



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:11 PM BST

PDB ID : 1BW5
Title : THE NMR SOLUTION STRUCTURE OF THE HOMEODOMAIN OF THE RAT INSULIN GENE ENHANCER PROTEIN ISL-1, 50 STRUCTURES
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Deposited on : 1998-09-29

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
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

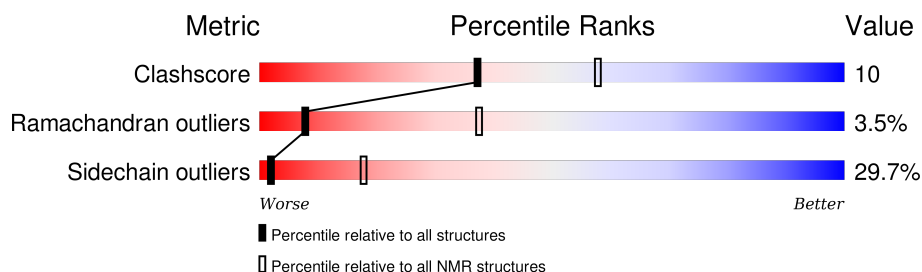
1 Overall quality at a glance

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	66	<div> <div></div> <div>32%</div> <div>29%</div> <div>6%</div> <div>33%</div> </div>

2 Ensemble composition and analysis

This entry contains 50 models. Model 32 is the overall representative, medoid model (most similar to other models). The authors have identified model 4 as representative.

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:12-A:55 (44)	0.34	32

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 9 clusters and 4 single-model clusters were found.

Cluster number	Models
1	3, 6, 9, 12, 16, 20, 23, 24, 29, 30, 32, 33, 34, 39, 40, 41, 42, 43, 44, 45, 46, 48
2	5, 22, 28, 36, 47
3	2, 10, 25, 35
4	7, 26, 31, 50
5	4, 14, 18
6	15, 19
7	13, 37
8	11, 38
9	17, 49
Single-model clusters	1; 8; 21; 27

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1136 atoms, of which 590 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INSULIN GENE ENHANCER PROTEIN ISL-1.

Mol	Chain	Residues	Atoms						Trace
1	A	66	Total	C	H	N	O	S	0
			1136	341	590	107	91	7	

There are 2 discrepancies between the modelled and reference sequences:

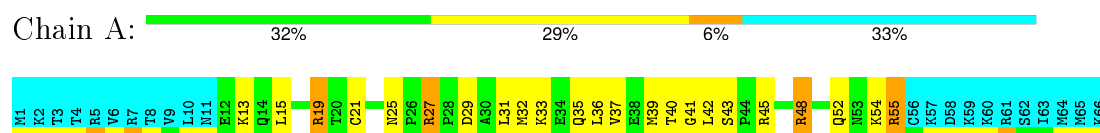
Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ARG	LYS	CONFLICT	UNP P50480
A	64	MET	LEU	CONFLICT	UNP P50480

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

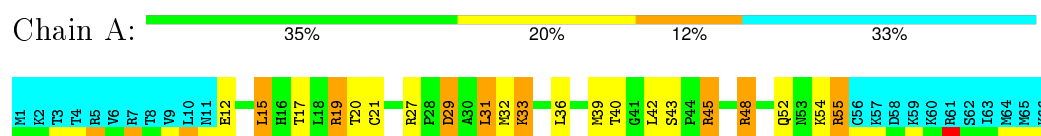


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

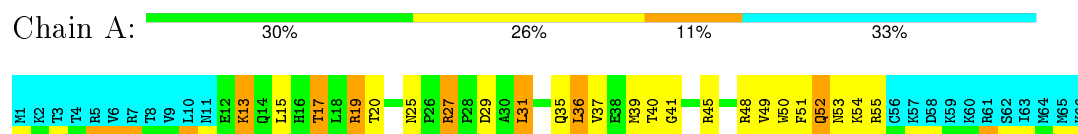
4.2.1 Score per residue for model 1

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



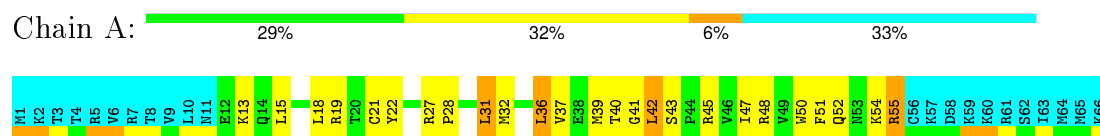
4.2.2 Score per residue for model 2

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



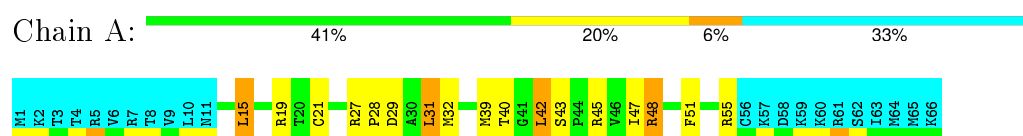
4.2.3 Score per residue for model 3

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



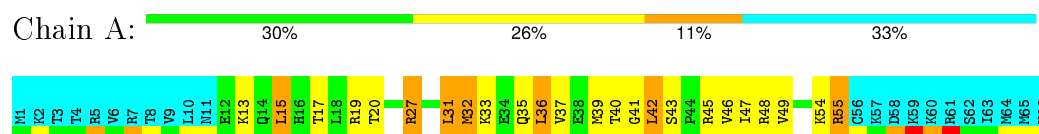
4.2.4 Score per residue for model 4

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



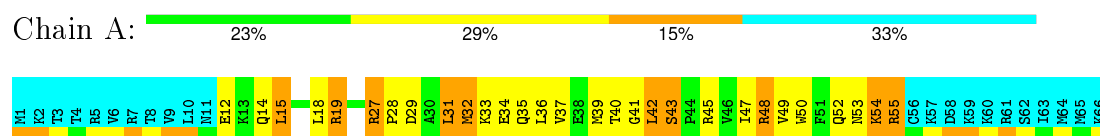
4.2.5 Score per residue for model 5

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



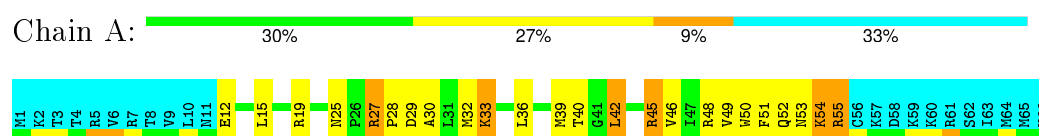
4.2.6 Score per residue for model 6

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



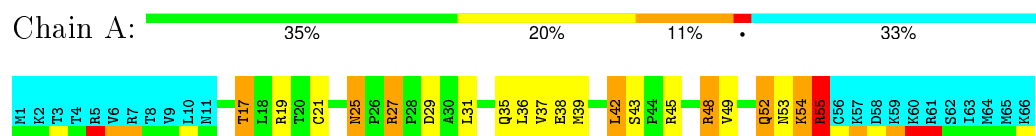
4.2.7 Score per residue for model 7

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



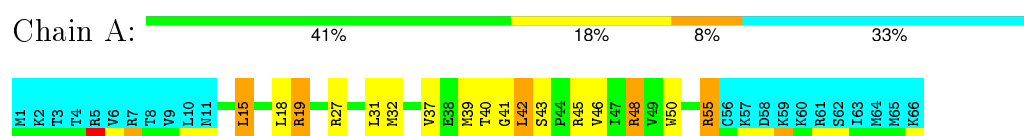
4.2.8 Score per residue for model 8

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



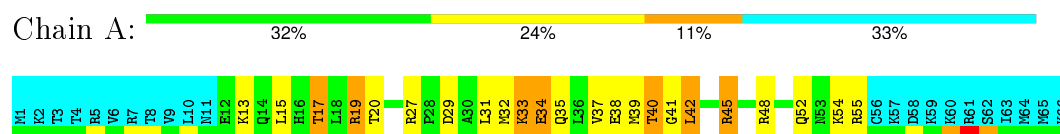
4.2.9 Score per residue for model 9

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



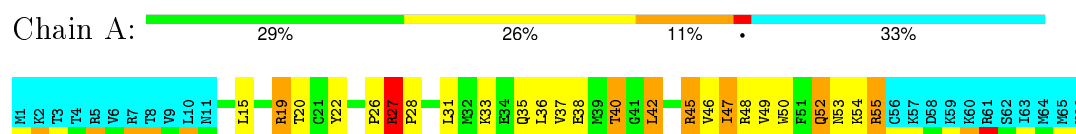
4.2.10 Score per residue for model 10

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



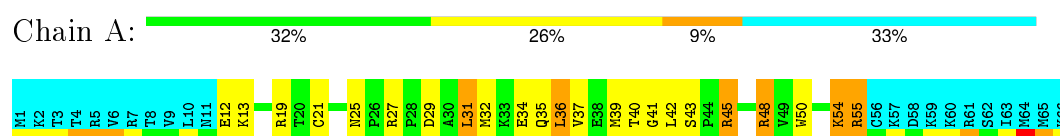
4.2.11 Score per residue for model 11

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



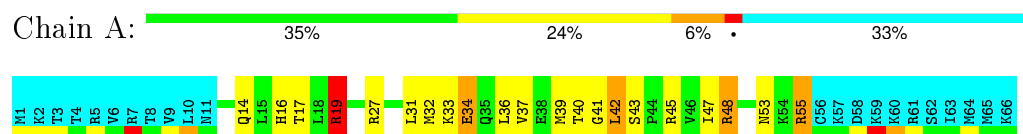
4.2.12 Score per residue for model 12

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



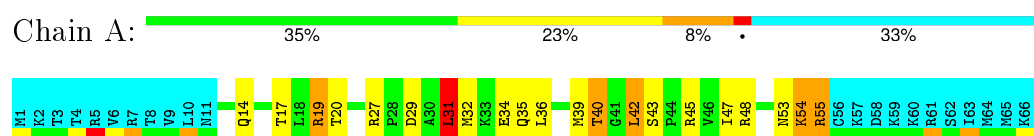
4.2.13 Score per residue for model 13

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



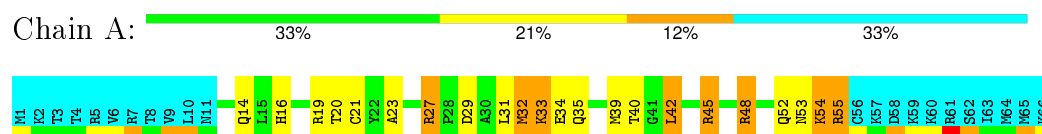
4.2.14 Score per residue for model 14

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



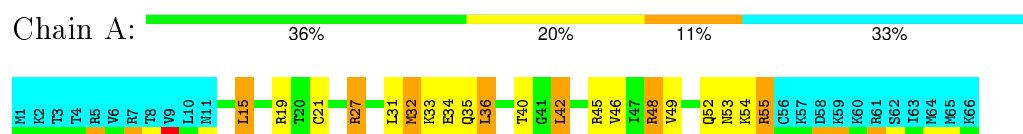
4.2.15 Score per residue for model 15

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



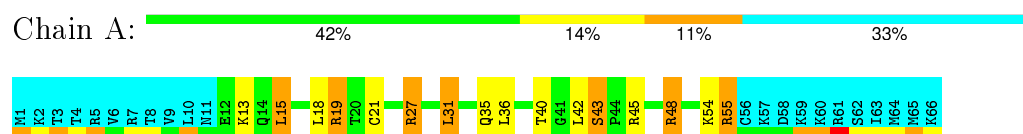
4.2.16 Score per residue for model 16

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



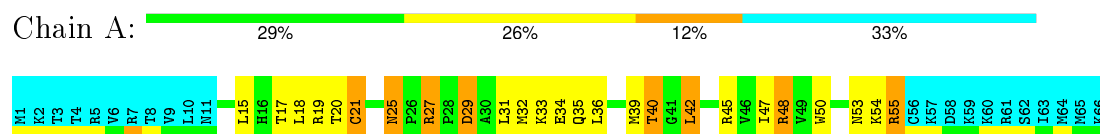
4.2.17 Score per residue for model 17

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



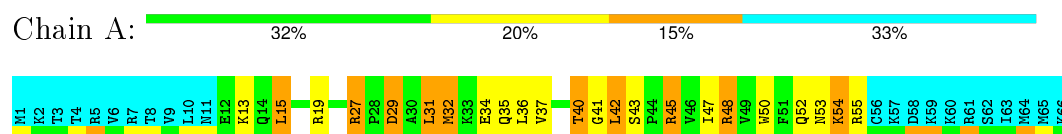
4.2.18 Score per residue for model 18

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



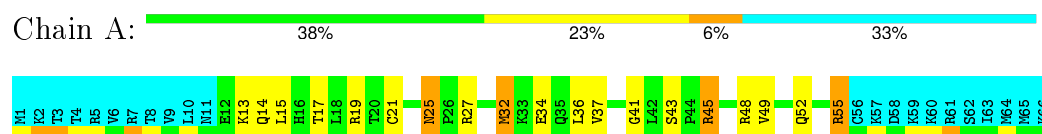
4.2.19 Score per residue for model 19

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



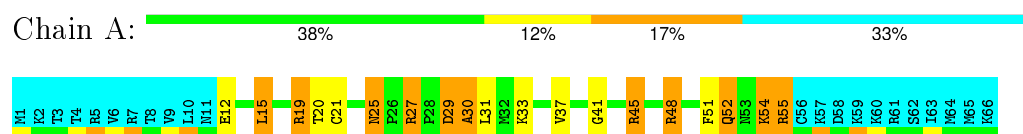
4.2.20 Score per residue for model 20

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



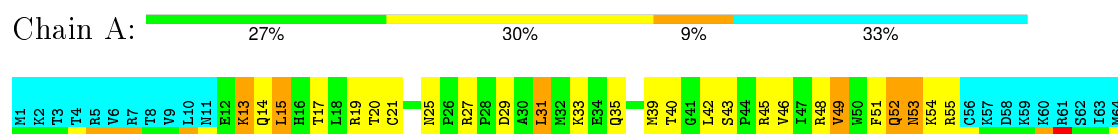
4.2.21 Score per residue for model 21

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



4.2.22 Score per residue for model 22

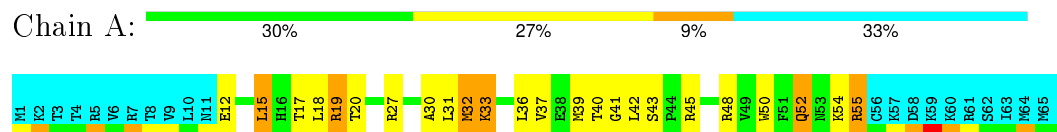
- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



M65
M66

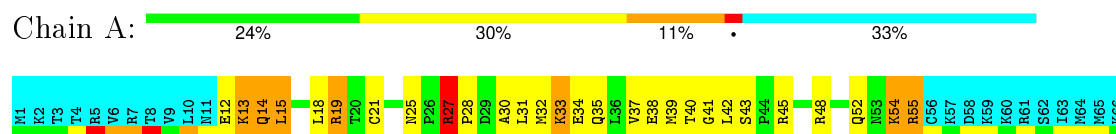
4.2.23 Score per residue for model 23

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



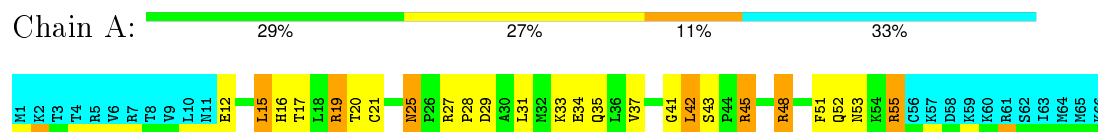
4.2.24 Score per residue for model 24

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



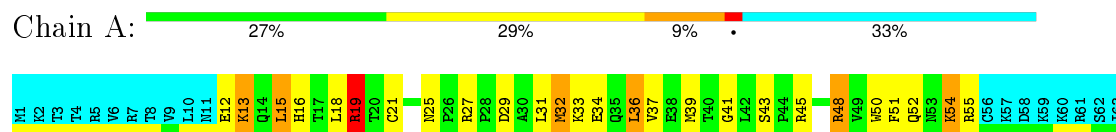
4.2.25 Score per residue for model 25

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



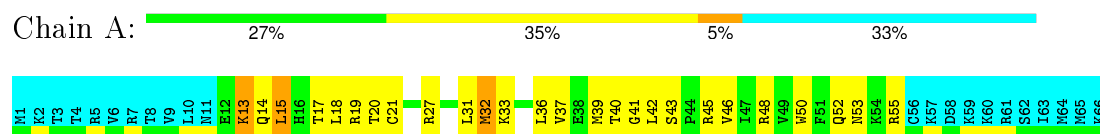
4.2.26 Score per residue for model 26

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

M64
M65
M66

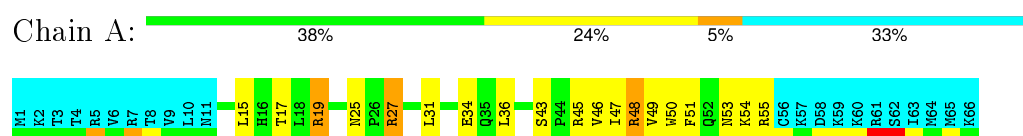
4.2.27 Score per residue for model 27

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



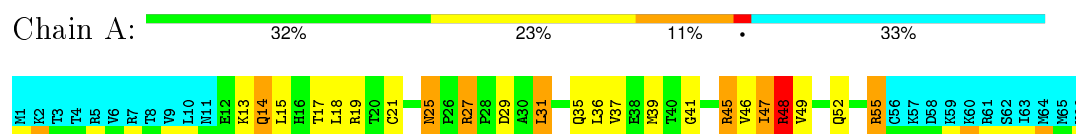
4.2.28 Score per residue for model 28

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



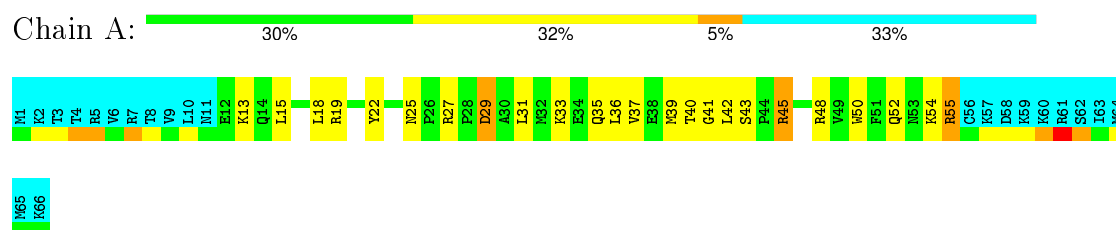
4.2.29 Score per residue for model 29

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



4.2.30 Score per residue for model 30

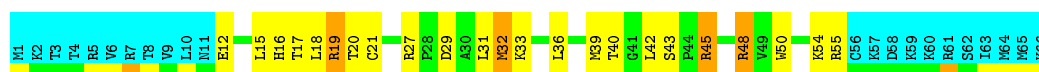
- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



4.2.31 Score per residue for model 31

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1





4.2.32 Score per residue for model 32 (medoid)

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 41% 20% 6% 33%



4.2.33 Score per residue for model 33

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

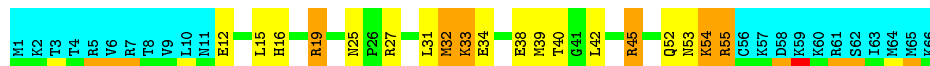
Chain A: 39% 18% 9% 33%



4.2.34 Score per residue for model 34

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 38% 20% 9% 33%



4.2.35 Score per residue for model 35

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 33% 29% 5% 33%



4.2.36 Score per residue for model 36

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

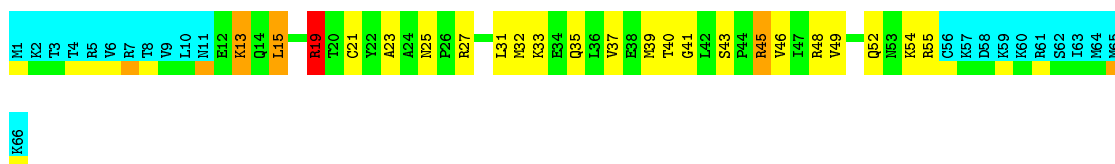
Chain A: 38% 17% 12% 33%



4.2.37 Score per residue for model 37

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

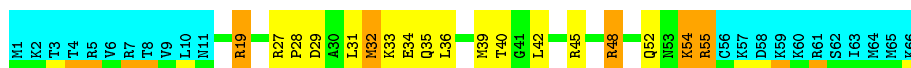
Chain A: 32% 29% 5% 33%



4.2.38 Score per residue for model 38

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 39% 20% 8% 33%



4.2.39 Score per residue for model 39

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 33% 21% 12% 33%



4.2.40 Score per residue for model 40

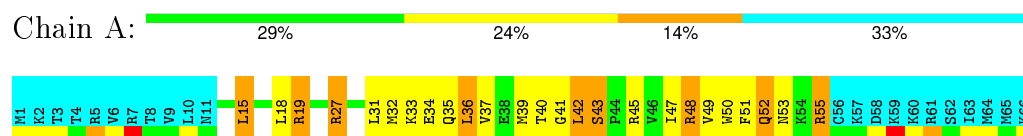
- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 41% 15% 11% 33%



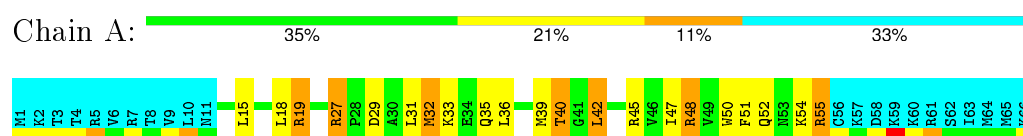
4.2.41 Score per residue for model 41

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



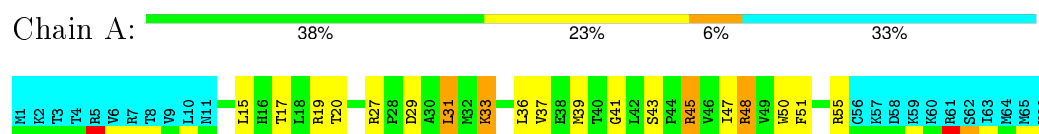
4.2.42 Score per residue for model 42

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



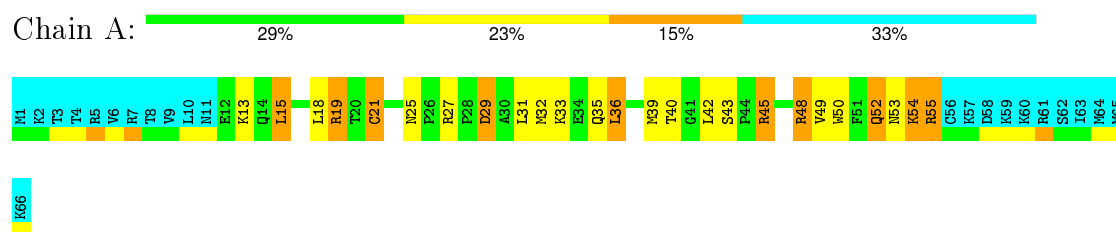
4.2.43 Score per residue for model 43

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



4.2.44 Score per residue for model 44

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1



4.2.45 Score per residue for model 45

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

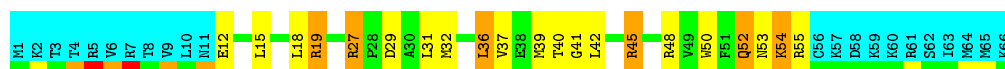




4.2.46 Score per residue for model 46

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

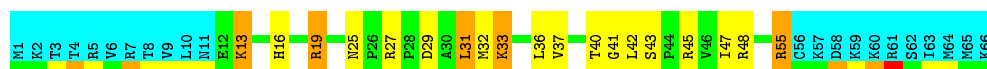
Chain A: 35% 23% 9% 33%



4.2.47 Score per residue for model 47

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 38% 21% 8% 33%



4.2.48 Score per residue for model 48

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 32% 29% 5% 33%



4.2.49 Score per residue for model 49

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

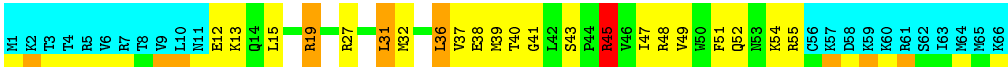
Chain A: 29% 27% 8% 33%



4.2.50 Score per residue for model 50

- Molecule 1: INSULIN GENE ENHANCER PROTEIN ISL-1

Chain A: 33% 27% 5% 33%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 50 calculated structures, 50 were deposited, based on the following criterion: *LOW RESTRAINT ENERGY*.

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

Software name	Classification	Version
XPLOR	refinement	3.851
BRUKER UXNMR	structure solution	UXNMR
XEASY	structure solution	
X-PLOR	structure solution	

No chemical shift data was provided. 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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.0±0.2
All	All	0	248

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	27	ARG	Sidechain	50
1	A	55	ARG	Sidechain	50
1	A	45	ARG	Sidechain	50
1	A	48	ARG	Sidechain	49
1	A	19	ARG	Sidechain	49

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	365	378	378	7±3
All	All	18250	18900	18900	368

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:THR:OG1	1:A:42:LEU:HD13	0.89	1.68	27	8
1:A:40:THR:OG1	1:A:42:LEU:HD22	0.85	1.71	10	5
1:A:17:THR:O	1:A:20:THR:HG22	0.82	1.75	31	9
1:A:42:LEU:O	1:A:42:LEU:HD23	0.81	1.76	11	5
1:A:42:LEU:HD21	1:A:47:ILE:HG12	0.78	1.53	5	8
1:A:32:MET:O	1:A:36:LEU:HD23	0.77	1.79	20	21
1:A:40:THR:CG2	1:A:42:LEU:HD22	0.76	2.10	41	6
1:A:42:LEU:HD23	1:A:42:LEU:O	0.74	1.80	42	11
1:A:42:LEU:HD23	1:A:42:LEU:C	0.73	2.03	11	10
1:A:40:THR:HG23	1:A:42:LEU:HG	0.73	1.60	49	1
1:A:27:ARG:N	1:A:28:PRO:CD	0.73	2.52	11	2
1:A:42:LEU:HD21	1:A:47:ILE:CG1	0.71	2.15	5	9
1:A:40:THR:HG23	1:A:42:LEU:HD22	0.71	1.63	41	5
1:A:18:LEU:HB3	1:A:50:TRP:CH2	0.68	2.24	40	13
1:A:45:ARG:O	1:A:49:VAL:HG12	0.65	1.92	50	3
1:A:40:THR:OG1	1:A:42:LEU:HD21	0.64	1.92	49	2
1:A:15:LEU:HD13	1:A:15:LEU:C	0.64	2.14	18	3
1:A:40:THR:HG23	1:A:42:LEU:HB3	0.63	1.70	39	1
1:A:51:PHE:O	1:A:53:ASN:N	0.62	2.30	22	1
1:A:42:LEU:HD12	1:A:43:SER:O	0.62	1.93	1	3
1:A:42:LEU:HD13	1:A:42:LEU:H	0.61	1.54	8	1
1:A:42:LEU:HD21	1:A:47:ILE:HD12	0.61	1.71	18	1
1:A:42:LEU:HD21	1:A:47:ILE:CD1	0.60	2.26	18	3
1:A:33:LYS:O	1:A:37:VAL:HG23	0.60	1.95	11	2
1:A:42:LEU:HD21	1:A:47:ILE:HD11	0.60	1.72	41	1
1:A:37:VAL:O	1:A:41:GLY:N	0.59	2.35	2	28
1:A:42:LEU:C	1:A:42:LEU:HD23	0.59	2.17	3	6
1:A:29:ASP:O	1:A:33:LYS:HB2	0.58	1.98	1	10
1:A:29:ASP:O	1:A:30:ALA:HB2	0.58	1.97	21	1
1:A:15:LEU:C	1:A:15:LEU:HD13	0.58	2.18	30	3
1:A:40:THR:O	1:A:42:LEU:HD13	0.57	1.99	47	7
1:A:26:PRO:O	1:A:27:ARG:CG	0.57	2.52	11	1
1:A:42:LEU:CD1	1:A:42:LEU:N	0.56	2.69	44	2
1:A:12:GLU:O	1:A:16:HIS:CD2	0.55	2.59	31	1
1:A:28:PRO:HG3	1:A:51:PHE:CZ	0.54	2.38	4	3
1:A:21:CYS:O	1:A:25:ASN:N	0.54	2.41	49	8
1:A:18:LEU:HB3	1:A:50:TRP:CZ2	0.53	2.38	40	2
1:A:50:TRP:O	1:A:54:LYS:HB2	0.52	2.05	12	1
1:A:42:LEU:HD12	1:A:42:LEU:N	0.52	2.19	22	2
1:A:53:ASN:OD1	1:A:54:LYS:N	0.52	2.43	19	5
1:A:42:LEU:CD2	1:A:42:LEU:C	0.51	2.71	11	1
1:A:17:THR:HG21	1:A:39:MET:O	0.51	2.05	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:O	1:A:40:THR:HG22	0.51	2.04	2	2
1:A:46:VAL:O	1:A:49:VAL:HG12	0.51	2.05	28	6
1:A:40:THR:OG1	1:A:42:LEU:CD2	0.51	2.58	17	2
1:A:27:ARG:CG	1:A:27:ARG:O	0.51	2.59	6	1
1:A:42:LEU:HD11	1:A:46:VAL:HB	0.50	1.83	7	1
1:A:36:LEU:HD12	1:A:47:ILE:HD12	0.50	1.83	41	2
1:A:54:LYS:HA	1:A:54:LYS:CE	0.50	2.37	26	1
1:A:30:ALA:O	1:A:33:LYS:HG3	0.50	2.07	7	1
1:A:15:LEU:O	1:A:15:LEU:HD13	0.50	2.07	30	2
1:A:40:THR:CG2	1:A:42:LEU:HG	0.49	2.37	49	1
1:A:42:LEU:C	1:A:42:LEU:CD2	0.49	2.80	8	4
1:A:32:MET:HB3	1:A:36:LEU:HD23	0.49	1.84	41	1
1:A:53:ASN:N	1:A:53:ASN:OD1	0.48	2.45	11	1
1:A:49:VAL:O	1:A:53:ASN:ND2	0.48	2.45	6	7
1:A:43:SER:OG	1:A:44:PRO:HD2	0.48	2.08	33	2
1:A:30:ALA:O	1:A:33:LYS:CG	0.48	2.61	7	1
1:A:50:TRP:O	1:A:53:ASN:ND2	0.48	2.47	41	1
1:A:40:THR:HG23	1:A:42:LEU:H	0.48	1.69	23	2
1:A:42:LEU:HG	1:A:43:SER:O	0.47	2.10	19	5
1:A:34:GLU:O	1:A:37:VAL:HB	0.47	2.09	13	1
1:A:18:LEU:CB	1:A:50:TRP:CZ2	0.47	2.97	40	4
1:A:21:CYS:SG	1:A:36:LEU:HD21	0.47	2.50	44	1
1:A:54:LYS:HA	1:A:54:LYS:HE3	0.47	1.86	34	2
1:A:43:SER:O	1:A:47:ILE:HG12	0.47	2.09	43	1
1:A:29:ASP:N	1:A:29:ASP:OD1	0.47	2.47	8	1
1:A:40:THR:OG1	1:A:42:LEU:HB3	0.47	2.09	19	2
1:A:42:LEU:HD23	1:A:46:VAL:HG11	0.47	1.85	27	1
1:A:17:THR:O	1:A:20:THR:OG1	0.47	2.32	5	3
1:A:22:TYR:CE1	1:A:54:LYS:HG2	0.47	2.45	3	1
1:A:46:VAL:HA	1:A:49:VAL:CG1	0.47	2.40	37	2
1:A:16:HIS:O	1:A:19:ARG:HB3	0.47	2.10	13	2
1:A:40:THR:O	1:A:42:LEU:CD1	0.46	2.63	47	2
1:A:15:LEU:C	1:A:15:LEU:CD1	0.46	2.83	30	1
1:A:29:ASP:O	1:A:30:ALA:CB	0.46	2.64	21	1
1:A:53:ASN:O	1:A:54:LYS:C	0.46	2.54	7	4
1:A:33:LYS:CD	1:A:34:GLU:N	0.46	2.78	10	1
1:A:50:TRP:HZ3	1:A:51:PHE:CZ	0.46	2.29	26	2
1:A:28:PRO:O	1:A:29:ASP:OD1	0.45	2.34	40	1
1:A:18:LEU:O	1:A:21:CYS:N	0.45	2.49	31	4
1:A:30:ALA:HA	1:A:33:LYS:HG2	0.45	1.88	24	2
1:A:36:LEU:HD12	1:A:47:ILE:CD1	0.45	2.42	41	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:HIS:O	1:A:19:ARG:HB2	0.45	2.12	31	1
1:A:51:PHE:O	1:A:54:LYS:CG	0.45	2.65	21	1
1:A:29:ASP:O	1:A:33:LYS:HB3	0.45	2.11	43	1
1:A:29:ASP:OD1	1:A:29:ASP:N	0.45	2.50	19	3
1:A:50:TRP:O	1:A:53:ASN:OD1	0.45	2.35	7	3
1:A:29:ASP:O	1:A:33:LYS:CG	0.44	2.66	10	1
1:A:36:LEU:O	1:A:40:THR:HG23	0.44	2.13	11	2
1:A:46:VAL:O	1:A:50:TRP:HB2	0.44	2.12	9	1
1:A:42:LEU:HG	1:A:43:SER:N	0.44	2.28	19	3
1:A:14:GLN:OE1	1:A:40:THR:HB	0.44	2.13	27	1
1:A:27:ARG:NE	1:A:27:ARG:O	0.44	2.51	11	1
1:A:32:MET:C	1:A:36:LEU:HD23	0.44	2.32	19	2
1:A:29:ASP:OD1	1:A:31:LEU:HB2	0.44	2.13	14	1
1:A:28:PRO:O	1:A:29:ASP:CG	0.43	2.56	39	7
1:A:15:LEU:CD1	1:A:15:LEU:C	0.43	2.86	23	2
1:A:50:TRP:O	1:A:54:LYS:CB	0.43	2.65	12	1
1:A:51:PHE:O	1:A:54:LYS:HB3	0.43	2.14	2	3
1:A:50:TRP:HE3	1:A:51:PHE:CD1	0.43	2.32	28	1
1:A:27:ARG:N	1:A:28:PRO:HD2	0.43	2.24	11	1
1:A:51:PHE:HA	1:A:54:LYS:HG2	0.43	1.89	21	1
1:A:26:PRO:C	1:A:28:PRO:HD3	0.43	2.34	11	1
1:A:15:LEU:HD13	1:A:15:LEU:O	0.43	2.13	35	2
1:A:42:LEU:HD11	1:A:46:VAL:CG1	0.43	2.43	9	1
1:A:20:THR:HG23	1:A:21:CYS:N	0.43	2.28	27	1
1:A:40:THR:CG2	1:A:42:LEU:HB3	0.42	2.41	39	1
1:A:37:VAL:HG13	1:A:42:LEU:O	0.42	2.14	8	1
1:A:51:PHE:O	1:A:54:LYS:HG3	0.42	2.12	21	1
1:A:15:LEU:O	1:A:19:ARG:HB2	0.42	2.15	48	1
1:A:43:SER:HB3	1:A:44:PRO:HD2	0.42	1.91	32	1
1:A:22:TYR:CD1	1:A:22:TYR:C	0.42	2.92	11	1
1:A:20:THR:CG2	1:A:21:CYS:N	0.42	2.82	21	2
1:A:52:GLN:O	1:A:53:ASN:HB2	0.42	2.14	22	1
1:A:50:TRP:HE3	1:A:51:PHE:CD2	0.42	2.33	2	3
1:A:51:PHE:O	1:A:54:LYS:HB2	0.42	2.14	42	1
1:A:33:LYS:CD	1:A:33:LYS:C	0.42	2.88	43	1
1:A:32:MET:HG3	1:A:36:LEU:HD23	0.42	1.91	38	1
1:A:27:ARG:O	1:A:27:ARG:CG	0.42	2.68	49	1
1:A:47:ILE:HG22	1:A:48:ARG:N	0.41	2.29	29	2
1:A:32:MET:O	1:A:33:LYS:C	0.41	2.57	15	2
1:A:42:LEU:C	1:A:42:LEU:HD12	0.41	2.36	1	1
1:A:19:ARG:O	1:A:23:ALA:CB	0.41	2.69	37	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LYS:C	1:A:33:LYS:CD	0.41	2.88	33	1
1:A:46:VAL:HA	1:A:49:VAL:HG12	0.41	1.93	37	1
1:A:18:LEU:O	1:A:19:ARG:C	0.40	2.60	31	1
1:A:14:GLN:O	1:A:15:LEU:C	0.40	2.59	24	1
1:A:51:PHE:O	1:A:52:GLN:C	0.40	2.60	40	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	44/66 (67%)	34±2 (78±5%)	8±2 (19±4%)	2±1 (4±2%)	8	37
All	All	2200/3300 (67%)	1707 (78%)	415 (19%)	78 (4%)	8	37

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	31	LEU	42
1	A	52	GLN	16
1	A	13	LYS	11
1	A	55	ARG	2
1	A	48	ARG	1
1	A	23	ALA	1
1	A	12	GLU	1
1	A	53	ASN	1
1	A	27	ARG	1
1	A	34	GLU	1
1	A	30	ALA	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	40/62 (65%)	28±3 (70±6%)	12±3 (30±6%)	2	18
All	All	2000/3100 (65%)	1406 (70%)	594 (30%)	2	18

All 31 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	39	MET	39
1	A	55	ARG	32
1	A	54	LYS	31
1	A	19	ARG	30
1	A	15	LEU	29
1	A	32	MET	29
1	A	52	GLN	28
1	A	48	ARG	28
1	A	35	GLN	26
1	A	43	SER	26
1	A	31	LEU	26
1	A	33	LYS	25
1	A	42	LEU	22
1	A	27	ARG	22
1	A	45	ARG	21
1	A	25	ASN	21
1	A	34	GLU	21
1	A	36	LEU	20
1	A	40	THR	17
1	A	13	LYS	16
1	A	29	ASP	16
1	A	12	GLU	15
1	A	21	CYS	12
1	A	17	THR	10
1	A	38	GLU	8
1	A	53	ASN	7
1	A	20	THR	5
1	A	16	HIS	4
1	A	47	ILE	4
1	A	14	GLN	3
1	A	49	VAL	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided