



Full wwPDB NMR Structure Validation Report ⓘ

Mar 29, 2026 – 03:38 AM UTC

PDB ID : 5V7Z / pdb_00005v7z
BMRB ID : 30273
Title : SSNMR Structure of the Human RIP1/RIP3 Necrosome
Authors : Mompean, M.; Li, W.; Li, J.; Laage, S.; Siemer, A.B.; Wu, H.; McDermott, A.E.
Deposited on : 2017-03-21

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

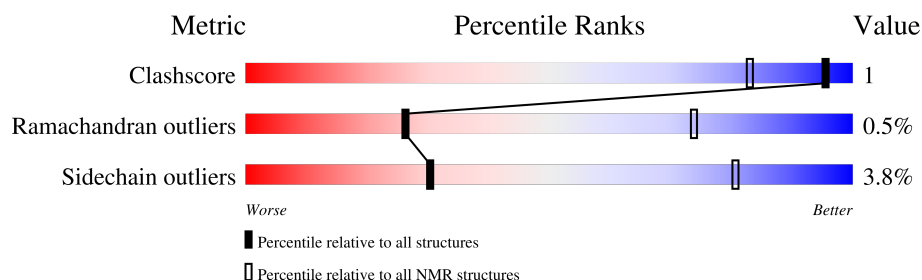
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 9%.

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	15	80% 20%
1	C	15	80% 20%
1	E	15	87% 13%
1	G	15	87% 13%
2	B	18	72% 28%
2	D	18	67% 33%
2	F	18	72% 28%
2	H	18	72% 28%

2 Ensemble composition and analysis

This entry contains 10 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

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:451-A:462, B:532-B:544, C:451-C:462, D:532-D:543, E:450-E:462, F:532-F:544, G:450-G:462, H:532-H:544 (101)	0.57	2

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 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 8, 9
2	3, 7
Single-model clusters	5; 6; 10

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1996 atoms, of which 980 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP.

Mol	Chain	Residues	Atoms						Trace
1	A	15	Total	C	H	N	O	S	0
			217	68	107	18	23	1	
1	C	15	Total	C	H	N	O	S	0
			217	68	107	18	23	1	
1	E	15	Total	C	H	N	O	S	0
			217	68	107	18	23	1	
1	G	15	Total	C	H	N	O	S	0
			217	68	107	18	23	1	

- Molecule 2 is a protein called THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE.

Mol	Chain	Residues	Atoms						Trace
2	B	18	Total	C	H	N	O	S	0
			282	92	138	21	30	1	
2	D	18	Total	C	H	N	O	S	0
			282	92	138	21	30	1	
2	F	18	Total	C	H	N	O	S	0
			282	92	138	21	30	1	
2	H	18	Total	C	H	N	O	S	0
			282	92	138	21	30	1	

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: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A: 



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C: 



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E: 



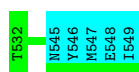
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G: 



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B: 



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

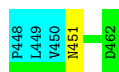


4.2 Scores per residue for each member of the ensemble

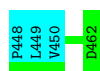
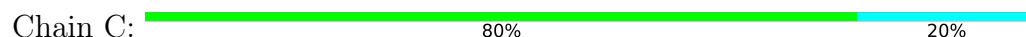
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  87% 13%



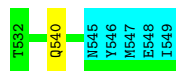
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  87% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  67% 6% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  61% 6% 33%



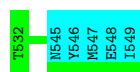
- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  72% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

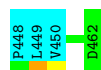
Chain H:  72% 28%



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  80% 7% 13%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  87% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  72% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  67% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  72% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain H:  72% 28%



4.2.3 Score per residue for model 3

- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  87% 13%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  87% 13%



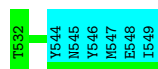
- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  61% 11% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  67% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  67% 6% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain H:  67% 6% 28%



4.2.4 Score per residue for model 4

- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  73% 7% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  73% 13% 13%



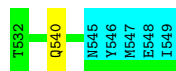
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  87% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  67% 6% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  67% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  72% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain H:  72% 28%



4.2.5 Score per residue for model 5

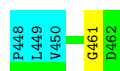
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  80% 20%



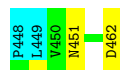
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  73% 7% 20%



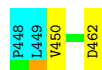
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  73% 13% 13%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  73% 13% 13%



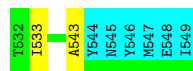
- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  61% 11% 28%



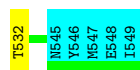
- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  56% 11% 33%



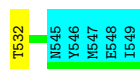
- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  67% 6% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

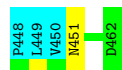
Chain H:  67% 6% 28%



4.2.6 Score per residue for model 6

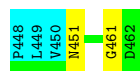
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  73% 7% 20%



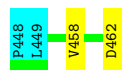
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  67% 13% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  73% 13% 13%



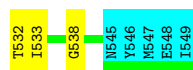
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  80% 7% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  56% 17% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  56% 11% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  67% 6% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

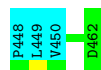
Chain H:  67% 6% 28%



4.2.7 Score per residue for model 7

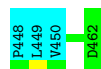
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  80% 20%



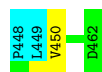
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  80% 7% 13%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  87% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  61% 11% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  56% 11% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  72% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

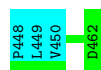
Chain H:  61% 11% 28%



4.2.8 Score per residue for model 8

- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  80% 20%



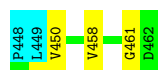
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  67% 20% 13%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  73% 13% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  61% 11% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  61% 6% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  72% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain H:  67% 6% 28%



4.2.9 Score per residue for model 9

- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  80% 20%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  87% 13%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  80% 7% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  61% 11% 28%



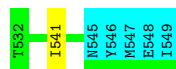
- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  56% 11% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  67% 6% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

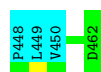
Chain H:  67% 6% 28%



4.2.10 Score per residue for model 10

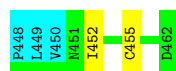
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain A:  80% 20%



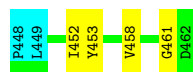
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain C:  67% 13% 20%



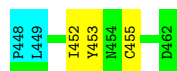
- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain E:  60% 27% 13%



- Molecule 1: PRO-LEU-VAL-ASN-ILE-TYR-ASN-CYS-SER-GLY-VAL-GLN-VAL-GLY-ASP

Chain G:  67% 20% 13%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain B:  61% 11% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain D:  61% 6% 33%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain F:  72% 28%



- Molecule 2: THR-ILE-TYR-ASN-SER-THR-GLY-ILE-GLN-ILE-GLY-ALA-TYR-ASN-TYR-MET-GLU-ILE

Chain H:  61% 11% 28%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics, molecular dynamics*.

Of the 100 calculated structures, 10 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
CYANA	structure calculation	3.97
Amber	refinement	

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	153
Number of shifts mapped to atoms	153
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	9%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality i

6.1 Standard geometry i

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	0.84±0.05	0±0/88 (0.0± 0.0%)	1.54±0.04	0±0/117 (0.0± 0.0%)
1	C	0.83±0.05	0±0/88 (0.0± 0.0%)	1.54±0.06	0±1/117 (0.2± 0.5%)
1	E	0.83±0.04	0±0/95 (0.0± 0.0%)	1.56±0.10	0±0/127 (0.2± 0.3%)
1	G	0.80±0.03	0±0/95 (0.0± 0.0%)	1.53±0.08	0±0/127 (0.1± 0.2%)
2	B	0.75±0.03	0±0/100 (0.0± 0.0%)	1.34±0.05	0±0/137 (0.2± 0.3%)
2	D	0.73±0.03	0±0/87 (0.0± 0.0%)	1.42±0.06	0±0/119 (0.1± 0.3%)
2	F	0.79±0.02	0±0/100 (0.0± 0.0%)	1.36±0.06	0±0/137 (0.0± 0.0%)
2	H	0.77±0.02	0±0/100 (0.0± 0.0%)	1.35±0.04	0±0/137 (0.1± 0.2%)
All	All	0.79	0/7530 (0.0%)	1.45	10/10180 (0.1%)

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	E	0.0±0.0	0.1±0.3
1	G	0.0±0.0	0.1±0.3
All	All	0	2

There are no bond-length outliers.

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	E	452	ILE	CB-CA-C	6.06	118.65	111.32	10	1
1	G	462	ASP	CA-CB-CG	5.42	118.03	112.60	5	1
2	H	532	THR	CA-CB-CG2	5.40	119.68	110.50	7	1
1	E	462	ASP	CA-CB-CG	5.36	117.96	112.60	5	1
1	C	461	GLY	CA-C-N	5.12	130.92	121.70	5	1
1	C	461	GLY	C-N-CA	5.12	130.92	121.70	5	1
2	B	540	GLN	OE1-CD-NE2	-5.09	117.51	122.60	1	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	D	540	GLN	OE1-CD-NE2	-5.07	117.53	122.60	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	G	461	GLY	Peptide	1
1	E	461	GLY	Peptide	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	C	88	78	78	0±0
1	G	95	87	87	0±0
1	A	88	78	78	0±0
1	E	95	87	87	0±0
2	H	98	97	94	0±0
2	B	98	97	94	1±1
2	D	86	88	85	1±1
2	F	98	97	94	0±0
All	All	7460	7090	6970	15

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:532:THR:HG23	2:D:543:ALA:HB3	0.53	1.80	7	2
2:B:533:ILE:HD11	1:C:461:GLY:HA2	0.50	1.81	6	1
1:E:461:GLY:CA	2:H:533:ILE:HD11	0.45	2.42	8	1
1:G:452:ILE:HD11	1:G:455:CYS:SG	0.44	2.53	10	2
2:B:542:GLY:HA3	2:D:533:ILE:HD11	0.43	1.90	5	1
1:C:452:ILE:HD11	1:C:455:CYS:SG	0.43	2.52	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:543:ALA:HB3	2:D:532:THR:CG2	0.43	2.44	7	1
2:F:533:ILE:HD11	2:H:542:GLY:HA2	0.42	1.89	6	1
2:H:532:THR:HB	2:H:533:ILE:HD12	0.42	1.89	10	1
2:B:532:THR:HA	1:E:451:ASN:OD1	0.42	2.15	5	1
2:B:532:THR:HB	2:B:533:ILE:HD12	0.42	1.91	3	1
2:B:543:ALA:HB3	2:D:532:THR:HG23	0.41	1.92	7	1
2:B:532:THR:CG2	2:D:543:ALA:HB3	0.41	2.45	7	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	11/15 (73%)	9±1 (82±11%)	2±1 (18±11%)	0±0 (0±0%)	100	100
1	C	11/15 (73%)	9±1 (82±8%)	2±1 (18±8%)	0±0 (0±0%)	100	100
1	E	12/15 (80%)	9±1 (74±7%)	3±1 (24±8%)	0±0 (2±3%)	9	53
1	G	12/15 (80%)	8±1 (71±9%)	3±1 (28±9%)	0±0 (1±3%)	18	68
2	B	12/18 (67%)	10±0 (81±4%)	2±1 (18±5%)	0±0 (1±3%)	18	68
2	D	11/18 (61%)	8±1 (75±8%)	3±1 (25±9%)	0±0 (1±3%)	16	66
2	F	12/18 (67%)	10±2 (84±13%)	2±2 (16±13%)	0±0 (0±0%)	100	100
2	H	12/18 (67%)	11±1 (89±9%)	1±1 (11±9%)	0±0 (0±0%)	100	100
All	All	930/1320 (70%)	741 (80%)	184 (20%)	5 (1%)	26	74

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)
2	B	538	GLY	1
2	D	538	GLY	1
1	E	450	VAL	1
1	E	453	TYR	1
1	G	453	TYR	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	10/13 (77%)	10±0 (97±5%)	0±0 (3±5%)	37	85
1	C	10/13 (77%)	10±0 (99±3%)	0±0 (1±3%)	65	95
1	E	11/13 (85%)	10±1 (93±8%)	1±1 (7±8%)	15	63
1	G	11/13 (85%)	11±0 (99±3%)	0±0 (1±3%)	68	95
2	B	10/15 (67%)	9±1 (94±8%)	1±1 (6±8%)	19	68
2	D	9/15 (60%)	8±1 (94±7%)	0±1 (6±7%)	21	70
2	F	10/15 (67%)	10±0 (97±5%)	0±0 (3±5%)	37	85
2	H	10/15 (67%)	10±0 (96±5%)	0±0 (4±5%)	29	79
All	All	810/1120 (72%)	779 (96%)	31 (4%)	30	81

All 20 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	E	458	VAL	4
1	A	451	ASN	3
1	E	462	ASP	3
2	B	537	THR	3
2	H	532	THR	2
2	D	532	THR	2
2	F	536	SER	1
2	F	532	THR	1
2	B	532	THR	1
1	C	451	ASN	1
1	G	462	ASP	1
2	H	536	SER	1
2	D	537	THR	1
1	E	450	VAL	1
2	B	541	ILE	1
2	D	541	ILE	1
2	F	541	ILE	1
2	H	541	ILE	1
2	B	535	ASN	1
2	D	535	ASN	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 [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 9% for the well-defined parts and 9% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *shift_set_1*

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	153
Number of shifts mapped to atoms	153
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	31	0.08 ± 0.31	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	28	-0.47 ± 0.55	None needed (< 0.5 ppm)
$^{13}\text{C}'$	27	0.86 ± 0.23	Should be applied
^{15}N	27	-1.05 ± 0.49	Should be applied

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 9%, i.e. 116 atoms were assigned a chemical shift out of a possible 1241. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	70/521 (13%)	0/218 (0%)	47/202 (23%)	23/101 (23%)
Sidechain	46/621 (7%)	0/408 (0%)	45/193 (23%)	1/20 (5%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	0/99 (0%)	0/44 (0%)	0/55 (0%)	0/0 (—%)
Overall	116/1241 (9%)	0/670 (0%)	92/450 (20%)	24/121 (20%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 9%, i.e. 151 atoms were assigned a chemical shift out of a possible 1704. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	85/668 (13%)	0/276 (0%)	58/264 (22%)	27/128 (21%)
Sidechain	66/892 (7%)	0/588 (0%)	65/280 (23%)	1/24 (4%)
Aromatic	0/144 (0%)	0/64 (0%)	0/80 (0%)	0/0 (—%)
Overall	151/1704 (9%)	0/928 (0%)	123/624 (20%)	28/152 (18%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

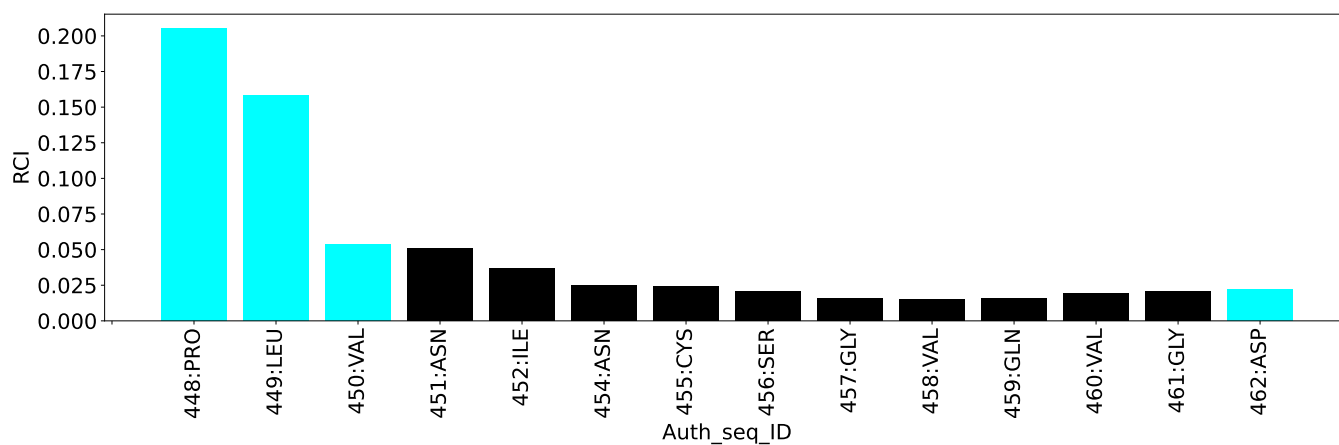
7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots ⓘ

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:



Random coil index (RCI) for chain B:

