Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2GLG
Title	:	NMR structure of the [L23,A24]-sCT mutant
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Deposited on	:	2006-04-04

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

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

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

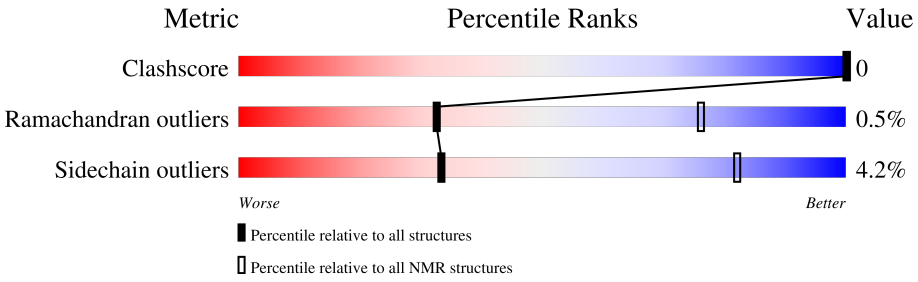
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	33	79% · 18%

2 Ensemble composition and analysis (i)

This entry contains 100 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 55 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 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:4-A:30 (27)	0.37	55

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 10 clusters and 4 single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 6, 7, 10, 11, 13, 14, 15, 16, 21, 22, 25, 28, 32, 33, 35, 36, 38, 39, 42, 45, 46, 49, 52, 53, 55, 56, 58, 59, 60, 63, 64, 67, 81, 85, 86, 87, 96, 98, 99
2	19, 24, 26, 27, 34, 40, 41, 43, 44, 57, 61, 62, 65, 66, 68, 69, 70
3	18, 20, 47, 48, 50, 51, 54, 76, 88, 94, 95
4	23, 30, 71, 72, 73, 74, 75, 77
5	17, 91, 92, 93
6	8, 9, 12
7	1, 90, 100
8	78, 79, 80
9	29, 31
10	89, 97
Single-model clusters	37; 82; 83; 84

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 471 atoms, of which 237 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calcitonin-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	33	471	143	237	41	48	2	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	PRO	engineered mutation	UNP P01263
A	24	ALA	ARG	engineered mutation	UNP P01263

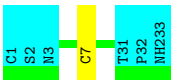
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Calcitonin-1

Chain A: 



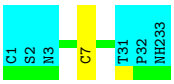
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Calcitonin-1

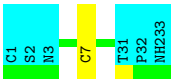
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: Calcitonin-1

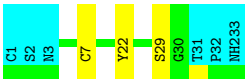
Chain A: 



4.2.3 Score per residue for model 3

• Molecule 1: Calcitonin-1

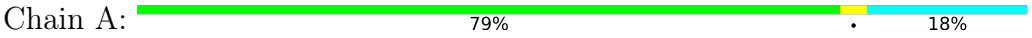
Chain A:

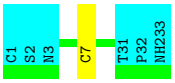


4.2.4 Score per residue for model 4

• Molecule 1: Calcitonin-1

Chain A:

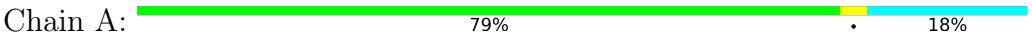


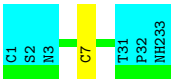


4.2.5 Score per residue for model 5

• Molecule 1: Calcitonin-1

Chain A:

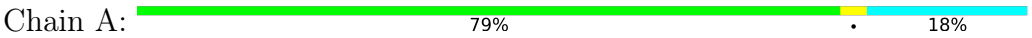


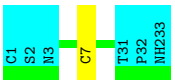


4.2.6 Score per residue for model 6

• Molecule 1: Calcitonin-1

Chain A:

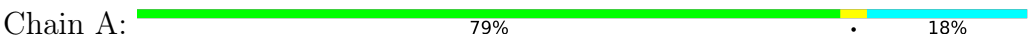


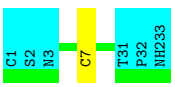


4.2.7 Score per residue for model 7

• Molecule 1: Calcitonin-1

Chain A:

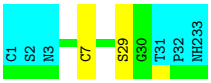




4.2.8 Score per residue for model 8

• Molecule 1: Calcitonin-1

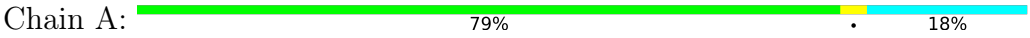
Chain A:

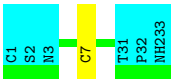


4.2.9 Score per residue for model 9

• Molecule 1: Calcitonin-1

Chain A:

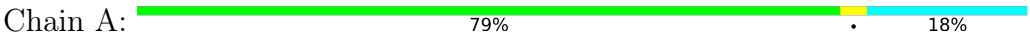


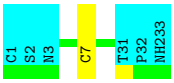


4.2.10 Score per residue for model 10

• Molecule 1: Calcitonin-1

Chain A:

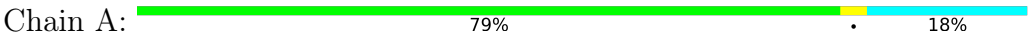


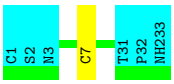


4.2.11 Score per residue for model 11

• Molecule 1: Calcitonin-1

Chain A:

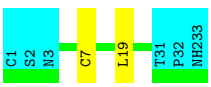




4.2.12 Score per residue for model 12

• Molecule 1: Calcitonin-1

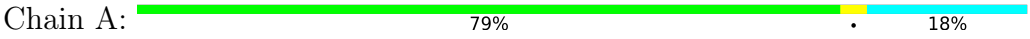
Chain A:

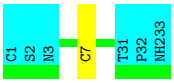


4.2.13 Score per residue for model 13

• Molecule 1: Calcitonin-1

Chain A:

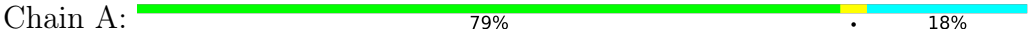


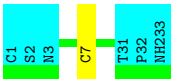


4.2.14 Score per residue for model 14

• Molecule 1: Calcitonin-1

Chain A:





4.2.15 Score per residue for model 15

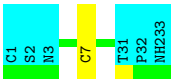
• Molecule 1: Calcitonin-1

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: Calcitonin-1

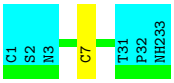
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Calcitonin-1

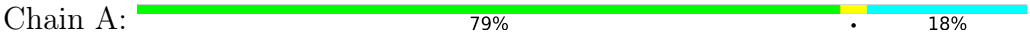
Chain A:

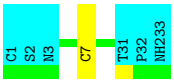


4.2.18 Score per residue for model 18

• Molecule 1: Calcitonin-1

Chain A:

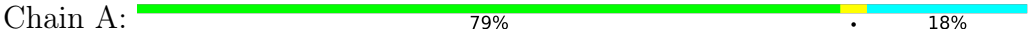


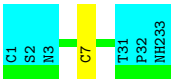


4.2.19 Score per residue for model 19

• Molecule 1: Calcitonin-1

Chain A:





4.2.20 Score per residue for model 20

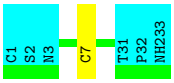
• Molecule 1: Calcitonin-1

Chain A:

4.2.21 Score per residue for model 21

• Molecule 1: Calcitonin-1

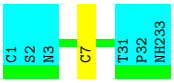
Chain A:



4.2.22 Score per residue for model 22

• Molecule 1: Calcitonin-1

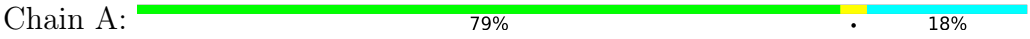
Chain A:

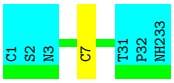


4.2.23 Score per residue for model 23

• Molecule 1: Calcitonin-1

Chain A:





4.2.24 Score per residue for model 24

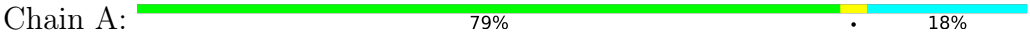
• Molecule 1: Calcitonin-1

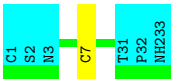
Chain A:

4.2.25 Score per residue for model 25

• Molecule 1: Calcitonin-1

Chain A:

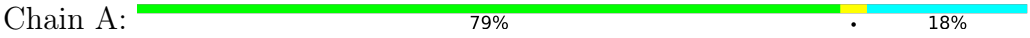


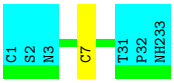


4.2.26 Score per residue for model 26

• Molecule 1: Calcitonin-1

Chain A:

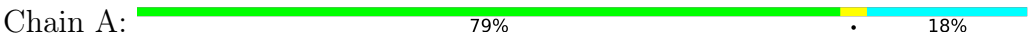


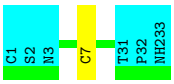


4.2.27 Score per residue for model 27

• Molecule 1: Calcitonin-1

Chain A:

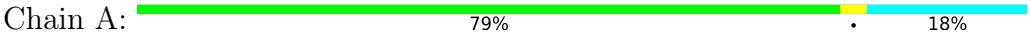


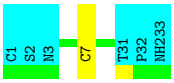


4.2.28 Score per residue for model 28

• Molecule 1: Calcitonin-1

Chain A:





4.2.29 Score per residue for model 29

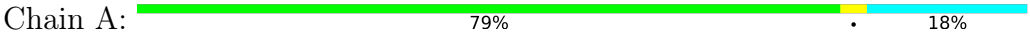
• Molecule 1: Calcitonin-1

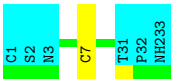
Chain A:

4.2.30 Score per residue for model 30

• Molecule 1: Calcitonin-1

Chain A:





4.2.31 Score per residue for model 31

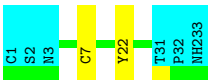
• Molecule 1: Calcitonin-1

Chain A:

4.2.32 Score per residue for model 32

• Molecule 1: Calcitonin-1

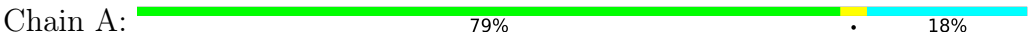
Chain A:

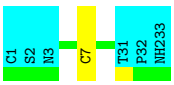


4.2.33 Score per residue for model 33

• Molecule 1: Calcitonin-1

Chain A:

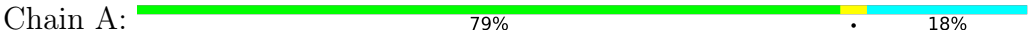


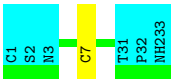


4.2.34 Score per residue for model 34

• Molecule 1: Calcitonin-1

Chain A:

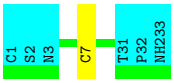




4.2.35 Score per residue for model 35

• Molecule 1: Calcitonin-1

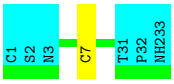
Chain A:



4.2.36 Score per residue for model 36

• Molecule 1: Calcitonin-1

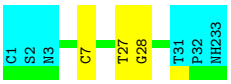
Chain A:



4.2.37 Score per residue for model 37

• Molecule 1: Calcitonin-1

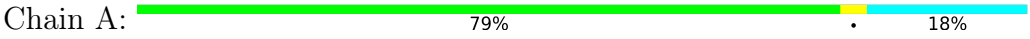
Chain A:

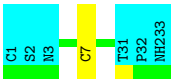


4.2.38 Score per residue for model 38

• Molecule 1: Calcitonin-1

Chain A:

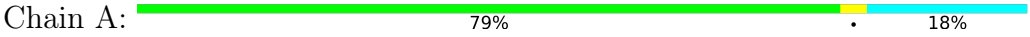


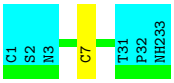


4.2.39 Score per residue for model 39

• Molecule 1: Calcitonin-1

Chain A:

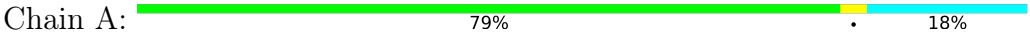


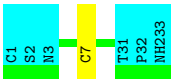


4.2.40 Score per residue for model 40

• Molecule 1: Calcitonin-1

Chain A:

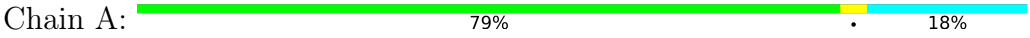


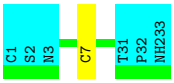


4.2.41 Score per residue for model 41

• Molecule 1: Calcitonin-1

Chain A:

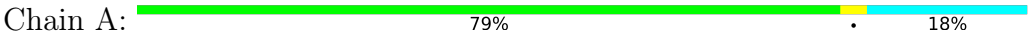


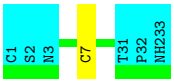


4.2.42 Score per residue for model 42

• Molecule 1: Calcitonin-1

Chain A:

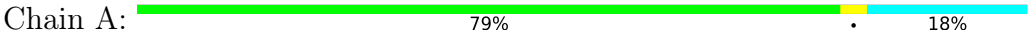


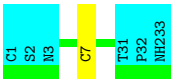


4.2.43 Score per residue for model 43

• Molecule 1: Calcitonin-1

Chain A:

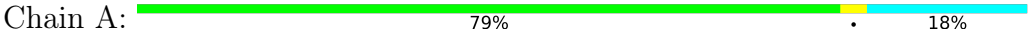


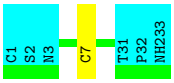


4.2.44 Score per residue for model 44

• Molecule 1: Calcitonin-1

Chain A:

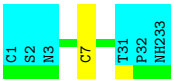




4.2.45 Score per residue for model 45

• Molecule 1: Calcitonin-1

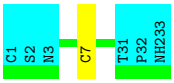
Chain A:



4.2.46 Score per residue for model 46

• Molecule 1: Calcitonin-1

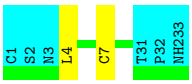
Chain A:



4.2.47 Score per residue for model 47

• Molecule 1: Calcitonin-1

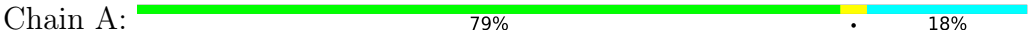
Chain A:

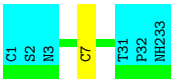


4.2.48 Score per residue for model 48

• Molecule 1: Calcitonin-1

Chain A:

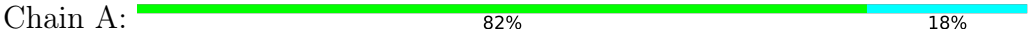


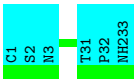


4.2.49 Score per residue for model 49

• Molecule 1: Calcitonin-1

Chain A:





4.2.50 Score per residue for model 50

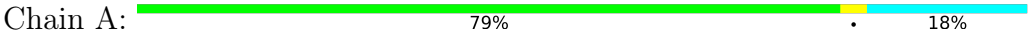
• Molecule 1: Calcitonin-1

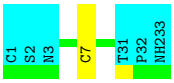
Chain A:

4.2.51 Score per residue for model 51

• Molecule 1: Calcitonin-1

Chain A:

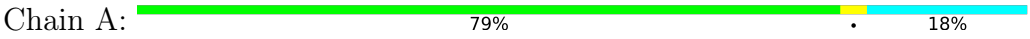


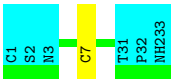


4.2.52 Score per residue for model 52

• Molecule 1: Calcitonin-1

Chain A:

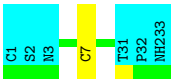




4.2.53 Score per residue for model 53

• Molecule 1: Calcitonin-1

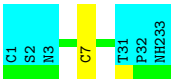
Chain A: 



4.2.54 Score per residue for model 54

• Molecule 1: Calcitonin-1

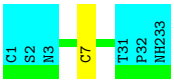
Chain A: 



4.2.55 Score per residue for model 55 (medoid)

• Molecule 1: Calcitonin-1

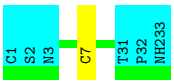
Chain A: 



4.2.56 Score per residue for model 56

• Molecule 1: Calcitonin-1

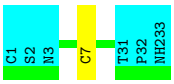
Chain A: 



4.2.57 Score per residue for model 57

• Molecule 1: Calcitonin-1

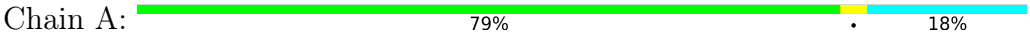
Chain A: 

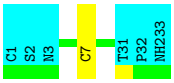


4.2.58 Score per residue for model 58

• Molecule 1: Calcitonin-1

Chain A:

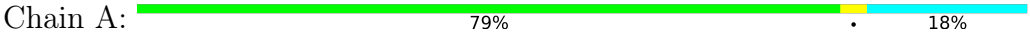


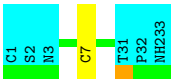


4.2.59 Score per residue for model 59

• Molecule 1: Calcitonin-1

Chain A:

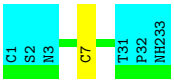




4.2.60 Score per residue for model 60

• Molecule 1: Calcitonin-1

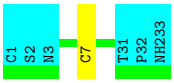
Chain A:



4.2.61 Score per residue for model 61

• Molecule 1: Calcitonin-1

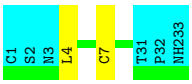
Chain A:



4.2.62 Score per residue for model 62

• Molecule 1: Calcitonin-1

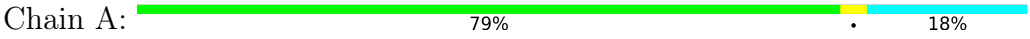
Chain A:

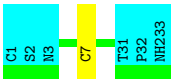


4.2.63 Score per residue for model 63

• Molecule 1: Calcitonin-1

Chain A:





4.2.64 Score per residue for model 64

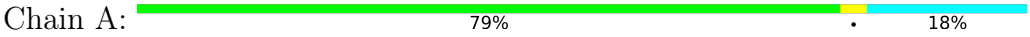
• Molecule 1: Calcitonin-1

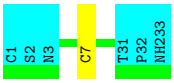
Chain A:

4.2.65 Score per residue for model 65

• Molecule 1: Calcitonin-1

Chain A:

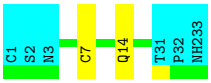




4.2.66 Score per residue for model 66

• Molecule 1: Calcitonin-1

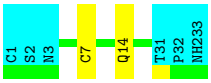
Chain A:



4.2.67 Score per residue for model 67

• Molecule 1: Calcitonin-1

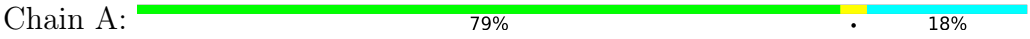
Chain A:

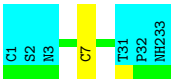


4.2.68 Score per residue for model 68

• Molecule 1: Calcitonin-1

Chain A:

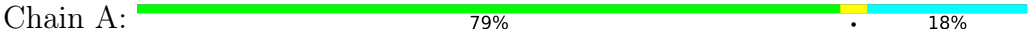


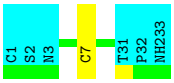


4.2.69 Score per residue for model 69

• Molecule 1: Calcitonin-1

Chain A:





4.2.70 Score per residue for model 70

• Molecule 1: Calcitonin-1

Chain A:

4.2.71 Score per residue for model 71

• Molecule 1: Calcitonin-1

Chain A:

4.2.72 Score per residue for model 72

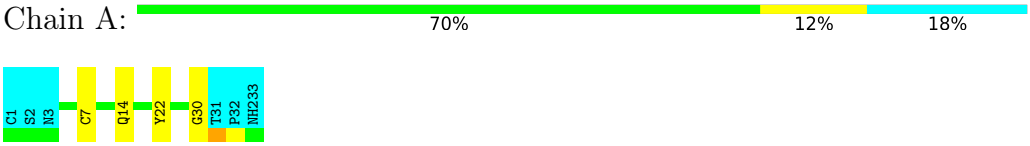
• Molecule 1: Calcitonin-1

Chain A:

4.2.73 Score per residue for model 73

• Molecule 1: Calcitonin-1

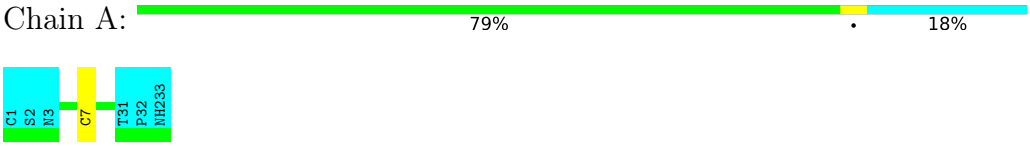
Chain A:



4.2.74 Score per residue for model 74

• Molecule 1: Calcitonin-1

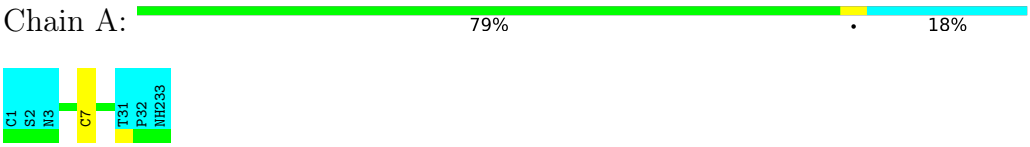
Chain A:



4.2.75 Score per residue for model 75

• Molecule 1: Calcitonin-1

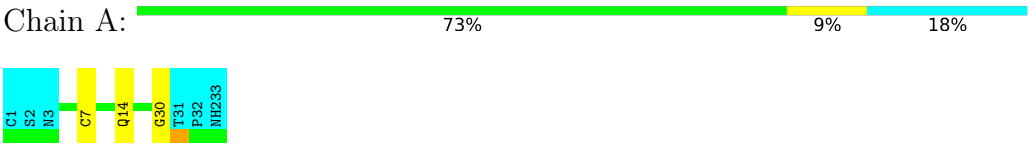
Chain A:



4.2.76 Score per residue for model 76

• Molecule 1: Calcitonin-1

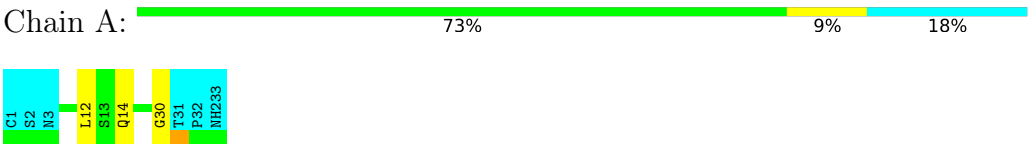
Chain A:



4.2.77 Score per residue for model 77

• Molecule 1: Calcitonin-1

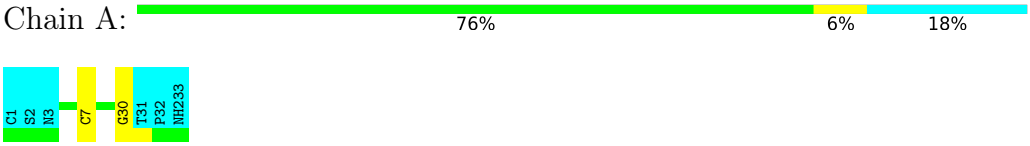
Chain A:



4.2.78 Score per residue for model 78

• Molecule 1: Calcitonin-1

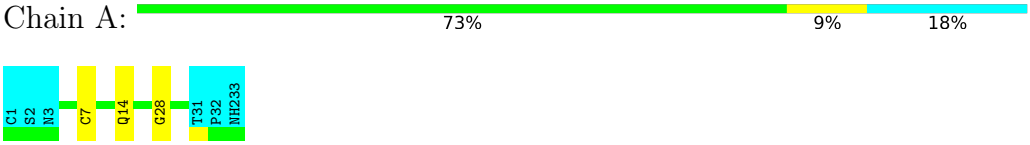
Chain A:



4.2.79 Score per residue for model 79

• Molecule 1: Calcitonin-1

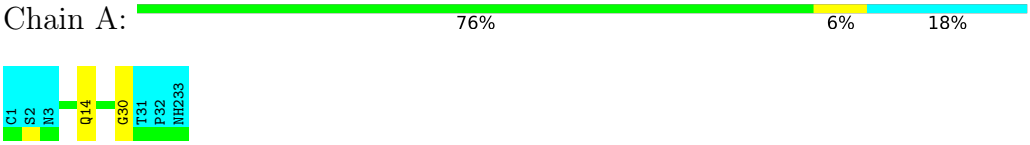
Chain A:



4.2.80 Score per residue for model 80

• Molecule 1: Calcitonin-1

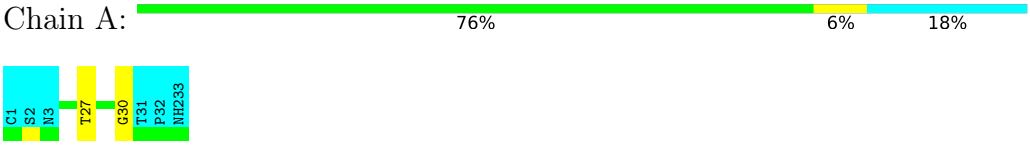
Chain A:



4.2.81 Score per residue for model 81

• Molecule 1: Calcitonin-1

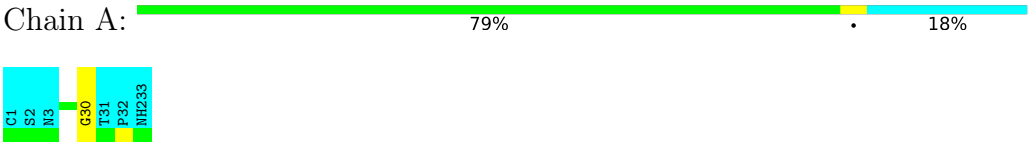
Chain A:



4.2.82 Score per residue for model 82

• Molecule 1: Calcitonin-1

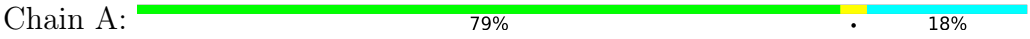
Chain A:

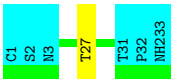


4.2.83 Score per residue for model 83

• Molecule 1: Calcitonin-1

Chain A:

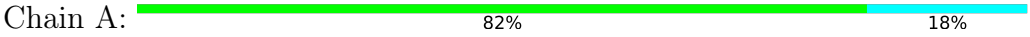


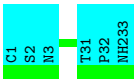


4.2.84 Score per residue for model 84

• Molecule 1: Calcitonin-1

Chain A:

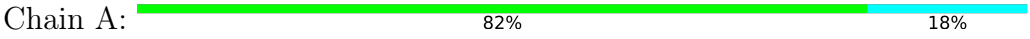


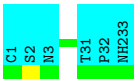


4.2.85 Score per residue for model 85

• Molecule 1: Calcitonin-1

Chain A:

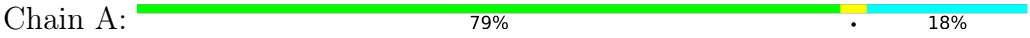


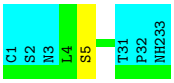


4.2.86 Score per residue for model 86

• Molecule 1: Calcitonin-1

Chain A:

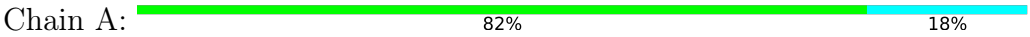


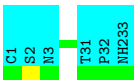


4.2.87 Score per residue for model 87

• Molecule 1: Calcitonin-1

Chain A:

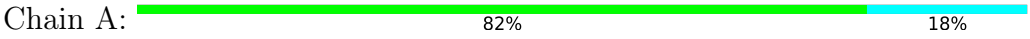


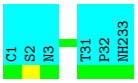


4.2.88 Score per residue for model 88

• Molecule 1: Calcitonin-1

Chain A:

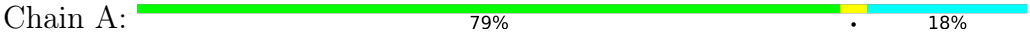


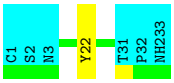


4.2.89 Score per residue for model 89

• Molecule 1: Calcitonin-1

Chain A:





4.2.90 Score per residue for model 90

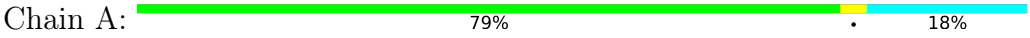
• Molecule 1: Calcitonin-1

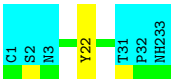
Chain A:

4.2.91 Score per residue for model 91

• Molecule 1: Calcitonin-1

Chain A:

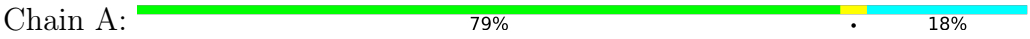


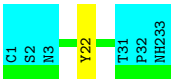


4.2.92 Score per residue for model 92

• Molecule 1: Calcitonin-1

Chain A:

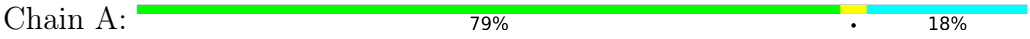


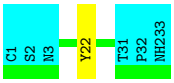


4.2.93 Score per residue for model 93

• Molecule 1: Calcitonin-1

Chain A:

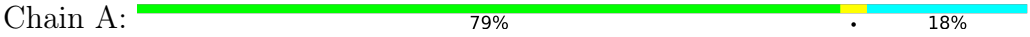


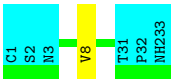


4.2.94 Score per residue for model 94

• Molecule 1: Calcitonin-1

Chain A:

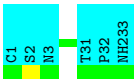




4.2.95 Score per residue for model 95

• Molecule 1: Calcitonin-1

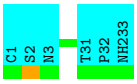
Chain A:



4.2.96 Score per residue for model 96

• Molecule 1: Calcitonin-1

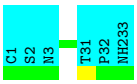
Chain A:



4.2.97 Score per residue for model 97

• Molecule 1: Calcitonin-1

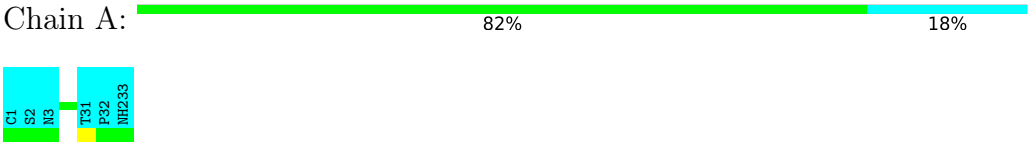
Chain A:



4.2.98 Score per residue for model 98

• Molecule 1: Calcitonin-1

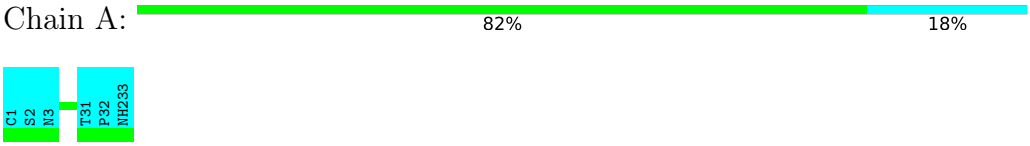
Chain A:



4.2.99 Score per residue for model 99

• Molecule 1: Calcitonin-1

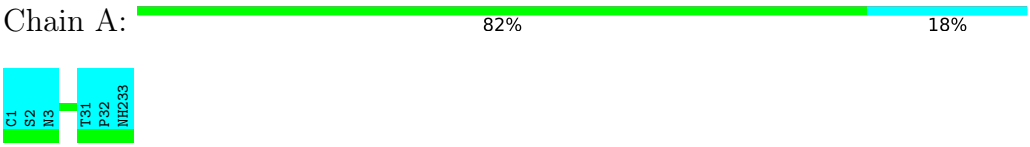
Chain A:



4.2.100 Score per residue for model 100

• Molecule 1: Calcitonin-1

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained simulated annealing/energy minimization followed by unrestrained molecular dynamics*.

Of the 100 calculated structures, 100 were deposited, based on the following criterion: *periodically sampled unrestrained molecular dynamics structures*.

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

Software name	Classification	Version
Amber	structure solution	6.0
Amber	refinement	6.0

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.67±0.04	0±0/201 (0.0± 0.0%)	0.91±0.05	0±0/272 (0.0± 0.1%)
All	All	0.67	0/20100 (0.0%)	0.91	12/27200 (0.0%)

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	0.0±0.1
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	22	TYR	CB-CG-CD2	-6.10	117.34	121.00	64	12

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	22	TYR	Sidechain	1

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	199	206	206	0±0
All	All	19900	20600	20600	-

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 -.

There are no clashes.

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	27/33 (82%)	26±1 (95±2%)	1±1 (4±2%)	0±0 (0±1%)	32	76
All	All	2700/3300 (82%)	2566 (95%)	121 (4%)	13 (0%)	32	76

All 5 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	30	GLY	7
1	A	29	SER	2
1	A	28	GLY	2
1	A	27	THR	1
1	A	5	SER	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	23/28 (82%)	22±1 (96±2%)	1±1 (4±2%)	33 82
All	All	2300/2800 (82%)	2203 (96%)	97 (4%)	33 82

All 10 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	7	CYS	77
1	A	14	GLN	7
1	A	17	HIS	4
1	A	4	LEU	2
1	A	27	THR	2
1	A	19	LEU	1
1	A	22	TYR	1
1	A	13	SER	1
1	A	12	LEU	1
1	A	8	VAL	1

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 monosaccharides 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

No chemical shift data were provided