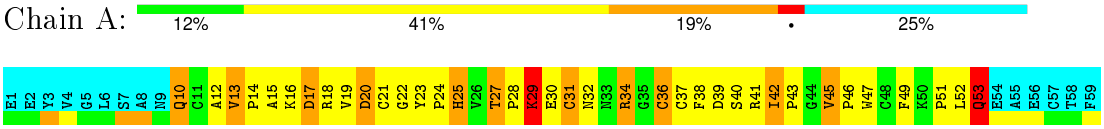
• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:

4.2.43 Score per residue for model 43

• Molecule 1: INTESTINAL TREFOIL FACTOR

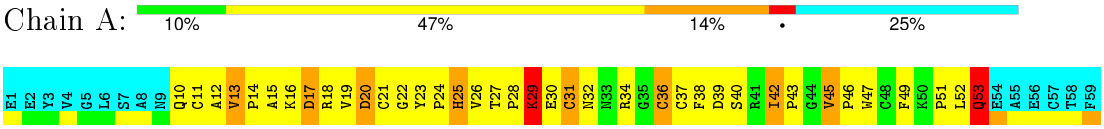
Chain A:



4.2.44 Score per residue for model 44

• Molecule 1: INTESTINAL TREFOIL FACTOR

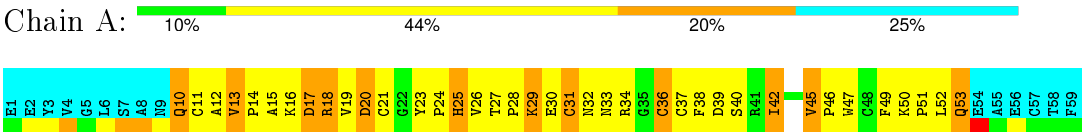
Chain A:



4.2.45 Score per residue for model 45

• Molecule 1: INTESTINAL TREFOIL FACTOR

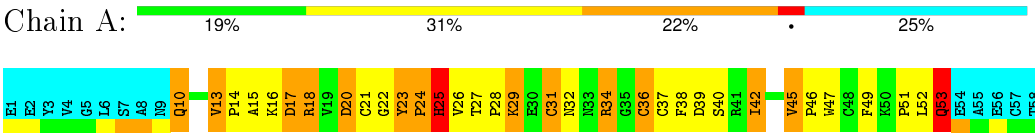
Chain A:



4.2.46 Score per residue for model 46

• Molecule 1: INTESTINAL TREFOIL FACTOR

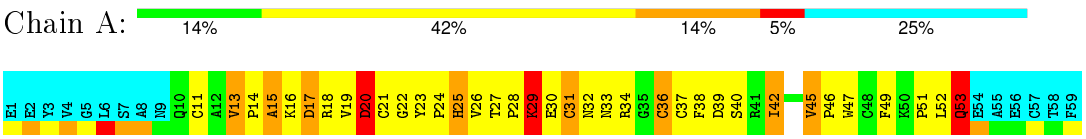
Chain A:



4.2.47 Score per residue for model 47

• Molecule 1: INTESTINAL TREFOIL FACTOR

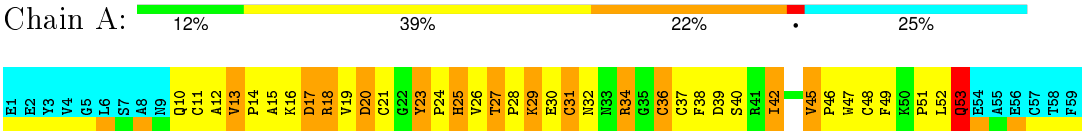
Chain A:



4.2.48 Score per residue for model 48

• Molecule 1: INTESTINAL TREFOIL FACTOR

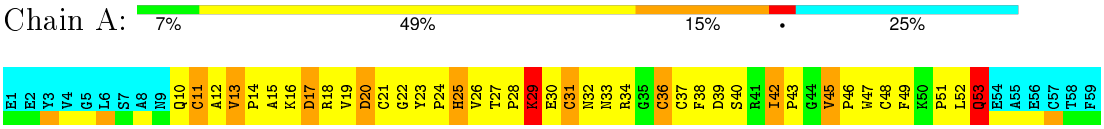
Chain A:



4.2.49 Score per residue for model 49

• Molecule 1: INTESTINAL TREFOIL FACTOR

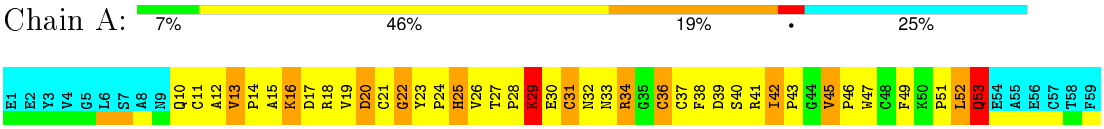
Chain A:



4.2.50 Score per residue for model 50

• Molecule 1: INTESTINAL TREFOIL FACTOR

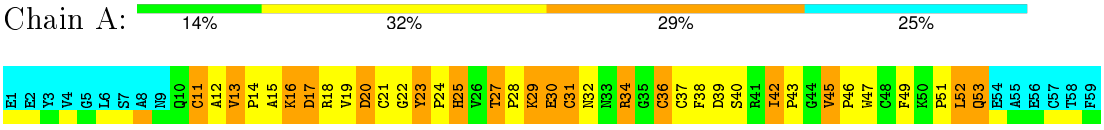
Chain A:



4.2.51 Score per residue for model 51

• Molecule 1: INTESTINAL TREFOIL FACTOR

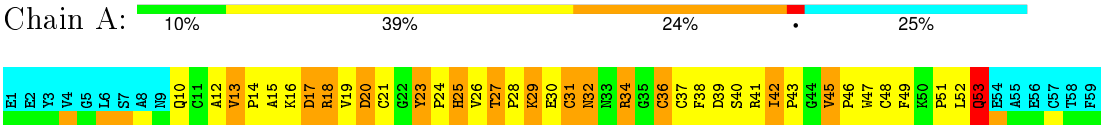
Chain A:



4.2.52 Score per residue for model 52

• Molecule 1: INTESTINAL TREFOIL FACTOR

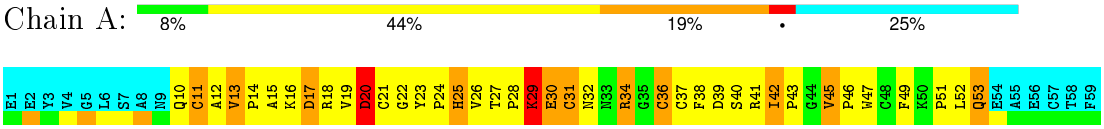
Chain A:



4.2.53 Score per residue for model 53

• Molecule 1: INTESTINAL TREFOIL FACTOR

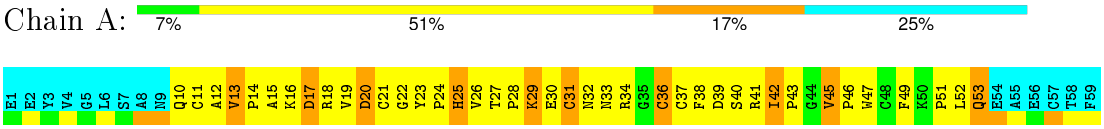
Chain A:



4.2.54 Score per residue for model 54

• Molecule 1: INTESTINAL TREFOIL FACTOR

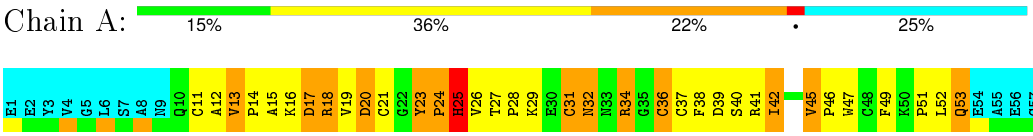
Chain A:



4.2.55 Score per residue for model 55

• Molecule 1: INTESTINAL TREFOIL FACTOR

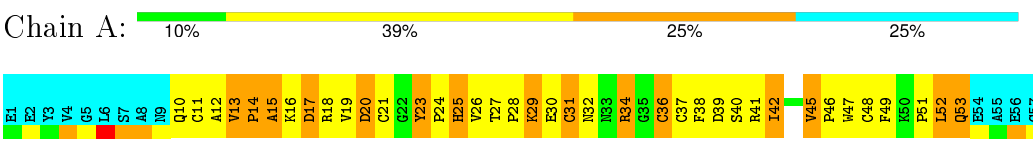
Chain A:



4.2.56 Score per residue for model 56

• Molecule 1: INTESTINAL TREFOIL FACTOR

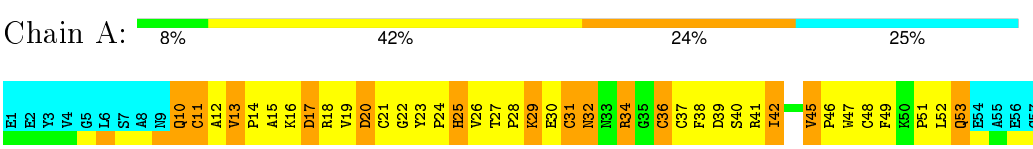
Chain A:



4.2.57 Score per residue for model 57

• Molecule 1: INTESTINAL TREFOIL FACTOR

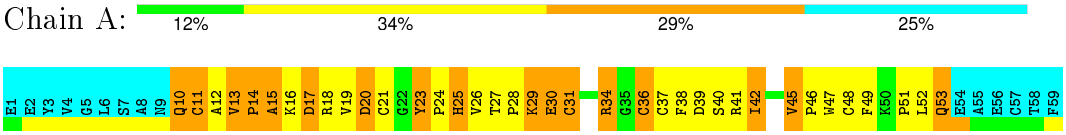
Chain A:



4.2.58 Score per residue for model 58

• Molecule 1: INTESTINAL TREFOIL FACTOR

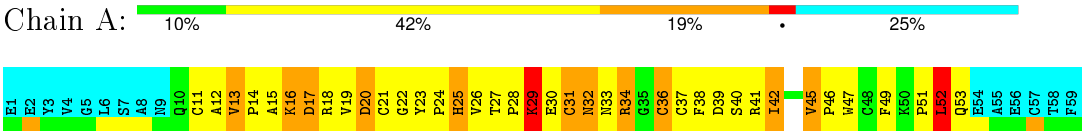
Chain A:



4.2.59 Score per residue for model 59

• Molecule 1: INTESTINAL TREFOIL FACTOR

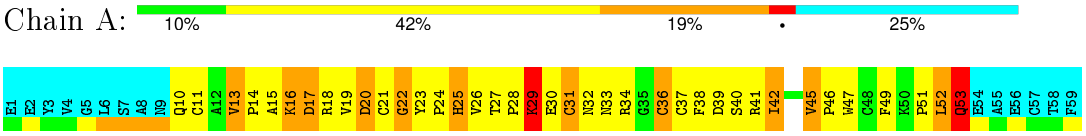
Chain A:



4.2.60 Score per residue for model 60

• Molecule 1: INTESTINAL TREFOIL FACTOR

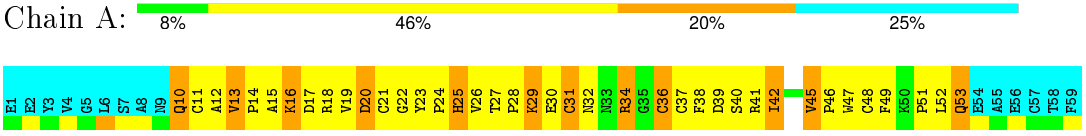
Chain A:



4.2.61 Score per residue for model 61

• Molecule 1: INTESTINAL TREFOIL FACTOR

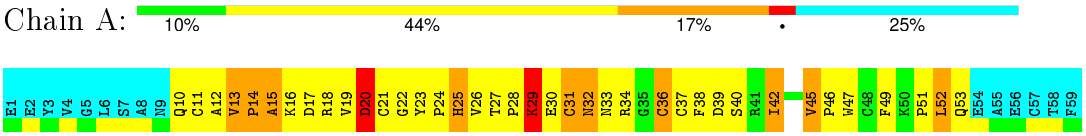
Chain A:



4.2.62 Score per residue for model 62

• Molecule 1: INTESTINAL TREFOIL FACTOR

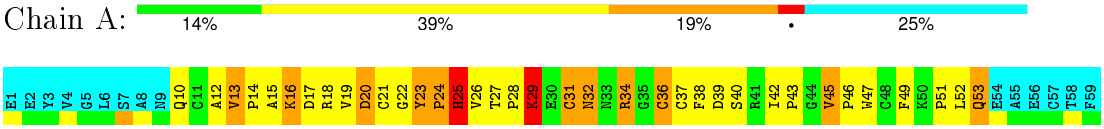
Chain A:



4.2.63 Score per residue for model 63

• Molecule 1: INTESTINAL TREFOIL FACTOR

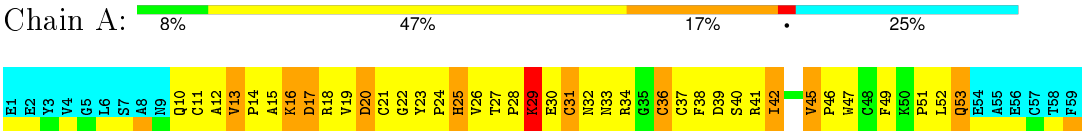
Chain A:



4.2.64 Score per residue for model 64

• Molecule 1: INTESTINAL TREFOIL FACTOR

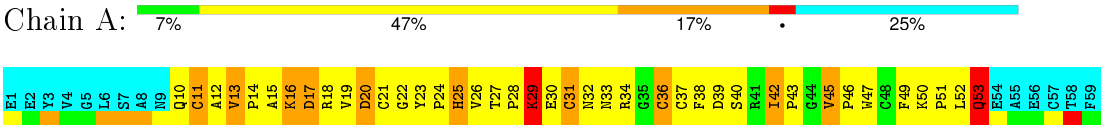
Chain A:



4.2.65 Score per residue for model 65

• Molecule 1: INTESTINAL TREFOIL FACTOR

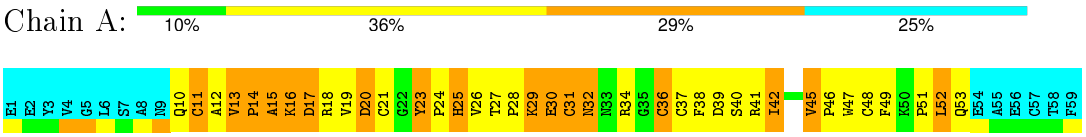
Chain A:



4.2.66 Score per residue for model 66

• Molecule 1: INTESTINAL TREFOIL FACTOR

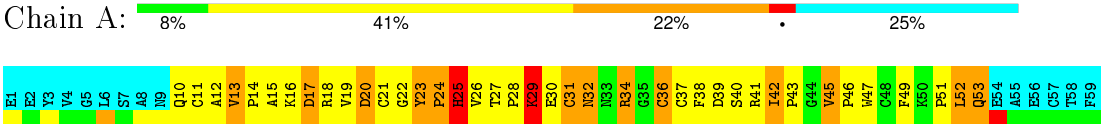
Chain A:



4.2.67 Score per residue for model 67

• Molecule 1: INTESTINAL TREFOIL FACTOR

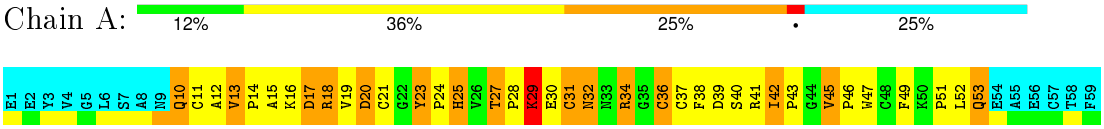
Chain A:



4.2.68 Score per residue for model 68

• Molecule 1: INTESTINAL TREFOIL FACTOR

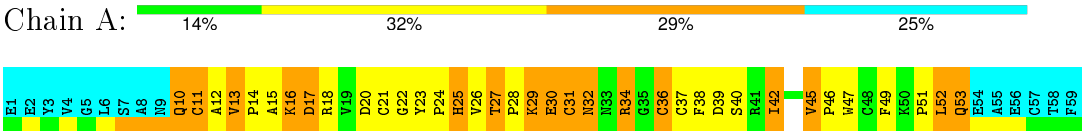
Chain A:



4.2.69 Score per residue for model 69

• Molecule 1: INTESTINAL TREFOIL FACTOR

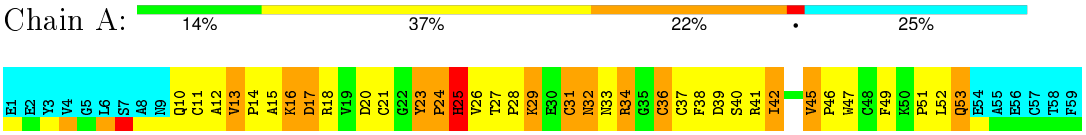
Chain A:



4.2.70 Score per residue for model 70

• Molecule 1: INTESTINAL TREFOIL FACTOR

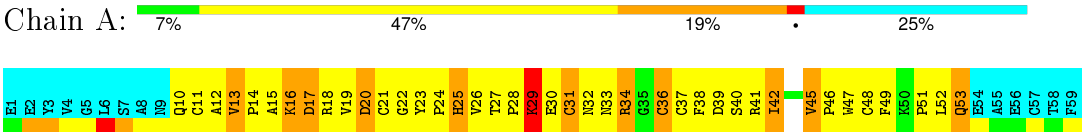
Chain A:



4.2.71 Score per residue for model 71

• Molecule 1: INTESTINAL TREFOIL FACTOR

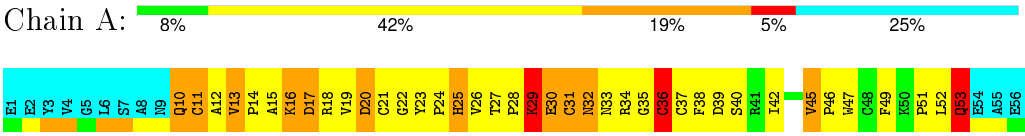
Chain A:



4.2.72 Score per residue for model 72

• Molecule 1: INTESTINAL TREFOIL FACTOR

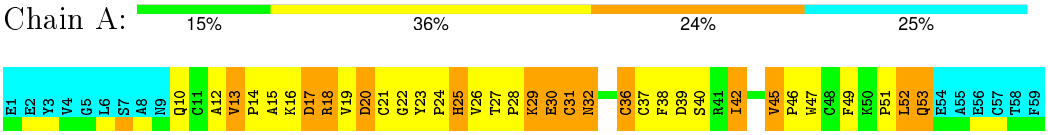
Chain A:



4.2.73 Score per residue for model 73

• Molecule 1: INTESTINAL TREFOIL FACTOR

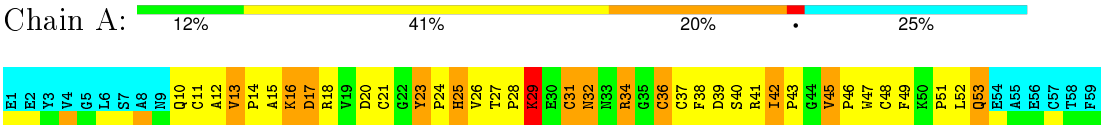
Chain A:



4.2.74 Score per residue for model 74

• Molecule 1: INTESTINAL TREFOIL FACTOR

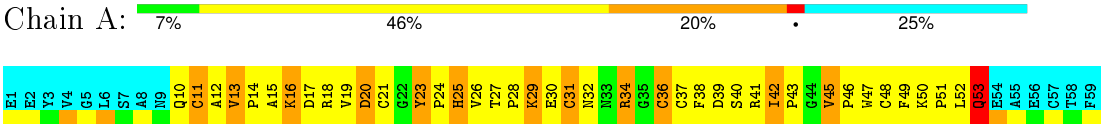
Chain A:



4.2.75 Score per residue for model 75

• Molecule 1: INTESTINAL TREFOIL FACTOR

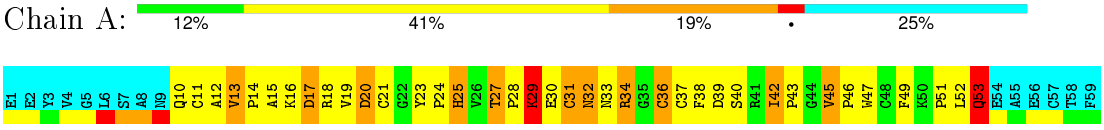
Chain A:



4.2.76 Score per residue for model 76

• Molecule 1: INTESTINAL TREFOIL FACTOR

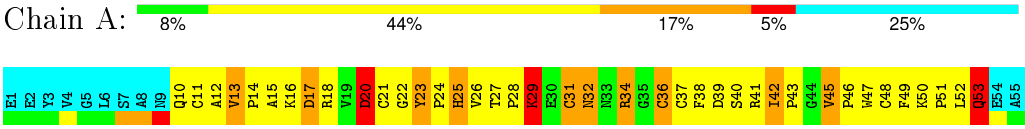
Chain A:



4.2.77 Score per residue for model 77

• Molecule 1: INTESTINAL TREFOIL FACTOR

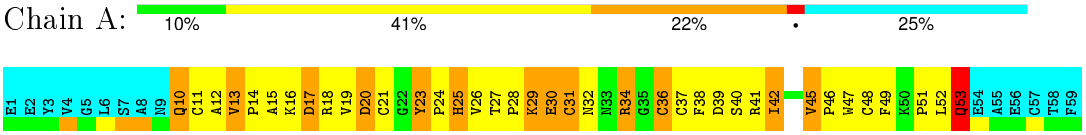
Chain A:



4.2.78 Score per residue for model 78

• Molecule 1: INTESTINAL TREFOIL FACTOR

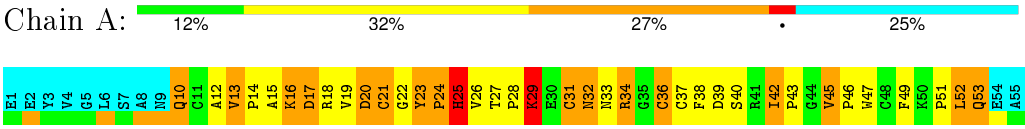
Chain A:



4.2.79 Score per residue for model 79

• Molecule 1: INTESTINAL TREFOIL FACTOR

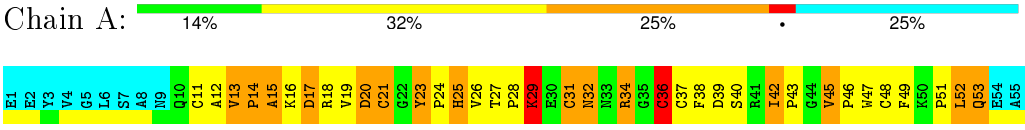
Chain A:



4.2.80 Score per residue for model 80

• Molecule 1: INTESTINAL TREFOIL FACTOR

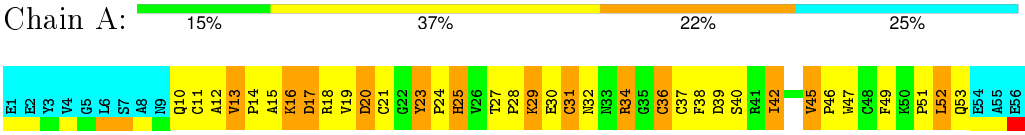
Chain A:



4.2.81 Score per residue for model 81

• Molecule 1: INTESTINAL TREFOIL FACTOR

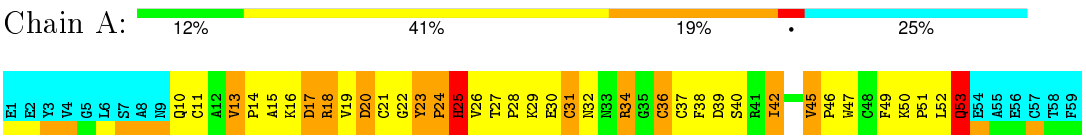
Chain A:



4.2.82 Score per residue for model 82

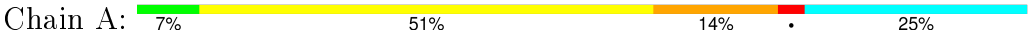
• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A:



4.2.83 Score per residue for model 83

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 

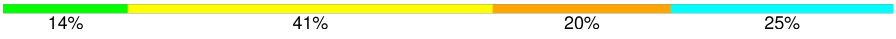
4.2.84 Score per residue for model 84

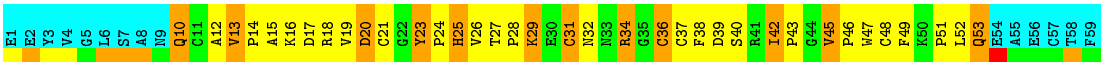
• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 

4.2.85 Score per residue for model 85

• Molecule 1: INTESTINAL TREFOIL FACTOR

Chain A: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING COMBINED WITH TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 85 were deposited, based on the following criterion: *CONSISTENCY WITH THE NMR STRUCTURAL DATA*.

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

Software name	Classification	Version
DYANA	refinement	
XEASY	structure solution	
DYANA	structure solution	

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

Chemical shift file(s)	BMRB entry 5771
Number of chemical shift lists	1
Total number of shifts	367
Number of shifts mapped to atoms	367
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

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

6 Model quality

6.1 Standard geometry

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

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	342	324	323	48±4
All	All	29070	27540	27455	4044

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 72.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ALA:HB1	1:A:45:VAL:HG11	1.06	1.26	39	85
1:A:18:ARG:CZ	1:A:49:PHE:CE2	0.85	2.60	81	68
1:A:13:VAL:HG12	1:A:14:PRO:HD2	0.85	1.49	26	85
1:A:42:ILE:HD13	1:A:45:VAL:CG1	0.74	2.13	58	67
1:A:18:ARG:NH1	1:A:49:PHE:CZ	0.74	2.54	11	39
1:A:52:LEU:C	1:A:52:LEU:HD23	0.73	2.03	44	37
1:A:25:HIS:O	1:A:25:HIS:CD2	0.73	2.41	56	45
1:A:52:LEU:HD23	1:A:52:LEU:C	0.72	2.05	58	43
1:A:25:HIS:CG	1:A:25:HIS:O	0.71	2.43	69	43
1:A:13:VAL:HG12	1:A:17:ASP:HB3	0.71	1.63	62	10
1:A:18:ARG:HD2	1:A:49:PHE:CD2	0.71	2.20	58	85
1:A:25:HIS:CD2	1:A:25:HIS:O	0.71	2.43	58	39
1:A:52:LEU:HD23	1:A:53:GLN:N	0.71	1.99	23	46
1:A:25:HIS:O	1:A:25:HIS:CG	0.71	2.44	43	31

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:O	1:A:52:LEU:HD23	0.70	1.86	73	4
1:A:14:PRO:O	1:A:15:ALA:HB2	0.69	1.88	15	20
1:A:14:PRO:O	1:A:15:ALA:HB3	0.69	1.86	53	65
1:A:18:ARG:NH1	1:A:49:PHE:CE2	0.68	2.61	83	85
1:A:42:ILE:HD13	1:A:45:VAL:HG13	0.67	1.65	1	67
1:A:18:ARG:NH1	1:A:45:VAL:HG21	0.66	2.05	3	46
1:A:32:ASN:C	1:A:32:ASN:OD1	0.66	2.34	3	4
1:A:32:ASN:OD1	1:A:32:ASN:C	0.65	2.35	50	2
1:A:27:THR:O	1:A:31:CYS:HB3	0.64	1.93	66	79
1:A:38:PHE:CD1	1:A:39:ASP:N	0.64	2.65	82	3
1:A:18:ARG:NH1	1:A:49:PHE:CD2	0.63	2.66	49	28
1:A:25:HIS:CE1	1:A:30:GLU:CD	0.63	2.72	73	50
1:A:23:TYR:CZ	1:A:34:ARG:HG3	0.63	2.28	67	21
1:A:27:THR:O	1:A:38:PHE:CD2	0.63	2.52	82	3
1:A:28:PRO:HA	1:A:38:PHE:CD1	0.62	2.29	82	3
1:A:27:THR:O	1:A:38:PHE:CD1	0.62	2.52	71	73
1:A:28:PRO:HA	1:A:38:PHE:CD2	0.62	2.30	79	82
1:A:23:TYR:CE1	1:A:34:ARG:CG	0.61	2.84	37	19
1:A:38:PHE:CD2	1:A:39:ASP:N	0.61	2.68	74	82
1:A:27:THR:C	1:A:38:PHE:CD2	0.61	2.75	75	3
1:A:53:GLN:NE2	1:A:53:GLN:H	0.60	1.94	71	2
1:A:23:TYR:CB	1:A:26:VAL:CG1	0.60	2.80	22	56
1:A:18:ARG:NH1	1:A:45:VAL:CG2	0.60	2.65	59	46
1:A:27:THR:C	1:A:38:PHE:CD1	0.60	2.75	71	81
1:A:14:PRO:O	1:A:15:ALA:CB	0.60	2.50	76	85
1:A:46:PRO:O	1:A:47:TRP:C	0.60	2.40	76	85
1:A:27:THR:O	1:A:38:PHE:CG	0.59	2.55	33	76
1:A:15:ALA:HA	1:A:18:ARG:NE	0.59	2.13	75	81
1:A:25:HIS:CE1	1:A:30:GLU:OE2	0.59	2.56	8	13
1:A:38:PHE:CG	1:A:39:ASP:N	0.58	2.71	74	85
1:A:39:ASP:O	1:A:47:TRP:CG	0.58	2.57	65	85
1:A:40:SER:HA	1:A:47:TRP:CE2	0.58	2.34	38	85
1:A:53:GLN:O	1:A:53:GLN:CG	0.56	2.53	71	1
1:A:27:THR:CA	1:A:38:PHE:CE2	0.56	2.88	75	1
1:A:18:ARG:HD2	1:A:49:PHE:CG	0.56	2.36	83	79
1:A:13:VAL:HG12	1:A:14:PRO:CD	0.56	2.26	58	18
1:A:27:THR:CA	1:A:38:PHE:CE1	0.56	2.89	39	75
1:A:16:LYS:C	1:A:16:LYS:CD	0.56	2.74	81	13
1:A:16:LYS:CD	1:A:16:LYS:C	0.56	2.74	79	19
1:A:17:ASP:CG	1:A:17:ASP:O	0.55	2.44	23	7
1:A:17:ASP:O	1:A:17:ASP:CG	0.55	2.44	50	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:GLN:CG	1:A:53:GLN:O	0.55	2.53	13	1
1:A:23:TYR:HB2	1:A:26:VAL:CG1	0.55	2.31	11	56
1:A:52:LEU:C	1:A:52:LEU:CD2	0.55	2.75	44	36
1:A:23:TYR:CE1	1:A:34:ARG:HG2	0.55	2.36	50	16
1:A:21:CYS:CB	1:A:36:CYS:SG	0.54	2.95	80	1
1:A:27:THR:HA	1:A:38:PHE:CE1	0.54	2.38	51	66
1:A:52:LEU:CD2	1:A:52:LEU:C	0.54	2.76	26	33
1:A:23:TYR:CE2	1:A:25:HIS:CD2	0.54	2.96	83	7
1:A:15:ALA:HA	1:A:18:ARG:CG	0.53	2.33	82	85
1:A:23:TYR:CE2	1:A:34:ARG:HG3	0.53	2.38	79	12
1:A:51:PRO:O	1:A:52:LEU:C	0.53	2.47	62	85
1:A:23:TYR:CE1	1:A:34:ARG:CZ	0.53	2.92	75	1
1:A:32:ASN:N	1:A:32:ASN:OD1	0.53	2.42	83	1
1:A:23:TYR:CE1	1:A:34:ARG:HB3	0.52	2.39	71	7
1:A:27:THR:HA	1:A:38:PHE:CE2	0.52	2.40	75	1
1:A:13:VAL:CG1	1:A:17:ASP:OD2	0.52	2.58	62	1
1:A:31:CYS:SG	1:A:37:CYS:O	0.51	2.68	35	85
1:A:27:THR:OG1	1:A:30:GLU:CB	0.51	2.59	58	12
1:A:27:THR:HG1	1:A:30:GLU:H	0.51	1.46	58	4
1:A:29:LYS:O	1:A:32:ASN:OD1	0.51	2.29	50	30
1:A:25:HIS:CE1	1:A:30:GLU:OE1	0.51	2.64	53	5
1:A:29:LYS:O	1:A:33:ASN:N	0.51	2.44	60	14
1:A:32:ASN:OD1	1:A:38:PHE:CB	0.51	2.59	83	10
1:A:53:GLN:OE1	1:A:53:GLN:O	0.50	2.29	14	5
1:A:18:ARG:CD	1:A:49:PHE:CD2	0.50	2.93	45	37
1:A:23:TYR:CD2	1:A:48:CYS:SG	0.50	3.05	61	8
1:A:34:ARG:CD	1:A:34:ARG:O	0.50	2.59	51	8
1:A:53:GLN:O	1:A:53:GLN:OE1	0.50	2.29	41	5
1:A:21:CYS:SG	1:A:49:PHE:C	0.50	2.90	80	2
1:A:21:CYS:SG	1:A:49:PHE:CA	0.50	2.99	80	1
1:A:26:VAL:HG11	1:A:48:CYS:HB2	0.50	1.83	78	9
1:A:23:TYR:CE1	1:A:34:ARG:NH2	0.50	2.80	75	1
1:A:13:VAL:CG1	1:A:17:ASP:HB3	0.49	2.37	39	80
1:A:42:ILE:HD13	1:A:45:VAL:CG2	0.49	2.37	38	19
1:A:39:ASP:O	1:A:47:TRP:CB	0.49	2.60	65	28
1:A:40:SER:HB2	1:A:47:TRP:CH2	0.49	2.43	3	25
1:A:30:GLU:CD	1:A:30:GLU:C	0.49	2.71	64	1
1:A:23:TYR:HB3	1:A:26:VAL:CG1	0.49	2.38	40	68
1:A:26:VAL:C	1:A:27:THR:CG2	0.49	2.80	73	47
1:A:29:LYS:N	1:A:32:ASN:HD22	0.49	2.05	47	9
1:A:23:TYR:CE2	1:A:34:ARG:HG2	0.49	2.42	83	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:CZ	1:A:34:ARG:HG2	0.49	2.43	69	7
1:A:10:GLN:O	1:A:52:LEU:N	0.49	2.45	1	35
1:A:25:HIS:CE1	1:A:30:GLU:HG2	0.49	2.42	54	2
1:A:25:HIS:CE1	1:A:30:GLU:CG	0.49	2.95	54	4
1:A:34:ARG:O	1:A:34:ARG:CD	0.49	2.61	17	13
1:A:39:ASP:CB	1:A:49:PHE:CE2	0.49	2.96	38	45
1:A:29:LYS:N	1:A:32:ASN:ND2	0.49	2.60	47	10
1:A:24:PRO:O	1:A:26:VAL:N	0.48	2.46	46	8
1:A:28:PRO:CA	1:A:38:PHE:CD2	0.48	2.97	34	66
1:A:29:LYS:O	1:A:33:ASN:CB	0.48	2.61	60	13
1:A:10:GLN:N	1:A:10:GLN:CD	0.47	2.66	49	1
1:A:19:VAL:HG12	1:A:19:VAL:O	0.47	2.09	33	3
1:A:25:HIS:NE2	1:A:30:GLU:OE2	0.47	2.47	64	1
1:A:19:VAL:O	1:A:20:ASP:O	0.47	2.32	82	80
1:A:52:LEU:HD23	1:A:53:GLN:C	0.47	2.29	60	30
1:A:30:GLU:OE1	1:A:31:CYS:N	0.47	2.48	64	1
1:A:42:ILE:CD1	1:A:45:VAL:HG22	0.47	2.40	13	14
1:A:32:ASN:ND2	1:A:32:ASN:C	0.47	2.69	79	8
1:A:23:TYR:CB	1:A:26:VAL:HG12	0.46	2.40	38	45
1:A:23:TYR:CE2	1:A:25:HIS:NE2	0.46	2.83	83	1
1:A:53:GLN:NE2	1:A:53:GLN:N	0.46	2.64	13	1
1:A:10:GLN:N	1:A:10:GLN:OE1	0.46	2.48	72	1
1:A:32:ASN:C	1:A:32:ASN:ND2	0.46	2.69	12	4
1:A:53:GLN:N	1:A:53:GLN:CD	0.46	2.68	71	1
1:A:23:TYR:OH	1:A:34:ARG:NE	0.46	2.48	74	2
1:A:13:VAL:CG1	1:A:17:ASP:CB	0.46	2.94	64	16
1:A:32:ASN:CG	1:A:32:ASN:O	0.45	2.55	80	17
1:A:19:VAL:O	1:A:19:VAL:HG12	0.45	2.11	26	4
1:A:51:PRO:O	1:A:53:GLN:N	0.45	2.50	73	1
1:A:18:ARG:NH2	1:A:39:ASP:CG	0.45	2.69	82	1
1:A:53:GLN:CD	1:A:53:GLN:N	0.45	2.69	13	1
1:A:25:HIS:O	1:A:30:GLU:OE1	0.45	2.34	64	1
1:A:42:ILE:HD13	1:A:45:VAL:HG22	0.45	1.87	12	3
1:A:42:ILE:CD1	1:A:45:VAL:CG2	0.45	2.94	13	13
1:A:28:PRO:CA	1:A:38:PHE:CD1	0.45	3.00	75	1
1:A:23:TYR:CZ	1:A:34:ARG:CG	0.44	3.00	67	1
1:A:20:ASP:OD1	1:A:22:GLY:N	0.44	2.50	77	4
1:A:32:ASN:OD1	1:A:38:PHE:HB2	0.44	2.12	83	1
1:A:25:HIS:ND1	1:A:30:GLU:OE1	0.44	2.50	37	8
1:A:23:TYR:OH	1:A:34:ARG:CZ	0.44	2.66	78	1
1:A:14:PRO:O	1:A:18:ARG:NH2	0.44	2.50	38	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:THR:OG1	1:A:30:GLU:N	0.44	2.48	78	6
1:A:32:ASN:OD1	1:A:38:PHE:N	0.44	2.50	66	2
1:A:13:VAL:HB	1:A:18:ARG:HD3	0.44	1.89	61	19
1:A:18:ARG:NE	1:A:49:PHE:CD2	0.44	2.86	45	5
1:A:53:GLN:N	1:A:53:GLN:NE2	0.44	2.63	71	1
1:A:23:TYR:CZ	1:A:34:ARG:HB3	0.44	2.48	35	3
1:A:26:VAL:CG1	1:A:48:CYS:HB2	0.44	2.42	56	10
1:A:27:THR:C	1:A:38:PHE:CE2	0.44	2.92	75	1
1:A:20:ASP:HB2	1:A:46:PRO:CG	0.44	2.43	79	1
1:A:32:ASN:OD1	1:A:32:ASN:N	0.43	2.50	72	2
1:A:29:LYS:O	1:A:32:ASN:ND2	0.43	2.50	22	2
1:A:32:ASN:O	1:A:32:ASN:CG	0.43	2.56	26	8
1:A:16:LYS:NZ	1:A:17:ASP:OD2	0.43	2.51	71	1
1:A:17:ASP:O	1:A:17:ASP:OD1	0.43	2.37	62	1
1:A:26:VAL:HG11	1:A:48:CYS:CB	0.43	2.44	56	2
1:A:19:VAL:HG11	1:A:50:LYS:HD3	0.43	1.90	82	1
1:A:23:TYR:CE2	1:A:34:ARG:CG	0.43	3.02	55	2
1:A:43:PRO:O	1:A:45:VAL:O	0.43	2.37	67	35
1:A:50:LYS:HB3	1:A:51:PRO:HD2	0.42	1.90	14	5
1:A:10:GLN:CD	1:A:11:CYS:SG	0.42	2.97	72	1
1:A:39:ASP:HB2	1:A:49:PHE:CE2	0.42	2.49	38	3
1:A:53:GLN:O	1:A:53:GLN:HG2	0.42	2.14	71	1
1:A:40:SER:HA	1:A:47:TRP:CD2	0.42	2.49	13	13
1:A:10:GLN:OE1	1:A:11:CYS:SG	0.42	2.78	72	1
1:A:29:LYS:O	1:A:33:ASN:HB2	0.42	2.15	60	11
1:A:15:ALA:HA	1:A:18:ARG:CD	0.42	2.45	9	12
1:A:13:VAL:HG22	1:A:52:LEU:HB2	0.42	1.90	39	1
1:A:53:GLN:HG2	1:A:53:GLN:O	0.42	2.14	13	1
1:A:27:THR:C	1:A:38:PHE:CE1	0.42	2.93	58	2
1:A:10:GLN:O	1:A:51:PRO:HA	0.42	2.14	39	2
1:A:23:TYR:OH	1:A:34:ARG:CG	0.42	2.68	67	1
1:A:17:ASP:OD2	1:A:53:GLN:NE2	0.41	2.52	69	1
1:A:15:ALA:C	1:A:18:ARG:HG2	0.41	2.35	58	2
1:A:33:ASN:OD1	1:A:33:ASN:C	0.41	2.58	42	2
1:A:30:GLU:OE1	1:A:30:GLU:C	0.41	2.58	64	1
1:A:18:ARG:NH1	1:A:45:VAL:HG23	0.41	2.30	61	1
1:A:18:ARG:CB	1:A:46:PRO:HG2	0.41	2.45	82	2
1:A:23:TYR:OH	1:A:34:ARG:HG2	0.41	2.15	83	1
1:A:27:THR:OG1	1:A:30:GLU:HB2	0.41	2.16	66	1
1:A:19:VAL:HG11	1:A:50:LYS:CD	0.41	2.45	16	1
1:A:19:VAL:O	1:A:20:ASP:C	0.41	2.59	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ARG:HE	1:A:45:VAL:HG21	0.41	1.76	81	1
1:A:32:ASN:ND2	1:A:32:ASN:O	0.41	2.53	74	1
1:A:33:ASN:OD1	1:A:33:ASN:O	0.41	2.38	25	1
1:A:43:PRO:HA	1:A:47:TRP:NE1	0.41	2.31	80	1
1:A:13:VAL:HG23	1:A:49:PHE:CE1	0.41	2.51	62	1
1:A:27:THR:CG2	1:A:30:GLU:HB2	0.40	2.46	69	2
1:A:34:ARG:HD2	1:A:34:ARG:O	0.40	2.16	67	1
1:A:16:LYS:HD2	1:A:16:LYS:C	0.40	2.36	79	1
1:A:10:GLN:NE2	1:A:37:CYS:SG	0.40	2.94	50	1
1:A:43:PRO:O	1:A:44:GLY:C	0.40	2.60	83	1
1:A:35:GLY:O	1:A:36:CYS:HB2	0.40	2.16	39	1
1:A:10:GLN:OE1	1:A:37:CYS:SG	0.40	2.80	43	1
1:A:35:GLY:O	1:A:36:CYS:CB	0.40	2.69	72	1
1:A:10:GLN:CG	1:A:51:PRO:HB3	0.40	2.46	68	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	44/59 (75%)	27±1 (62±2%)	10±1 (24±3%)	6±1 (14±2%)	1	5
All	All	3740/5015 (75%)	2334 (62%)	884 (24%)	522 (14%)	1	5

All 11 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	36	CYS	85
1	A	29	LYS	85
1	A	20	ASP	85
1	A	24	PRO	85
1	A	53	GLN	62
1	A	22	GLY	61
1	A	15	ALA	21
1	A	14	PRO	20

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Mol	Chain	Res	Type	Models (Total)
1	A	25	HIS	9
1	A	52	LEU	8
1	A	35	GLY	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	39/51 (76%)	23±2 (60±4%)	16±2 (40±4%)	1 5
All	All	3315/4335 (76%)	1996 (60%)	1319 (40%)	1 5

All 23 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	25	HIS	85
1	A	31	CYS	85
1	A	45	VAL	85
1	A	16	LYS	85
1	A	13	VAL	85
1	A	42	ILE	85
1	A	36	CYS	85
1	A	21	CYS	85
1	A	53	GLN	84
1	A	34	ARG	78
1	A	29	LYS	71
1	A	17	ASP	70
1	A	11	CYS	66
1	A	41	ARG	54
1	A	10	GLN	49
1	A	32	ASN	47
1	A	23	TYR	24
1	A	52	LEU	24
1	A	30	GLU	23
1	A	20	ASP	14
1	A	18	ARG	13
1	A	50	LYS	12

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Mol	Chain	Res	Type	Models (Total)
1	A	27	THR	10

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 46% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5771

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	367
Number of shifts mapped to atoms	367
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	50	-0.17 ± 0.53	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 47%, i.e. 256 atoms were assigned a chemical shift out of a possible 540. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	115/208 (55%)	78/82 (95%)	0/88 (0%)	37/38 (97%)
Sidechain	127/286 (44%)	122/173 (71%)	0/97 (0%)	5/16 (31%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	14/46 (30%)	13/24 (54%)	0/19 (0%)	1/3 (33%)
Overall	256/540 (47%)	213/279 (76%)	0/204 (0%)	43/57 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 321 atoms were assigned a chemical shift out of a possible 702. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	153/283 (54%)	103/112 (92%)	0/118 (0%)	50/53 (94%)
Sidechain	152/356 (43%)	146/213 (69%)	0/126 (0%)	6/17 (35%)
Aromatic	16/63 (25%)	15/33 (45%)	0/27 (0%)	1/3 (33%)
Overall	321/702 (46%)	264/358 (74%)	0/271 (0%)	57/73 (78%)

7.1.4 Statistically unusual chemical shifts (i)

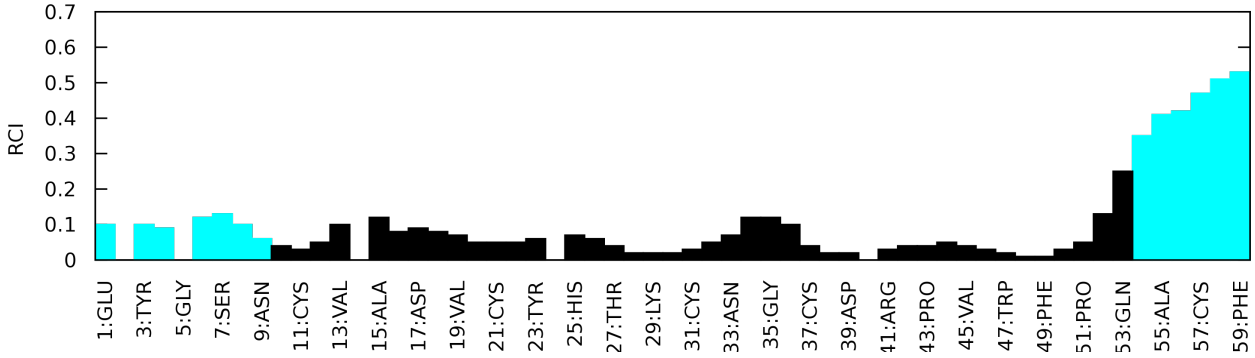
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	18	ARG	NE	107.70	92.63 – 76.73	14.5
1	A	18	ARG	HD3	1.82	4.36 – 1.86	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:


RCI
0.7
0.6
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0
1:GLU
3:TYR
5:GLY
7:SER
9:ASN
11:CYS
13:VAL
15:ALA
17:ASP
19:VAL
21:CYS
23:TYR
25:HIS
27:THR
29:LYS
31:CYS
33:ASN
35:GLY
37:CYS
39:ASP
41:ARG
43:PRO
45:VAL
47:TRP
49:PHE
51:PRO
53:GLN
55:ALA
57:CYS
59:PHE