



Full wwPDB NMR Structure Validation Report ⓘ

Mar 10, 2026 – 09:21 PM UTC

PDB ID : 2KQ0 / pdb_00002kq0
BMRB ID : 16575
Title : Human NEDD4 3rd WW Domain Complex with Ebola Zaire Virus Matrix Protein VP40 Derived Peptide ILPTAPPEYMEA
Authors : Iglesias-Bexiga, M.; Macias, M.; Bonet, R.; Blanco, F.J.; Cobos, E.S.; Luque, I.
Deposited on : 2009-10-23

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

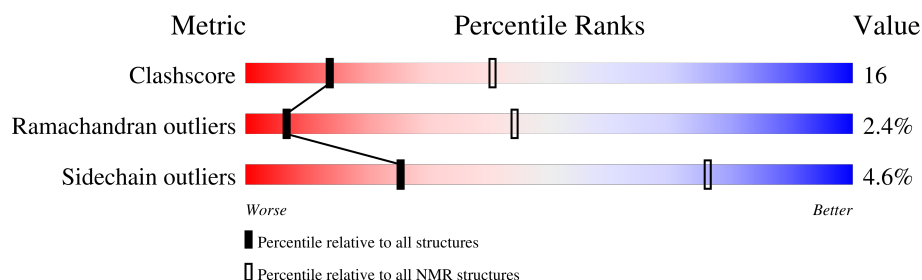
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 54%.

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	49	
2	B	12	

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:14-A:42, B:114-B:120 (36)	0.67	15

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 5 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 723 atoms, of which 354 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called E3 ubiquitin-protein ligase NEDD4.

Mol	Chain	Residues	Atoms					Trace
1	A	35	Total	C	H	N	O	0
			592	195	293	55	49	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P46934
A	2	ALA	-	expression tag	UNP P46934
A	3	MET	-	expression tag	UNP P46934
A	4	GLY	-	expression tag	UNP P46934

- Molecule 2 is a protein called 12-mer from Matrix protein VP40.

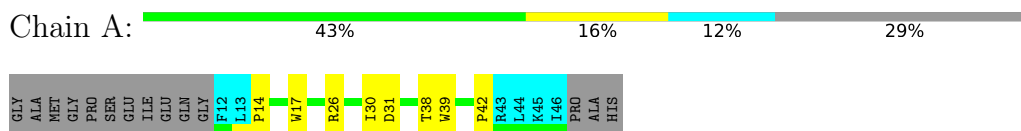
Mol	Chain	Residues	Atoms						Trace
2	B	9	Total	C	H	N	O	S	0
			131	44	61	9	16	1	

4 Residue-property plots [i](#)

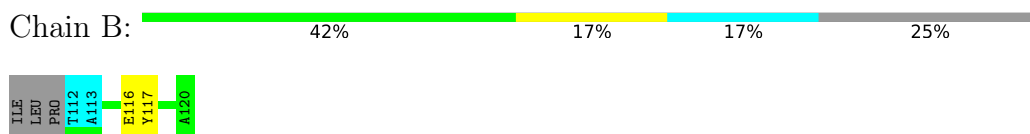
4.1 Average score per residue in the NMR ensemble

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: E3 ubiquitin-protein ligase NEDD4



- Molecule 2: 12-mer from Matrix protein VP40

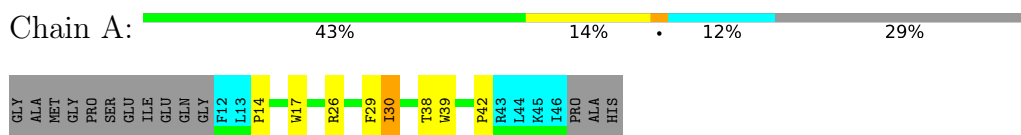


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

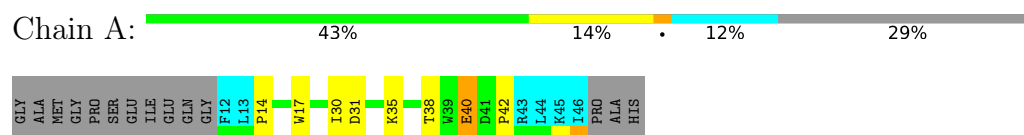


- Molecule 2: 12-mer from Matrix protein VP40

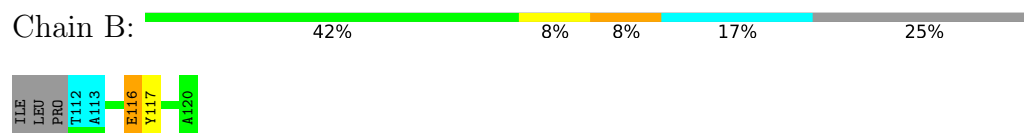


4.2.2 Score per residue for model 2

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

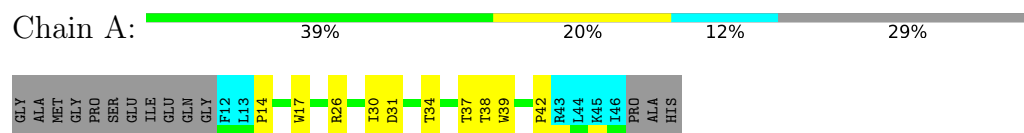


- Molecule 2: 12-mer from Matrix protein VP40

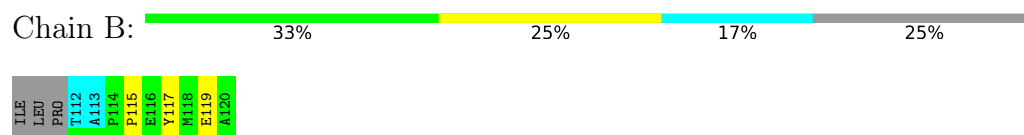


4.2.3 Score per residue for model 3

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

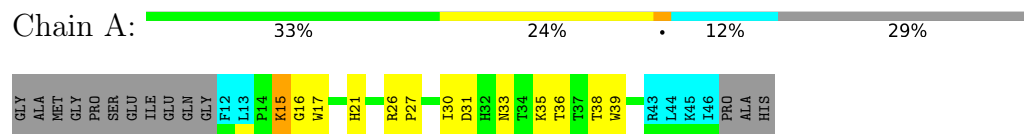


- Molecule 2: 12-mer from Matrix protein VP40

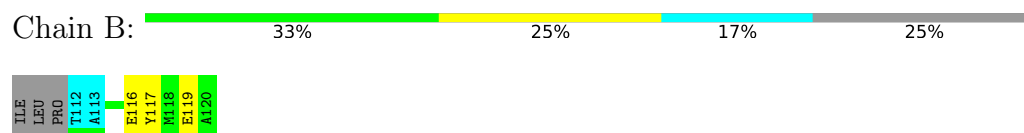


4.2.4 Score per residue for model 4

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

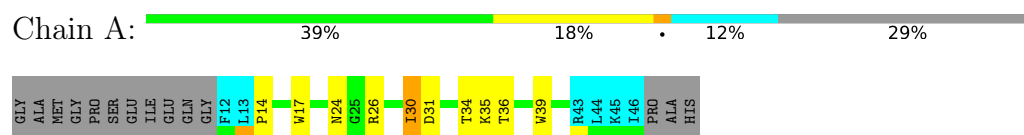


- Molecule 2: 12-mer from Matrix protein VP40

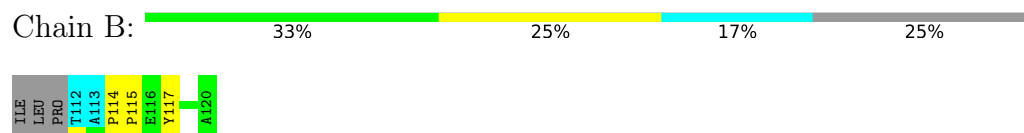


4.2.5 Score per residue for model 5

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

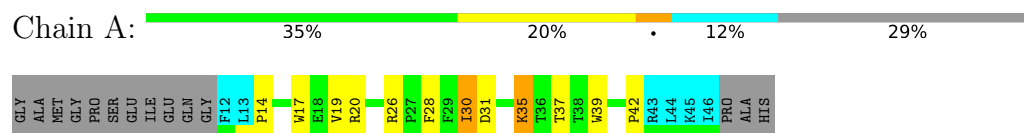


- Molecule 2: 12-mer from Matrix protein VP40

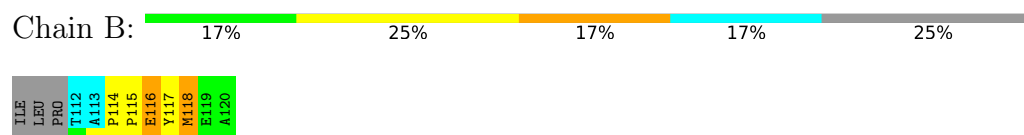


4.2.6 Score per residue for model 6

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

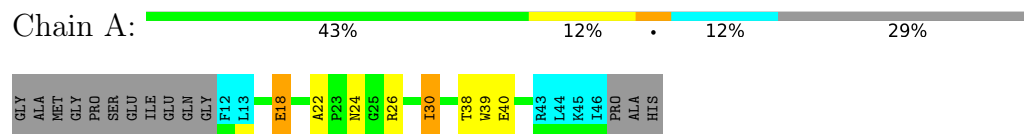


- Molecule 2: 12-mer from Matrix protein VP40

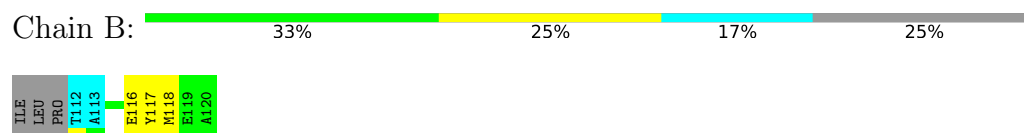


4.2.7 Score per residue for model 7

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

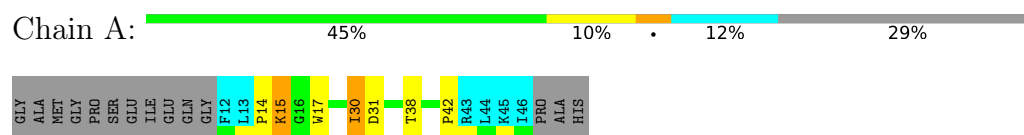


- Molecule 2: 12-mer from Matrix protein VP40



4.2.8 Score per residue for model 8

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

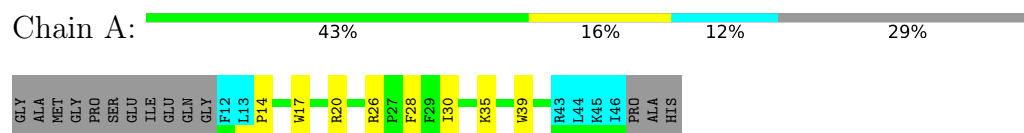


- Molecule 2: 12-mer from Matrix protein VP40



4.2.9 Score per residue for model 9

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

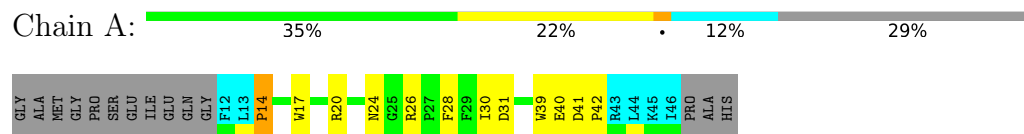


- Molecule 2: 12-mer from Matrix protein VP40

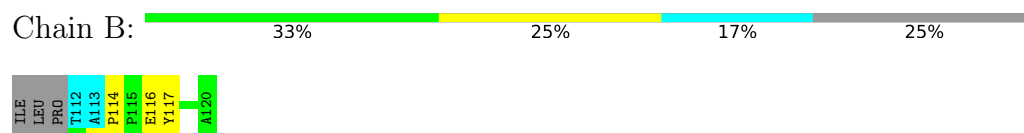


4.2.10 Score per residue for model 10

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

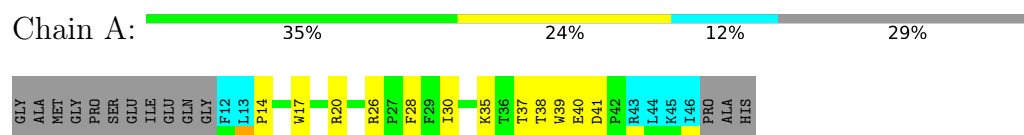


- Molecule 2: 12-mer from Matrix protein VP40

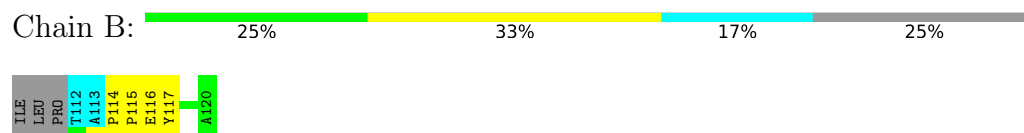


4.2.11 Score per residue for model 11

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

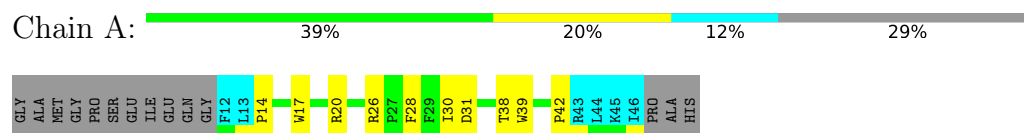


- Molecule 2: 12-mer from Matrix protein VP40

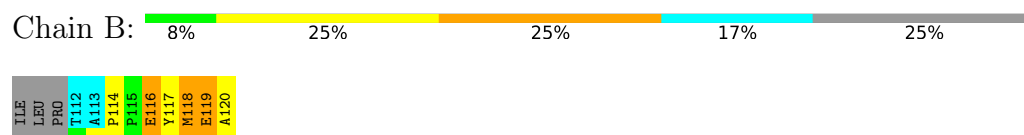


4.2.12 Score per residue for model 12

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

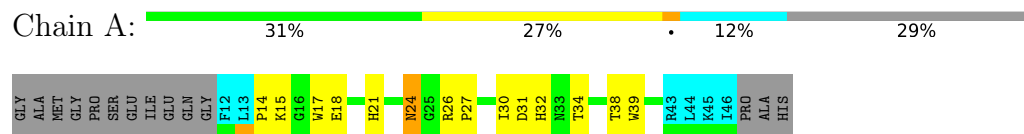


- Molecule 2: 12-mer from Matrix protein VP40

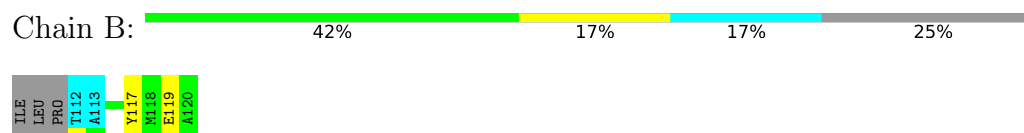


4.2.13 Score per residue for model 13

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

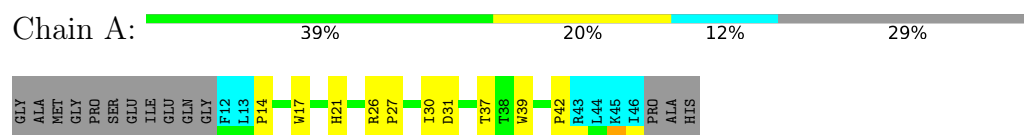


- Molecule 2: 12-mer from Matrix protein VP40

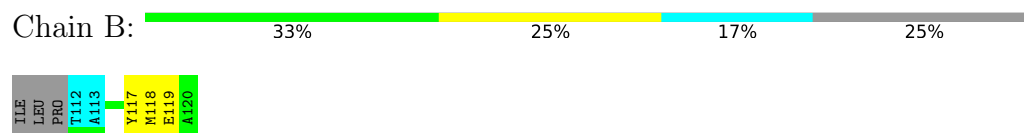


4.2.14 Score per residue for model 14

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

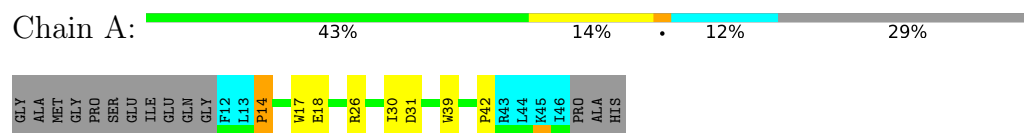


- Molecule 2: 12-mer from Matrix protein VP40

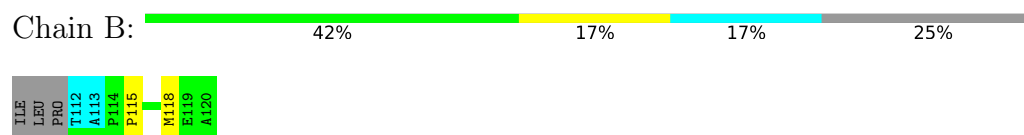


4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

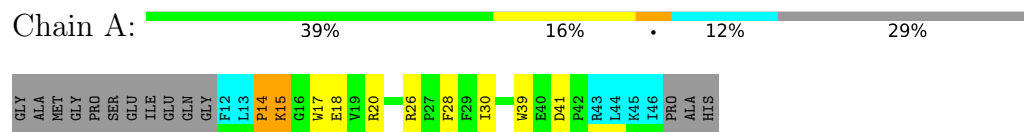


- Molecule 2: 12-mer from Matrix protein VP40

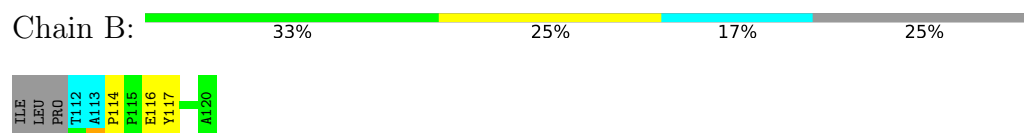


4.2.16 Score per residue for model 16

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

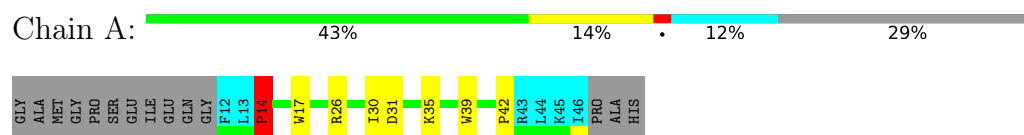


- Molecule 2: 12-mer from Matrix protein VP40



4.2.17 Score per residue for model 17

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

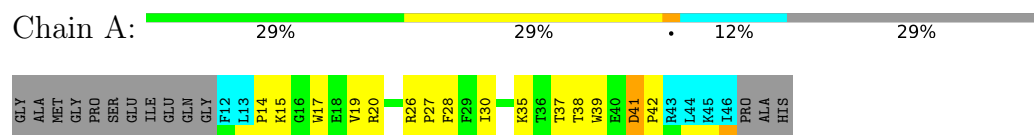


- Molecule 2: 12-mer from Matrix protein VP40

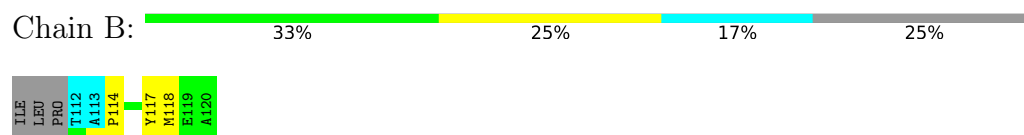


4.2.18 Score per residue for model 18

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

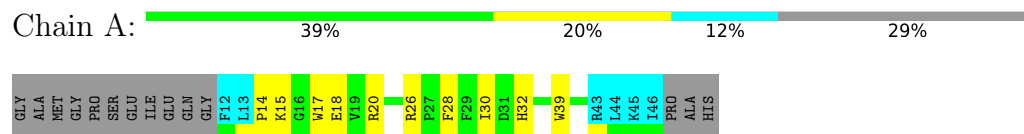


- Molecule 2: 12-mer from Matrix protein VP40



4.2.19 Score per residue for model 19

- Molecule 1: E3 ubiquitin-protein ligase NEDD4

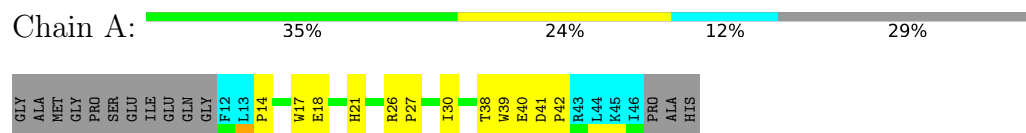


- Molecule 2: 12-mer from Matrix protein VP40



4.2.20 Score per residue for model 20

- Molecule 1: E3 ubiquitin-protein ligase NEDD4



- Molecule 2: 12-mer from Matrix protein VP40



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 120 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
CNSSOLVE	structure solution	
CNSSOLVE	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	443
Number of shifts mapped to atoms	345
Number of unparsed shifts	0
Number of shifts with mapping errors	98
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

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	0.40±0.02	0±0/256 (0.0± 0.0%)	0.81±0.04	0±0/351 (0.1± 0.1%)
2	B	0.43±0.05	0±0/60 (0.0± 0.0%)	0.76±0.08	0±0/79 (0.0± 0.0%)
All	All	0.41	0/6320 (0.0%)	0.80	4/8600 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	30	ILE	N-CA-C	6.07	116.76	107.77	7	4

There are no chirality outliers.

There are no planarity outliers.

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	244	225	223	8±2
2	B	58	49	49	3±1
All	All	6040	5480	5440	181

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:ILE:HB	2:B:117:TYR:HE2	0.95	1.21	17	12
1:A:14:PRO:HG2	1:A:42:PRO:HB2	0.93	1.40	12	5
1:A:14:PRO:HG2	1:A:42:PRO:HG2	0.88	1.44	10	6
1:A:30:ILE:HB	2:B:117:TYR:CE2	0.79	2.12	11	17
1:A:26:ARG:HG2	1:A:39:TRP:CE3	0.68	2.24	19	16
1:A:14:PRO:HB2	1:A:17:TRP:CD1	0.66	2.26	19	9
1:A:17:TRP:HA	1:A:30:ILE:O	0.64	1.93	19	16
1:A:35:LYS:HD3	2:B:118:MET:HA	0.62	1.71	6	1
1:A:26:ARG:HG2	1:A:39:TRP:HE3	0.61	1.55	11	4
1:A:17:TRP:CE2	1:A:31:ASP:HB2	0.60	2.32	4	10
1:A:35:LYS:HG3	2:B:117:TYR:HD1	0.60	1.55	11	1
2:B:117:TYR:HE1	2:B:119:GLU:HB2	0.58	1.58	14	1
1:A:38:THR:OG1	1:A:40:GLU:HG2	0.57	2.00	11	1
1:A:30:ILE:CB	2:B:117:TYR:HE2	0.56	2.09	8	3
1:A:17:TRP:CZ3	1:A:38:THR:HG22	0.56	2.35	13	7
1:A:30:ILE:HB	2:B:117:TYR:CE1	0.55	2.36	1	1
1:A:37:THR:HG21	2:B:115:PRO:HG2	0.55	1.76	6	2
1:A:37:THR:HG21	2:B:115:PRO:HD2	0.54	1.78	11	1
1:A:29:PHE:HB2	1:A:38:THR:OG1	0.53	2.03	1	1
1:A:18:GLU:HB2	1:A:30:ILE:HG13	0.53	1.80	7	3
1:A:15:LYS:HA	1:A:15:LYS:HE3	0.52	1.81	4	1
1:A:18:GLU:HB2	1:A:32:HIS:CE1	0.52	2.39	19	1
1:A:35:LYS:HG3	2:B:117:TYR:CD1	0.52	2.38	11	1
1:A:39:TRP:CZ2	2:B:115:PRO:HD3	0.52	2.40	15	1
1:A:30:ILE:HG22	1:A:37:THR:HG22	0.51	1.83	6	2
1:A:20:ARG:HD2	1:A:28:PHE:CZ	0.50	2.41	10	6
1:A:16:GLY:O	1:A:31:ASP:HA	0.50	2.07	4	1
1:A:26:ARG:CG	1:A:39:TRP:CE3	0.48	2.96	10	6
1:A:15:LYS:HD3	1:A:15:LYS:H	0.48	1.68	8	1
1:A:35:LYS:HA	2:B:117:TYR:CD1	0.48	2.43	17	4
2:B:117:TYR:CZ	2:B:119:GLU:HB2	0.48	2.43	4	1
2:B:117:TYR:HD1	2:B:118:MET:N	0.47	2.08	14	4
1:A:30:ILE:CG2	1:A:37:THR:HG22	0.47	2.40	6	1
1:A:18:GLU:O	1:A:30:ILE:HG12	0.47	2.10	16	2
2:B:117:TYR:CD1	2:B:117:TYR:C	0.47	2.93	19	1
1:A:20:ARG:HB3	1:A:28:PHE:CE1	0.47	2.44	11	2
1:A:20:ARG:HD2	1:A:28:PHE:HZ	0.47	1.71	12	2
1:A:30:ILE:HB	2:B:117:TYR:HE1	0.46	1.70	1	1
1:A:26:ARG:HD2	1:A:27:PRO:HD2	0.46	1.86	18	1
1:A:21:HIS:HA	1:A:27:PRO:HA	0.46	1.88	4	4
2:B:119:GLU:HG2	2:B:120:ALA:N	0.45	2.26	12	1
1:A:15:LYS:H	1:A:15:LYS:CD	0.45	2.25	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:116:GLU:CD	2:B:116:GLU:H	0.45	2.18	2	3
1:A:30:ILE:HG22	2:B:117:TYR:CE2	0.44	2.47	7	1
1:A:26:ARG:HG2	1:A:39:TRP:CZ3	0.44	2.47	15	2
1:A:15:LYS:O	1:A:15:LYS:HG3	0.44	2.13	16	1
1:A:30:ILE:HG22	1:A:37:THR:HB	0.44	1.90	18	1
1:A:35:LYS:HB3	2:B:117:TYR:CD1	0.43	2.49	2	1
1:A:32:HIS:CE1	2:B:119:GLU:HG3	0.42	2.49	13	1
1:A:38:THR:HB	1:A:40:GLU:OE2	0.42	2.15	2	1
1:A:35:LYS:HA	2:B:117:TYR:CE1	0.41	2.51	4	2
2:B:114:PRO:HA	2:B:115:PRO:HD3	0.41	1.78	5	1
2:B:117:TYR:C	2:B:117:TYR:CD1	0.41	2.99	13	2
1:A:24:ASN:C	1:A:26:ARG:N	0.41	2.79	10	1
1:A:22:ALA:C	1:A:24:ASN:H	0.40	2.24	7	1
1:A:26:ARG:NE	1:A:39:TRP:CE3	0.40	2.89	14	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	29/49 (59%)	21±8 (74±29%)	3±1 (10±5%)	1±1 (2±2%)	8	48
2	B	6/12 (50%)	5±1 (78±20%)	1±1 (14±10%)	0±0 (2±6%)	6	43
All	All	613/1220 (50%)	523 (85%)	75 (12%)	15 (2%)	7	44

All 6 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	14	PRO	4
2	B	118	MET	3
1	A	15	LYS	3
1	A	35	LYS	2
1	A	41	ASP	2
1	A	40	GLU	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	26/41 (63%)	23±6 (90±23%)	1±1 (3±4%)	34	83
2	B	6/10 (60%)	5±1 (91±11%)	1±1 (9±11%)	11	56
All	All	605/1020 (59%)	577 (95%)	28 (5%)	25	76

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)
2	B	116	GLU	8
1	A	34	THR	3
1	A	15	LYS	3
2	B	119	GLU	2
1	A	36	THR	2
1	A	31	ASP	2
1	A	30	ILE	1
1	A	40	GLU	1
1	A	33	ASN	1
2	B	118	MET	1
1	A	18	GLU	1
1	A	38	THR	1
1	A	24	ASN	1
1	A	14	PRO	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 54% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_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	443
Number of shifts mapped to atoms	345
Number of unparsed shifts	0
Number of shifts with mapping errors	98
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

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

- No matching atom found in the structure. All 98 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	PRO	HA	4.266	0.100	1
1	A	5	PRO	HB2	2.104	0.100	1
1	A	5	PRO	HB3	1.642	0.100	1
1	A	5	PRO	HD2	3.718	0.100	2
1	A	5	PRO	HD3	3.46	0.100	2
1	A	5	PRO	HG2	1.831	0.100	2
1	A	5	PRO	HG3	1.78	0.100	2
1	A	6	SER	H	8.491	0.100	1
1	A	6	SER	HA	4.257	0.100	1
1	A	6	SER	HB2	3.77	0.100	1
1	A	6	SER	HB3	3.696	0.100	1
1	A	6	SER	N	116.118	0.300	1
1	A	7	GLU	H	8.409	0.100	1
1	A	7	GLU	HA	4.073	0.100	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	7	GLU	HB2	1.802	0.100	1
1	A	7	GLU	HB3	1.767	0.100	1
1	A	7	GLU	HG2	2.094	0.100	2
1	A	7	GLU	HG3	1.878	0.100	2
1	A	7	GLU	N	122.503	0.300	1
1	A	8	ILE	H	8.041	0.100	1
1	A	8	ILE	HA	3.902	0.100	1
1	A	8	ILE	HB	1.648	0.100	1
1	A	8	ILE	HD11	0.633	0.100	1
1	A	8	ILE	HD12	0.633	0.100	1
1	A	8	ILE	HD13	0.633	0.100	1
1	A	8	ILE	HG12	1.281	0.100	2
1	A	8	ILE	HG13	0.985	0.100	2
1	A	8	ILE	HG21	0.694	0.100	1
1	A	8	ILE	HG22	0.694	0.100	1
1	A	8	ILE	HG23	0.694	0.100	1
1	A	8	ILE	N	120.387	0.300	1
1	A	9	GLU	H	8.215	0.100	1
1	A	9	GLU	HA	4.073	0.100	1
1	A	9	GLU	HB2	1.843	0.100	1
1	A	9	GLU	HB3	1.75	0.100	1
1	A	9	GLU	HG2	2.193	0.100	2
1	A	9	GLU	HG3	2.087	0.100	2
1	A	9	GLU	N	123.95	0.300	1
1	A	10	GLN	H	8.2145	0.100	1
1	A	10	GLN	HA	4.079	0.100	1
1	A	10	GLN	HB2	1.931	0.100	1
1	A	10	GLN	HB3	1.765	0.100	1
1	A	10	GLN	HE21	7.14	0.100	2
1	A	10	GLN	HE22	7.142	0.100	2
1	A	10	GLN	HG2	2.192	0.100	2
1	A	10	GLN	HG3	2.074	0.100	2
1	A	10	GLN	N	120.301	0.300	1
1	A	10	GLN	NE2	112.517	0.300	1
1	A	11	GLY	H	8.1565	0.100	1
1	A	11	GLY	HA2	3.709	0.100	2
1	A	11	GLY	HA3	3.659	0.100	2
1	A	11	GLY	N	108.313	0.300	1
1	A	47	PRO	HA	4.171	0.100	1
1	A	47	PRO	HB2	1.839	0.100	1
1	A	47	PRO	HB3	2.0775	0.100	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	47	PRO	HD2	3.696	0.100	2
1	A	47	PRO	HD3	3.457	0.100	2
1	A	47	PRO	HG3	1.766	0.100	2
1	A	48	ALA	H	8.3635	0.100	1
1	A	48	ALA	HA	4.047	0.100	1
1	A	48	ALA	HB1	1.175	0.100	1
1	A	48	ALA	HB2	1.175	0.100	1
1	A	48	ALA	HB3	1.175	0.100	1
1	A	48	ALA	N	125.145	0.300	1
1	A	49	HIS	H	7.8775	0.100	1
1	A	49	HIS	HA	4.273	0.100	1
1	A	49	HIS	HB2	3.022	0.100	1
1	A	49	HIS	HB3	2.895	0.100	1
1	A	49	HIS	N	122.616	0.300	1
1	B	109	ILE	H	8.022	0.100	1
1	B	109	ILE	HA	3.899	0.100	1
1	B	109	ILE	HB	1.599	0.100	1
1	B	109	ILE	HD11	0.672	0.100	1
1	B	109	ILE	HD12	0.672	0.100	1
1	B	109	ILE	HD13	0.672	0.100	1
1	B	109	ILE	HG12	1.291	0.100	2
1	B	109	ILE	HG13	0.991	0.100	2
1	B	109	ILE	HG21	0.697	0.100	1
1	B	109	ILE	HG22	0.697	0.100	1
1	B	109	ILE	HG23	0.697	0.100	1
1	B	110	LEU	H	8.231	0.100	1
1	B	110	LEU	HA	4.484	0.100	1
1	B	110	LEU	HB2	1.509	0.100	1
1	B	110	LEU	HB3	1.448	0.100	1
1	B	110	LEU	HD11	0.755	0.100	2
1	B	110	LEU	HD12	0.755	0.100	2
1	B	110	LEU	HD13	0.755	0.100	2
1	B	110	LEU	HD21	0.716	0.100	2
1	B	110	LEU	HD22	0.716	0.100	2
1	B	110	LEU	HD23	0.716	0.100	2
1	B	110	LEU	HG	1.383	0.100	1
1	B	111	PRO	HA	4.313	0.100	1
1	B	111	PRO	HB2	2.135	0.100	2
1	B	111	PRO	HB3	1.856	0.100	2
1	B	111	PRO	HD2	3.698	0.100	2
1	B	111	PRO	HD3	3.499	0.100	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	111	PRO	HG2	1.767	0.100	2
1	B	111	PRO	HG3	1.737	0.100	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	39	0.38 ± 0.82	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 54%, i.e. 267 atoms were assigned a chemical shift out of a possible 491. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	91/170 (54%)	66/68 (97%)	0/72 (0%)	25/30 (83%)
Sidechain	145/252 (58%)	142/161 (88%)	0/81 (0%)	3/10 (30%)
Aromatic	31/69 (45%)	29/34 (85%)	0/29 (0%)	2/6 (33%)
Overall	267/491 (54%)	237/263 (90%)	0/182 (0%)	30/46 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 55%, i.e. 345 atoms were assigned a chemical shift out of a possible 624. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	113/210 (54%)	82/84 (98%)	0/88 (0%)	31/38 (82%)
Sidechain	196/335 (59%)	193/216 (89%)	0/105 (0%)	3/14 (21%)
Aromatic	36/79 (46%)	34/39 (87%)	0/34 (0%)	2/6 (33%)
Overall	345/624 (55%)	309/339 (91%)	0/227 (0%)	36/58 (62%)

7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules con-

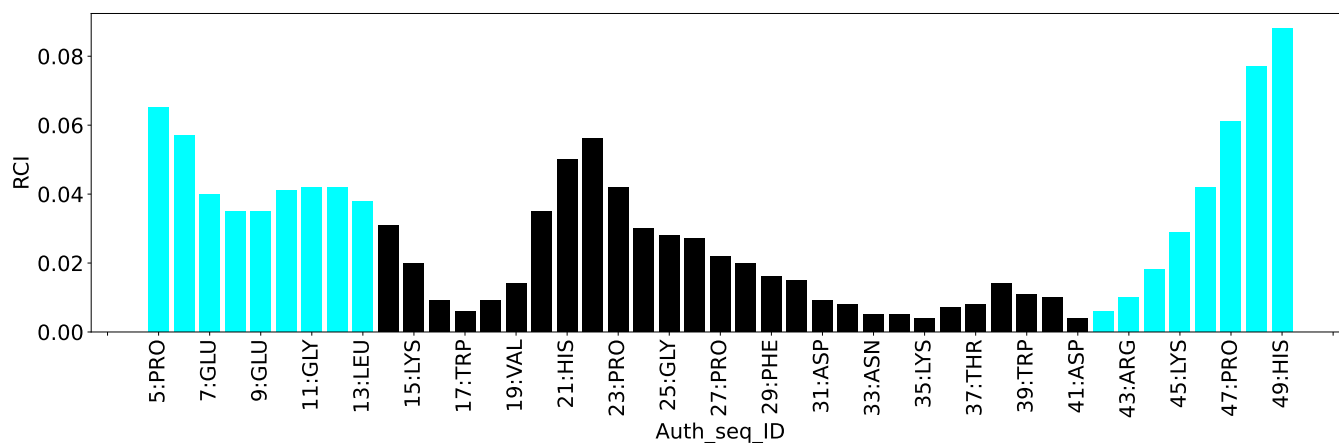
taining paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	20	ARG	NE	113.10	76.53 – 92.65	17.7
1	A	31	ASP	HB3	-0.23	1.32 – 4.00	-10.8
1	A	41	ASP	HA	2.23	3.04 – 6.12	-7.6
1	A	42	PRO	HG3	-0.01	0.33 – 3.48	-6.1
1	A	20	ARG	HB3	0.26	0.43 – 3.11	-5.6
1	A	26	ARG	HD3	1.66	1.81 – 4.39	-5.6
1	A	35	LYS	HA	2.11	2.15 – 6.37	-5.1

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:



Random coil index (RCI) for chain B:

