



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 09:55 pm BST

PDB ID : 2GO0  
Title : NMR solution structure of human pancreatitis-associated protein  
Authors : Chen, C.P.; Ho, M.R.; Lou, Y.C.  
Deposited on : 2006-04-12

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

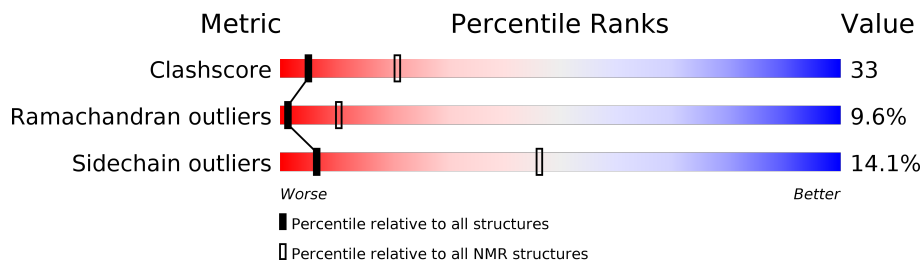
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 86%.

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  $\geq 3$ , 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	137	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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:6-A:55, A:62-A:69, A:82-A:85, A:89-A:96, A:107-A:135 (99)	0.14	11

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 4 clusters and 4 single-model clusters were found.

Cluster number	Models
1	1, 3, 4, 10, 11, 13, 14, 18
2	2, 7, 19
3	9, 15, 20
4	12, 16
Single-model clusters	5; 6; 8; 17

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2069 atoms, of which 1001 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Regenerating islet-derived protein 3 alpha.

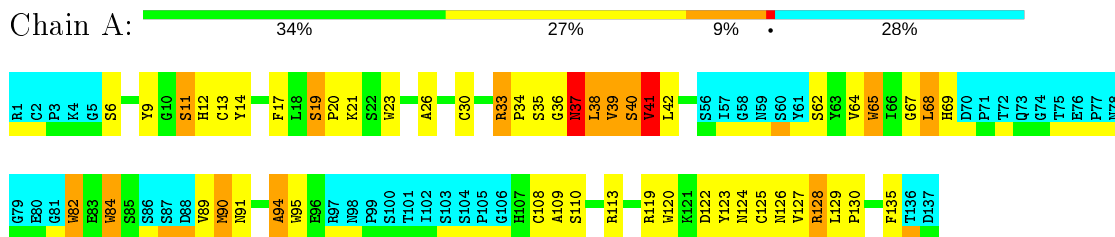
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	137	2069	674	1001	183	204	7	0

## 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: Regenerating islet-derived protein 3 alpha

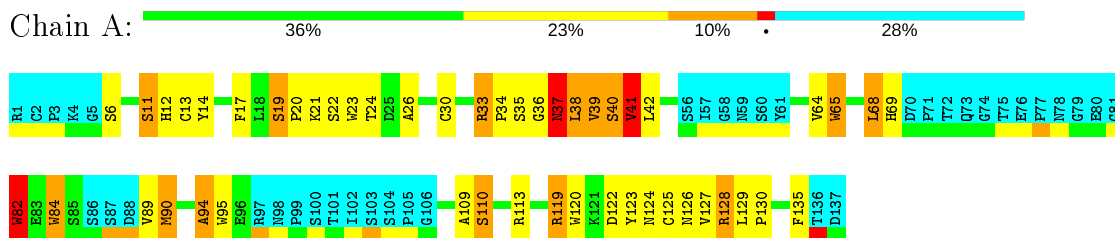


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

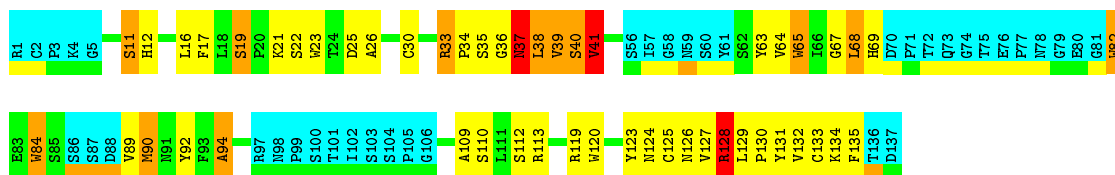
- Molecule 1: Regenerating islet-derived protein 3 alpha



#### 4.2.2 Score per residue for model 2

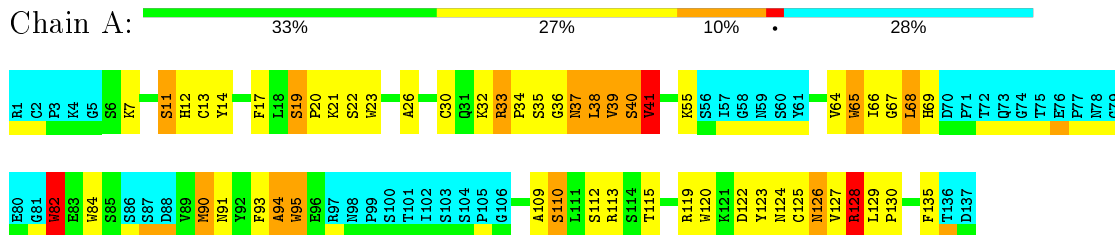
- Molecule 1: Regenerating islet-derived protein 3 alpha





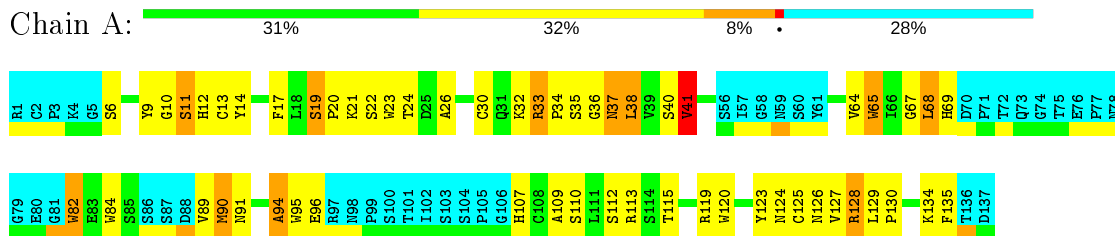
#### 4.2.3 Score per residue for model 3

- Molecule 1: Regenerating islet-derived protein 3 alpha



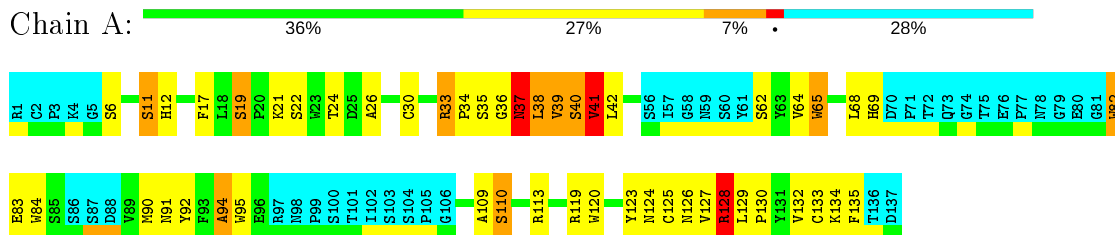
#### 4.2.4 Score per residue for model 4

- Molecule 1: Regenerating islet-derived protein 3 alpha



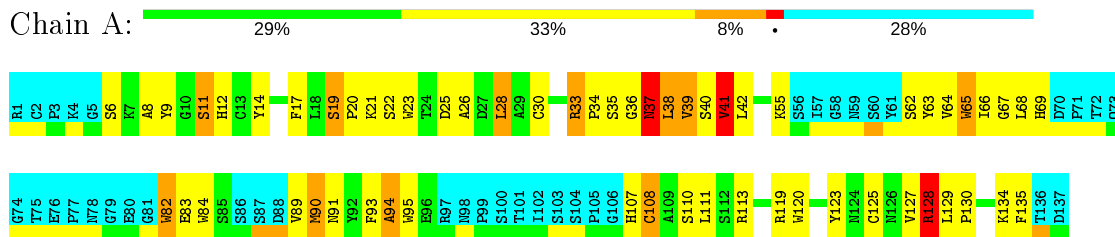
#### 4.2.5 Score per residue for model 5

- Molecule 1: Regenerating islet-derived protein 3 alpha



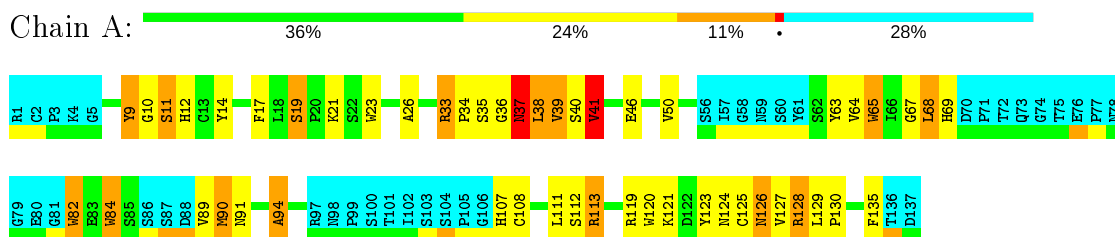
#### 4.2.6 Score per residue for model 6

- Molecule 1: Regenerating islet-derived protein 3 alpha



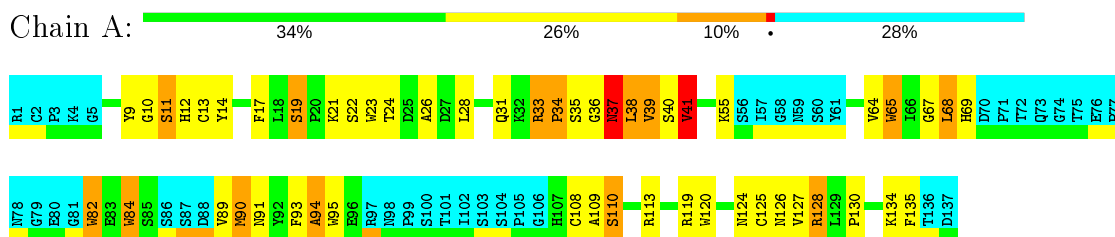
#### 4.2.7 Score per residue for model 7

- Molecule 1: Regenerating islet-derived protein 3 alpha



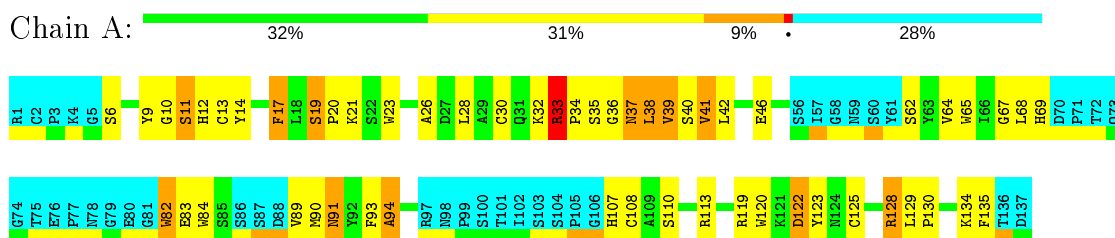
#### 4.2.8 Score per residue for model 8

- Molecule 1: Regenerating islet-derived protein 3 alpha



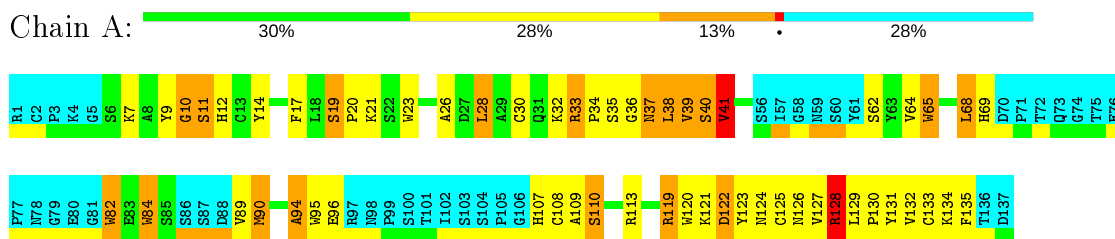
#### 4.2.9 Score per residue for model 9

- Molecule 1: Regenerating islet-derived protein 3 alpha



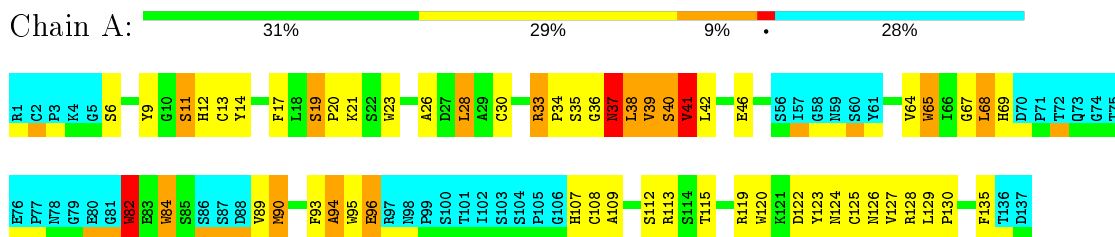
#### 4.2.10 Score per residue for model 10

- Molecule 1: Regenerating islet-derived protein 3 alpha



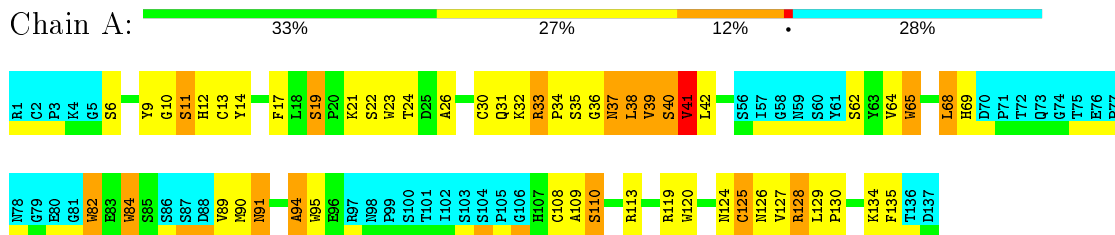
#### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Regenerating islet-derived protein 3 alpha



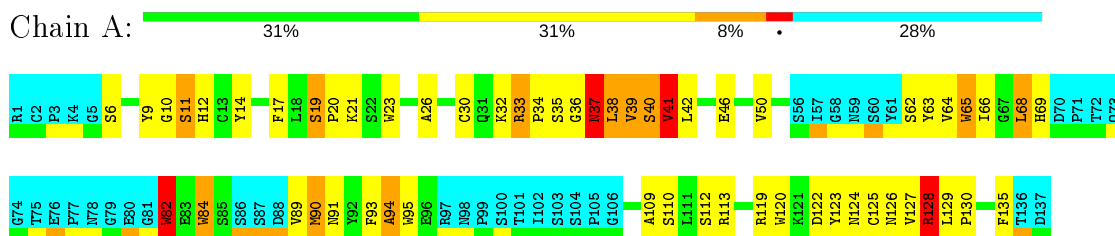
#### 4.2.12 Score per residue for model 12

- Molecule 1: Regenerating islet-derived protein 3 alpha



#### 4.2.13 Score per residue for model 13

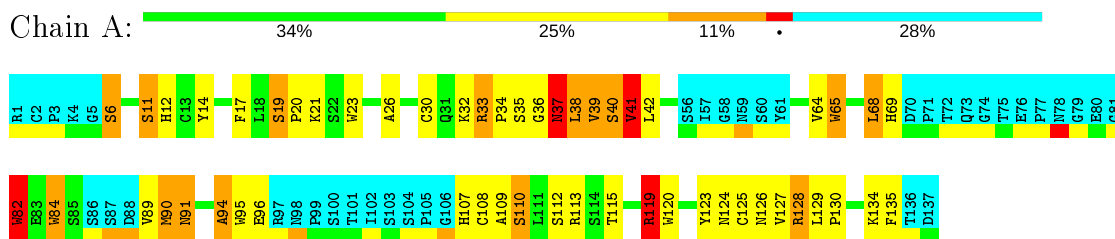
- Molecule 1: Regenerating islet-derived protein 3 alpha





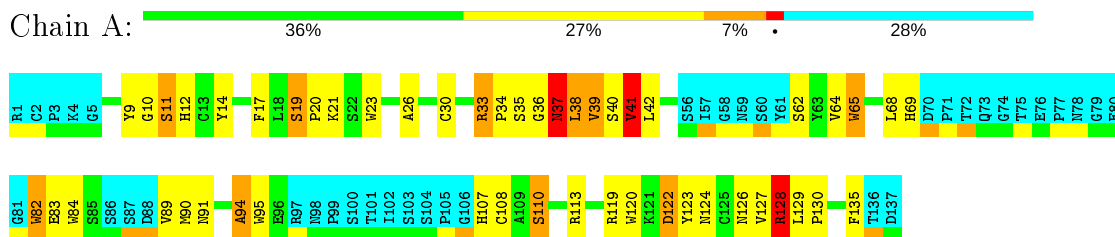
#### 4.2.14 Score per residue for model 14

- Molecule 1: Regenerating islet-derived protein 3 alpha



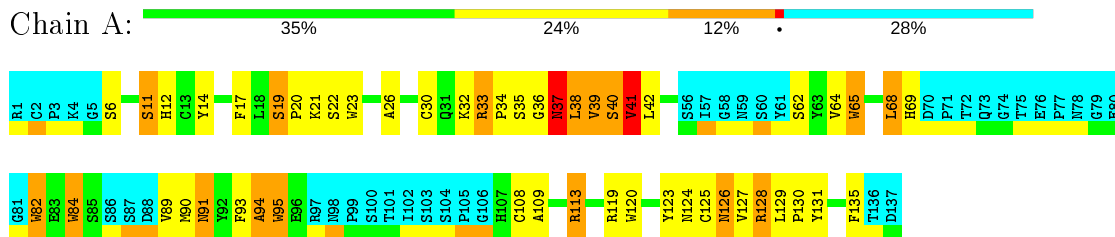
#### 4.2.15 Score per residue for model 15

- Molecule 1: Regenerating islet-derived protein 3 alpha



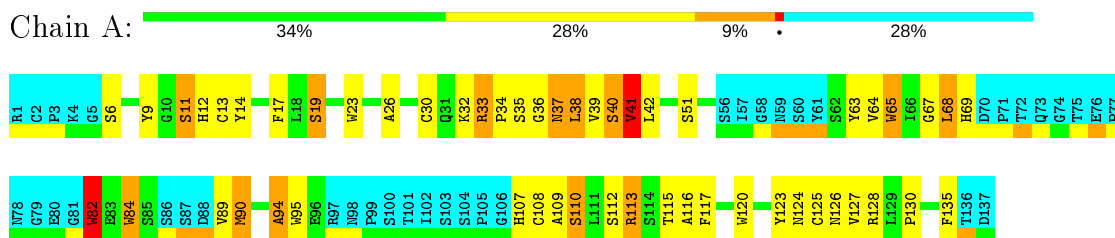
#### 4.2.16 Score per residue for model 16

- Molecule 1: Regenerating islet-derived protein 3 alpha



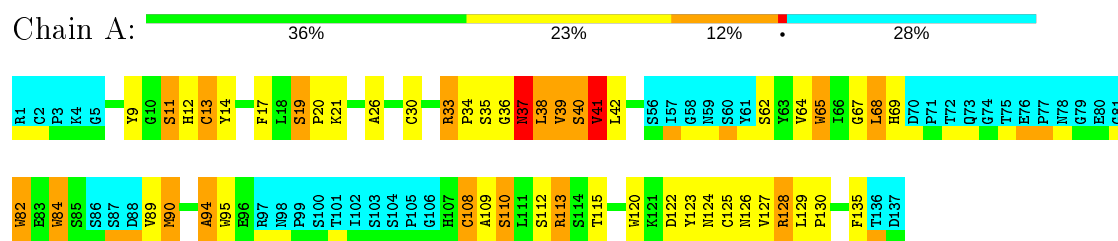
#### 4.2.17 Score per residue for model 17

- Molecule 1: Regenerating islet-derived protein 3 alpha



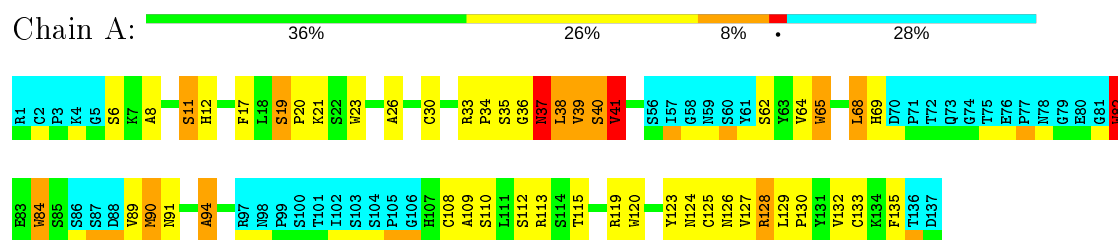
### 4.2.18 Score per residue for model 18

- Molecule 1: Regenerating islet-derived protein 3 alpha



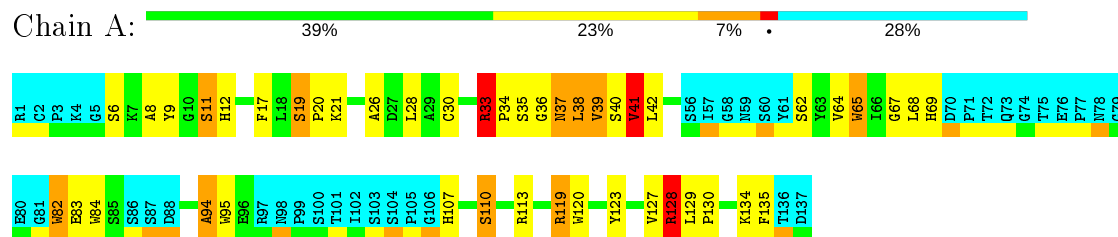
### 4.2.19 Score per residue for model 19

- Molecule 1: Regenerating islet-derived protein 3 alpha



### 4.2.20 Score per residue for model 20

- Molecule 1: Regenerating islet-derived protein 3 alpha



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
X-PLOR	structure solution	2.9.4a
X-PLOR	refinement	2.9.4a

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1549
Number of shifts mapped to atoms	1549
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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	3.6±0.7
All	All	0	72

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	113	ARG	Sidechain	19
1	A	128	ARG	Sidechain	18
1	A	33	ARG	Sidechain	18
1	A	119	ARG	Sidechain	17

### 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	798	759	759	51±6
All	All	15960	15180	15180	1015

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ALA:HB3	1:A:120:TRP:CZ2	0.79	2.13	4	20
1:A:94:ALA:HB3	1:A:120:TRP:CH2	0.79	2.13	16	17
1:A:30:CYS:SG	1:A:37:ASN:N	0.73	2.61	1	15
1:A:108:CYS:SG	1:A:125:CYS:N	0.72	2.61	18	2
1:A:89:VAL:HG22	1:A:90:MET:H	0.70	1.47	15	2
1:A:68:LEU:HD23	1:A:84:TRP:CE3	0.70	2.22	10	15
1:A:82:TRP:CD1	1:A:82:TRP:N	0.70	2.58	11	9
1:A:46:GLU:O	1:A:50:VAL:HG23	0.68	1.88	13	2
1:A:82:TRP:N	1:A:82:TRP:CD1	0.68	2.62	3	8
1:A:89:VAL:HG22	1:A:90:MET:N	0.66	2.05	15	11
1:A:33:ARG:O	1:A:35:SER:N	0.65	2.30	8	20
1:A:95:TRP:N	1:A:95:TRP:CD1	0.64	2.64	3	1
1:A:89:VAL:HG12	1:A:90:MET:H	0.64	1.52	12	2
1:A:95:TRP:CH2	1:A:109:ALA:HB2	0.63	2.28	8	2
1:A:89:VAL:HG12	1:A:90:MET:N	0.63	2.08	14	3
1:A:37:ASN:O	1:A:38:LEU:C	0.63	2.37	3	20
1:A:68:LEU:HD13	1:A:69:HIS:N	0.62	2.09	10	15
1:A:33:ARG:NH1	1:A:135:PHE:CE2	0.62	2.67	4	2
1:A:32:LYS:NZ	1:A:33:ARG:HH11	0.62	1.93	10	1
1:A:12:HIS:CE1	1:A:134:LYS:NZ	0.62	2.68	12	1
1:A:30:CYS:SG	1:A:37:ASN:C	0.61	2.79	6	15
1:A:41:VAL:O	1:A:84:TRP:CZ3	0.61	2.54	19	13
1:A:68:LEU:CD2	1:A:84:TRP:CE3	0.60	2.84	1	15
1:A:84:TRP:NE1	1:A:89:VAL:O	0.60	2.34	16	13
1:A:12:HIS:CG	1:A:134:LYS:NZ	0.60	2.69	12	1
1:A:64:VAL:HG13	1:A:130:PRO:O	0.60	1.96	8	20
1:A:41:VAL:O	1:A:84:TRP:CH2	0.60	2.55	2	15
1:A:135:PHE:O	1:A:135:PHE:CD2	0.59	2.55	3	6
1:A:82:TRP:CE2	1:A:90:MET:SD	0.59	2.95	12	2
1:A:42:LEU:HD21	1:A:84:TRP:NE1	0.59	2.12	9	6
1:A:82:TRP:CD2	1:A:90:MET:SD	0.59	2.95	14	3
1:A:135:PHE:CD2	1:A:135:PHE:O	0.59	2.56	1	5
1:A:26:ALA:CB	1:A:38:LEU:HD21	0.59	2.27	8	20
1:A:9:TYR:O	1:A:11:SER:N	0.59	2.36	8	12
1:A:30:CYS:SG	1:A:37:ASN:CA	0.59	2.90	17	15
1:A:94:ALA:N	1:A:120:TRP:CZ3	0.59	2.70	14	18
1:A:82:TRP:CZ3	1:A:95:TRP:NE1	0.59	2.70	20	3
1:A:82:TRP:CE3	1:A:90:MET:SD	0.59	2.96	4	6
1:A:84:TRP:N	1:A:84:TRP:CD1	0.59	2.71	8	2
1:A:96:GLU:CB	1:A:119:ARG:HE	0.59	2.09	14	1
1:A:36:GLY:O	1:A:37:ASN:ND2	0.58	2.36	10	7
1:A:82:TRP:CZ3	1:A:90:MET:SD	0.58	2.96	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:CD2	1:A:84:TRP:CD2	0.58	2.87	3	2
1:A:124:ASN:H	1:A:124:ASN:HD22	0.58	1.40	8	1
1:A:23:TRP:CG	1:A:108:CYS:SG	0.58	2.97	9	9
1:A:116:ALA:C	1:A:117:PHE:CG	0.58	2.78	17	1
1:A:12:HIS:CD2	1:A:134:LYS:NZ	0.57	2.72	12	2
1:A:84:TRP:CD1	1:A:84:TRP:N	0.57	2.73	7	4
1:A:135:PHE:CD1	1:A:135:PHE:O	0.57	2.57	13	5
1:A:116:ALA:O	1:A:117:PHE:CG	0.57	2.57	17	1
1:A:112:SER:CB	1:A:119:ARG:NH1	0.57	2.68	14	1
1:A:124:ASN:O	1:A:126:ASN:N	0.57	2.38	3	17
1:A:22:SER:OG	1:A:24:THR:HG22	0.57	2.00	4	5
1:A:63:TYR:CZ	1:A:112:SER:OG	0.57	2.58	17	4
1:A:68:LEU:CD1	1:A:69:HIS:N	0.56	2.69	4	15
1:A:68:LEU:HD22	1:A:84:TRP:CZ3	0.56	2.35	6	4
1:A:135:PHE:O	1:A:135:PHE:CD1	0.56	2.59	12	3
1:A:89:VAL:O	1:A:91:ASN:N	0.55	2.40	6	3
1:A:32:LYS:HZ2	1:A:33:ARG:HH11	0.55	1.43	10	1
1:A:82:TRP:CE3	1:A:95:TRP:CD1	0.55	2.94	15	1
1:A:12:HIS:CG	1:A:134:LYS:HZ3	0.55	2.20	12	1
1:A:17:PHE:C	1:A:19:SER:H	0.54	2.06	19	20
1:A:37:ASN:O	1:A:38:LEU:O	0.54	2.24	14	20
1:A:82:TRP:CZ2	1:A:90:MET:SD	0.54	3.01	12	1
1:A:108:CYS:SG	1:A:123:TYR:O	0.54	2.66	18	2
1:A:11:SER:O	1:A:12:HIS:CG	0.54	2.61	9	4
1:A:68:LEU:HB3	1:A:109:ALA:HB3	0.54	1.79	3	14
1:A:13:CYS:O	1:A:135:PHE:CE1	0.54	2.60	8	1
1:A:122:ASP:O	1:A:123:TYR:CD2	0.53	2.61	18	4
1:A:122:ASP:O	1:A:123:TYR:CD1	0.53	2.62	1	3
1:A:65:TRP:NE1	1:A:127:VAL:O	0.53	2.38	8	19
1:A:116:ALA:C	1:A:117:PHE:CD1	0.53	2.82	17	1
1:A:37:ASN:OD1	1:A:37:ASN:N	0.53	2.42	2	3
1:A:23:TRP:NE1	1:A:66:ILE:O	0.53	2.41	6	2
1:A:9:TYR:CD1	1:A:46:GLU:OE1	0.53	2.62	11	2
1:A:22:SER:O	1:A:25:ASP:N	0.52	2.42	6	1
1:A:9:TYR:CG	1:A:46:GLU:OE1	0.52	2.63	11	1
1:A:62:SER:O	1:A:63:TYR:CD1	0.52	2.63	6	1
1:A:11:SER:OG	1:A:12:HIS:CD2	0.52	2.63	7	1
1:A:40:SER:C	1:A:41:VAL:HG22	0.51	2.25	11	13
1:A:62:SER:OG	1:A:113:ARG:NE	0.51	2.42	16	1
1:A:36:GLY:O	1:A:37:ASN:OD1	0.51	2.28	13	10
1:A:132:VAL:O	1:A:133:CYS:SG	0.51	2.69	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:TRP:O	1:A:90:MET:CG	0.51	2.58	15	3
1:A:11:SER:C	1:A:12:HIS:CD2	0.51	2.84	19	16
1:A:42:LEU:HD22	1:A:91:ASN:CB	0.51	2.36	12	5
1:A:89:VAL:CG2	1:A:90:MET:N	0.51	2.74	15	4
1:A:82:TRP:O	1:A:90:MET:SD	0.51	2.69	16	2
1:A:90:MET:SD	1:A:90:MET:O	0.51	2.69	5	3
1:A:40:SER:OG	1:A:134:LYS:NZ	0.51	2.41	6	1
1:A:32:LYS:NZ	1:A:33:ARG:NH1	0.51	2.58	10	1
1:A:82:TRP:CZ3	1:A:95:TRP:CD1	0.50	2.99	6	2
1:A:26:ALA:HB1	1:A:38:LEU:HD21	0.50	1.84	8	1
1:A:93:PHE:CD1	1:A:93:PHE:O	0.50	2.64	6	1
1:A:68:LEU:HD23	1:A:84:TRP:CZ3	0.50	2.41	4	2
1:A:89:VAL:CG2	1:A:90:MET:H	0.50	2.19	15	1
1:A:90:MET:SD	1:A:92:TYR:O	0.50	2.69	5	2
1:A:84:TRP:HE1	1:A:89:VAL:C	0.49	2.10	7	11
1:A:23:TRP:CD2	1:A:108:CYS:SG	0.49	3.05	9	9
1:A:12:HIS:CD2	1:A:134:LYS:HZ3	0.49	2.25	12	1
1:A:107:HIS:CD2	1:A:107:HIS:N	0.49	2.80	4	2
1:A:126:ASN:HD22	1:A:126:ASN:N	0.49	2.05	16	1
1:A:64:VAL:O	1:A:110:SER:CB	0.49	2.61	17	2
1:A:23:TRP:O	1:A:23:TRP:CE3	0.49	2.66	4	6
1:A:21:LYS:N	1:A:128:ARG:HB3	0.49	2.23	14	7
1:A:39:VAL:HG22	1:A:40:SER:N	0.49	2.23	7	2
1:A:28:LEU:O	1:A:28:LEU:HD13	0.49	2.08	11	1
1:A:107:HIS:C	1:A:108:CYS:SG	0.49	2.91	6	1
1:A:116:ALA:O	1:A:117:PHE:CD2	0.49	2.65	17	1
1:A:31:GLN:C	1:A:33:ARG:N	0.48	2.66	8	1
1:A:42:LEU:HD22	1:A:91:ASN:HB2	0.48	1.83	14	4
1:A:89:VAL:CG1	1:A:90:MET:N	0.48	2.75	14	2
1:A:96:GLU:CB	1:A:119:ARG:NE	0.48	2.76	14	1
1:A:65:TRP:CZ3	1:A:110:SER:OG	0.48	2.62	10	9
1:A:68:LEU:HD13	1:A:69:HIS:H	0.48	1.67	7	7
1:A:26:ALA:HB3	1:A:38:LEU:HD21	0.48	1.86	12	19
1:A:39:VAL:CG2	1:A:40:SER:N	0.48	2.76	7	2
1:A:36:GLY:C	1:A:37:ASN:CG	0.48	2.72	2	3
1:A:28:LEU:HD23	1:A:28:LEU:O	0.48	2.09	9	2
1:A:120:TRP:CD1	1:A:120:TRP:N	0.47	2.82	3	1
1:A:68:LEU:HD23	1:A:84:TRP:CD2	0.47	2.44	3	1
1:A:6:SER:CB	1:A:14:TYR:O	0.47	2.63	14	1
1:A:90:MET:SD	1:A:90:MET:C	0.47	2.93	10	1
1:A:126:ASN:N	1:A:126:ASN:HD22	0.47	2.08	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:PHE:C	1:A:19:SER:N	0.47	2.68	19	14
1:A:31:GLN:O	1:A:31:GLN:NE2	0.47	2.48	12	1
1:A:93:PHE:N	1:A:93:PHE:CD1	0.47	2.83	3	1
1:A:40:SER:OG	1:A:41:VAL:N	0.46	2.49	19	4
1:A:13:CYS:O	1:A:135:PHE:CD1	0.46	2.68	8	3
1:A:122:ASP:N	1:A:122:ASP:OD1	0.46	2.48	9	2
1:A:96:GLU:OE2	1:A:121:LYS:NZ	0.46	2.43	10	1
1:A:36:GLY:O	1:A:37:ASN:CB	0.46	2.62	9	19
1:A:20:PRO:O	1:A:21:LYS:CG	0.46	2.64	20	13
1:A:68:LEU:CD1	1:A:83:GLU:C	0.46	2.84	6	5
1:A:93:PHE:CD1	1:A:93:PHE:N	0.46	2.82	9	4
1:A:28:LEU:O	1:A:28:LEU:HD23	0.46	2.10	10	2
1:A:124:ASN:C	1:A:126:ASN:N	0.46	2.69	3	15
1:A:23:TRP:CE3	1:A:23:TRP:O	0.46	2.69	2	1
1:A:38:LEU:O	1:A:39:VAL:C	0.46	2.54	20	18
1:A:31:GLN:O	1:A:33:ARG:N	0.46	2.49	8	1
1:A:33:ARG:N	1:A:33:ARG:NE	0.46	2.64	9	1
1:A:30:CYS:O	1:A:36:GLY:C	0.46	2.54	2	5
1:A:112:SER:OG	1:A:115:THR:OG1	0.46	2.34	4	5
1:A:55:LYS:O	1:A:55:LYS:CG	0.46	2.64	3	2
1:A:82:TRP:CE2	1:A:95:TRP:CH2	0.46	3.04	3	1
1:A:124:ASN:HD22	1:A:126:ASN:H	0.46	1.54	17	1
1:A:23:TRP:CD2	1:A:23:TRP:O	0.46	2.69	2	6
1:A:38:LEU:O	1:A:39:VAL:O	0.46	2.34	7	4
1:A:126:ASN:O	1:A:126:ASN:ND2	0.45	2.45	3	1
1:A:63:TYR:HA	1:A:111:LEU:O	0.45	2.11	7	1
1:A:11:SER:O	1:A:12:HIS:CD2	0.45	2.69	9	1
1:A:112:SER:CB	1:A:119:ARG:HH11	0.45	2.24	14	1
1:A:67:GLY:O	1:A:84:TRP:HA	0.45	2.12	3	3
1:A:23:TRP:O	1:A:23:TRP:CD2	0.45	2.69	14	7
1:A:39:VAL:CG1	1:A:66:ILE:HG22	0.45	2.42	13	1
1:A:33:ARG:CA	1:A:33:ARG:NE	0.45	2.79	9	1
1:A:21:LYS:N	1:A:128:ARG:HB2	0.45	2.26	3	11
1:A:40:SER:C	1:A:41:VAL:CG2	0.45	2.85	16	17
1:A:124:ASN:C	1:A:126:ASN:H	0.45	2.15	7	15
1:A:41:VAL:O	1:A:84:TRP:CZ2	0.45	2.70	5	3
1:A:32:LYS:C	1:A:33:ARG:HE	0.45	2.16	9	1
1:A:68:LEU:CD1	1:A:68:LEU:C	0.45	2.85	4	5
1:A:69:HIS:CD2	1:A:83:GLU:O	0.45	2.70	6	4
1:A:68:LEU:HD11	1:A:83:GLU:N	0.45	2.27	6	5
1:A:10:GLY:O	1:A:11:SER:OG	0.44	2.33	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LEU:HD13	1:A:28:LEU:O	0.44	2.13	6	1
1:A:90:MET:C	1:A:90:MET:SD	0.44	2.95	2	1
1:A:112:SER:OG	1:A:119:ARG:NH1	0.44	2.51	14	1
1:A:32:LYS:CG	1:A:32:LYS:O	0.44	2.65	3	3
1:A:96:GLU:OE1	1:A:96:GLU:O	0.44	2.36	11	1
1:A:12:HIS:ND1	1:A:134:LYS:NZ	0.44	2.66	12	1
1:A:115:THR:OG1	1:A:119:ARG:CG	0.44	2.66	14	1
1:A:22:SER:OG	1:A:25:ASP:CG	0.43	2.57	2	1
1:A:14:TYR:N	1:A:14:TYR:CD1	0.43	2.86	17	11
1:A:82:TRP:CD2	1:A:95:TRP:NE1	0.43	2.86	15	1
1:A:82:TRP:CE3	1:A:95:TRP:NE1	0.43	2.87	15	1
1:A:22:SER:OG	1:A:126:ASN:O	0.43	2.36	3	2
1:A:21:LYS:O	1:A:22:SER:C	0.43	2.54	8	1
1:A:11:SER:O	1:A:11:SER:OG	0.43	2.36	3	2
1:A:33:ARG:HE	1:A:33:ARG:N	0.43	2.12	9	1
1:A:20:PRO:O	1:A:21:LYS:HG2	0.43	2.13	19	1
1:A:132:VAL:HG12	1:A:133:CYS:N	0.43	2.29	5	2
1:A:40:SER:HG	1:A:134:LYS:HD3	0.43	1.74	12	1
1:A:63:TYR:CD2	1:A:111:LEU:O	0.43	2.71	6	1
1:A:14:TYR:CD1	1:A:14:TYR:N	0.43	2.87	6	5
1:A:107:HIS:O	1:A:125:CYS:SG	0.43	2.77	9	1
1:A:36:GLY:CA	1:A:134:LYS:O	0.42	2.67	8	3
1:A:11:SER:OG	1:A:11:SER:O	0.42	2.34	15	1
1:A:22:SER:OG	1:A:25:ASP:OD1	0.42	2.36	2	1
1:A:16:LEU:HD12	1:A:131:TYR:O	0.42	2.14	2	1
1:A:9:TYR:CD1	1:A:46:GLU:CD	0.42	2.93	9	1
1:A:38:LEU:HB3	1:A:67:GLY:N	0.42	2.30	9	9
1:A:68:LEU:HD22	1:A:84:TRP:HA	0.42	1.91	10	2
1:A:124:ASN:N	1:A:124:ASN:ND2	0.42	2.67	8	1
1:A:96:GLU:OE1	1:A:115:THR:HG21	0.42	2.14	4	1
1:A:68:LEU:C	1:A:68:LEU:CD1	0.42	2.88	12	2
1:A:65:TRP:CD1	1:A:129:LEU:HB2	0.42	2.50	6	1
1:A:11:SER:C	1:A:12:HIS:CG	0.42	2.93	9	3
1:A:32:LYS:O	1:A:32:LYS:CG	0.41	2.66	16	3
1:A:84:TRP:HE1	1:A:90:MET:HA	0.41	1.76	2	1
1:A:126:ASN:N	1:A:126:ASN:ND2	0.41	2.68	14	1
1:A:115:THR:O	1:A:116:ALA:HB3	0.41	2.16	17	1
1:A:34:PRO:O	1:A:35:SER:CB	0.41	2.68	8	1
1:A:36:GLY:HA2	1:A:134:LYS:O	0.41	2.15	8	2
1:A:94:ALA:HB3	1:A:120:TRP:CE2	0.41	2.48	4	1
1:A:131:TYR:N	1:A:131:TYR:CD1	0.41	2.89	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ALA:HB3	1:A:120:TRP:CZ3	0.41	2.51	15	1
1:A:62:SER:OG	1:A:113:ARG:NH2	0.41	2.54	16	1
1:A:32:LYS:NZ	1:A:33:ARG:NH2	0.41	2.69	17	1
1:A:135:PHE:O	1:A:135:PHE:CG	0.40	2.74	9	2
1:A:12:HIS:CE1	1:A:134:LYS:HZ2	0.40	2.35	12	1
1:A:22:SER:OG	1:A:125:CYS:O	0.40	2.38	12	1
1:A:55:LYS:CG	1:A:55:LYS:O	0.40	2.69	6	1
1:A:42:LEU:HD22	1:A:91:ASN:HB3	0.40	1.93	13	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	99/137 (72%)	84±1 (85±1%)	6±1 (6±1%)	10±1 (10±1%)	1	10
All	All	1980/2740 (72%)	1674 (85%)	115 (6%)	191 (10%)	1	10

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	11	SER	20
1	A	34	PRO	20
1	A	94	ALA	20
1	A	38	LEU	20
1	A	41	VAL	20
1	A	37	ASN	20
1	A	39	VAL	19
1	A	90	MET	15
1	A	82	TRP	15
1	A	125	CYS	15
1	A	10	GLY	7

### 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	86/118 (73%)	74±2 (86±2%)	12±2 (14±2%)	<b>6</b> 46
All	All	1720/2360 (73%)	1478 (86%)	242 (14%)	<b>6</b> 46

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	19	SER	20
1	A	65	TRP	20
1	A	41	VAL	19
1	A	129	LEU	17
1	A	110	SER	17
1	A	40	SER	15
1	A	68	LEU	15
1	A	37	ASN	13
1	A	84	TRP	13
1	A	82	TRP	12
1	A	128	ARG	10
1	A	123	TYR	10
1	A	91	ASN	9
1	A	62	SER	9
1	A	13	CYS	7
1	A	119	ARG	5
1	A	113	ARG	4
1	A	33	ARG	3
1	A	28	LEU	3
1	A	95	TRP	3
1	A	122	ASP	3
1	A	126	ASN	3
1	A	6	SER	2
1	A	108	CYS	2
1	A	7	LYS	2
1	A	121	LYS	1
1	A	51	SER	1
1	A	96	GLU	1
1	A	93	PHE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	17	PHE	1
1	A	9	TYR	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 87% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping [i](#)

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	1549
Number of shifts mapped to atoms	1549
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
<sup>13</sup> C <sub>α</sub>	137	1.08 $\pm$ 0.09	Should be applied
<sup>13</sup> C <sub>β</sub>	126	1.42 $\pm$ 0.17	Should be applied
<sup>13</sup> C'	137	0.23 $\pm$ 0.13	None needed (< 0.5 ppm)
<sup>15</sup> N	129	1.08 $\pm$ 0.23	Should be applied

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 86%, i.e. 1055 atoms were assigned a chemical shift out of a possible 1222. 4 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	489/489 (100%)	195/195 (100%)	198/198 (100%)	96/96 (100%)
Sidechain	476/547 (87%)	295/326 (90%)	177/198 (89%)	4/23 (17%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	90/186 (48%)	48/97 (49%)	36/80 (45%)	6/9 (67%)
Overall	1055/1222 (86%)	538/618 (87%)	411/476 (86%)	106/128 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1416 atoms were assigned a chemical shift out of a possible 1622. 4 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	669/669 (100%)	266/266 (100%)	274/274 (100%)	129/129 (100%)
Sidechain	649/759 (86%)	407/454 (90%)	234/271 (86%)	8/34 (24%)
Aromatic	98/194 (51%)	52/101 (51%)	40/84 (48%)	6/9 (67%)
Overall	1416/1622 (87%)	725/821 (88%)	548/629 (87%)	143/172 (83%)

#### 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	94	ALA	H	3.53	11.19 – 5.19	-7.8
1	A	129	LEU	HD23	-1.03	2.14 – -0.66	-6.3
1	A	129	LEU	HD22	-1.03	2.14 – -0.66	-6.3
1	A	129	LEU	HD21	-1.03	2.14 – -0.66	-6.3
1	A	9	TYR	HB2	0.91	4.76 – 1.06	-5.4
1	A	94	ALA	HB2	0.03	2.61 – 0.11	-5.3
1	A	94	ALA	HB3	0.03	2.61 – 0.11	-5.3
1	A	94	ALA	HB1	0.03	2.61 – 0.11	-5.3
1	A	17	PHE	HB2	1.05	4.85 – 1.15	-5.3
1	A	41	VAL	H	4.72	11.69 – 4.89	-5.2
1	A	27	ASP	HB3	1.22	4.07 – 1.27	-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:

