



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 10:46 PM UTC

PDB ID : 6TF4 / pdb_00006tf4
BMRB ID : 34450
Title : Solution structure of RfaH C-terminal domain from *Vibrio cholerae*
Authors : Zuber, P.K.; Schweimer, K.; Knauer, S.H.
Deposited on : 2019-11-13

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

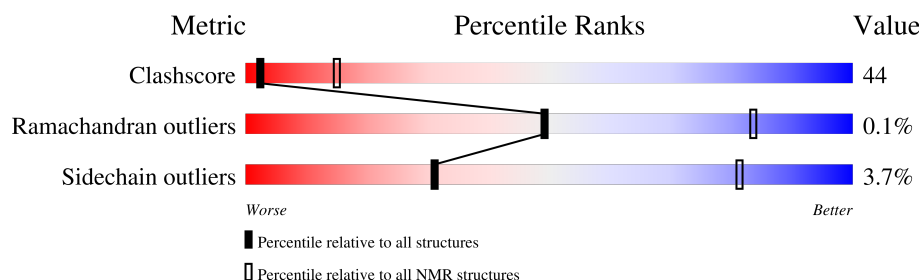
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	67	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:112-A:165 (54)	0.43	3

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 2 clusters and 14 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 900 atoms, of which 452 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription/translation regulatory transformer protein RfaH.

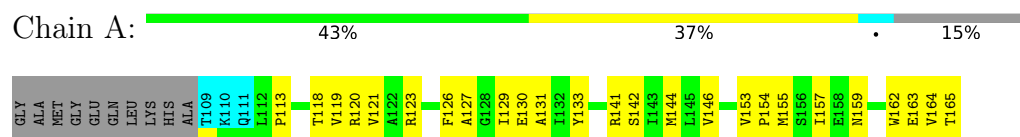
Mol	Chain	Residues	Atoms							Trace
1	A	57	Total	C	H	N	O	S		0
			900	280	452	76	89	3		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	GLY	-	expression tag	UNP A0A557GAU8
A	100	ALA	-	expression tag	UNP A0A557GAU8
A	101	MET	-	expression tag	UNP A0A557GAU8
A	102	GLY	-	expression tag	UNP A0A557GAU8

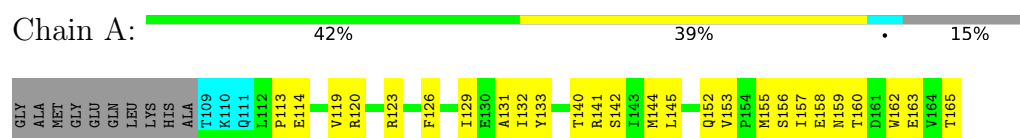
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



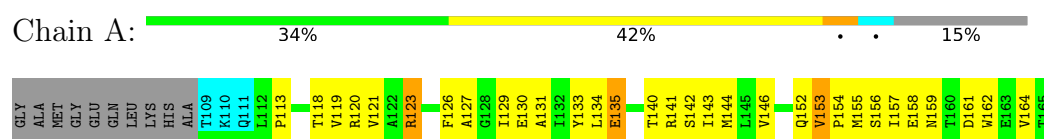
4.2.4 Score per residue for model 4

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



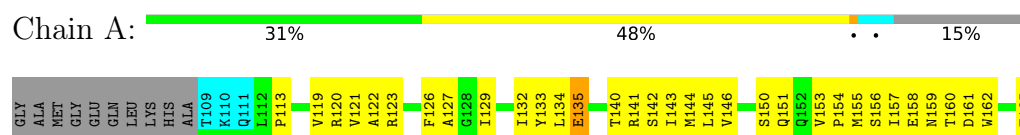
4.2.5 Score per residue for model 5

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



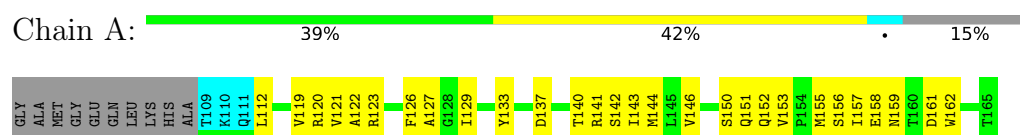
4.2.6 Score per residue for model 6

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



4.2.7 Score per residue for model 7

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



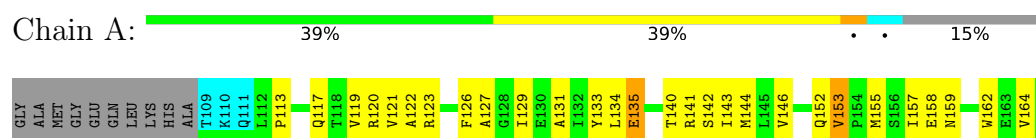
4.2.8 Score per residue for model 8

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



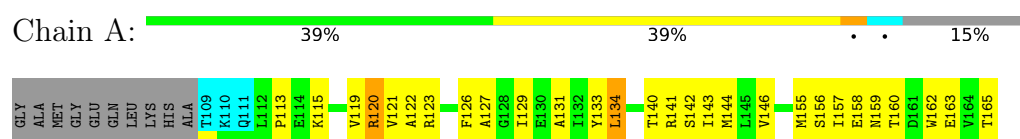
4.2.9 Score per residue for model 9

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



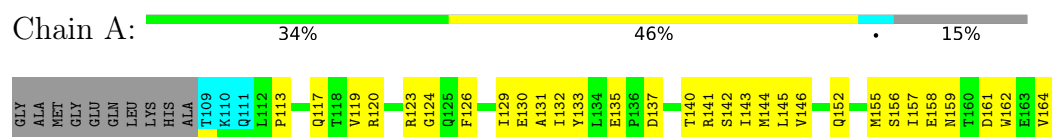
4.2.10 Score per residue for model 10

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



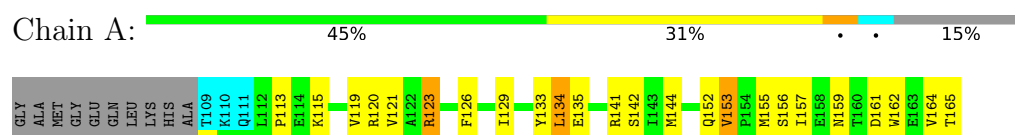
4.2.11 Score per residue for model 11

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



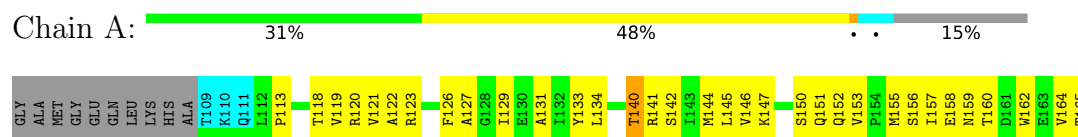
4.2.12 Score per residue for model 12

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



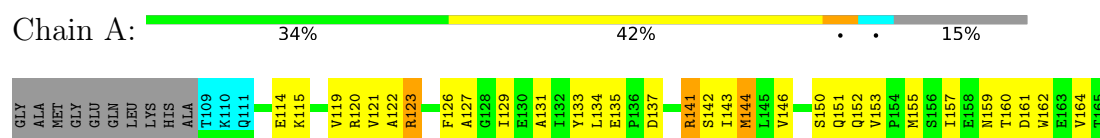
4.2.13 Score per residue for model 13

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



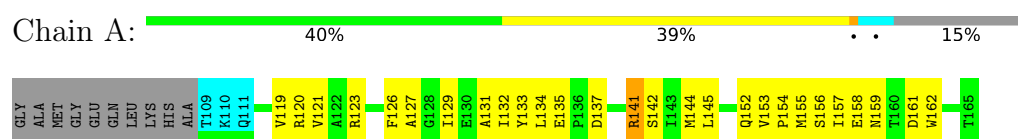
4.2.14 Score per residue for model 14

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



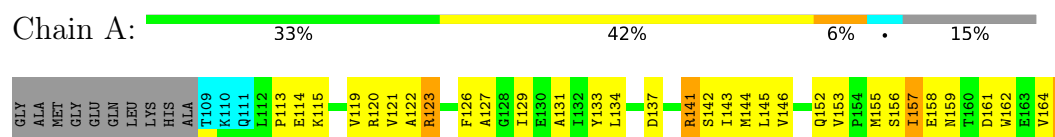
4.2.15 Score per residue for model 15

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



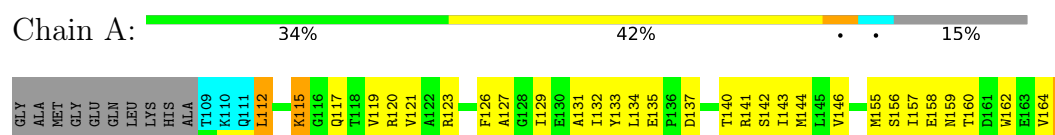
4.2.16 Score per residue for model 16

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



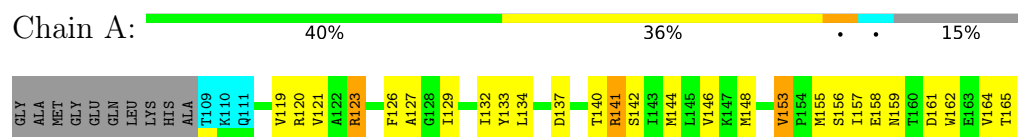
4.2.17 Score per residue for model 17

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



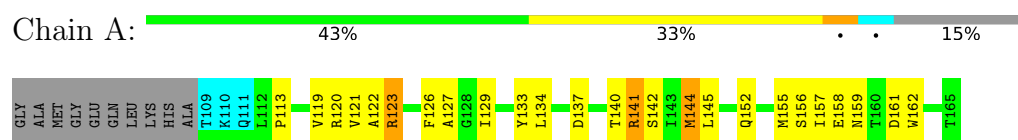
4.2.18 Score per residue for model 18

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



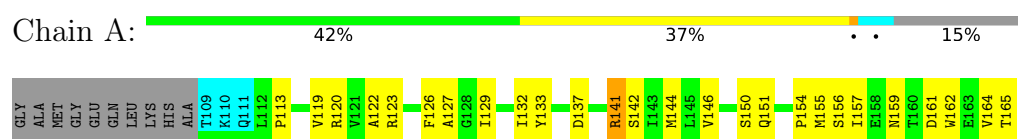
4.2.19 Score per residue for model 19

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



4.2.20 Score per residue for model 20

- Molecule 1: Transcription/translation regulatory transformer protein RfaH



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	v1.2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	831
Number of shifts mapped to atoms	723
Number of unparsed shifts	0
Number of shifts with mapping errors	108
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	3.0±0.2
All	All	0	59

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	120	ARG	Sidechain	20
1	A	141	ARG	Sidechain	20
1	A	123	ARG	Sidechain	19

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	423	424	424	37±6
All	All	8460	8480	8480	744

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 44.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:TYR:O	1:A:134:LEU:HD23	0.93	1.63	5	3
1:A:119:VAL:HG11	1:A:144:MET:CE	0.93	1.93	13	7
1:A:144:MET:HE1	1:A:162:TRP:CD1	0.91	2.00	11	6
1:A:126:PHE:CE1	1:A:155:MET:HE1	0.90	2.00	9	6
1:A:133:TYR:C	1:A:134:LEU:HD12	0.90	1.92	15	3
1:A:119:VAL:HG21	1:A:144:MET:CE	0.88	1.98	7	6
1:A:119:VAL:HG11	1:A:144:MET:HE2	0.87	1.44	3	7
1:A:119:VAL:HG11	1:A:144:MET:SD	0.85	2.11	8	6
1:A:126:PHE:CE2	1:A:155:MET:HE1	0.84	2.07	2	5
1:A:126:PHE:O	1:A:129:ILE:HG22	0.83	1.72	19	19
1:A:126:PHE:CZ	1:A:155:MET:HE1	0.82	2.10	10	10
1:A:122:ALA:O	1:A:127:ALA:HB1	0.78	1.77	8	11
1:A:126:PHE:CD2	1:A:129:ILE:HD12	0.78	2.14	5	1
1:A:146:VAL:HG21	1:A:155:MET:HE3	0.76	1.57	1	8
1:A:118:THR:HG21	1:A:130:GLU:OE1	0.75	1.82	5	1
1:A:119:VAL:HG23	1:A:164:VAL:HG12	0.74	1.59	13	4
1:A:119:VAL:HG21	1:A:144:MET:HE2	0.73	1.59	7	3
1:A:134:LEU:C	1:A:134:LEU:HD13	0.73	2.08	9	1
1:A:133:TYR:O	1:A:134:LEU:HD12	0.73	1.81	6	5
1:A:145:LEU:C	1:A:145:LEU:HD13	0.71	2.11	13	1
1:A:146:VAL:HG21	1:A:155:MET:SD	0.71	2.24	13	2
1:A:117:GLN:NE2	1:A:164:VAL:HG11	0.71	2.00	9	2
1:A:156:SER:O	1:A:157:ILE:HD13	0.70	1.86	20	7
1:A:144:MET:HE1	1:A:162:TRP:CG	0.70	2.21	11	6
1:A:157:ILE:HG22	1:A:161:ASP:HB2	0.69	1.64	7	7
1:A:119:VAL:HG12	1:A:131:ALA:O	0.68	1.89	17	12
1:A:144:MET:HE1	1:A:162:TRP:CD2	0.67	2.24	7	11
1:A:146:VAL:HG21	1:A:155:MET:CG	0.67	2.20	6	3
1:A:113:PRO:HB3	1:A:164:VAL:HG11	0.66	1.67	5	3
1:A:126:PHE:CZ	1:A:155:MET:HE2	0.66	2.25	6	1
1:A:117:GLN:NE2	1:A:164:VAL:HG21	0.65	2.07	9	1
1:A:119:VAL:CG2	1:A:164:VAL:HG12	0.64	2.21	13	4
1:A:126:PHE:CZ	1:A:155:MET:CE	0.64	2.81	3	9
1:A:164:VAL:C	1:A:165:THR:HG22	0.64	2.17	2	1
1:A:145:LEU:HD21	1:A:152:GLN:CD	0.64	2.17	4	1
1:A:144:MET:CE	1:A:162:TRP:CE2	0.63	2.81	16	9
1:A:144:MET:CE	1:A:162:TRP:CD1	0.63	2.80	10	5
1:A:113:PRO:HB3	1:A:164:VAL:HG21	0.63	1.71	8	1
1:A:153:VAL:HG13	1:A:153:VAL:O	0.63	1.93	16	1
1:A:145:LEU:HD21	1:A:152:GLN:CG	0.62	2.24	4	1
1:A:148:MET:SD	1:A:153:VAL:HG21	0.62	2.34	18	1
1:A:119:VAL:HG23	1:A:164:VAL:CG1	0.62	2.25	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:VAL:HG21	1:A:162:TRP:CE3	0.61	2.29	2	6
1:A:117:GLN:HE22	1:A:164:VAL:HG21	0.61	1.56	9	1
1:A:144:MET:HE1	1:A:162:TRP:CE2	0.60	2.30	16	1
1:A:145:LEU:HD21	1:A:152:GLN:HB3	0.60	1.72	19	2
1:A:129:ILE:CD1	1:A:146:VAL:HG11	0.59	2.27	17	2
1:A:146:VAL:HG21	1:A:155:MET:CE	0.59	2.26	1	7
1:A:119:VAL:HG23	1:A:163:GLU:O	0.59	1.97	1	4
1:A:157:ILE:HG22	1:A:161:ASP:CB	0.59	2.27	15	4
1:A:121:VAL:HG22	1:A:162:TRP:HB3	0.59	1.75	5	3
1:A:159:ASN:OD1	1:A:162:TRP:CH2	0.58	2.56	18	3
1:A:146:VAL:CG2	1:A:155:MET:CG	0.57	2.81	6	2
1:A:137:ASP:CB	1:A:143:ILE:HD11	0.57	2.29	11	3
1:A:162:TRP:CE3	1:A:162:TRP:O	0.57	2.57	1	4
1:A:144:MET:SD	1:A:162:TRP:CD1	0.57	2.98	3	8
1:A:162:TRP:O	1:A:162:TRP:CE3	0.57	2.57	9	16
1:A:126:PHE:CZ	1:A:155:MET:SD	0.57	2.98	9	14
1:A:113:PRO:O	1:A:133:TYR:CE2	0.57	2.58	9	1
1:A:126:PHE:CE1	1:A:155:MET:SD	0.57	2.98	7	2
1:A:134:LEU:C	1:A:134:LEU:HD23	0.56	2.26	18	1
1:A:153:VAL:HG23	1:A:153:VAL:O	0.56	1.98	8	2
1:A:126:PHE:CD2	1:A:129:ILE:HD13	0.55	2.37	6	6
1:A:123:ARG:C	1:A:127:ALA:HB2	0.55	2.25	16	1
1:A:133:TYR:C	1:A:134:LEU:HD23	0.55	2.25	5	1
1:A:121:VAL:HG12	1:A:127:ALA:HA	0.55	1.77	7	11
1:A:153:VAL:HG23	1:A:154:PRO:HD2	0.54	1.79	6	2
1:A:165:THR:O	1:A:165:THR:HG23	0.54	2.02	11	1
1:A:146:VAL:HG21	1:A:155:MET:HB2	0.54	1.79	5	2
1:A:152:GLN:C	1:A:153:VAL:CG2	0.53	2.82	9	2
1:A:144:MET:HE2	1:A:162:TRP:NE1	0.53	2.19	10	3
1:A:139:ASP:OD2	1:A:140:THR:HG23	0.53	2.04	2	1
1:A:144:MET:SD	1:A:157:ILE:HD12	0.53	2.44	14	2
1:A:144:MET:CE	1:A:162:TRP:CD2	0.53	2.92	3	5
1:A:119:VAL:HG23	1:A:164:VAL:HG22	0.53	1.81	9	1
1:A:133:TYR:CE1	1:A:142:SER:HB3	0.53	2.39	11	3
1:A:134:LEU:CB	1:A:143:ILE:O	0.53	2.57	14	2
1:A:140:THR:O	1:A:158:GLU:CB	0.53	2.57	10	11
1:A:133:TYR:CE2	1:A:142:SER:HB3	0.53	2.40	2	2
1:A:134:LEU:C	1:A:134:LEU:CD2	0.53	2.82	18	1
1:A:126:PHE:HD2	1:A:129:ILE:HD13	0.52	1.64	6	4
1:A:144:MET:HE2	1:A:162:TRP:CD1	0.52	2.39	10	2
1:A:119:VAL:HG12	1:A:164:VAL:HG12	0.52	1.79	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:PRO:HG2	1:A:133:TYR:CE2	0.52	2.39	8	9
1:A:119:VAL:HG11	1:A:144:MET:HE1	0.52	1.80	4	3
1:A:145:LEU:C	1:A:145:LEU:CD1	0.52	2.81	13	1
1:A:133:TYR:CE1	1:A:142:SER:HB2	0.52	2.40	4	4
1:A:150:SER:O	1:A:151:GLN:NE2	0.52	2.43	20	3
1:A:133:TYR:CE2	1:A:142:SER:HB2	0.52	2.40	8	10
1:A:119:VAL:HG21	1:A:144:MET:SD	0.52	2.45	5	2
1:A:113:PRO:HG2	1:A:133:TYR:CD2	0.52	2.40	2	6
1:A:129:ILE:HD11	1:A:146:VAL:HG11	0.51	1.83	17	1
1:A:159:ASN:HA	1:A:162:TRP:CE2	0.51	2.39	16	20
1:A:159:ASN:HA	1:A:162:TRP:CZ2	0.51	2.39	18	13
1:A:153:VAL:HG12	1:A:154:PRO:HD2	0.51	1.82	5	1
1:A:144:MET:SD	1:A:162:TRP:NE1	0.51	2.84	11	1
1:A:153:VAL:O	1:A:153:VAL:CG1	0.51	2.58	16	1
1:A:157:ILE:HB	1:A:162:TRP:CD1	0.51	2.40	20	20
1:A:162:TRP:C	1:A:162:TRP:CE3	0.51	2.89	16	1
1:A:126:PHE:O	1:A:129:ILE:CG2	0.51	2.57	6	17
1:A:126:PHE:HE2	1:A:146:VAL:HG11	0.51	1.66	5	1
1:A:161:ASP:OD1	1:A:162:TRP:N	0.51	2.43	16	1
1:A:133:TYR:CZ	1:A:142:SER:HB3	0.50	2.41	17	3
1:A:118:THR:CG2	1:A:130:GLU:OE1	0.50	2.57	5	2
1:A:119:VAL:HG22	1:A:162:TRP:HB2	0.50	1.84	1	1
1:A:133:TYR:CE2	1:A:144:MET:HE2	0.50	2.42	16	1
1:A:159:ASN:HA	1:A:162:TRP:CD2	0.50	2.42	16	9
1:A:134:LEU:N	1:A:143:ILE:O	0.50	2.43	10	3
1:A:146:VAL:CG2	1:A:155:MET:SD	0.49	2.98	13	1
1:A:153:VAL:O	1:A:153:VAL:CG2	0.49	2.61	8	1
1:A:133:TYR:CZ	1:A:142:SER:HB2	0.49	2.43	6	7
1:A:159:ASN:OD1	1:A:160:THR:N	0.49	2.46	17	6
1:A:164:VAL:O	1:A:165:THR:HG23	0.49	2.07	16	1
1:A:140:THR:O	1:A:158:GLU:CG	0.49	2.60	1	5
1:A:159:ASN:O	1:A:162:TRP:O	0.49	2.31	6	19
1:A:145:LEU:C	1:A:145:LEU:HD23	0.49	2.33	19	3
1:A:152:GLN:C	1:A:153:VAL:CG1	0.49	2.85	13	3
1:A:152:GLN:C	1:A:153:VAL:HG13	0.49	2.32	14	3
1:A:115:LYS:CD	1:A:134:LEU:O	0.48	2.60	17	1
1:A:158:GLU:CD	1:A:160:THR:HG1	0.48	2.15	17	1
1:A:152:GLN:O	1:A:153:VAL:HG13	0.48	2.08	7	2
1:A:164:VAL:O	1:A:165:THR:CB	0.48	2.59	2	1
1:A:119:VAL:CG1	1:A:164:VAL:HG12	0.48	2.38	5	1
1:A:129:ILE:HD11	1:A:146:VAL:CG1	0.48	2.38	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:GLN:O	1:A:153:VAL:CG2	0.48	2.62	15	1
1:A:133:TYR:CD2	1:A:144:MET:HE2	0.48	2.43	16	1
1:A:113:PRO:HG2	1:A:133:TYR:CG	0.48	2.44	16	4
1:A:152:GLN:O	1:A:153:VAL:CG1	0.48	2.62	14	3
1:A:113:PRO:HG2	1:A:133:TYR:CZ	0.48	2.44	4	8
1:A:114:GLU:O	1:A:115:LYS:C	0.48	2.57	14	3
1:A:119:VAL:CG1	1:A:144:MET:SD	0.48	2.98	2	3
1:A:142:SER:N	1:A:157:ILE:O	0.48	2.46	14	2
1:A:159:ASN:HA	1:A:162:TRP:CH2	0.48	2.43	20	7
1:A:142:SER:O	1:A:157:ILE:N	0.48	2.43	14	2
1:A:135:GLU:O	1:A:143:ILE:N	0.48	2.47	6	2
1:A:122:ALA:O	1:A:127:ALA:CB	0.47	2.59	8	2
1:A:143:ILE:CD1	1:A:156:SER:OG	0.47	2.63	16	1
1:A:129:ILE:CD1	1:A:146:VAL:CG1	0.47	2.92	17	2
1:A:146:VAL:HG21	1:A:155:MET:HG3	0.47	1.86	6	1
1:A:135:GLU:HG3	1:A:143:ILE:CG1	0.47	2.40	9	1
1:A:146:VAL:HG21	1:A:155:MET:CB	0.47	2.39	6	2
1:A:143:ILE:CD1	1:A:156:SER:CB	0.47	2.92	6	1
1:A:132:ILE:O	1:A:134:LEU:CD1	0.47	2.62	15	1
1:A:119:VAL:HG22	1:A:131:ALA:O	0.47	2.09	15	2
1:A:152:GLN:C	1:A:153:VAL:HG23	0.47	2.35	15	1
1:A:123:ARG:N	1:A:161:ASP:O	0.46	2.43	2	2
1:A:143:ILE:HD12	1:A:156:SER:OG	0.46	2.10	16	1
1:A:158:GLU:CD	1:A:160:THR:OG1	0.46	2.58	17	1
1:A:113:PRO:CG	1:A:133:TYR:CD2	0.46	2.99	5	1
1:A:119:VAL:HG21	1:A:144:MET:HE1	0.46	1.87	15	4
1:A:137:ASP:HB2	1:A:143:ILE:CG1	0.46	2.41	17	4
1:A:137:ASP:HB2	1:A:143:ILE:HD11	0.46	1.88	11	1
1:A:144:MET:HE3	1:A:162:TRP:CE2	0.46	2.45	12	5
1:A:143:ILE:CD1	1:A:156:SER:HB3	0.46	2.41	6	3
1:A:113:PRO:HG2	1:A:133:TYR:CD1	0.46	2.46	10	1
1:A:134:LEU:HD13	1:A:135:GLU:HB3	0.46	1.85	9	1
1:A:145:LEU:HD21	1:A:152:GLN:OE1	0.46	2.11	11	1
1:A:158:GLU:O	1:A:161:ASP:N	0.46	2.44	18	1
1:A:134:LEU:C	1:A:134:LEU:CD1	0.46	2.80	9	1
1:A:154:PRO:O	1:A:155:MET:SD	0.45	2.75	20	2
1:A:158:GLU:O	1:A:161:ASP:CG	0.45	2.59	16	1
1:A:143:ILE:HD13	1:A:156:SER:CB	0.45	2.42	17	1
1:A:133:TYR:CE2	1:A:142:SER:OG	0.45	2.58	5	1
1:A:126:PHE:CD2	1:A:129:ILE:CD1	0.45	2.95	5	1
1:A:123:ARG:O	1:A:161:ASP:O	0.45	2.34	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:VAL:CG1	1:A:127:ALA:HA	0.45	2.42	16	1
1:A:158:GLU:OE1	1:A:160:THR:OG1	0.45	2.33	17	1
1:A:164:VAL:O	1:A:165:THR:O	0.45	2.34	17	1
1:A:113:PRO:HG2	1:A:133:TYR:CE1	0.45	2.46	13	4
1:A:157:ILE:CG2	1:A:161:ASP:CB	0.44	2.95	7	1
1:A:158:GLU:O	1:A:159:ASN:C	0.44	2.59	18	2
1:A:121:VAL:HG23	1:A:129:ILE:O	0.44	2.12	2	2
1:A:133:TYR:O	1:A:134:LEU:CD1	0.44	2.62	6	1
1:A:164:VAL:C	1:A:165:THR:OG1	0.44	2.57	16	1
1:A:121:VAL:HG21	1:A:129:ILE:CG2	0.44	2.43	15	3
1:A:140:THR:O	1:A:158:GLU:HG3	0.44	2.12	17	1
1:A:119:VAL:HG11	1:A:144:MET:HE3	0.44	1.90	11	1
1:A:132:ILE:O	1:A:145:LEU:N	0.43	2.49	6	1
1:A:121:VAL:CG1	1:A:126:PHE:O	0.43	2.65	10	2
1:A:162:TRP:CE3	1:A:162:TRP:C	0.43	2.96	8	6
1:A:158:GLU:C	1:A:162:TRP:NE1	0.43	2.76	16	1
1:A:130:GLU:O	1:A:146:VAL:HG13	0.43	2.12	11	1
1:A:137:ASP:HB2	1:A:143:ILE:CD1	0.43	2.43	11	1
1:A:137:ASP:O	1:A:141:ARG:O	0.43	2.37	19	2
1:A:129:ILE:HG21	1:A:146:VAL:HG13	0.43	1.91	5	1
1:A:113:PRO:O	1:A:133:TYR:CD2	0.43	2.72	9	1
1:A:137:ASP:O	1:A:141:ARG:CB	0.43	2.66	18	3
1:A:126:PHE:CD1	1:A:129:ILE:HD13	0.43	2.49	7	2
1:A:148:MET:SD	1:A:153:VAL:CG2	0.43	3.05	18	1
1:A:126:PHE:CD1	1:A:157:ILE:HD11	0.43	2.49	20	1
1:A:143:ILE:HD13	1:A:156:SER:OG	0.43	2.14	10	1
1:A:146:VAL:HB	1:A:155:MET:HE2	0.43	1.91	10	1
1:A:119:VAL:HG23	1:A:164:VAL:CG2	0.43	2.43	9	1
1:A:142:SER:O	1:A:156:SER:HA	0.42	2.14	17	5
1:A:153:VAL:CG2	1:A:154:PRO:HD2	0.42	2.43	6	1
1:A:142:SER:HG	1:A:162:TRP:HZ2	0.42	1.55	3	1
1:A:140:THR:O	1:A:158:GLU:HB3	0.42	2.15	9	11
1:A:126:PHE:CE2	1:A:146:VAL:HG11	0.42	2.49	5	2
1:A:123:ARG:HG2	1:A:124:GLY:N	0.42	2.29	11	1
1:A:134:LEU:O	1:A:135:GLU:CD	0.42	2.62	2	1
1:A:126:PHE:HD1	1:A:129:ILE:HG21	0.42	1.75	10	1
1:A:133:TYR:CE2	1:A:142:SER:CB	0.42	3.03	17	2
1:A:132:ILE:O	1:A:144:MET:HA	0.42	2.15	6	7
1:A:115:LYS:CB	1:A:134:LEU:O	0.41	2.68	10	1
1:A:115:LYS:HE2	1:A:134:LEU:HD13	0.41	1.91	12	1
1:A:152:GLN:O	1:A:153:VAL:HG23	0.41	2.15	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:SER:C	1:A:151:GLN:HG3	0.41	2.41	14	4
1:A:153:VAL:CG1	1:A:154:PRO:HD2	0.41	2.44	5	1
1:A:137:ASP:CB	1:A:143:ILE:CD1	0.41	2.99	11	1
1:A:153:VAL:HG13	1:A:154:PRO:HD2	0.41	1.91	15	1
1:A:137:ASP:O	1:A:141:ARG:HB2	0.41	2.16	16	2
1:A:164:VAL:HG22	1:A:165:THR:N	0.41	2.30	3	1
1:A:145:LEU:HD21	1:A:152:GLN:NE2	0.41	2.30	4	1
1:A:117:GLN:NE2	1:A:164:VAL:CG1	0.41	2.80	9	1
1:A:121:VAL:HB	1:A:126:PHE:O	0.41	2.16	16	2
1:A:134:LEU:HB3	1:A:143:ILE:O	0.41	2.16	8	1
1:A:152:GLN:O	1:A:153:VAL:HG22	0.41	2.15	9	1
1:A:122:ALA:C	1:A:127:ALA:HB1	0.41	2.39	13	1
1:A:121:VAL:HA	1:A:162:TRP:CB	0.41	2.46	17	1
1:A:134:LEU:HD23	1:A:134:LEU:O	0.41	2.15	18	1
1:A:114:GLU:N	1:A:114:GLU:OE2	0.41	2.54	4	1
1:A:164:VAL:C	1:A:165:THR:HG1	0.41	2.23	16	1
1:A:140:THR:O	1:A:158:GLU:HG2	0.40	2.16	13	3
1:A:147:LYS:HD3	1:A:152:GLN:NE2	0.40	2.31	13	1
1:A:144:MET:CE	1:A:162:TRP:NE1	0.40	2.84	17	1
1:A:133:TYR:CE1	1:A:142:SER:CB	0.40	3.04	11	1
1:A:142:SER:C	1:A:143:ILE:HD13	0.40	2.41	5	1
1:A:120:ARG:O	1:A:120:ARG:CG	0.40	2.70	10	1
1:A:135:GLU:O	1:A:143:ILE:HG12	0.40	2.17	17	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	53/67 (79%)	50±1 (95±1%)	3±1 (5±1%)	0±0 (0±0%)	49	83
All	All	1060/1340 (79%)	1007 (95%)	52 (5%)	1 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	112	LEU	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	47/56 (84%)	45±1 (96±2%)	2±1 (4±2%)	31	81
All	All	940/1120 (84%)	905 (96%)	35 (4%)	31	81

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	165	THR	11
1	A	135	GLU	9
1	A	153	VAL	4
1	A	144	MET	3
1	A	118	THR	2
1	A	134	LEU	2
1	A	112	LEU	1
1	A	140	THR	1
1	A	157	ILE	1
1	A	115	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 92% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *vcrfah-ctd.bmrB*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	831
Number of shifts mapped to atoms	723
Number of unparsed shifts	0
Number of shifts with mapping errors	108
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 108 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	99	GLY	C	172.16	0.20	1
1	A	100	ALA	HA	4.37	0.03	1
1	A	100	ALA	HB1	1.4	0.03	1
1	A	100	ALA	HB2	1.4	0.03	1
1	A	100	ALA	HB3	1.4	0.03	1
1	A	100	ALA	C	178.02	0.20	1
1	A	100	ALA	CA	52.62	0.20	1
1	A	100	ALA	CB	19.43	0.20	1
1	A	100	ALA	N	123.89	0.20	1
1	A	101	MET	H	8.59	0.03	1
1	A	101	MET	HA	4.49	0.03	1
1	A	101	MET	HB2	2.12	0.03	2
1	A	101	MET	HB3	2.05	0.03	2
1	A	101	MET	HE1	2.11	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	MET	HE2	2.11	0.03	1
1	A	101	MET	HE3	2.11	0.03	1
1	A	101	MET	HG2	2.64	0.03	2
1	A	101	MET	HG3	2.58	0.03	2
1	A	101	MET	C	176.95	0.20	1
1	A	101	MET	CA	55.83	0.20	1
1	A	101	MET	CB	32.77	0.20	1
1	A	101	MET	CE	16.93	0.20	1
1	A	101	MET	CG	32.05	0.20	1
1	A	101	MET	N	119.96	0.20	1
1	A	102	GLY	H	8.47	0.03	1
1	A	102	GLY	HA2	3.98	0.03	2
1	A	102	GLY	HA3	3.95	0.03	2
1	A	102	GLY	C	174.42	0.20	1
1	A	102	GLY	CA	45.47	0.20	1
1	A	102	GLY	N	110.25	0.20	1
1	A	103	GLU	H	8.31	0.03	1
1	A	103	GLU	HA	4.25	0.03	1
1	A	103	GLU	HB2	2.05	0.03	2
1	A	103	GLU	HB3	1.96	0.03	2
1	A	103	GLU	HG2	2.49	0.03	2
1	A	103	GLU	HG3	2.49	0.03	2
1	A	103	GLU	C	176.74	0.20	1
1	A	103	GLU	CA	56.9	0.20	1
1	A	103	GLU	CB	30.3	0.20	1
1	A	103	GLU	CG	36.94	0.20	1
1	A	103	GLU	N	120.97	0.20	1
1	A	104	GLN	H	8.49	0.03	1
1	A	104	GLN	HA	4.28	0.03	1
1	A	104	GLN	HB2	2.1	0.03	2
1	A	104	GLN	HB3	2.0	0.03	2
1	A	104	GLN	HG2	2.33	0.03	2
1	A	104	GLN	HG3	2.33	0.03	2
1	A	104	GLN	C	176.08	0.20	1
1	A	104	GLN	CA	56.17	0.20	1
1	A	104	GLN	CB	29.26	0.20	1
1	A	104	GLN	CG	33.82	0.20	1
1	A	104	GLN	N	121.22	0.20	1
1	A	105	LEU	H	8.21	0.03	1
1	A	105	LEU	HA	4.3	0.03	1
1	A	105	LEU	HB2	1.61	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	105	LEU	HB3	1.51	0.03	2
1	A	105	LEU	HD11	0.86	0.03	1
1	A	105	LEU	HD12	0.86	0.03	1
1	A	105	LEU	HD13	0.86	0.03	1
1	A	105	LEU	HD21	0.92	0.03	1
1	A	105	LEU	HD22	0.92	0.03	1
1	A	105	LEU	HD23	0.92	0.03	1
1	A	105	LEU	HG	1.59	0.03	1
1	A	105	LEU	C	177.37	0.20	1
1	A	105	LEU	CA	55.4	0.20	1
1	A	105	LEU	CB	42.21	0.20	1
1	A	105	LEU	CD1	23.48	0.20	2
1	A	105	LEU	CD2	24.95	0.20	2
1	A	105	LEU	CG	27.05	0.20	1
1	A	105	LEU	N	123.11	0.20	1
1	A	106	LYS	H	8.21	0.03	1
1	A	106	LYS	HA	4.24	0.03	1
1	A	106	LYS	HB2	1.73	0.03	2
1	A	106	LYS	HB3	1.73	0.03	2
1	A	106	LYS	HD2	1.65	0.03	2
1	A	106	LYS	HD3	1.65	0.03	2
1	A	106	LYS	HE2	2.98	0.03	2
1	A	106	LYS	HE3	2.98	0.03	2
1	A	106	LYS	HG2	1.31	0.03	2
1	A	106	LYS	HG3	1.37	0.03	2
1	A	106	LYS	C	176.32	0.20	1
1	A	106	LYS	CA	56.39	0.20	1
1	A	106	LYS	CB	32.96	0.20	1
1	A	106	LYS	CD	29.07	0.20	1
1	A	106	LYS	CE	42.66	0.20	1
1	A	106	LYS	CG	24.68	0.20	1
1	A	106	LYS	N	121.8	0.20	1
1	A	107	HIS	H	8.25	0.03	1
1	A	107	HIS	HA	4.59	0.03	1
1	A	107	HIS	HB2	3.11	0.03	2
1	A	107	HIS	HB3	3.03	0.03	2
1	A	107	HIS	HD2	6.98	0.03	1
1	A	107	HIS	HE1	7.76	0.03	1
1	A	107	HIS	C	175.29	0.20	1
1	A	107	HIS	CA	56.23	0.20	1
1	A	107	HIS	CB	31.23	0.20	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	107	HIS	CD2	120.04	0.20	1
1	A	107	HIS	CE1	138.64	0.20	1
1	A	107	HIS	N	120.05	0.20	1
1	A	108	ALA	H	8.31	0.03	1
1	A	108	ALA	HA	4.37	0.03	1
1	A	108	ALA	HB1	1.38	0.03	1
1	A	108	ALA	HB2	1.38	0.03	1
1	A	108	ALA	HB3	1.38	0.03	1
1	A	108	ALA	C	177.74	0.20	1
1	A	108	ALA	CA	52.67	0.20	1
1	A	108	ALA	CB	19.42	0.20	1
1	A	108	ALA	N	125.36	0.20	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	66	-0.11 ± 0.37	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	61	0.15 ± 0.44	None needed (< 0.5 ppm)
$^{13}\text{C}'$	67	0.14 ± 0.23	None needed (< 0.5 ppm)
^{15}N	66	-0.14 ± 0.79	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 681 atoms were assigned a chemical shift out of a possible 738. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	268/268 (100%)	109/109 (100%)	108/108 (100%)	51/51 (100%)
Sidechain	383/439 (87%)	261/286 (91%)	121/137 (88%)	1/16 (6%)
Aromatic	30/31 (97%)	15/15 (100%)	14/15 (93%)	1/1 (100%)
Overall	681/738 (92%)	385/410 (94%)	243/260 (93%)	53/68 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 720 atoms were assigned a chemical shift out of a possible 782. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	283/283 (100%)	115/115 (100%)	114/114 (100%)	54/54 (100%)
Sidechain	407/468 (87%)	277/304 (91%)	129/146 (88%)	1/18 (6%)
Aromatic	30/31 (97%)	15/15 (100%)	14/15 (93%)	1/1 (100%)
Overall	720/782 (92%)	407/434 (94%)	257/275 (93%)	56/73 (77%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

