Full wwPDB NMR Structure Validation Report (i)

Mar 3, 2022 – 08:33 AM EST

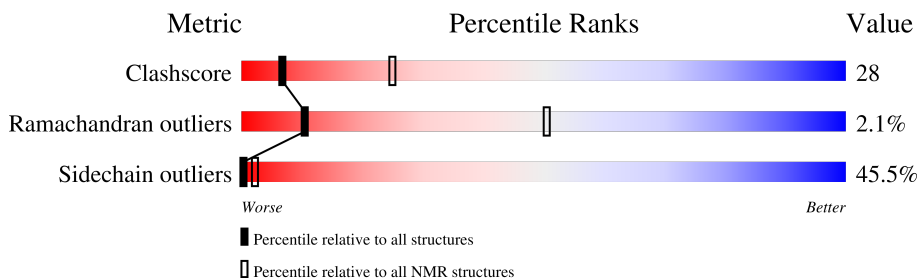|		
PDB ID	:	2I2H
Title	:	NMR structure of TPC3 in TFE
Authors	:	Syvitski, R.T.; Jakeman, D.L.; Li, Y.
Deposited on	:	2006-08-16

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	Percentile Ranks	Value
Clashscore		28
Ramachandran outliers		2.1%
Sidechain outliers		45.5%

Worse ——————————————————— *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	19	11% 53% 16% 21%

2   Ensemble composition and analysis ⓘ

This entry contains 22 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:4-A:18 (15)	0.25	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 and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 7, 9, 15
2	10, 12, 13, 18, 20
3	3, 4, 17
4	11, 14, 21
5	16, 22
Single-model clusters	6; 8; 19

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 294 atoms, of which 146 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called signaling peptide TCP3.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	19	294	95	146	27	26	1

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: signaling peptide TCP3

Chain A: 11%   53%   16%   21%

S1 G2 T3 L4 S5 T6 F7 F8 R9 L10 F11 N12 R13 S14 F15 T16 Q17 A18 NH219
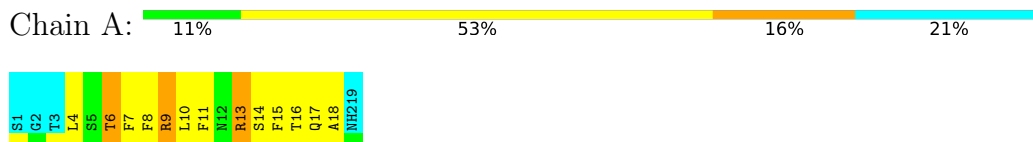
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: signaling peptide TCP3

Chain A: 16%   42%   21%   21%

S1 G2 T3 L4 S5 T6 F7 F8 R9 L10 F11 N12 R13 S14 F15 T16 Q17 A18 NH219
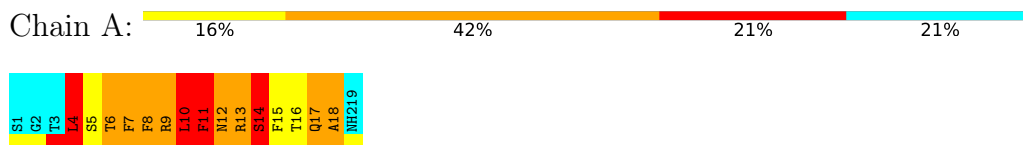
4.2.2 Score per residue for model 2

- Molecule 1: signaling peptide TCP3

Chain A: 37%   16%   26%   21%

S1 G2 T3 L4 S5 T6 F7 F8 R9 L10 F11 N12 R13 S14 F15 NH219

4.2.3 Score per residue for model 3

• Molecule 1: signaling peptide TCP3

Chain A:

4.2.4 Score per residue for model 4

• Molecule 1: signaling peptide TCP3

Chain A:

4.2.5 Score per residue for model 5

• Molecule 1: signaling peptide TCP3

Chain A:

4.2.6 Score per residue for model 6

• Molecule 1: signaling peptide TCP3

Chain A:

4.2.7 Score per residue for model 7

• Molecule 1: signaling peptide TCP3

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: signaling peptide TCP3

Chain A:

4.2.9 Score per residue for model 9

• Molecule 1: signaling peptide TCP3

Chain A:
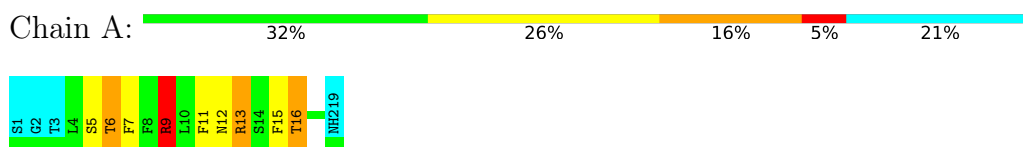
4.2.10 Score per residue for model 10

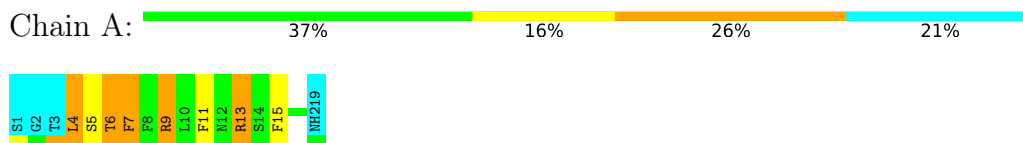• Molecule 1: signaling peptide TCP3

Chain A:
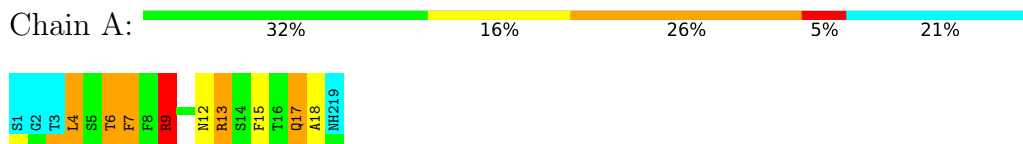
4.2.11 Score per residue for model 11

• Molecule 1: signaling peptide TCP3
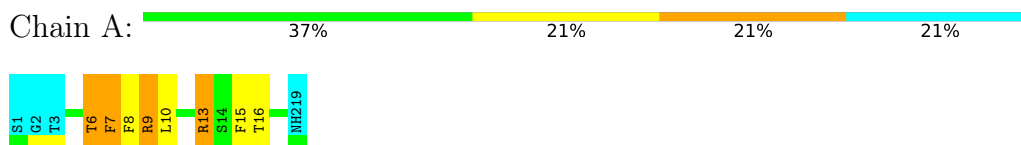
Chain A:
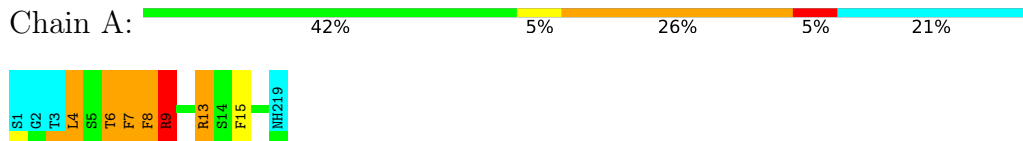
4.2.12 Score per residue for model 12

• Molecule 1: signaling peptide TCP3

Chain A:
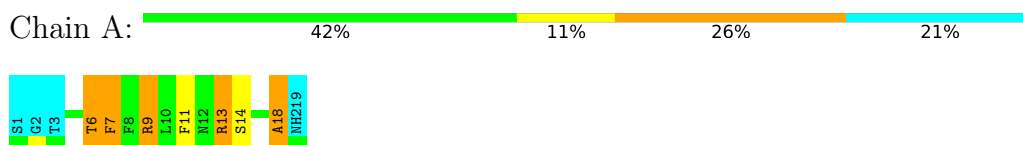
4.2.13   Score per residue for model 13

• Molecule 1: signaling peptide TCP3

Chain A:
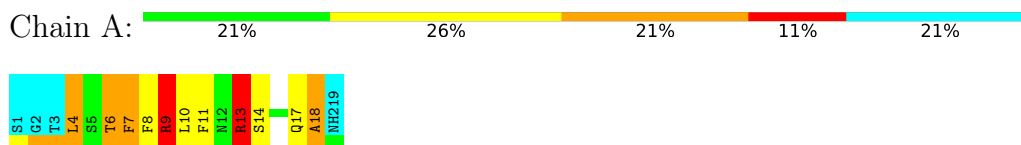
4.2.14   Score per residue for model 14

• Molecule 1: signaling peptide TCP3

Chain A:
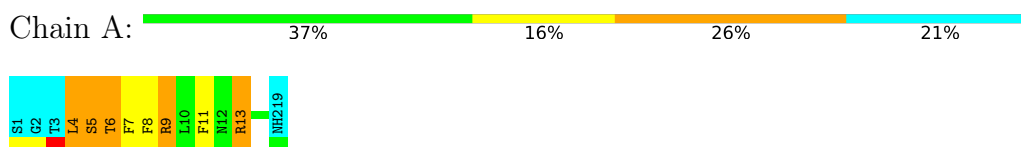
4.2.15   Score per residue for model 15

• Molecule 1: signaling peptide TCP3

Chain A:
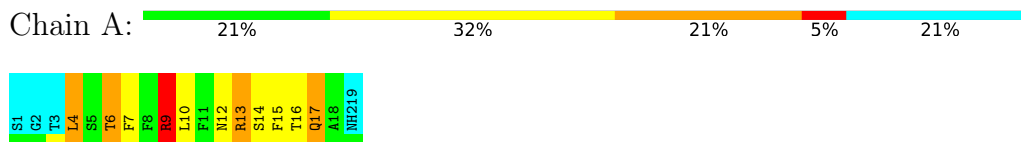
4.2.16   Score per residue for model 16

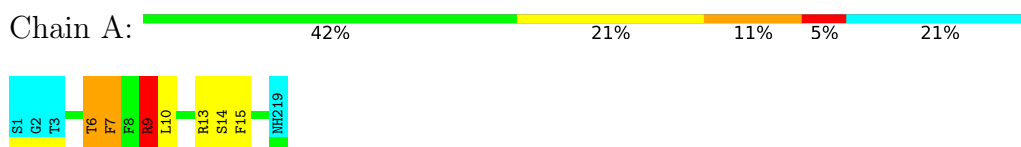• Molecule 1: signaling peptide TCP3

Chain A:
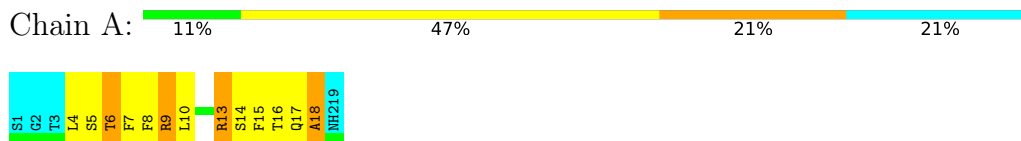
4.2.17   Score per residue for model 17

• Molecule 1: signaling peptide TCP3

Chain A:
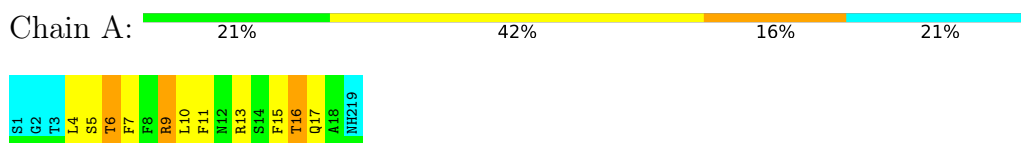
4.2.18 Score per residue for model 18

• Molecule 1: signaling peptide TCP3

Chain A:
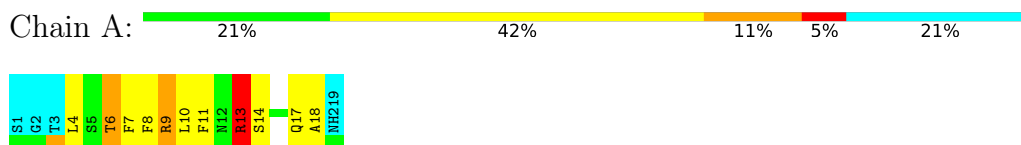
4.2.19 Score per residue for model 19

• Molecule 1: signaling peptide TCP3

Chain A:
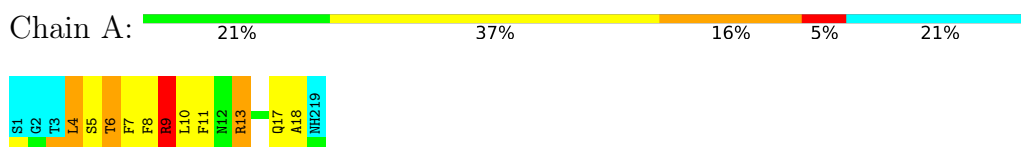
4.2.20 Score per residue for model 20

• Molecule 1: signaling peptide TCP3

Chain A:
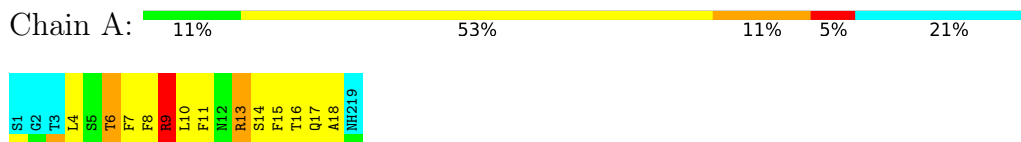
4.2.21 Score per residue for model 21
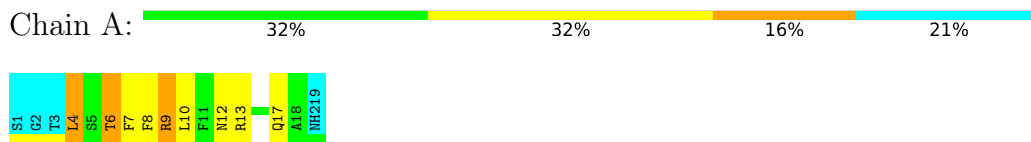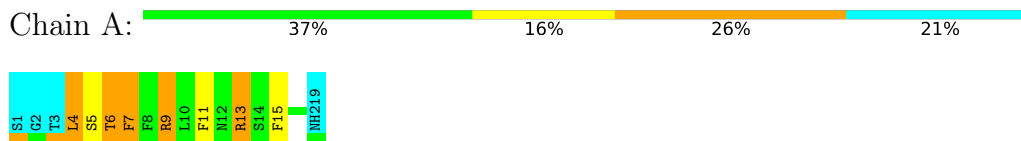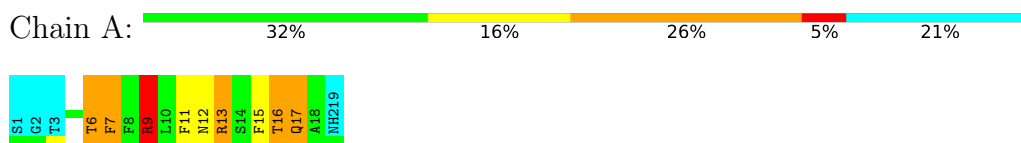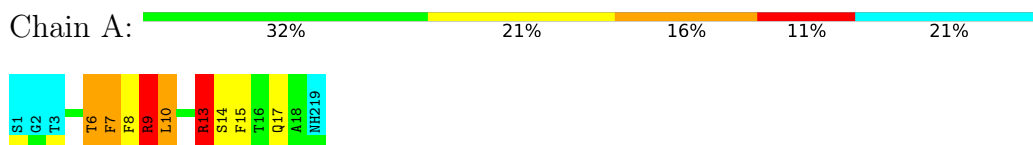
• Molecule 1: signaling peptide TCP3

Chain A:
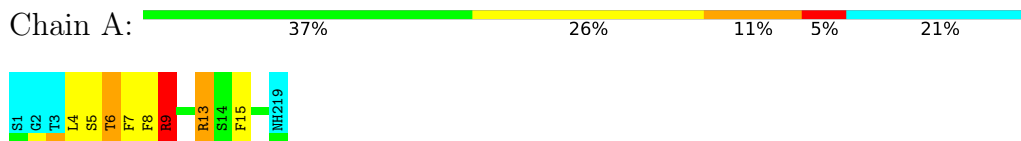
4.2.22 Score per residue for model 22

• Molecule 1: signaling peptide TCP3

Chain A:
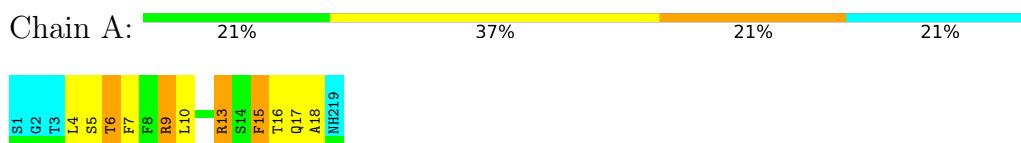
5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 22 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	1.86±3.86	3±13/133 (2.1± 9.6%)	1.65±1.72	2±11/177 (1.3± 6.0%)
All	All	4.28	61/2926 (2.1%)	2.38	51/3894 (1.3%)

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±0.2	1.9±0.4
All	All	1	42

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	13	ARG	CZ-NH2	-65.14	0.48	1.33	1	1
1	A	14	SER	CB-OG	-58.53	0.66	1.42	1	1
1	A	9	ARG	CZ-NH1	-55.95	0.60	1.33	1	1
1	A	18	ALA	C-O	-54.83	0.19	1.23	1	1
1	A	9	ARG	NE-CZ	-50.50	0.67	1.33	1	1
1	A	17	GLN	CD-OE1	-46.33	0.22	1.24	1	1
1	A	9	ARG	CZ-NH2	-45.48	0.73	1.33	1	1
1	A	13	ARG	NE-CZ	-45.13	0.74	1.33	1	1
1	A	13	ARG	CD-NE	-45.13	0.69	1.46	1	1
1	A	13	ARG	CZ-NH1	-45.08	0.74	1.33	1	1
1	A	5	SER	CB-OG	-44.09	0.84	1.42	1	1
1	A	9	ARG	CD-NE	-43.39	0.72	1.46	1	1
1	A	18	ALA	CA-C	-42.72	0.41	1.52	1	1
1	A	18	ALA	CA-CB	-39.12	0.70	1.52	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models Worst	Total
1	A	8	PHE	CG-CD2	-37.21	0.82	1.38	1	1
1	A	15	PHE	CG-CD2	-32.93	0.89	1.38	1	1
1	A	17	GLN	CD-NE2	-32.92	0.50	1.32	1	1
1	A	12	ASN	CG-OD1	-30.80	0.56	1.24	1	1
1	A	17	GLN	CG-CD	-30.44	0.81	1.51	1	1
1	A	8	PHE	CE1-CZ	-28.64	0.82	1.37	1	1
1	A	15	PHE	CG-CD1	-27.09	0.98	1.38	1	1
1	A	8	PHE	CG-CD1	-25.69	1.00	1.38	1	1
1	A	15	PHE	CE1-CZ	-25.26	0.89	1.37	1	1
1	A	13	ARG	CG-CD	-24.77	0.90	1.51	1	1
1	A	9	ARG	CG-CD	-22.52	0.95	1.51	1	1
1	A	12	ASN	CG-ND2	-21.32	0.79	1.32	1	1
1	A	15	PHE	CE2-CZ	-20.65	0.98	1.37	1	1
1	A	10	LEU	CG-CD2	-20.10	0.77	1.51	1	1
1	A	8	PHE	CE2-CZ	-19.55	1.00	1.37	1	1
1	A	16	THR	CB-OG1	-19.34	1.04	1.43	1	1
1	A	11	PHE	CG-CD1	-18.71	1.10	1.38	1	1
1	A	4	LEU	CG-CD1	-18.36	0.83	1.51	1	1
1	A	17	GLN	CB-CG	-18.25	1.03	1.52	1	1
1	A	4	LEU	CG-CD2	-18.12	0.84	1.51	1	1
1	A	10	LEU	CG-CD1	-18.09	0.84	1.51	1	1
1	A	17	GLN	C-N	-17.10	0.94	1.34	1	1
1	A	11	PHE	CG-CD2	-16.69	1.13	1.38	1	1
1	A	7	PHE	CG-CD2	-16.56	1.14	1.38	1	1
1	A	7	PHE	CG-CD1	-16.10	1.14	1.38	1	1
1	A	17	GLN	CA-CB	-14.90	1.21	1.53	1	1
1	A	17	GLN	C-O	-14.60	0.95	1.23	1	1
1	A	11	PHE	CE2-CZ	-14.05	1.10	1.37	1	1
1	A	4	LEU	CB-CG	-13.74	1.12	1.52	1	1
1	A	8	PHE	CB-CG	-12.81	1.29	1.51	1	1
1	A	11	PHE	CE1-CZ	-12.44	1.13	1.37	1	1
1	A	16	THR	CB-CG2	-12.32	1.11	1.52	1	1
1	A	7	PHE	CE1-CZ	-12.32	1.14	1.37	1	1
1	A	7	PHE	CE2-CZ	-12.01	1.14	1.37	1	1
1	A	18	ALA	N-CA	-11.82	1.22	1.46	1	1
1	A	17	GLN	CA-C	-10.21	1.26	1.52	1	1
1	A	13	ARG	CB-CG	-9.60	1.26	1.52	1	1
1	A	8	PHE	CD2-CE2	-9.54	1.20	1.39	1	1
1	A	8	PHE	CD1-CE1	-9.51	1.20	1.39	1	1
1	A	9	ARG	CB-CG	-8.99	1.28	1.52	1	1
1	A	15	PHE	CB-CG	-8.96	1.36	1.51	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	11	PHE	CB-CG	-8.04	1.37	1.51	1	1
1	A	15	PHE	CD1-CE1	-6.54	1.26	1.39	1	1
1	A	15	PHE	CD2-CE2	-6.54	1.26	1.39	1	1
1	A	11	PHE	CD2-CE2	-5.79	1.27	1.39	1	1
1	A	11	PHE	CD1-CE1	-5.76	1.27	1.39	1	1
1	A	7	PHE	CB-CG	-5.16	1.42	1.51	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	13	ARG	NE-CZ-NH1	43.85	142.23	120.30	1	1
1	A	9	ARG	CD-NE-CZ	37.05	175.47	123.60	1	1
1	A	17	GLN	OE1-CD-NE2	-34.27	43.09	121.90	1	1
1	A	13	ARG	CD-NE-CZ	32.17	168.65	123.60	1	1
1	A	18	ALA	N-CA-CB	27.35	148.38	110.10	1	1
1	A	12	ASN	OD1-CG-ND2	-25.92	62.29	121.90	1	1
1	A	9	ARG	CG-CD-NE	25.24	164.80	111.80	1	1
1	A	18	ALA	CB-CA-C	-23.77	74.44	110.10	1	1
1	A	13	ARG	NE-CZ-NH2	-23.27	108.67	120.30	1	1
1	A	8	PHE	CB-CG-CD1	23.22	137.06	120.80	1	1
1	A	9	ARG	NE-CZ-NH1	-21.87	109.36	120.30	1	1
1	A	17	GLN	CG-CD-NE2	20.77	166.55	116.70	1	1
1	A	15	PHE	CB-CG-CD1	20.59	135.21	120.80	1	1
1	A	18	ALA	CA-C-O	20.27	162.66	120.10	1	1
1	A	9	ARG	NE-CZ-NH2	19.24	129.92	120.30	1	1
1	A	13	ARG	CG-CD-NE	18.25	150.13	111.80	1	1
1	A	15	PHE	CD1-CG-CD2	-17.54	95.50	118.30	1	1
1	A	12	ASN	CB-CG-ND2	15.32	153.47	116.70	1	1
1	A	8	PHE	CD1-CG-CD2	-15.26	98.46	118.30	1	1
1	A	8	PHE	CG-CD1-CE1	14.73	137.00	120.80	1	1
1	A	17	GLN	CG-CD-OE1	14.38	150.36	121.60	1	1
1	A	8	PHE	CZ-CE2-CD2	14.17	137.10	120.10	1	1
1	A	15	PHE	CE1-CZ-CE2	-13.61	95.50	120.00	1	1
1	A	10	LEU	CB-CG-CD1	13.20	133.44	111.00	1	1
1	A	15	PHE	CG-CD1-CE1	13.10	135.21	120.80	1	1
1	A	17	GLN	CB-CG-CD	12.60	144.36	111.60	1	1
1	A	15	PHE	CZ-CE2-CD2	12.58	135.20	120.10	1	1
1	A	15	PHE	CB-CG-CD2	12.13	129.29	120.80	1	1
1	A	8	PHE	CE1-CZ-CE2	-12.00	98.41	120.00	1	1
1	A	4	LEU	CB-CG-CD1	11.63	130.78	111.00	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models Worst	Models Total
1	A	12	ASN	CB-CG-OD1	11.32	144.24	121.60	1	1
1	A	4	LEU	CD1-CG-CD2	-10.92	77.75	110.50	1	1
1	A	13	ARG	CB-CG-CD	10.54	138.99	111.60	1	1
1	A	9	ARG	CB-CG-CD	10.26	138.27	111.60	1	1
1	A	10	LEU	CD1-CG-CD2	-9.80	81.08	110.50	1	1
1	A	13	ARG	NH1-CZ-NH2	-9.36	109.11	119.40	1	1
1	A	14	SER	CA-CB-OG	9.24	136.14	111.20	1	1
1	A	10	LEU	CB-CG-CD2	7.87	124.38	111.00	1	1
1	A	15	PHE	CG-CD2-CE2	7.73	129.31	120.80	1	1
1	A	15	PHE	CD1-CE1-CZ	7.66	129.30	120.10	1	1
1	A	11	PHE	CB-CG-CD2	7.15	125.81	120.80	1	1
1	A	4	LEU	CB-CG-CD2	7.04	122.96	111.00	1	1
1	A	7	PHE	CD1-CG-CD2	-6.92	109.31	118.30	1	1
1	A	7	PHE	CB-CG-CD1	6.82	125.57	120.80	1	1
1	A	7	PHE	CB-CG-CD2	6.17	125.12	120.80	1	1
1	A	7	PHE	CE1-CZ-CE2	-5.95	109.29	120.00	1	1
1	A	11	PHE	CD1-CG-CD2	-5.84	110.71	118.30	1	1
1	A	18	ALA	N-CA-C	5.77	126.59	111.00	1	1
1	A	5	SER	CA-CB-OG	5.28	125.47	111.20	1	1
1	A	8	PHE	CB-CG-CD2	5.26	124.48	120.80	1	1
1	A	11	PHE	CE1-CZ-CE2	-5.19	110.66	120.00	1	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
1	A	18	ALA	CA	1

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	21
1	A	13	ARG	Sidechain	21

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	130	127	127	7±14
All	All	2860	2794	2791	156

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 28.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:17:GLN:CD	1:A:17:GLN:CB	1.53	1.75	1	1
1:A:10:LEU:CD2	1:A:10:LEU:CB	1.42	1.94	1	1
1:A:13:ARG:CD	1:A:13:ARG:CB	1.35	2.02	1	1
1:A:18:ALA:CB	1:A:18:ALA:N	1.34	1.85	1	1
1:A:10:LEU:CB	1:A:10:LEU:CD1	1.27	2.07	1	1
1:A:18:ALA:N	1:A:18:ALA:O	1.27	1.68	1	1
1:A:12:ASN:OD1	1:A:12:ASN:CB	1.21	1.88	1	1
1:A:12:ASN:CB	1:A:12:ASN:ND2	1.11	2.14	1	1
1:A:18:ALA:CB	1:A:18:ALA:O	1.06	0.76	1	1
1:A:18:ALA:O	1:A:18:ALA:HB3	1.06	1.30	1	1
1:A:14:SER:OG	1:A:14:SER:CA	1.05	2.05	1	1
1:A:14:SER:OG	1:A:14:SER:HB2	1.01	1.29	1	1
1:A:10:LEU:CD2	1:A:10:LEU:HG	1.00	1.59	1	1
1:A:18:ALA:O	1:A:18:ALA:HA	1.00	1.50	1	1
1:A:14:SER:OG	1:A:14:SER:HB3	1.00	1.29	1	1
1:A:10:LEU:CD1	1:A:10:LEU:HG	0.98	1.58	1	1
1:A:14:SER:OG	1:A:14:SER:CB	0.95	0.66	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD12	0.95	1.48	1	1
1:A:17:GLN:CD	1:A:17:GLN:HG2	0.93	1.37	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD11	0.93	1.48	1	1
1:A:13:ARG:CD	1:A:13:ARG:HG2	0.92	1.45	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD13	0.91	1.48	1	1
1:A:17:GLN:CD	1:A:17:GLN:HG3	0.91	1.37	1	1
1:A:18:ALA:CB	1:A:18:ALA:HA	0.90	1.46	1	1
1:A:18:ALA:O	1:A:18:ALA:CA	0.90	0.60	1	1
1:A:13:ARG:CD	1:A:13:ARG:CG	0.89	0.90	1	1
1:A:13:ARG:CD	1:A:13:ARG:HG3	0.89	1.45	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD22	0.88	1.43	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD23	0.88	1.43	1	1
1:A:10:LEU:CG	1:A:10:LEU:HD21	0.87	1.43	1	1
1:A:12:ASN:OD1	1:A:12:ASN:ND2	0.87	0.73	1	1
1:A:17:GLN:CD	1:A:17:GLN:CG	0.86	0.81	1	1
1:A:10:LEU:CD1	1:A:10:LEU:CG	0.84	0.84	1	1
1:A:18:ALA:HB2	1:A:18:ALA:CA	0.83	1.37	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:ARG:NE	1:A:13:ARG:HD2	0.83	1.28	1	1
1:A:12:ASN:CG	1:A:12:ASN:HD21	0.82	1.43	1	1
1:A:12:ASN:ND2	1:A:12:ASN:CG	0.82	0.79	1	1
1:A:18:ALA:HB3	1:A:18:ALA:CA	0.81	1.37	1	1
1:A:13:ARG:CG	1:A:13:ARG:HD2	0.81	1.42	1	1
1:A:12:ASN:CG	1:A:12:ASN:HD22	0.79	1.43	1	1
1:A:18:ALA:HB3	1:A:18:ALA:C	0.78	1.29	1	1
1:A:18:ALA:O	1:A:18:ALA:HB1	0.78	1.02	1	1
1:A:10:LEU:CD2	1:A:10:LEU:CG	0.77	0.77	1	1
1:A:12:ASN:OD1	1:A:12:ASN:CG	0.75	0.56	1	1
1:A:13:ARG:NE	1:A:13:ARG:HD3	0.74	1.28	1	1
1:A:13:ARG:CG	1:A:13:ARG:HD3	0.73	1.42	1	1
1:A:18:ALA:CB	1:A:18:ALA:CA	0.70	0.70	1	1
1:A:18:ALA:C	1:A:18:ALA:HB1	0.70	1.14	1	1
1:A:13:ARG:CZ	1:A:13:ARG:HH12	0.69	1.39	1	1
1:A:9:ARG:CZ	1:A:9:ARG:HH21	0.68	1.38	1	1
1:A:18:ALA:CB	1:A:18:ALA:C	0.68	0.71	1	1
1:A:9:ARG:CZ	1:A:9:ARG:HH22	0.67	1.38	1	1
1:A:4:LEU:HD23	1:A:8:PHE:CD1	0.66	2.26	11	1
1:A:13:ARG:CZ	1:A:13:ARG:HH11	0.66	1.39	1	1
1:A:12:ASN:O	1:A:16:THR:HG23	0.59	1.96	15	1
1:A:10:LEU:CD2	1:A:10:LEU:HB3	0.59	2.18	1	1
1:A:17:GLN:CD	1:A:17:GLN:HE22	0.59	1.19	1	1
1:A:17:GLN:O	1:A:18:ALA:HB3	0.59	1.97	20	5
1:A:13:ARG:CZ	1:A:13:ARG:NH1	0.59	0.74	1	1
1:A:9:ARG:CZ	1:A:9:ARG:NH2	0.58	0.73	1	1
1:A:17:GLN:CD	1:A:17:GLN:HE21	0.58	1.19	1	1
1:A:17:GLN:O	1:A:18:ALA:HB2	0.58	1.98	16	1
1:A:9:ARG:CZ	1:A:9:ARG:HH11	0.57	1.27	1	1
1:A:9:ARG:CZ	1:A:9:ARG:HH12	0.56	1.27	1	1
1:A:14:SER:CB	1:A:14:SER:HG	0.52	1.23	1	1
1:A:10:LEU:O	1:A:14:SER:CB	0.52	2.57	8	1
1:A:11:PHE:O	1:A:15:PHE:CB	0.52	2.57	6	1
1:A:15:PHE:CD1	1:A:15:PHE:C	0.52	2.82	7	1
1:A:14:SER:O	1:A:18:ALA:N	0.51	2.44	20	3
1:A:7:PHE:O	1:A:11:PHE:CD1	0.50	2.64	6	1
1:A:6:THR:O	1:A:9:ARG:N	0.49	2.45	4	22
1:A:4:LEU:HD23	1:A:8:PHE:HD1	0.48	1.67	11	1
1:A:13:ARG:CZ	1:A:13:ARG:HH22	0.47	1.18	1	1
1:A:4:LEU:CD1	1:A:4:LEU:N	0.46	2.78	22	1
1:A:13:ARG:CZ	1:A:13:ARG:HH21	0.46	1.18	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:PHE:CE2	1:A:11:PHE:CZ	0.46	3.04	6	1
1:A:13:ARG:O	1:A:16:THR:OG1	0.46	2.34	15	1
1:A:17:GLN:CD	1:A:17:GLN:NE2	0.45	0.50	1	1
1:A:9:ARG:O	1:A:13:ARG:CG	0.45	2.65	3	2
1:A:7:PHE:O	1:A:11:PHE:HB2	0.45	2.12	1	1
1:A:9:ARG:CZ	1:A:9:ARG:NH1	0.45	0.60	1	1
1:A:6:THR:O	1:A:7:PHE:C	0.44	2.56	8	22
1:A:15:PHE:O	1:A:15:PHE:CD1	0.44	2.70	17	1
1:A:4:LEU:HD13	1:A:7:PHE:HB3	0.44	1.90	13	1
1:A:9:ARG:O	1:A:13:ARG:HG2	0.44	2.13	8	1
1:A:13:ARG:O	1:A:17:GLN:CB	0.43	2.67	13	1
1:A:13:ARG:CD	1:A:13:ARG:NE	0.43	0.69	1	1
1:A:10:LEU:O	1:A:14:SER:HB2	0.43	2.13	1	1
1:A:12:ASN:O	1:A:16:THR:OG1	0.43	2.36	9	1
1:A:10:LEU:HA	1:A:13:ARG:CG	0.43	2.42	8	1
1:A:5:SER:OG	1:A:6:THR:N	0.43	2.50	14	3
1:A:15:PHE:O	1:A:16:THR:C	0.43	2.57	22	3
1:A:9:ARG:O	1:A:13:ARG:HG3	0.42	2.14	3	1
1:A:4:LEU:N	1:A:4:LEU:HD12	0.42	2.28	22	1
1:A:10:LEU:O	1:A:14:SER:HB3	0.42	2.14	8	1
1:A:16:THR:O	1:A:17:GLN:C	0.42	2.57	17	2
1:A:17:GLN:O	1:A:18:ALA:CB	0.41	2.65	16	1
1:A:9:ARG:O	1:A:13:ARG:HB2	0.41	2.15	18	1
1:A:15:PHE:O	1:A:17:GLN:N	0.41	2.53	22	1
1:A:4:LEU:CD1	1:A:7:PHE:HB3	0.41	2.46	13	1
1:A:4:LEU:O	1:A:8:PHE:CD1	0.41	2.74	18	1
1:A:13:ARG:CD	1:A:13:ARG:HH21	0.40	1.58	1	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	15/19 (79%)	12±1 (82±7%)	2±1 (16±6%)	0±0 (2±3%)	10	50
All	All	330/418 (79%)	270 (82%)	53 (16%)	7 (2%)	10	50

All 4 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	18	ALA	4
1	A	4	LEU	1
1	A	16	THR	1
1	A	17	GLN	1

6.3.2 Protein sidechains ⓘ

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	14/16 (88%)	8±1 (55±9%)	6±1 (45±9%)	0	2
All	All	308/352 (88%)	168 (55%)	140 (45%)	0	2

All 14 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	6	THR	22
1	A	13	ARG	16
1	A	10	LEU	13
1	A	4	LEU	12
1	A	8	PHE	11
1	A	11	PHE	11
1	A	9	ARG	11
1	A	7	PHE	10
1	A	15	PHE	10
1	A	5	SER	7
1	A	14	SER	5
1	A	17	GLN	5
1	A	16	THR	4
1	A	12	ASN	3

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 ⓘ

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	17:GLN	C	18:ALA	N	0.94
1	A	2:GLY	C	3:THR	N	0.63
1	A	3:THR	C	4:LEU	N	0.52
1	A	1:SER	C	2:GLY	N	0.44
1	A	18:ALA	C	19:NH2	N	0.17

7 Chemical shift validation ⓘ

No chemical shift data were provided