



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 05:48 PM UTC

PDB ID : 2I2J / pdb_00002i2j
Title : NMR structure of UA159sp in TFE
Authors : Syvitski, R.T.; Jakeman, D.L.; Li, Y.
Deposited on : 2006-08-16

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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

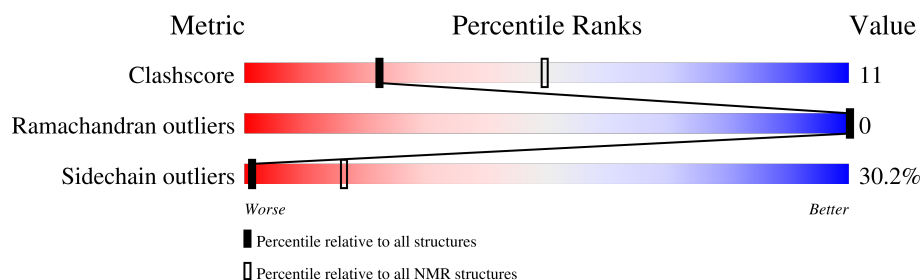
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	22	27% 14% 9% 50%

2 Ensemble composition and analysis

This entry contains 34 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:7-A:17 (11)	0.14	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 339 atoms, of which 171 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Competence stimulating peptide.

Mol	Chain	Residues	Atoms					Trace
1	A	22	Total	C	H	N	O	1
			339	108	171	31	29	

There is a discrepancy between the modelled and reference sequences:

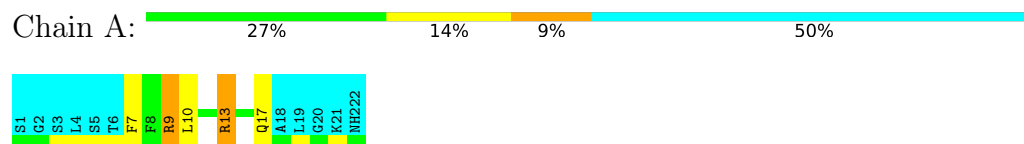
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	NH2	-	amidation	UNP Q1WBY9

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Competence stimulating peptide

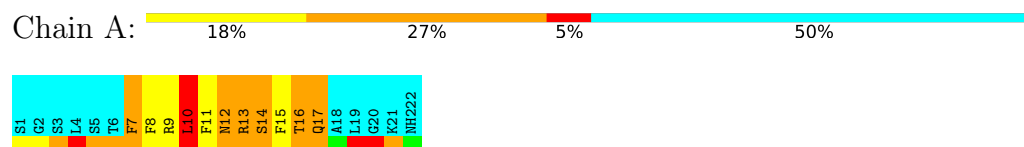


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

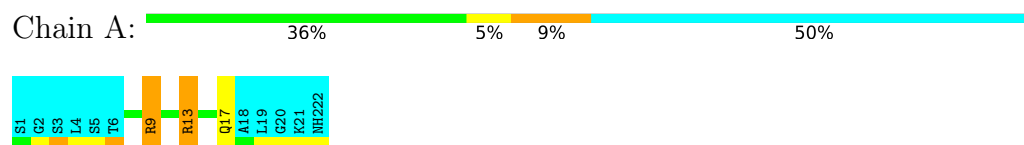
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Competence stimulating peptide



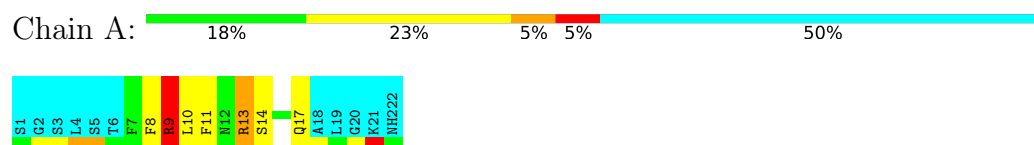
4.2.2 Score per residue for model 2

- Molecule 1: Competence stimulating peptide



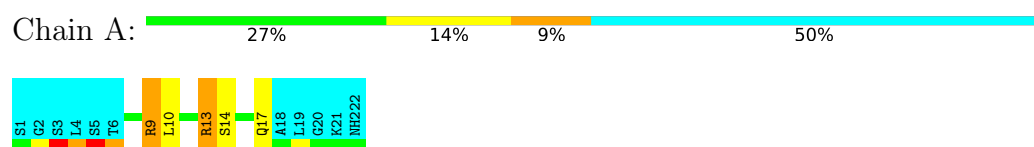
4.2.3 Score per residue for model 3

- Molecule 1: Competence stimulating peptide



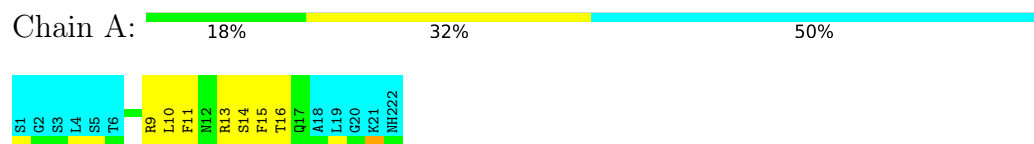
4.2.4 Score per residue for model 4

- Molecule 1: Competence stimulating peptide



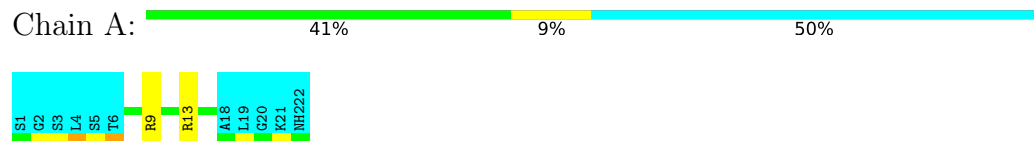
4.2.5 Score per residue for model 5

- Molecule 1: Competence stimulating peptide



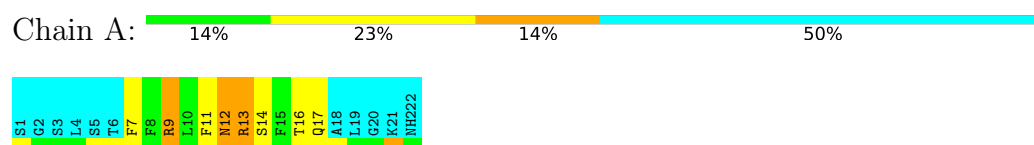
4.2.6 Score per residue for model 6

- Molecule 1: Competence stimulating peptide



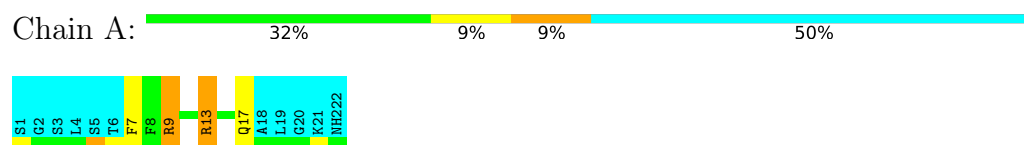
4.2.7 Score per residue for model 7

- Molecule 1: Competence stimulating peptide



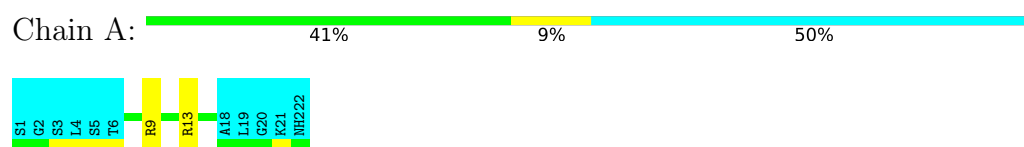
4.2.8 Score per residue for model 8

- Molecule 1: Competence stimulating peptide



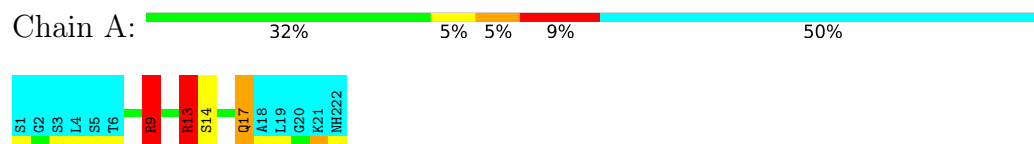
4.2.9 Score per residue for model 9

- Molecule 1: Competence stimulating peptide



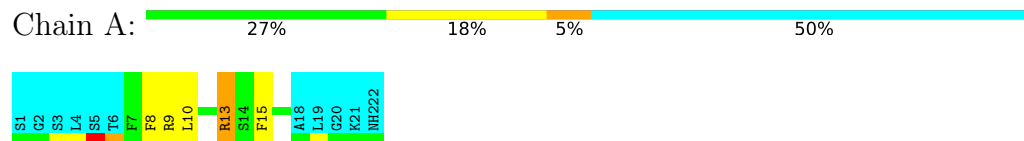
4.2.10 Score per residue for model 10

- Molecule 1: Competence stimulating peptide



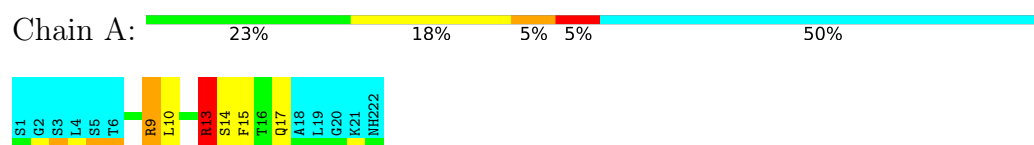
4.2.11 Score per residue for model 11

- Molecule 1: Competence stimulating peptide



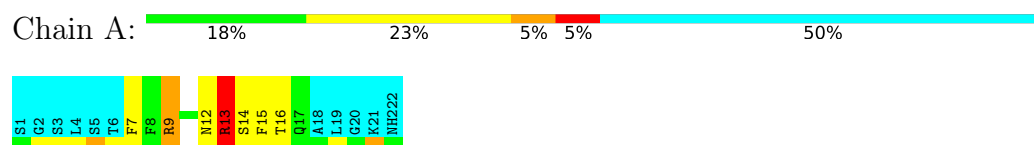
4.2.12 Score per residue for model 12

- Molecule 1: Competence stimulating peptide



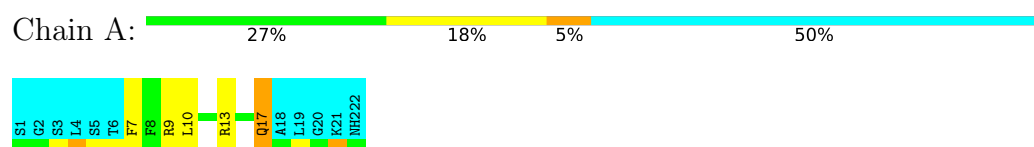
4.2.13 Score per residue for model 13

- Molecule 1: Competence stimulating peptide



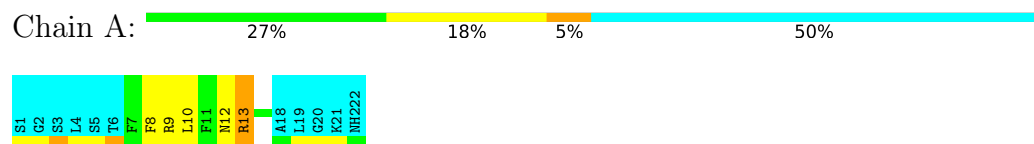
4.2.14 Score per residue for model 14

- Molecule 1: Competence stimulating peptide



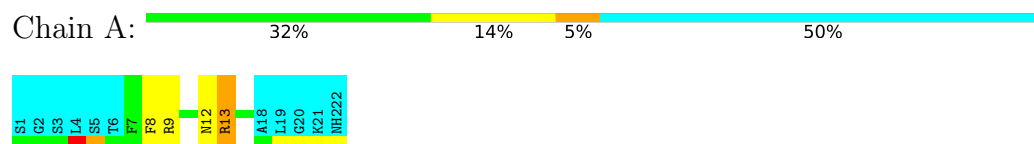
4.2.15 Score per residue for model 15

- Molecule 1: Competence stimulating peptide



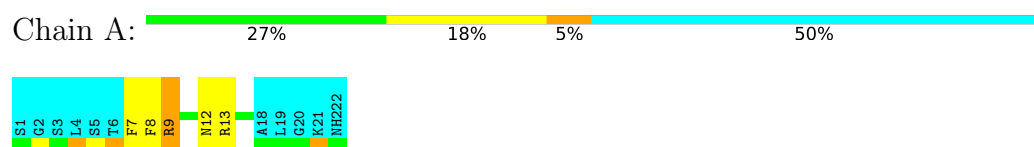
4.2.16 Score per residue for model 16

- Molecule 1: Competence stimulating peptide



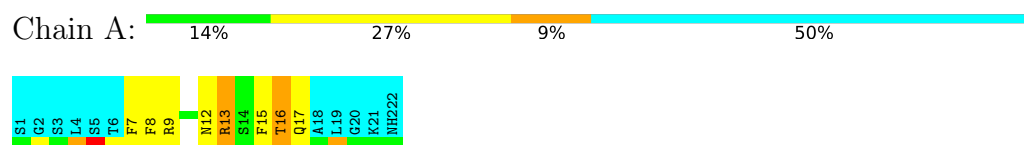
4.2.17 Score per residue for model 17

- Molecule 1: Competence stimulating peptide



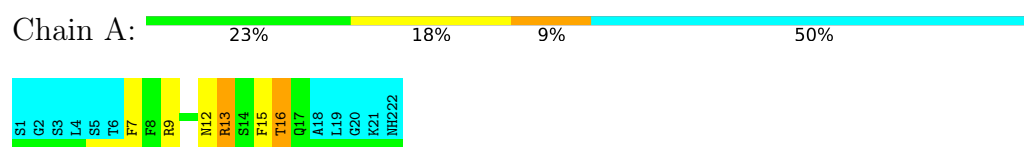
4.2.18 Score per residue for model 18

- Molecule 1: Competence stimulating peptide



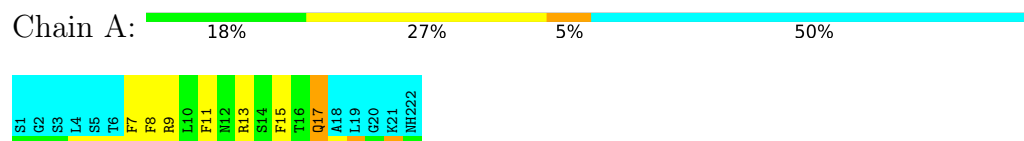
4.2.19 Score per residue for model 19

- Molecule 1: Competence stimulating peptide



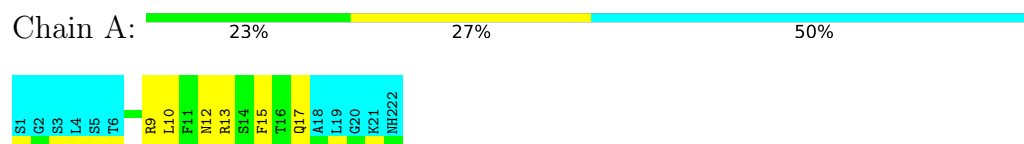
4.2.20 Score per residue for model 20

- Molecule 1: Competence stimulating peptide



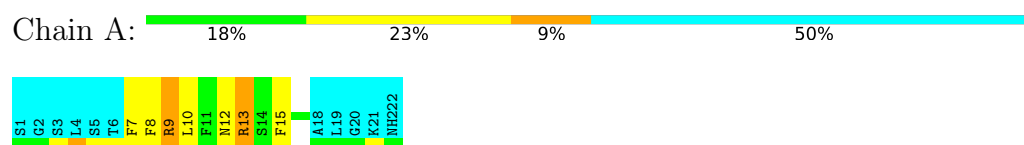
4.2.21 Score per residue for model 21

- Molecule 1: Competence stimulating peptide



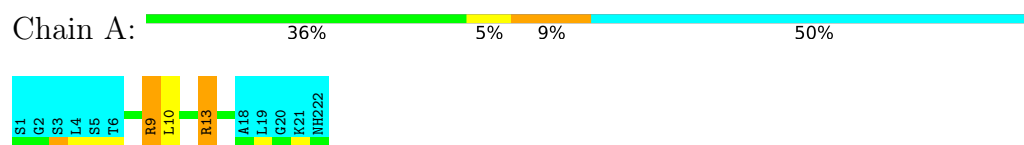
4.2.22 Score per residue for model 22

- Molecule 1: Competence stimulating peptide



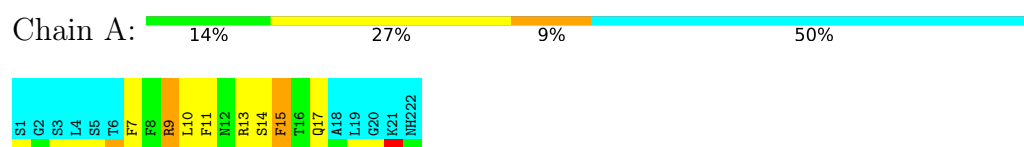
4.2.23 Score per residue for model 23

- Molecule 1: Competence stimulating peptide



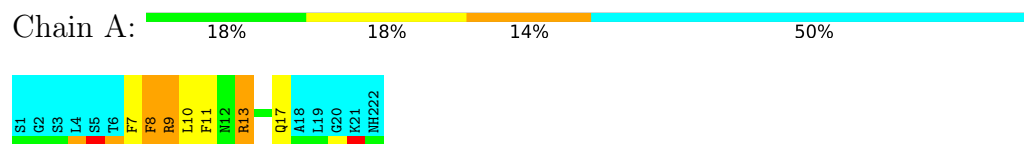
4.2.24 Score per residue for model 24

- Molecule 1: Competence stimulating peptide



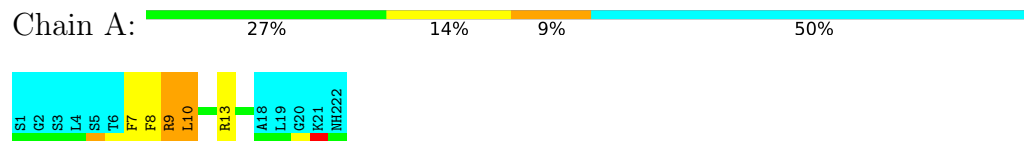
4.2.25 Score per residue for model 25

- Molecule 1: Competence stimulating peptide



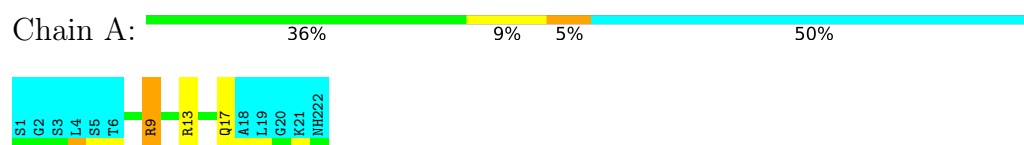
4.2.26 Score per residue for model 26

- Molecule 1: Competence stimulating peptide



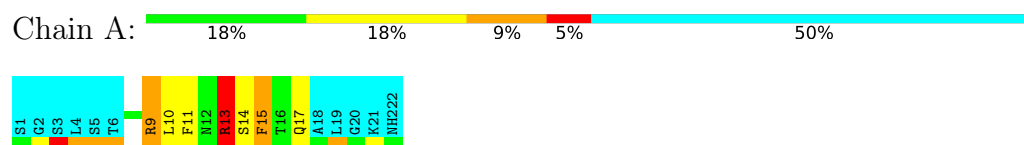
4.2.27 Score per residue for model 27

- Molecule 1: Competence stimulating peptide



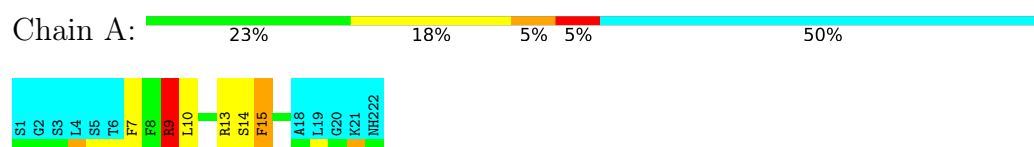
4.2.28 Score per residue for model 28

- Molecule 1: Competence stimulating peptide



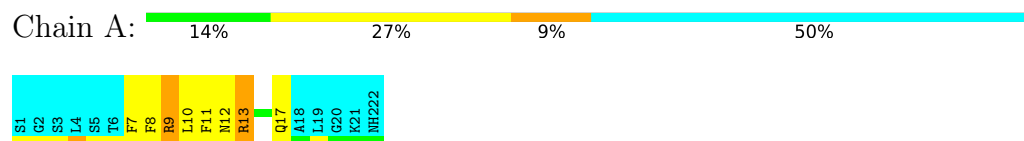
4.2.29 Score per residue for model 29

- Molecule 1: Competence stimulating peptide



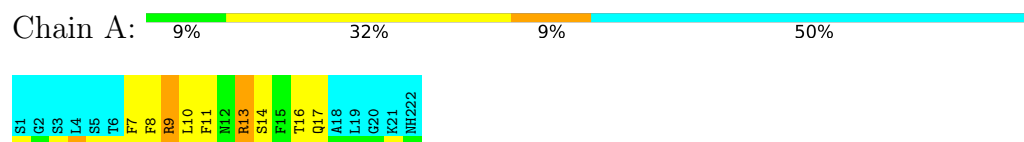
4.2.30 Score per residue for model 30

- Molecule 1: Competence stimulating peptide



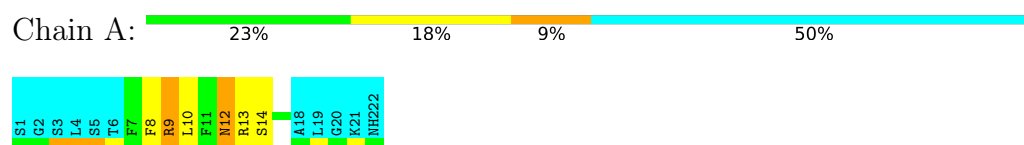
4.2.31 Score per residue for model 31

- Molecule 1: Competence stimulating peptide



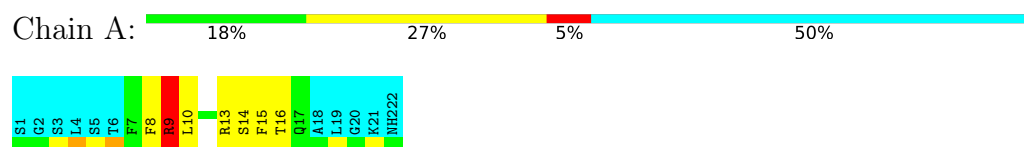
4.2.32 Score per residue for model 32

- Molecule 1: Competence stimulating peptide



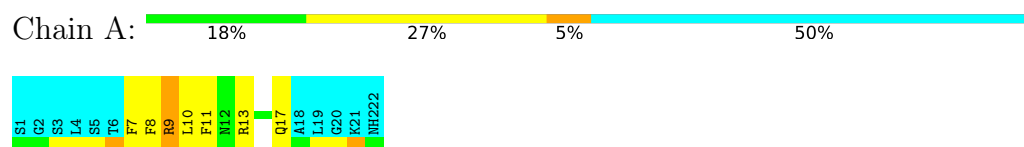
4.2.33 Score per residue for model 33

- Molecule 1: Competence stimulating peptide



4.2.34 Score per residue for model 34

- Molecule 1: Competence stimulating peptide



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 34 were deposited, based on the following criterion: *non-violating structures*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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	1.96±2.99	2±9/108 (1.4± 8.3%)	1.83±1.82	1±6/144 (0.7± 4.1%)
All	All	3.58	53/3672 (1.4%)	2.58	35/4896 (0.7%)

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	1.9±0.3
All	All	0	66

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	9	ARG	CZ-NH2	-61.23	0.53	1.33	1	1
1	A	9	ARG	NE-CZ	-60.30	0.66	1.33	1	1
1	A	13	ARG	NE-CZ	-58.62	0.68	1.33	1	1
1	A	9	ARG	CD-NE	-54.52	0.69	1.46	1	1
1	A	13	ARG	CZ-NH2	-54.30	0.62	1.33	1	1
1	A	17	GLN	CD-OE1	-53.84	0.21	1.23	1	1
1	A	13	ARG	CD-NE	-49.41	0.77	1.46	1	1
1	A	12	ASN	CG-OD1	-41.03	0.45	1.23	1	1
1	A	13	ARG	CZ-NH1	-39.20	0.77	1.32	1	1
1	A	9	ARG	CZ-NH1	-38.59	0.78	1.32	1	1
1	A	14	SER	CB-OG	-37.53	0.67	1.42	1	1
1	A	17	GLN	CD-NE2	-35.69	0.58	1.33	1	1
1	A	12	ASN	CG-ND2	-30.97	0.68	1.33	1	1
1	A	7	PHE	CG-CD2	-30.57	0.74	1.38	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	16	THR	CB-OG1	-25.70	1.02	1.43	1	1
1	A	17	GLN	CG-CD	-25.29	0.88	1.52	1	1
1	A	10	LEU	CG-CD2	-23.07	0.76	1.52	1	1
1	A	13	ARG	CG-CD	-22.13	0.86	1.52	1	1
1	A	7	PHE	CE1-CZ	-21.34	0.74	1.38	1	1
1	A	9	ARG	CG-CD	-20.55	0.90	1.52	1	1
1	A	11	PHE	CG-CD2	-19.80	0.97	1.38	1	1
1	A	10	LEU	CG-CD1	-19.41	0.88	1.52	1	1
1	A	8	PHE	CG-CD2	-18.68	0.99	1.38	1	1
1	A	15	PHE	CG-CD1	-18.63	0.99	1.38	1	1
1	A	11	PHE	CG-CD1	-18.28	1.00	1.38	1	1
1	A	8	PHE	CG-CD1	-17.25	1.02	1.38	1	1
1	A	15	PHE	CG-CD2	-16.79	1.03	1.38	1	1
1	A	7	PHE	CG-CD1	-14.91	1.07	1.38	1	1
1	A	11	PHE	CE1-CZ	-13.76	0.97	1.38	1	1
1	A	8	PHE	CE1-CZ	-13.02	0.99	1.38	1	1
1	A	15	PHE	CE2-CZ	-12.97	0.99	1.38	1	1
1	A	16	THR	CB-CG2	-12.89	1.10	1.52	1	1
1	A	11	PHE	CE2-CZ	-12.75	1.00	1.38	1	1
1	A	8	PHE	CE2-CZ	-12.02	1.02	1.38	1	1
1	A	15	PHE	CE1-CZ	-11.69	1.03	1.38	1	1
1	A	12	ASN	CB-CG	-10.75	1.25	1.52	1	1
1	A	7	PHE	CE2-CZ	-10.38	1.07	1.38	1	1
1	A	17	GLN	CB-CG	-10.22	1.21	1.52	1	1
1	A	9	ARG	CB-CG	-9.34	1.24	1.52	1	1
1	A	7	PHE	CB-CG	-9.08	1.29	1.50	1	1
1	A	10	LEU	CB-CG	-8.78	1.35	1.53	1	1
1	A	11	PHE	CB-CG	-8.22	1.31	1.50	1	1
1	A	8	PHE	CB-CG	-8.17	1.31	1.50	1	1
1	A	13	ARG	CB-CG	-8.04	1.28	1.52	1	1
1	A	15	PHE	CB-CG	-7.71	1.32	1.50	1	1
1	A	7	PHE	CD1-CE1	-6.09	1.20	1.38	1	1
1	A	7	PHE	CD2-CE2	-6.09	1.20	1.38	1	1
1	A	11	PHE	CD1-CE1	-5.49	1.22	1.38	1	1
1	A	11	PHE	CD2-CE2	-5.49	1.22	1.38	1	1
1	A	8	PHE	CD1-CE1	-5.46	1.22	1.38	1	1
1	A	8	PHE	CD2-CE2	-5.44	1.22	1.38	1	1
1	A	15	PHE	CD1-CE1	-5.14	1.23	1.38	1	1
1	A	15	PHE	CD2-CE2	-5.14	1.23	1.38	1	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	17	GLN	OE1-CD-NE2	-78.87	43.73	122.60	1	1
1	A	12	ASN	OD1-CG-ND2	-74.64	47.96	122.60	1	1
1	A	13	ARG	CD-NE-CZ	37.69	177.16	124.40	1	1
1	A	17	GLN	CG-CD-NE2	34.48	168.11	116.40	1	1
1	A	9	ARG	CD-NE-CZ	32.01	169.21	124.40	1	1
1	A	12	ASN	CB-CG-ND2	29.12	160.08	116.40	1	1
1	A	13	ARG	CG-CD-NE	22.71	161.95	112.00	1	1
1	A	9	ARG	NE-CZ-NH2	-22.26	99.17	119.20	1	1
1	A	9	ARG	CG-CD-NE	21.84	160.04	112.00	1	1
1	A	17	GLN	CB-CG-CD	18.24	143.61	112.60	1	1
1	A	9	ARG	NE-CZ-NH1	16.09	137.59	121.50	1	1
1	A	12	ASN	CB-CG-OD1	15.58	151.96	120.80	1	1
1	A	13	ARG	CB-CG-CD	15.50	146.96	111.30	1	1
1	A	9	ARG	CB-CG-CD	14.01	143.53	111.30	1	1
1	A	17	GLN	CG-CD-OE1	13.68	148.16	120.80	1	1
1	A	10	LEU	CD1-CG-CD2	-13.18	81.81	110.80	1	1
1	A	13	ARG	NE-CZ-NH2	-13.01	107.49	119.20	1	1
1	A	7	PHE	CD1-CG-CD2	-12.91	99.23	118.60	1	1
1	A	7	PHE	CB-CG-CD1	12.80	142.46	120.70	1	1
1	A	7	PHE	CG-CD1-CE1	12.79	142.45	120.70	1	1
1	A	7	PHE	CZ-CE2-CD2	12.41	142.34	120.00	1	1
1	A	14	SER	CA-CB-OG	12.27	135.63	111.10	1	1
1	A	7	PHE	CE1-CZ-CE2	-11.47	99.36	120.00	1	1
1	A	11	PHE	CD1-CG-CD2	-9.92	103.72	118.60	1	1
1	A	11	PHE	CE1-CZ-CE2	-9.05	103.70	120.00	1	1
1	A	15	PHE	CD1-CG-CD2	-8.86	105.31	118.60	1	1
1	A	8	PHE	CD1-CG-CD2	-8.73	105.50	118.60	1	1
1	A	10	LEU	CB-CG-CD1	8.47	136.10	110.70	1	1
1	A	13	ARG	NE-CZ-NH1	8.24	129.74	121.50	1	1
1	A	15	PHE	CE1-CZ-CE2	-8.16	105.31	120.00	1	1
1	A	8	PHE	CE1-CZ-CE2	-8.02	105.56	120.00	1	1
1	A	16	THR	CA-CB-OG1	5.72	118.18	109.60	1	1
1	A	11	PHE	CZ-CE2-CD2	5.15	129.27	120.00	1	1
1	A	11	PHE	CB-CG-CD1	5.02	129.24	120.70	1	1
1	A	11	PHE	CG-CD1-CE1	5.02	129.23	120.70	1	1

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	9	ARG	Sidechain	33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group	Models (Total)
1	A	13	ARG	Sidechain	33

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	104	99	99	2±8
All	All	3536	3366	3365	79

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:LEU:CD2	1:A:10:LEU:CB	1.53	1.87	1	1
1:A:12:ASN:OD1	1:A:12:ASN:CB	1.43	1.66	1	1
1:A:17:GLN:CD	1:A:17:GLN:CB	1.35	1.99	1	1
1:A:12:ASN:CB	1:A:12:ASN:ND2	1.35	1.90	1	1
1:A:13:ARG:CD	1:A:13:ARG:CB	1.34	2.05	1	1
1:A:10:LEU:CB	1:A:10:LEU:CD1	1.19	2.08	1	1
1:A:14:SER:OG	1:A:14:SER:HB2	1.03	1.29	1	1
1:A:14:SER:OG	1:A:14:SER:CA	1.03	2.05	1	1
1:A:14:SER:OG	1:A:14:SER:HB3	1.02	1.29	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD12	0.98	1.51	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD11	0.97	1.51	1	1
1:A:14:SER:OG	1:A:14:SER:CB	0.97	0.67	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD13	0.95	1.51	1	1
1:A:10:LEU:CD2	1:A:10:LEU:HG	0.94	1.59	1	1
1:A:10:LEU:CD1	1:A:10:LEU:HG	0.94	1.59	1	1
1:A:17:GLN:CD	1:A:17:GLN:HG2	0.94	1.43	1	1
1:A:17:GLN:CD	1:A:17:GLN:CG	0.93	0.88	1	1
1:A:17:GLN:CD	1:A:17:GLN:HG3	0.91	1.43	1	1
1:A:10:LEU:CD1	1:A:10:LEU:CG	0.88	0.88	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD21	0.87	1.42	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD22	0.87	1.42	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD23	0.87	1.42	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ARG:CD	1:A:13:ARG:HG2	0.87	1.40	1	1
1:A:13:ARG:CD	1:A:13:ARG:HG3	0.86	1.40	1	1
1:A:13:ARG:CD	1:A:13:ARG:CG	0.84	0.86	1	1
1:A:13:ARG:CG	1:A:13:ARG:HD3	0.76	1.35	1	1
1:A:10:LEU:CD2	1:A:10:LEU:CG	0.76	0.76	1	1
1:A:13:ARG:CG	1:A:13:ARG:HD2	0.73	1.35	1	1
1:A:13:ARG:CZ	1:A:13:ARG:HH11	0.71	1.42	1	1
1:A:13:ARG:CZ	1:A:13:ARG:HH12	0.71	1.42	1	1
1:A:12:ASN:ND2	1:A:12:ASN:CG	0.71	0.68	1	1
1:A:13:ARG:HD3	1:A:13:ARG:NE	0.68	1.29	1	1
1:A:10:LEU:CD2	1:A:10:LEU:HB3	0.67	2.11	1	1
1:A:12:ASN:CG	1:A:12:ASN:HD21	0.67	1.33	1	1
1:A:12:ASN:CG	1:A:12:ASN:HD22	0.66	1.33	1	1
1:A:12:ASN:OD1	1:A:12:ASN:CG	0.65	0.45	1	1
1:A:13:ARG:HD2	1:A:13:ARG:NE	0.65	1.29	1	1
1:A:12:ASN:OD1	1:A:12:ASN:ND2	0.64	0.50	1	1
1:A:13:ARG:CZ	1:A:13:ARG:NH1	0.62	0.77	1	1
1:A:17:GLN:CD	1:A:17:GLN:HE22	0.60	1.25	1	1
1:A:17:GLN:CD	1:A:17:GLN:HE21	0.59	1.25	1	1
1:A:13:ARG:CZ	1:A:13:ARG:HH22	0.57	1.29	1	1
1:A:13:ARG:CZ	1:A:13:ARG:HH21	0.57	1.29	1	1
1:A:11:PHE:CZ	1:A:15:PHE:CE1	0.55	2.95	24	1
1:A:12:ASN:O	1:A:16:THR:HG23	0.55	2.00	7	1
1:A:8:PHE:CE1	1:A:12:ASN:OD1	0.54	2.61	15	2
1:A:15:PHE:CD1	1:A:15:PHE:C	0.54	2.85	18	2
1:A:13:ARG:C	1:A:13:ARG:CD	0.53	2.82	12	1
1:A:10:LEU:HD23	1:A:10:LEU:C	0.53	2.29	31	1
1:A:14:SER:CB	1:A:14:SER:HG	0.52	1.23	1	1
1:A:10:LEU:C	1:A:10:LEU:CD2	0.49	2.84	31	1
1:A:17:GLN:CD	1:A:17:GLN:NE2	0.48	0.58	1	1
1:A:9:ARG:HD2	1:A:13:ARG:NH2	0.47	2.24	10	1
1:A:13:ARG:CZ	1:A:13:ARG:NH2	0.47	0.62	1	1
1:A:8:PHE:C	1:A:8:PHE:CD1	0.47	2.92	33	1
1:A:9:ARG:HG3	1:A:10:LEU:N	0.47	2.23	26	1
1:A:10:LEU:HD23	1:A:10:LEU:O	0.46	2.09	31	1
1:A:13:ARG:HG2	1:A:17:GLN:NE2	0.46	2.26	28	1
1:A:8:PHE:O	1:A:12:ASN:OD1	0.46	2.34	22	1
1:A:13:ARG:C	1:A:13:ARG:HD3	0.45	2.36	12	1
1:A:7:PHE:O	1:A:8:PHE:C	0.44	2.60	25	4
1:A:9:ARG:CG	1:A:10:LEU:N	0.44	2.80	26	1
1:A:12:ASN:O	1:A:16:THR:OG1	0.44	2.34	18	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ARG:CA	1:A:13:ARG:NE	0.43	2.80	13	1
1:A:17:GLN:CD	1:A:17:GLN:C	0.42	2.87	4	1
1:A:8:PHE:O	1:A:9:ARG:C	0.42	2.62	26	1
1:A:13:ARG:CD	1:A:13:ARG:HH21	0.42	1.63	1	1
1:A:11:PHE:CE1	1:A:15:PHE:CD2	0.41	3.08	28	1
1:A:12:ASN:OD1	1:A:12:ASN:C	0.41	2.63	21	1
1:A:10:LEU:O	1:A:14:SER:CB	0.41	2.68	5	1
1:A:14:SER:O	1:A:17:GLN:HG2	0.41	2.16	3	1
1:A:11:PHE:C	1:A:14:SER:HG	0.41	2.24	5	1
1:A:17:GLN:O	1:A:17:GLN:NE2	0.40	2.54	4	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	11/22 (50%)	11±0 (96±4%)	0±0 (4±4%)	0±0 (0±0%)	100	100
All	All	374/748 (50%)	360 (96%)	14 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	11/18 (61%)	8±2 (70±15%)	3±2 (30±15%)	1	16
All	All	374/612 (61%)	261 (70%)	113 (30%)	1	16

All 11 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	9	ARG	20
1	A	13	ARG	19
1	A	10	LEU	16
1	A	17	GLN	14
1	A	14	SER	9
1	A	15	PHE	9
1	A	11	PHE	7
1	A	7	PHE	6
1	A	12	ASN	6
1	A	16	THR	5
1	A	8	PHE	2

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1-A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	20:GLY	C	21:LYS	N	0.83
1	A	3:SER	C	4:LEU	N	0.64
1	A	2:GLY	C	3:SER	N	0.36
1	A	1:SER	C	2:GLY	N	0.32
1	A	21:LYS	C	22:NH2	N	0.09

7 Chemical shift validation

No chemical shift data were provided