



Full wwPDB NMR Structure Validation Report ⓘ

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BMRB ID : 17595
Title : Solution structure of the endonuclease Nob1 from P.horikoshii
Authors : Veith, T.; Martin, R.; Wurm, J.P.; Weis, B.; Duchardt-Ferner, E.; Saffertal, C.; Hennig, R.; Mirus, O.; Bohnsack, M.T.; Woehnert, J.; Schleiff, E.
Deposited on : 2011-05-05

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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

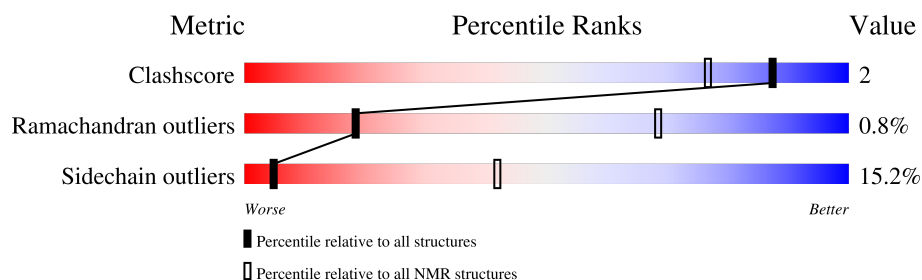
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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	165	

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:116 (110)	0.44	8
2	A:127-A:157 (31)	0.40	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 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2600 atoms, of which 1338 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Putative toxin VapC6.

Mol	Chain	Residues	Atoms						Trace
1	A	161	Total	C	H	N	O	S	0
			2599	806	1338	217	233	5	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP O58440
A	-2	SER	-	expression tag	UNP O58440
A	-1	MET	-	expression tag	UNP O58440
A	0	GLY	-	expression tag	UNP O58440

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

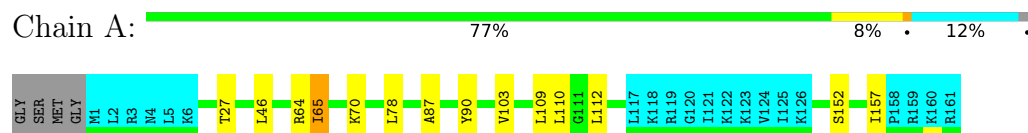
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: Putative toxin VapC6

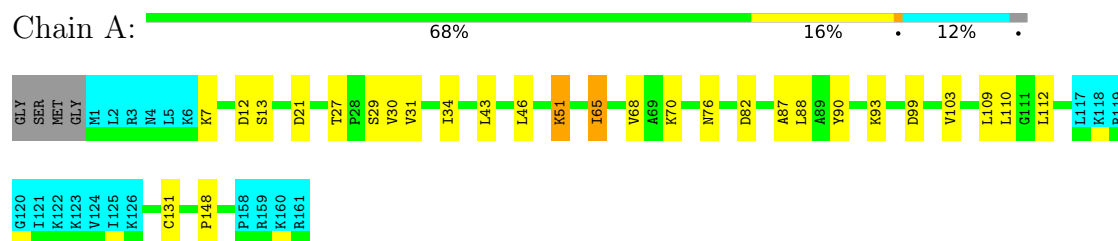


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

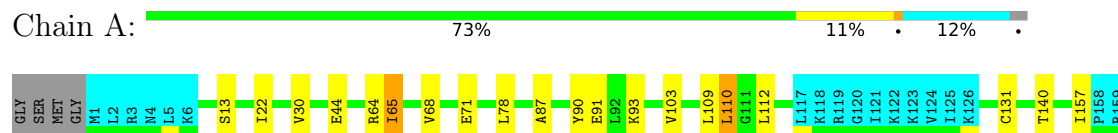
4.2.1 Score per residue for model 1

- Molecule 1: Putative toxin VapC6



4.2.2 Score per residue for model 2

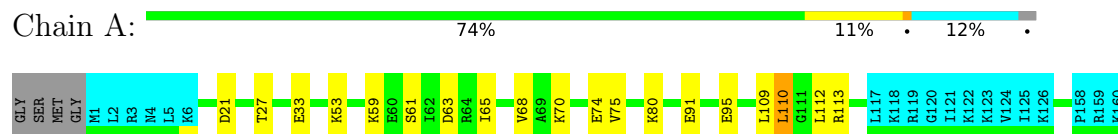
- Molecule 1: Putative toxin VapC6





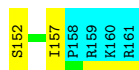
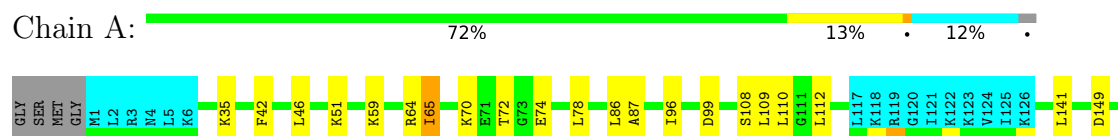
4.2.3 Score per residue for model 3

- Molecule 1: Putative toxin VapC6



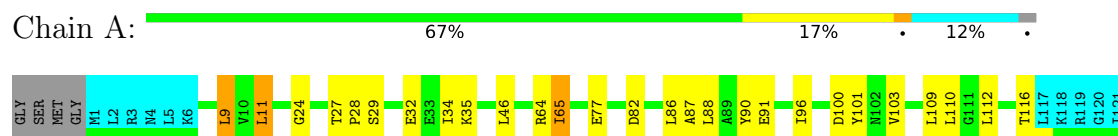
4.2.4 Score per residue for model 4

- Molecule 1: Putative toxin VapC6



4.2.5 Score per residue for model 5

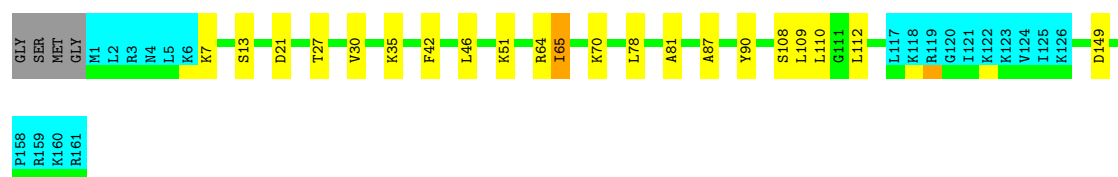
- Molecule 1: Putative toxin VapC6



4.2.6 Score per residue for model 6

- Molecule 1: Putative toxin VapC6

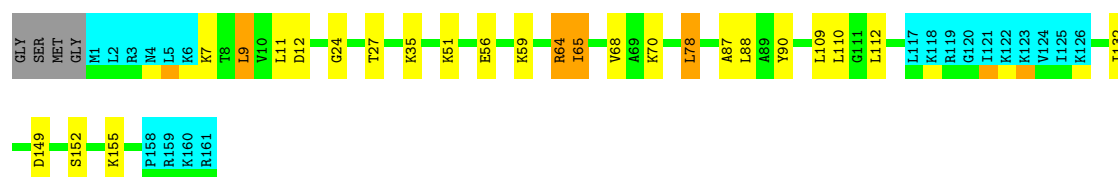




4.2.7 Score per residue for model 7

- Molecule 1: Putative toxin VapC6

Chain A: 70% 13% 12%



4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Putative toxin VapC6

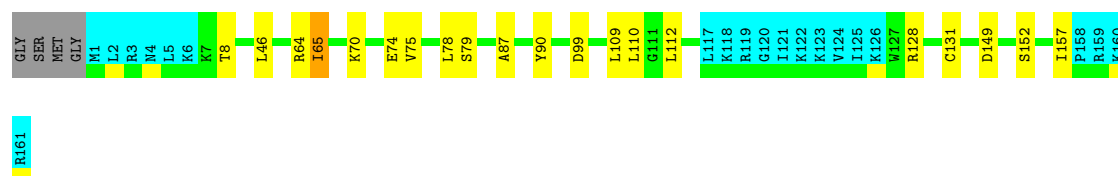
Chain A: 72% 13% 12%



4.2.9 Score per residue for model 9

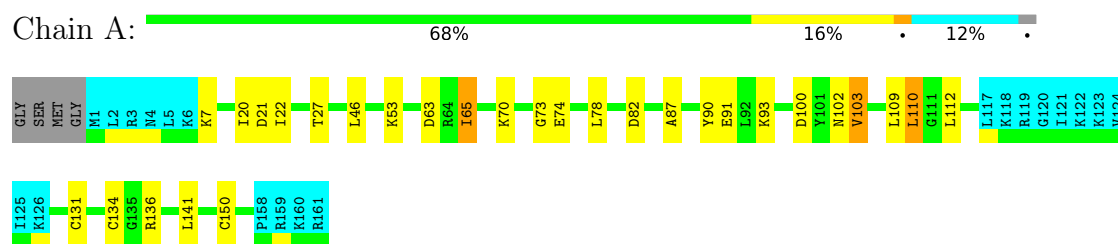
- Molecule 1: Putative toxin VapC6

Chain A: 73% 12% 12%



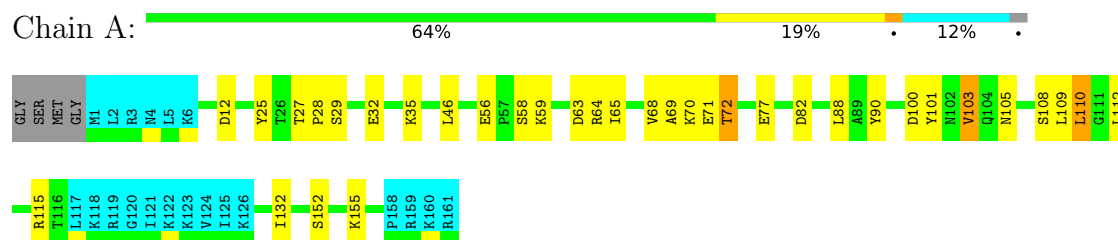
4.2.10 Score per residue for model 10

- Molecule 1: Putative toxin VapC6



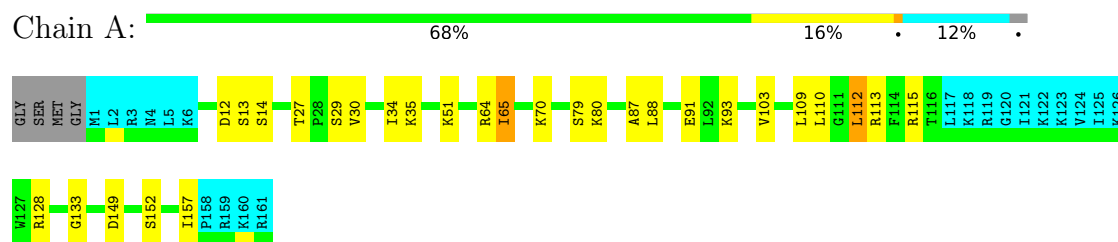
4.2.11 Score per residue for model 11

- Molecule 1: Putative toxin VapC6



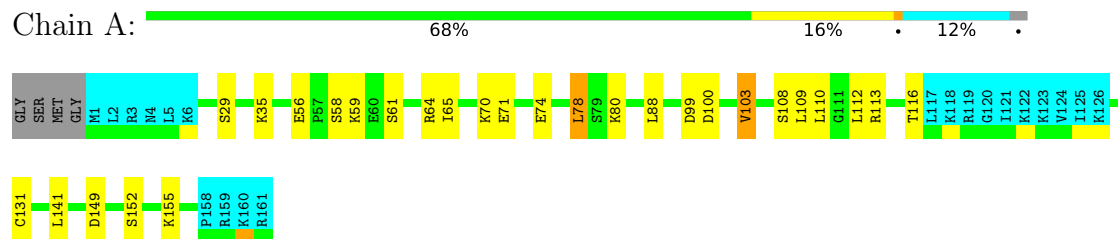
4.2.12 Score per residue for model 12

- Molecule 1: Putative toxin VapC6



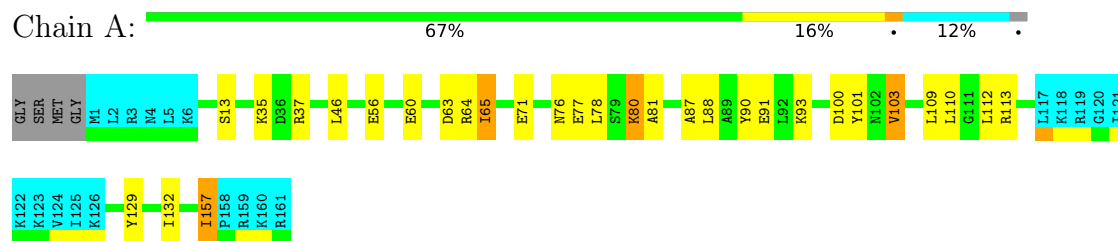
4.2.13 Score per residue for model 13

- Molecule 1: Putative toxin VapC6



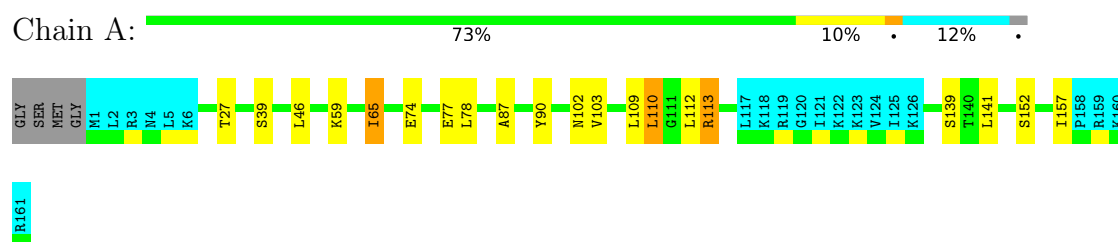
4.2.14 Score per residue for model 14

- Molecule 1: Putative toxin VapC6



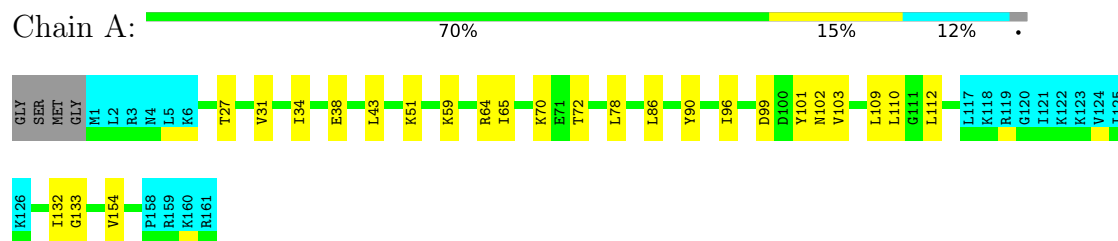
4.2.15 Score per residue for model 15

- Molecule 1: Putative toxin VapC6



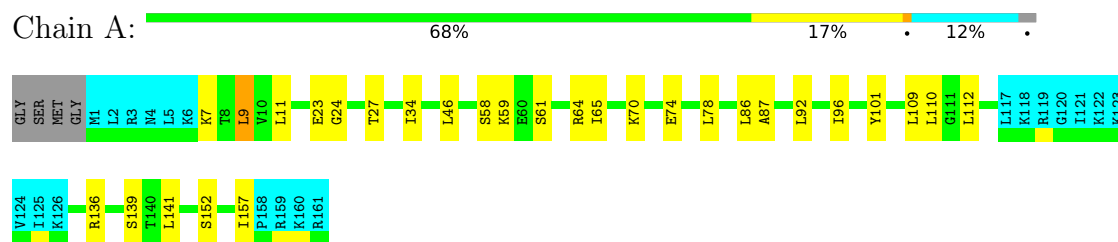
4.2.16 Score per residue for model 16

- Molecule 1: Putative toxin VapC6



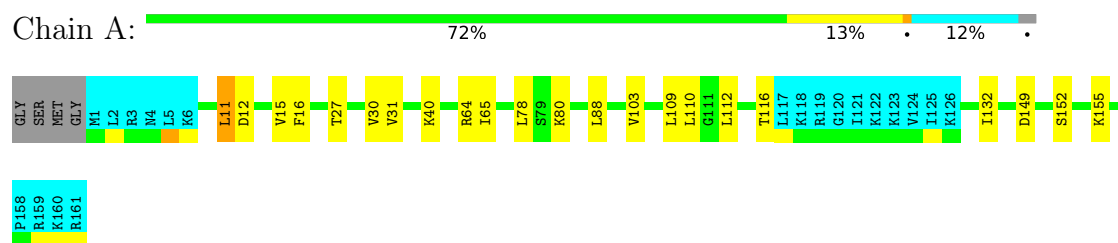
4.2.17 Score per residue for model 17

- Molecule 1: Putative toxin VapC6



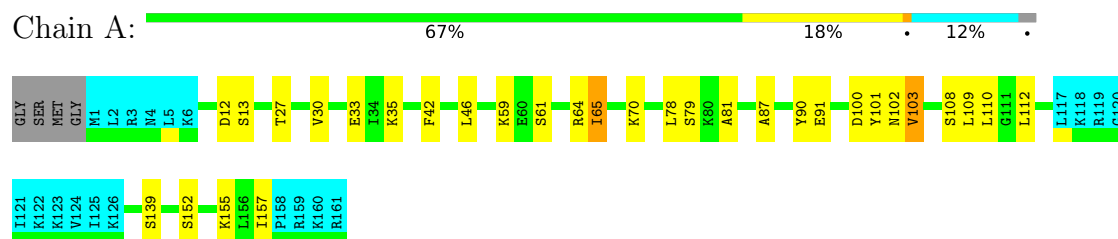
4.2.18 Score per residue for model 18

- Molecule 1: Putative toxin VapC6



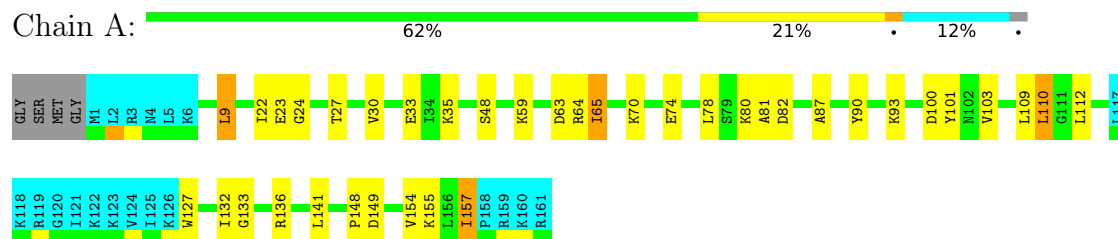
4.2.19 Score per residue for model 19

- Molecule 1: Putative toxin VapC6



4.2.20 Score per residue for model 20

- Molecule 1: Putative toxin VapC6



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
OPALp	refinement	
CYANA	structure solution	3.0
TALOS+	structure solution	
CANDID	structure solution	
ATNOS	refinement	
CANDID	refinement	
CYANA	refinement	3.0

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	1961
Number of shifts mapped to atoms	1961
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.59±0.01	0±0/1105 (0.0± 0.0%)	1.35±0.03	1±1/1493 (0.1± 0.1%)
All	All	0.59	0/22100 (0.0%)	1.35	21/29860 (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	A	0.0±0.0	0.9±0.9
All	All	0	19

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	A	28	PRO	CA-C-N	7.14	130.18	120.54	11	2
1	A	28	PRO	C-N-CA	7.14	130.18	120.54	11	2
1	A	99	ASP	CA-CB-CG	5.92	118.52	112.60	4	2
1	A	34	ILE	CB-CA-C	5.85	118.00	111.80	1	1
1	A	12	ASP	CA-C-N	5.74	129.42	120.82	1	1
1	A	12	ASP	C-N-CA	5.74	129.42	120.82	1	1
1	A	157	ILE	CA-CB-CG2	5.61	120.03	110.50	14	1
1	A	12	ASP	CA-CB-CG	5.58	118.18	112.60	19	1
1	A	22	ILE	CB-CA-C	5.43	119.77	110.38	20	1
1	A	51	LYS	N-CA-C	-5.32	104.38	112.04	6	1
1	A	31	VAL	CA-CB-CG1	5.29	119.39	110.40	18	1
1	A	72	THR	CB-CA-C	5.27	119.01	110.37	4	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	38	GLU	CA-C-N	5.25	127.27	120.44	16	1
1	A	38	GLU	C-N-CA	5.25	127.27	120.44	16	1
1	A	56	GLU	CA-C-N	5.23	125.23	120.21	13	2
1	A	56	GLU	C-N-CA	5.23	125.23	120.21	13	2

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	101	TYR	Sidechain	7
1	A	64	ARG	Sidechain	3
1	A	113	ARG	Sidechain	3
1	A	136	ARG	Sidechain	2
1	A	115	ARG	Sidechain	2
1	A	25	TYR	Sidechain	1
1	A	37	ARG	Sidechain	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	1089	1119	1119	4±2
All	All	21800	22380	22380	90

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:VAL:HG11	1:A:110:LEU:HD21	0.82	1.50	11	3
1:A:11:LEU:HB3	1:A:15:VAL:HG11	0.74	1.59	18	1
1:A:65:ILE:HD11	1:A:87:ALA:HA	0.62	1.70	6	15
1:A:78:LEU:HD12	1:A:78:LEU:H	0.53	1.64	7	4
1:A:9:LEU:HD23	1:A:24:GLY:HA3	0.52	1.79	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:ASP:O	1:A:15:VAL:HG12	0.51	2.05	18	1
1:A:90:TYR:CE2	1:A:110:LEU:HG	0.50	2.41	8	13
1:A:42:PHE:CZ	1:A:46:LEU:HD11	0.50	2.42	6	3
1:A:9:LEU:HD22	1:A:23:GLU:O	0.49	2.07	20	1
1:A:9:LEU:CD2	1:A:24:GLY:HA3	0.49	2.38	20	1
1:A:9:LEU:HD21	1:A:11:LEU:HD11	0.47	1.85	7	2
1:A:65:ILE:HD12	1:A:90:TYR:CE2	0.47	2.45	10	7
1:A:112:LEU:HD13	1:A:113:ARG:N	0.46	2.25	12	1
1:A:100:ASP:H	1:A:103:VAL:HG12	0.46	1.71	10	4
1:A:42:PHE:CE2	1:A:46:LEU:HD11	0.46	2.45	6	2
1:A:51:LYS:HA	1:A:51:LYS:HE3	0.45	1.89	1	1
1:A:86:LEU:HD23	1:A:96:ILE:HD13	0.44	1.88	4	4
1:A:31:VAL:HG23	1:A:43:LEU:HD21	0.44	1.88	1	1
1:A:100:ASP:H	1:A:103:VAL:CG1	0.44	2.25	14	3
1:A:129:TYR:C	1:A:157:ILE:HD11	0.44	2.37	14	1
1:A:65:ILE:HD11	1:A:87:ALA:CA	0.43	2.44	14	3
1:A:13:SER:HB2	1:A:30:VAL:HG21	0.43	1.90	2	1
1:A:31:VAL:HG23	1:A:43:LEU:HD13	0.43	1.89	16	1
1:A:134:CYS:SG	1:A:150:CYS:SG	0.43	3.17	10	1
1:A:86:LEU:CD1	1:A:96:ILE:HD13	0.42	2.45	17	1
1:A:30:VAL:HG22	1:A:81:ALA:CB	0.42	2.45	20	2
1:A:15:VAL:HG13	1:A:16:PHE:CD1	0.41	2.50	18	1
1:A:30:VAL:HG22	1:A:81:ALA:HB1	0.41	1.92	6	1
1:A:9:LEU:HD23	1:A:9:LEU:C	0.41	2.41	20	1
1:A:69:ALA:HA	1:A:72:THR:HG22	0.41	1.91	11	1
1:A:31:VAL:HG23	1:A:43:LEU:CD2	0.41	2.46	1	1
1:A:80:LYS:HE3	1:A:81:ALA:N	0.41	2.31	14	1
1:A:78:LEU:HD12	1:A:78:LEU:N	0.40	2.31	19	2
1:A:127:TRP:CH2	1:A:157:ILE:HD13	0.40	2.52	20	1
1:A:15:VAL:HG13	1:A:16:PHE:CE1	0.40	2.52	18	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	141/165 (85%)	129±2 (92±1%)	10±2 (7±1%)	1±1 (1±1%)	18	68
All	All	2820/3300 (85%)	2587 (92%)	210 (7%)	23 (1%)	18	68

All 10 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	74	GLU	6
1	A	34	ILE	4
1	A	133	GLY	3
1	A	7	LYS	2
1	A	148	PRO	2
1	A	132	ILE	2
1	A	22	ILE	1
1	A	75	VAL	1
1	A	128	ARG	1
1	A	73	GLY	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	123/144 (85%)	104±4 (85±3%)	19±4 (15±3%)	5	42
All	All	2460/2880 (85%)	2085 (85%)	375 (15%)	5	42

All 71 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	109	LEU	20
1	A	112	LEU	20
1	A	65	ILE	19
1	A	70	LYS	15
1	A	27	THR	14
1	A	103	VAL	14
1	A	64	ARG	14
1	A	78	LEU	11

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Mol	Chain	Res	Type	Models (Total)
1	A	110	LEU	11
1	A	152	SER	11
1	A	59	LYS	10
1	A	35	LYS	10
1	A	46	LEU	9
1	A	88	LEU	9
1	A	157	ILE	9
1	A	149	ASP	9
1	A	91	GLU	8
1	A	141	LEU	7
1	A	93	LYS	6
1	A	131	CYS	6
1	A	80	LYS	6
1	A	155	LYS	6
1	A	13	SER	5
1	A	29	SER	5
1	A	51	LYS	5
1	A	82	ASP	5
1	A	63	ASP	5
1	A	108	SER	5
1	A	77	GLU	5
1	A	21	ASP	4
1	A	71	GLU	4
1	A	61	SER	4
1	A	9	LEU	4
1	A	116	THR	4
1	A	139	SER	4
1	A	132	ILE	4
1	A	102	ASN	4
1	A	30	VAL	3
1	A	76	ASN	3
1	A	33	GLU	3
1	A	53	LYS	3
1	A	113	ARG	3
1	A	11	LEU	3
1	A	7	LYS	3
1	A	12	ASP	3
1	A	79	SER	3
1	A	99	ASP	3
1	A	58	SER	3
1	A	68	VAL	2
1	A	74	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	32	GLU	2
1	A	100	ASP	2
1	A	56	GLU	2
1	A	14	SER	2
1	A	72	THR	2
1	A	154	VAL	2
1	A	44	GLU	1
1	A	140	THR	1
1	A	95	GLU	1
1	A	8	THR	1
1	A	75	VAL	1
1	A	22	ILE	1
1	A	105	ASN	1
1	A	128	ARG	1
1	A	60	GLU	1
1	A	39	SER	1
1	A	23	GLU	1
1	A	92	LEU	1
1	A	136	ARG	1
1	A	40	LYS	1
1	A	48	SER	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 91% for the well-defined parts and 87% 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	1961
Number of shifts mapped to atoms	1961
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
$^{13}\text{C}_\alpha$	159	-0.13 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	146	0.01 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	158	0.07 ± 0.09	None needed (< 0.5 ppm)
^{15}N	152	0.21 ± 0.35	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 91%, i.e. 1735 atoms were assigned a chemical shift out of a possible 1916. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	703/706 (100%)	287/288 (100%)	281/282 (100%)	135/136 (99%)
Sidechain	956/1112 (86%)	642/725 (89%)	308/351 (88%)	6/36 (17%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	76/98 (78%)	47/47 (100%)	28/50 (56%)	1/1 (100%)
Overall	1735/1916 (91%)	976/1060 (92%)	617/683 (90%)	142/173 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 87%, i.e. 1961 atoms were assigned a chemical shift out of a possible 2266. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	792/805 (98%)	323/328 (98%)	317/322 (98%)	152/155 (98%)
Sidechain	1093/1363 (80%)	727/886 (82%)	359/422 (85%)	7/55 (13%)
Aromatic	76/98 (78%)	47/47 (100%)	28/50 (56%)	1/1 (100%)
Overall	1961/2266 (87%)	1097/1261 (87%)	704/794 (89%)	160/211 (76%)

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:

