



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 10:04 AM UTC

PDB ID : 8OSQ / pdb_00008osq
BMRB ID : 34809
Title : Why does the herpes simplex 1 virus-encoded UL49.5 protein fail to inhibit the TAP-dependent antigen presentation?
Authors : Zhukov, I.; Krupa, P.; Karska, N.; Rodziewicz-Motowidlo, S.; Lipinska, A.D.
Deposited on : 2023-04-19

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
Mogul : 2022.3.0, CSD as543be (2022)
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

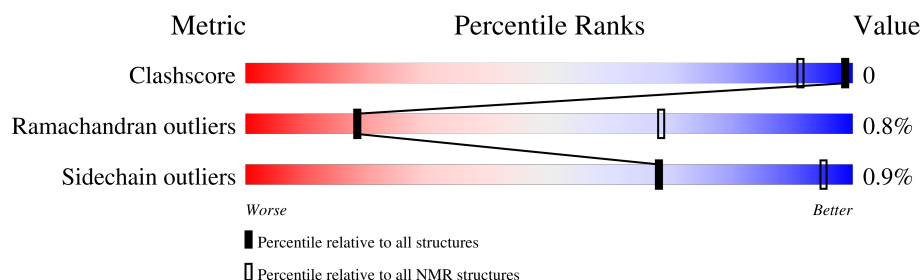
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 43%.

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	35	40% 34% 26%

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:22, A:24-A:30, A:32-A:34 (26)	0.72	5

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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 453 atoms, of which 216 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Envelope glycoprotein N.

Mol	Chain	Residues	Atoms					Trace
1	A	35	Total	C	H	N	O	0
			453	136	216	47	54	

There are 2 discrepancies between the modelled and reference sequences:

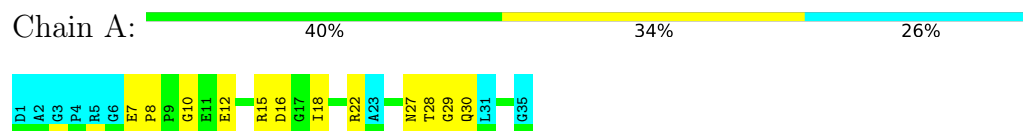
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ABA	CYS	engineered mutation	UNP O09800
A	31	NLE	MET	engineered mutation	UNP O09800

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: Envelope glycoprotein N

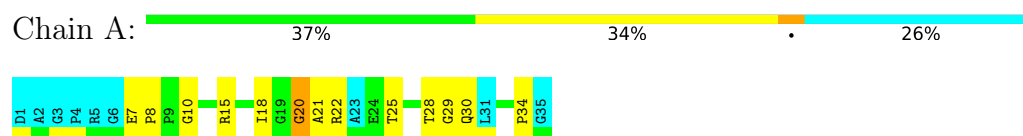


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

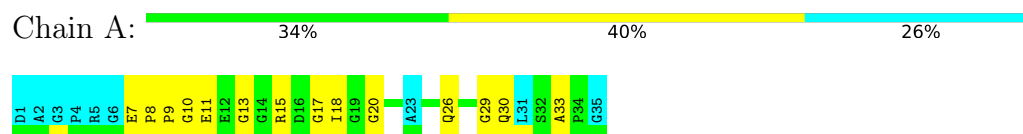
4.2.1 Score per residue for model 1

- Molecule 1: Envelope glycoprotein N



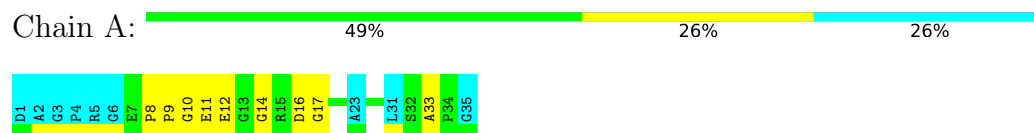
4.2.2 Score per residue for model 2

- Molecule 1: Envelope glycoprotein N



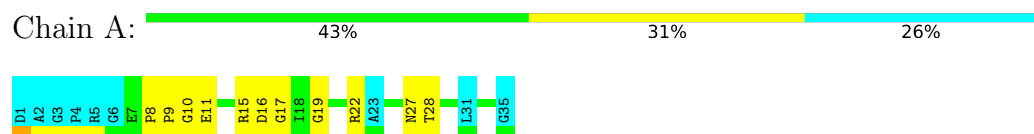
4.2.3 Score per residue for model 3

- Molecule 1: Envelope glycoprotein N



4.2.4 Score per residue for model 4

- Molecule 1: Envelope glycoprotein N



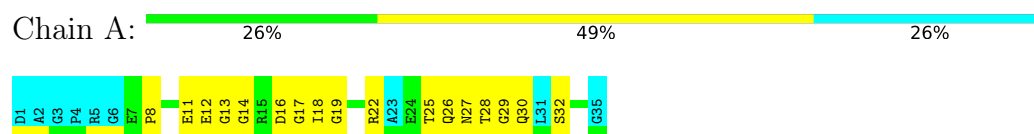
4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Envelope glycoprotein N



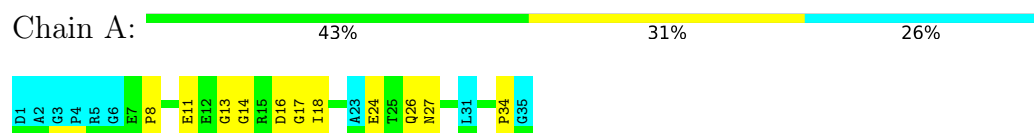
4.2.6 Score per residue for model 6

- Molecule 1: Envelope glycoprotein N



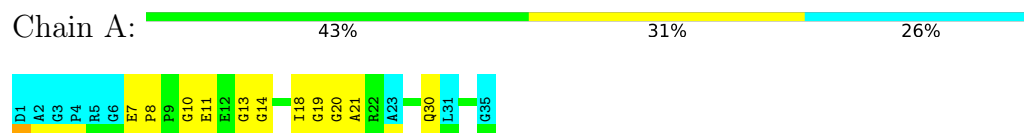
4.2.7 Score per residue for model 7

- Molecule 1: Envelope glycoprotein N



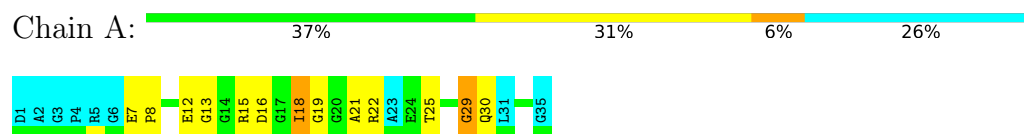
4.2.8 Score per residue for model 8

- Molecule 1: Envelope glycoprotein N



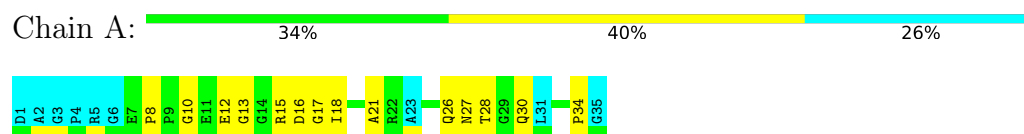
4.2.9 Score per residue for model 9

- Molecule 1: Envelope glycoprotein N



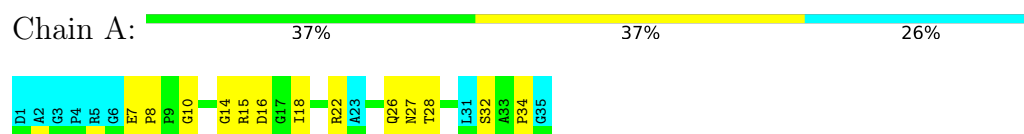
4.2.10 Score per residue for model 10

- Molecule 1: Envelope glycoprotein N



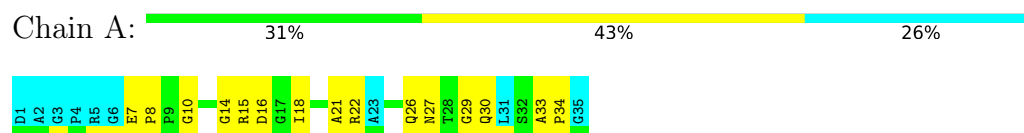
4.2.11 Score per residue for model 11

- Molecule 1: Envelope glycoprotein N



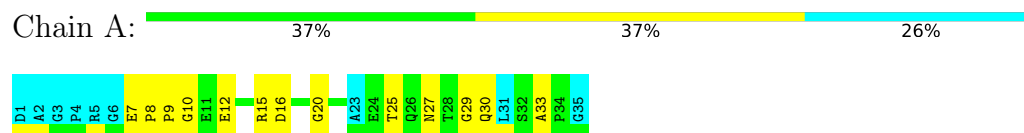
4.2.12 Score per residue for model 12

- Molecule 1: Envelope glycoprotein N



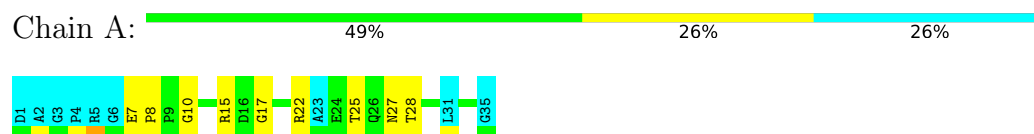
4.2.13 Score per residue for model 13

- Molecule 1: Envelope glycoprotein N



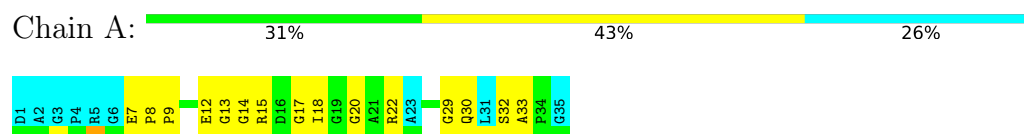
4.2.14 Score per residue for model 14

- Molecule 1: Envelope glycoprotein N



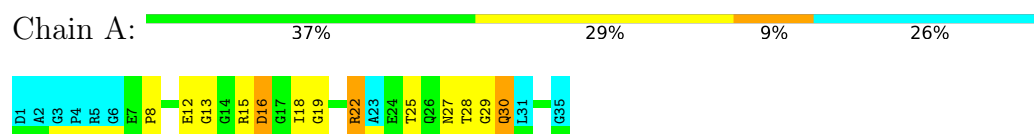
4.2.15 Score per residue for model 15

- Molecule 1: Envelope glycoprotein N



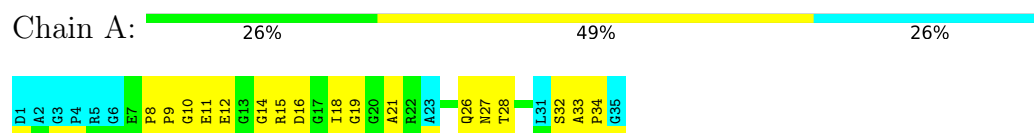
4.2.16 Score per residue for model 16

- Molecule 1: Envelope glycoprotein N



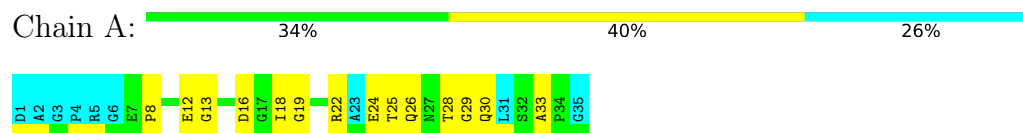
4.2.17 Score per residue for model 17

- Molecule 1: Envelope glycoprotein N



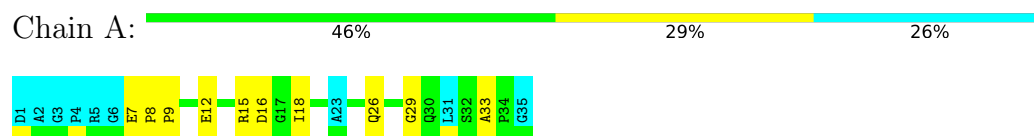
4.2.18 Score per residue for model 18

- Molecule 1: Envelope glycoprotein N



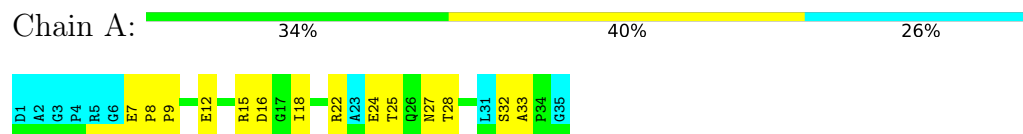
4.2.19 Score per residue for model 19

- Molecule 1: Envelope glycoprotein N



4.2.20 Score per residue for model 20

- Molecule 1: Envelope glycoprotein N



5 Refinement protocol and experimental data overview

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

Of the 10 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
Amber	structure calculation	

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	163
Number of shifts mapped to atoms	163
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

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: NLE, ABA

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	2.12±0.13	5±2/180 (2.8± 1.3%)	2.56±0.17	14±4/240 (5.9± 1.5%)
All	All	2.13	100/3600 (2.8%)	2.57	282/4800 (5.9%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.2±0.5
All	All	0	5

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	28	THR	CA-C	10.39	1.65	1.52	1	1
1	A	8	PRO	CA-C	10.02	1.61	1.52	4	5
1	A	18	ILE	N-CA	9.13	1.59	1.46	17	1
1	A	16	ASP	N-CA	8.73	1.56	1.46	10	3
1	A	34	PRO	CA-C	8.73	1.63	1.52	10	2
1	A	20	GLY	CA-C	8.55	1.62	1.52	8	1
1	A	33	ALA	CA-C	8.12	1.60	1.52	12	5
1	A	21	ALA	CA-C	7.61	1.62	1.52	10	2
1	A	17	GLY	CA-C	7.46	1.63	1.52	15	4
1	A	26	GLN	CA-C	7.29	1.61	1.52	2	1
1	A	15	ARG	CZ-NH1	-7.29	1.22	1.32	5	2
1	A	27	ASN	CA-C	7.18	1.62	1.52	17	2
1	A	15	ARG	CZ-NH2	-7.07	1.24	1.33	15	5
1	A	16	ASP	CA-C	6.96	1.62	1.52	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	13	GLY	C-O	-6.78	1.15	1.23	10	1
1	A	9	PRO	N-CA	6.78	1.56	1.47	19	2
1	A	15	ARG	CA-C	-6.76	1.44	1.52	4	1
1	A	14	GLY	N-CA	6.71	1.56	1.45	17	2
1	A	29	GLY	CA-C	6.49	1.57	1.52	6	2
1	A	25	THR	N-CA	6.34	1.54	1.45	9	1
1	A	13	GLY	CA-C	6.32	1.59	1.51	8	2
1	A	7	GLU	CA-C	-6.22	1.45	1.52	9	3
1	A	9	PRO	N-CD	6.14	1.56	1.47	13	1
1	A	10	GLY	N-CA	6.12	1.53	1.45	4	1
1	A	10	GLY	CA-C	6.09	1.60	1.51	12	2
1	A	21	ALA	CA-CB	6.09	1.60	1.52	9	1
1	A	18	ILE	CA-C	6.05	1.60	1.52	15	2
1	A	15	ARG	CD-NE	6.02	1.54	1.46	4	1
1	A	15	ARG	C-O	-6.02	1.17	1.24	15	1
1	A	20	GLY	N-CA	5.96	1.52	1.45	2	1
1	A	18	ILE	CA-CB	5.94	1.61	1.53	8	3
1	A	7	GLU	C-N	5.92	1.40	1.33	15	1
1	A	13	GLY	C-N	5.88	1.40	1.33	7	1
1	A	13	GLY	N-CA	5.81	1.53	1.45	16	1
1	A	28	THR	C-N	5.76	1.38	1.33	10	1
1	A	24	GLU	C-N	5.75	1.41	1.33	18	1
1	A	14	GLY	CA-C	5.71	1.58	1.51	3	2
1	A	34	PRO	N-CD	-5.70	1.39	1.47	11	1
1	A	18	ILE	C-N	5.69	1.40	1.33	6	1
1	A	33	ALA	N-CA	5.63	1.52	1.45	18	3
1	A	32	SER	CA-CB	5.54	1.64	1.53	17	1
1	A	12	GLU	N-CA	5.48	1.53	1.46	15	1
1	A	22	ARG	CD-NE	5.45	1.53	1.46	4	1
1	A	16	ASP	CA-CB	5.39	1.60	1.53	5	1
1	A	29	GLY	N-CA	5.38	1.52	1.45	2	1
1	A	7	GLU	C-O	5.37	1.30	1.24	11	1
1	A	7	GLU	CA-CB	5.36	1.60	1.53	14	1
1	A	16	ASP	C-O	-5.34	1.20	1.23	7	1
1	A	30	GLN	CA-C	5.32	1.64	1.52	5	1
1	A	10	GLY	C-N	5.31	1.41	1.33	2	1
1	A	29	GLY	C-N	5.31	1.40	1.33	15	1
1	A	25	THR	CA-CB	5.30	1.61	1.53	20	1
1	A	8	PRO	N-CA	5.27	1.57	1.46	15	1
1	A	30	GLN	N-CA	5.25	1.56	1.46	9	1
1	A	22	ARG	CZ-NH1	-5.25	1.25	1.32	15	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	19	GLY	CA-C	5.24	1.57	1.52	18	2
1	A	22	ARG	CZ-NH2	-5.21	1.26	1.33	11	1
1	A	29	GLY	C-O	5.15	1.29	1.23	13	1
1	A	17	GLY	N-CA	5.10	1.52	1.45	6	1
1	A	15	ARG	N-CA	5.09	1.52	1.46	14	1
1	A	16	ASP	C-N	5.04	1.39	1.33	18	1
1	A	32	SER	N-CA	5.02	1.55	1.46	6	1
1	A	11	GLU	C-O	-5.01	1.18	1.24	17	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	16	ASP	CA-CB-CG	11.44	124.04	112.60	16	5
1	A	34	PRO	CB-CA-C	10.37	120.84	111.40	1	2
1	A	8	PRO	N-CA-C	10.18	123.12	110.70	16	12
1	A	29	GLY	CA-C-O	-9.56	112.09	120.89	16	5
1	A	33	ALA	CA-C-N	9.55	131.77	119.84	20	2
1	A	33	ALA	C-N-CA	9.55	131.77	119.84	20	2
1	A	13	GLY	CA-C-N	9.48	130.70	119.99	16	2
1	A	13	GLY	C-N-CA	9.48	130.70	119.99	16	2
1	A	30	GLN	OE1-CD-NE2	-9.36	113.24	122.60	1	11
1	A	15	ARG	NE-CZ-NH2	8.98	127.28	119.20	5	1
1	A	29	GLY	N-CA-C	8.87	122.14	111.93	12	2
1	A	18	ILE	CA-C-N	8.70	129.57	120.00	6	6
1	A	18	ILE	C-N-CA	8.70	129.57	120.00	6	6
1	A	26	GLN	OE1-CD-NE2	-8.50	114.10	122.60	7	8
1	A	22	ARG	NH1-CZ-NH2	-8.25	108.58	119.30	18	1
1	A	33	ALA	N-CA-C	8.13	121.30	110.08	13	2
1	A	25	THR	N-CA-CB	-8.05	100.36	110.98	16	1
1	A	27	ASN	OD1-CG-ND2	-7.99	114.61	122.60	12	3
1	A	11	GLU	CA-C-N	7.92	131.23	120.38	8	2
1	A	11	GLU	C-N-CA	7.92	131.23	120.38	8	2
1	A	10	GLY	CA-C-N	7.84	133.65	121.19	4	8
1	A	10	GLY	C-N-CA	7.84	133.65	121.19	4	8
1	A	12	GLU	CA-C-N	7.81	128.81	119.99	17	6
1	A	12	GLU	C-N-CA	7.81	128.81	119.99	17	6
1	A	28	THR	CA-C-N	7.80	128.94	120.44	5	7
1	A	28	THR	C-N-CA	7.80	128.94	120.44	5	7
1	A	16	ASP	CA-C-N	7.64	128.76	120.44	19	3
1	A	16	ASP	C-N-CA	7.64	128.76	120.44	19	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	21	ALA	CB-CA-C	7.41	120.95	109.84	10	1
1	A	20	GLY	O-C-N	-7.30	116.53	122.81	1	2
1	A	12	GLU	N-CA-C	7.29	120.09	111.71	13	2
1	A	22	ARG	NE-CZ-NH1	7.28	128.78	121.50	16	4
1	A	27	ASN	CA-C-O	7.26	127.61	119.41	17	2
1	A	27	ASN	N-CA-CB	-7.25	100.56	111.15	13	3
1	A	22	ARG	CD-NE-CZ	7.17	134.44	124.40	6	4
1	A	14	GLY	CA-C-N	7.17	129.76	120.44	11	4
1	A	14	GLY	C-N-CA	7.17	129.76	120.44	11	4
1	A	19	GLY	N-CA-C	7.10	120.74	112.50	4	1
1	A	25	THR	CA-CB-OG1	7.04	120.16	109.60	16	2
1	A	8	PRO	N-CA-CB	7.00	109.87	103.08	3	5
1	A	19	GLY	CA-C-N	6.97	128.40	120.53	8	4
1	A	19	GLY	C-N-CA	6.97	128.40	120.53	8	4
1	A	18	ILE	O-C-N	-6.92	116.74	122.97	10	2
1	A	33	ALA	CA-C-O	-6.77	113.46	120.02	19	1
1	A	17	GLY	CA-C-N	6.74	132.55	122.98	14	2
1	A	17	GLY	C-N-CA	6.74	132.55	122.98	14	2
1	A	16	ASP	CA-C-O	6.69	126.26	119.97	10	2
1	A	15	ARG	CB-CA-C	6.65	121.21	110.96	13	1
1	A	11	GLU	CA-C-O	-6.64	113.38	120.42	2	2
1	A	20	GLY	CA-C-N	6.59	131.82	122.72	13	2
1	A	20	GLY	C-N-CA	6.59	131.82	122.72	13	2
1	A	22	ARG	NE-CZ-NH2	6.56	125.10	119.20	20	3
1	A	15	ARG	CA-C-O	-6.53	114.17	120.90	10	2
1	A	27	ASN	CA-C-N	6.46	129.88	120.71	16	1
1	A	27	ASN	C-N-CA	6.46	129.88	120.71	16	1
1	A	14	GLY	N-CA-C	6.44	121.55	114.40	7	1
1	A	12	GLU	CA-C-O	6.42	127.36	120.24	9	1
1	A	26	GLN	N-CA-CB	-6.38	99.45	111.00	2	2
1	A	15	ARG	NE-CZ-NH1	6.37	127.87	121.50	19	3
1	A	27	ASN	O-C-N	-6.36	114.13	122.59	16	2
1	A	15	ARG	NH1-CZ-NH2	-6.34	111.06	119.30	5	2
1	A	18	ILE	CA-CB-CG1	6.33	121.16	110.40	11	2
1	A	13	GLY	CA-C-O	-6.32	114.01	120.45	9	3
1	A	21	ALA	N-CA-CB	-6.31	100.53	110.06	1	1
1	A	9	PRO	N-CD-CG	6.30	112.64	103.20	4	1
1	A	29	GLY	O-C-N	-6.29	115.17	122.91	6	1
1	A	25	THR	N-CA-C	-6.29	103.96	111.69	14	1
1	A	12	GLU	N-CA-CB	-6.22	100.95	110.16	18	2
1	A	8	PRO	CB-CA-C	6.20	118.48	110.92	15	3

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	ILE	CA-C-O	6.19	126.53	120.27	16	3
1	A	8	PRO	N-CD-CG	6.16	112.44	103.20	12	2
1	A	16	ASP	N-CA-C	6.16	117.67	110.41	17	1
1	A	9	PRO	CA-C-N	6.10	126.71	119.94	2	1
1	A	9	PRO	C-N-CA	6.10	126.71	119.94	2	1
1	A	25	THR	CA-CB-CG2	6.07	120.81	110.50	6	1
1	A	10	GLY	N-CA-C	-6.04	105.27	113.37	3	2
1	A	28	THR	CA-CB-OG1	6.01	118.62	109.60	11	2
1	A	7	GLU	N-CA-CB	-5.94	102.63	110.17	12	1
1	A	15	ARG	N-CA-C	5.91	117.80	111.36	16	1
1	A	8	PRO	CA-C-O	-5.90	112.01	120.56	11	1
1	A	8	PRO	CA-C-N	5.82	125.44	119.56	17	1
1	A	8	PRO	C-N-CA	5.82	125.44	119.56	17	1
1	A	12	GLU	O-C-N	-5.80	115.44	122.22	19	1
1	A	7	GLU	CA-C-O	-5.79	114.42	120.38	14	2
1	A	9	PRO	N-CA-C	-5.77	106.64	113.86	5	1
1	A	21	ALA	CA-C-O	5.70	127.36	120.81	12	2
1	A	33	ALA	O-C-N	-5.69	116.70	121.54	12	1
1	A	11	GLU	N-CA-CB	-5.64	101.83	110.01	8	1
1	A	28	THR	O-C-N	-5.63	116.62	123.10	4	1
1	A	25	THR	CA-C-N	5.57	130.63	122.39	1	1
1	A	25	THR	C-N-CA	5.57	130.63	122.39	1	1
1	A	7	GLU	CB-CG-CD	5.54	122.02	112.60	13	1
1	A	7	GLU	CA-C-N	5.52	126.06	120.38	19	3
1	A	7	GLU	C-N-CA	5.52	126.06	120.38	19	3
1	A	12	GLU	CB-CA-C	5.49	119.50	110.88	6	1
1	A	18	ILE	CB-CA-C	5.46	117.16	111.09	1	3
1	A	28	THR	N-CA-C	5.44	118.12	110.23	16	1
1	A	27	ASN	CB-CA-C	5.41	121.30	109.99	4	1
1	A	32	SER	CA-C-N	5.41	128.88	120.60	20	2
1	A	32	SER	C-N-CA	5.41	128.88	120.60	20	2
1	A	9	PRO	CA-C-O	-5.37	111.48	119.00	3	1
1	A	34	PRO	N-CA-CB	5.34	108.86	103.25	7	2
1	A	17	GLY	CA-C-O	-5.33	115.16	122.31	2	1
1	A	8	PRO	CA-N-CD	-5.32	104.55	112.00	4	2
1	A	10	GLY	CA-C-O	-5.32	115.02	120.66	4	1
1	A	11	GLU	CB-CG-CD	5.30	121.61	112.60	4	1
1	A	33	ALA	CB-CA-C	5.29	118.24	109.56	3	1
1	A	24	GLU	CA-CB-CG	5.29	124.67	114.10	20	1
1	A	30	GLN	CG-CD-NE2	5.22	124.23	116.40	1	1
1	A	11	GLU	O-C-N	-5.20	115.88	122.27	3	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	ARG	CD-NE-CZ	5.16	131.63	124.40	12	1
1	A	9	PRO	CB-CA-C	-5.15	104.16	111.68	17	1
1	A	8	PRO	O-C-N	-5.10	115.44	121.46	6	1
1	A	13	GLY	O-C-N	-5.08	117.24	122.17	6	1
1	A	24	GLU	CA-C-O	-5.05	112.22	120.80	7	1
1	A	7	GLU	CA-CB-CG	5.04	124.18	114.10	19	1
1	A	30	GLN	CB-CG-CD	5.03	121.16	112.60	12	1
1	A	29	GLY	CA-C-N	5.02	130.73	121.70	6	1
1	A	29	GLY	C-N-CA	5.02	130.73	121.70	6	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	20	GLY	Mainchain	1
1	A	21	ALA	Mainchain	1
1	A	32	SER	Mainchain	1
1	A	22	ARG	Sidechain	1
1	A	30	GLN	Peptide	1

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	179	158	158	0±0
All	All	3580	3160	3160	1

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ILE:HG12	1:A:29:GLY:HA2	0.45	1.88	9	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	26/35 (74%)	23±1 (89±6%)	3±1 (10±6%)	0±0 (1±2%)	18	68
All	All	520/700 (74%)	462 (89%)	54 (10%)	4 (1%)	18	68

All 2 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	16	ASP	3
1	A	9	PRO	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	17/20 (85%)	17±0 (99±2%)	0±0 (1±2%)	68	95
All	All	340/400 (85%)	337 (99%)	3 (1%)	68	95

All 3 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	11	GLU	1
1	A	34	PRO	1
1	A	25	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	NLE	A	31	1	6,7,8	1.25±0.43	0±0 (8±8%)
1	ABA	A	23	1	4,5,6	1.06±0.36	0±0 (5±10%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	NLE	A	31	1	2,7,9	0.62±0.25	0±0 (0±0%)
1	ABA	A	23	1	1,5,7	0.74±0.56	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ABA	A	23	1	-	0±0,3,4,6	-
1	NLE	A	31	1	-	0±0,5,6,8	-

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	31	NLE	CB-CA	4.62	1.60	1.53	19	9

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	23	ABA	CB-CA	2.77	1.45	1.53	8	3
1	A	31	NLE	CA-N	2.56	1.55	1.48	3	1
1	A	23	ABA	O-C	2.03	1.27	1.20	16	1

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 43% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *chem_shift_list_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	163
Number of shifts mapped to atoms	163
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

No chemical shift referencing corrections were calculated (not enough data).

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 43%, i.e. 124 atoms were assigned a chemical shift out of a possible 289. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	53/131 (40%)	53/56 (95%)	0/52 (0%)	0/23 (0%)
Sidechain	71/158 (45%)	71/99 (72%)	0/50 (0%)	0/9 (0%)
Overall	124/289 (43%)	124/155 (80%)	0/102 (0%)	0/32 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 149 atoms were assigned a chemical shift out of a possible 360. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	67/167 (40%)	67/72 (93%)	0/66 (0%)	0/29 (0%)
Sidechain	82/193 (42%)	82/121 (68%)	0/60 (0%)	0/12 (0%)
Overall	149/360 (41%)	149/193 (77%)	0/126 (0%)	0/41 (0%)

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:

