WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Jan 25, 2024 – 07:18 pm GMT

PDB ID	:	3ZBE
BMRB ID	:	18841
Title	:	E. coli O157 ParE2-associated antitoxin 2 (PaaA2)
Authors	:	Sterckx, Y.G.J.; Van Nuland, N.A.J.; Vranken, W.F.; Loris, R.
Deposited on	:	2012-11-08

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 (i) 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 (i)) were used in the production of this report:

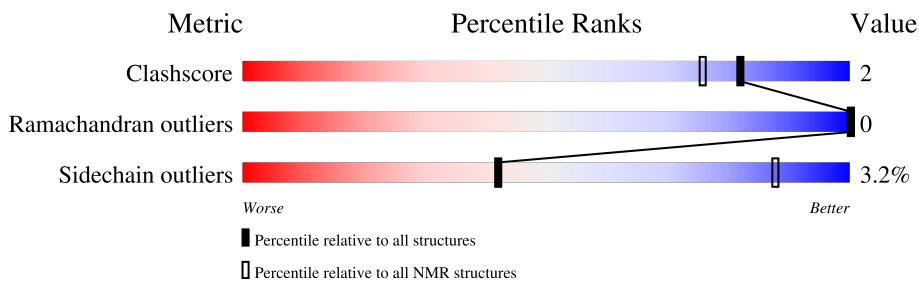|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 85%.

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		3.2%

Worse .... *Better*

■ Percentile relative to all structures

▯ Percentile relative to all NMR structures

Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	71	42% 58%

2 Ensemble composition and analysis ⓘ

This entry contains 50 models. Model 10 is the overall representative, medoid model (most similar to other models).

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:16-A:29 (14)	1.00	32
2	A:42-A:57 (16)	1.26	10

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 10 clusters and 2 single-model clusters were found.

Cluster number	Models
1	4, 6, 13, 14, 15, 17, 30, 31, 38
2	8, 21, 32, 33, 45, 49, 50
3	20, 24, 34, 35, 36, 46
4	1, 2, 25, 28, 41
5	22, 26, 42, 48
6	10, 23, 43, 47
7	3, 7, 19, 39
8	11, 12, 40, 44
9	9, 27, 37
10	5, 29
Single-model clusters	16; 18

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 1166 atoms, of which 574 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PAAA2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	71	1166	361	574	109	118	4	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q7ADP2
A	-6	ASP	-	expression tag	UNP Q7ADP2
A	-5	TYR	-	expression tag	UNP Q7ADP2
A	-4	LYS	-	expression tag	UNP Q7ADP2
A	-3	ASP	-	expression tag	UNP Q7ADP2
A	-2	ASP	-	expression tag	UNP Q7ADP2
A	-1	ASP	-	expression tag	UNP Q7ADP2
A	0	ASP	-	expression tag	UNP Q7ADP2
A	1	LYS	-	expression tag	UNP Q7ADP2

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: PAAA2

Chain A:
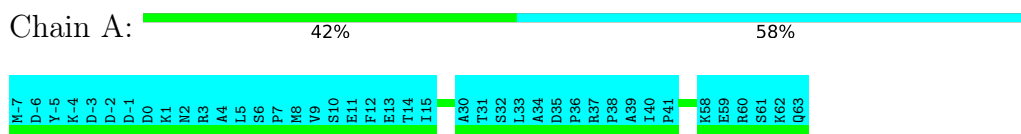
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PAAA2

Chain A:
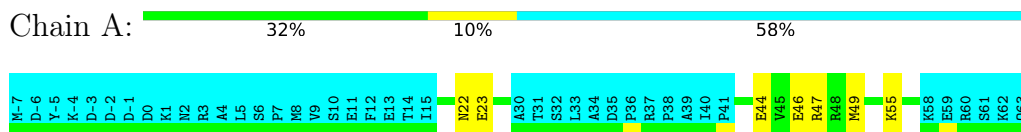
4.2.2 Score per residue for model 2

- Molecule 1: PAAA2

Chain A:
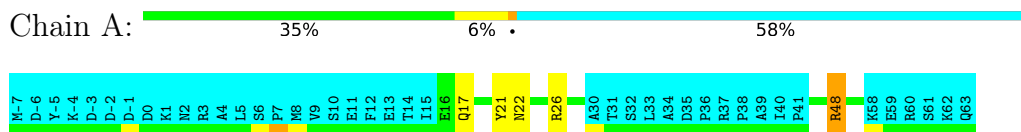
4.2.3 Score per residue for model 3

• Molecule 1: PAAA2

Chain A:
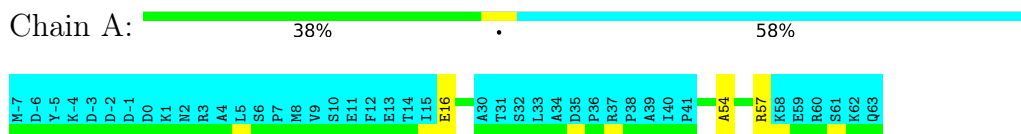
4.2.4 Score per residue for model 4

• Molecule 1: PAAA2

Chain A:
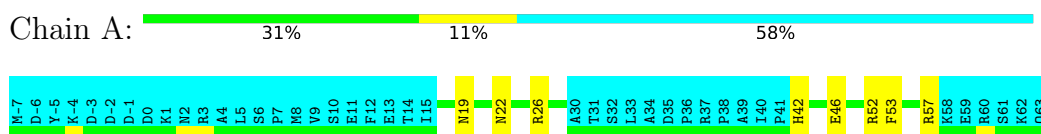
4.2.5 Score per residue for model 5

• Molecule 1: PAAA2

Chain A:
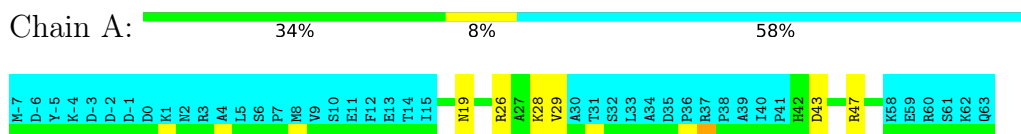
4.2.6 Score per residue for model 6

• Molecule 1: PAAA2

Chain A:
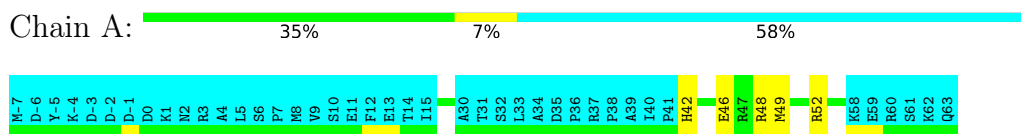
4.2.7 Score per residue for model 7

• Molecule 1: PAAA2

Chain A:
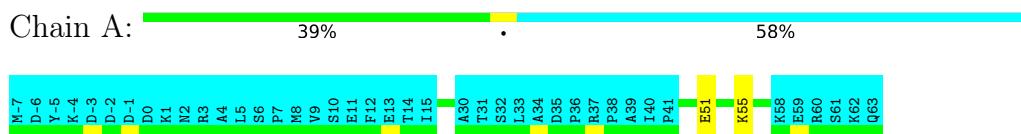
4.2.8 Score per residue for model 8

• Molecule 1: PAAA2

Chain A: 35% 6% 58%

M-7 D-6 Y-5 K-4 D-3 D-2 D-1 D0 K1 N2 R3 A4 L5 S6 P7 M8 V9 S10 E11 F12 E13 T14 I15 E16 A30 T31 S32 L33 A34 D35 P36 R37 P38 A39 I40 P41 H42 D43 R47 R52 K55 K58 E59 R60 S61 K62 Q63
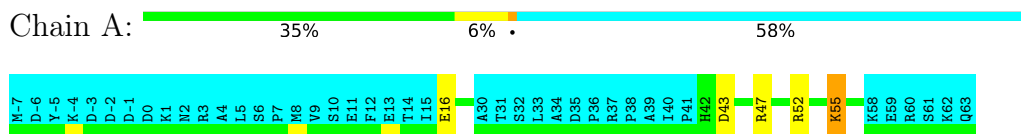
4.2.9 Score per residue for model 9

• Molecule 1: PAAA2

Chain A: 38% 58%

M-7 D-6 Y-5 K-4 D-3 D-2 D-1 D0 K1 N2 R3 A4 L5 S6 P7 M8 V9 S10 E11 F12 E13 T14 I15 N22 L25 R26 A30 T31 S32 L33 A34 D35 P36 R37 P38 A39 I40 P41 K58 E59 R60 S61 K62 Q63
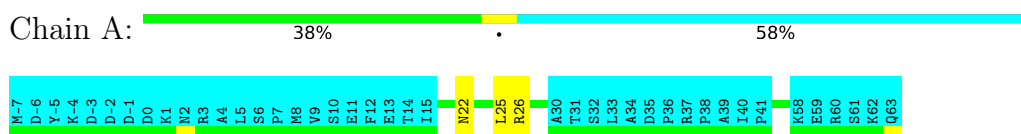
4.2.10 Score per residue for model 10 (medoid)

• Molecule 1: PAAA2

Chain A: 39% 58%

M-7 D-6 Y-5 K-4 D-3 D-2 D-1 D0 K1 N2 R3 A4 L5 S6 P7 M8 V9 S10 E11 F12 E13 T14 I15 E16 Q17 K28 V29 A30 T31 S32 L33 A34 D35 P36 R37 P38 A39 I40 P41 K58 E59 R60 S61 K62 Q63
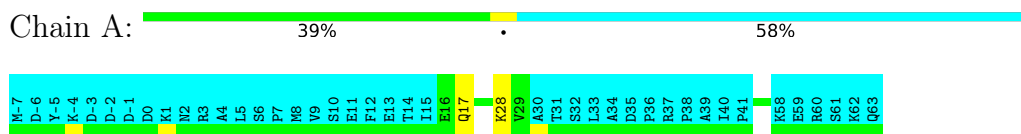
4.2.11 Score per residue for model 11

• Molecule 1: PAAA2

Chain A: 39% 58%

M-7 D-6 Y-5 K-4 D-3 D-2 D-1 D0 K1 N2 R3 A4 L5 S6 P7 M8 V9 S10 E11 F12 E13 T14 I15 E18 N19 S20 A30 T31 S32 L33 A34 D35 P36 R37 P38 A39 I40 P41 K58 E59 R60 S61 K62 Q63
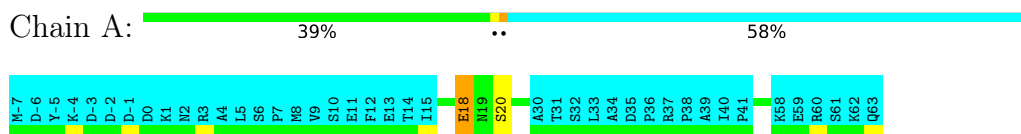
4.2.12 Score per residue for model 12

• Molecule 1: PAAA2

Chain A: 39% 58%

M-7 D-6 Y-5 K-4 D-3 D-2 D-1 D0 K1 N2 R3 A4 L5 S6 P7 M8 V9 S10 E11 F12 E13 T14 I15 A30 T31 S32 L33 A34 D35 P36 R37 P38 A39 I40 P41 H42 E46 K58 E59 R60 S61 K62 Q63
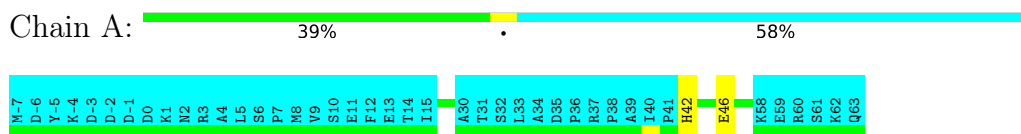
4.2.13   Score per residue for model 13

• Molecule 1: PAAA2

Chain A:
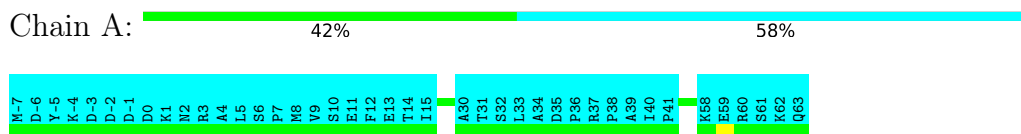
4.2.14   Score per residue for model 14

• Molecule 1: PAAA2

Chain A:
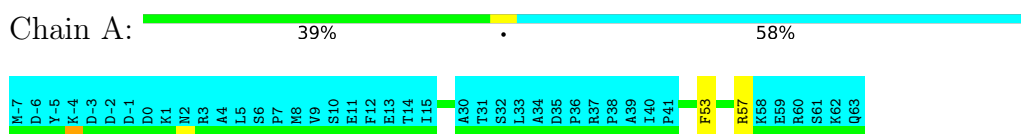
4.2.15   Score per residue for model 15

• Molecule 1: PAAA2

Chain A:
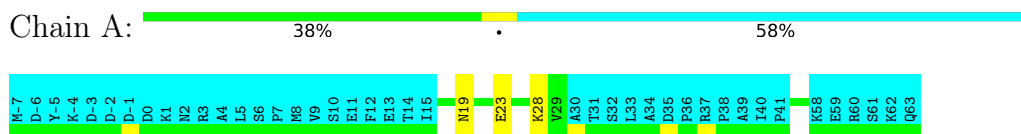
4.2.16   Score per residue for model 16

• Molecule 1: PAAA2

Chain A:
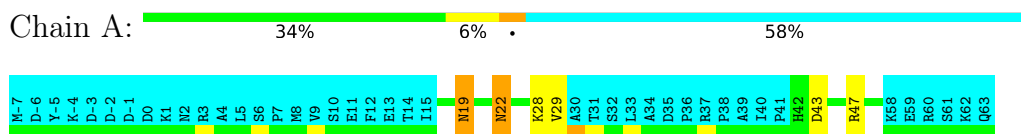
4.2.17   Score per residue for model 17

• Molecule 1: PAAA2

Chain A:
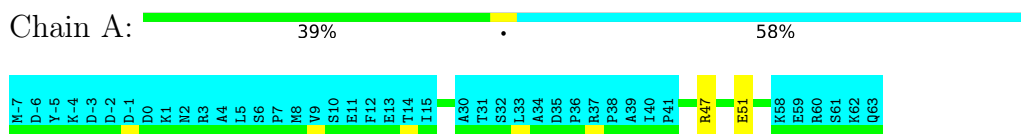
4.2.18 Score per residue for model 18

• Molecule 1: PAAA2

Chain A:
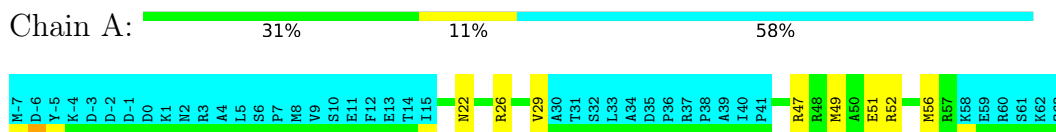
4.2.19 Score per residue for model 19

• Molecule 1: PAAA2

Chain A:
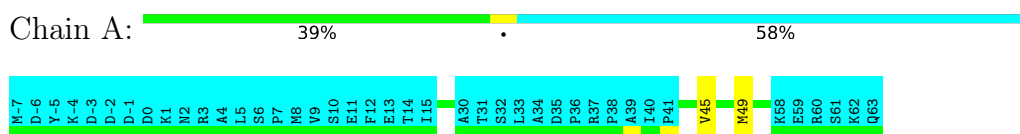
4.2.20 Score per residue for model 20

• Molecule 1: PAAA2

Chain A:
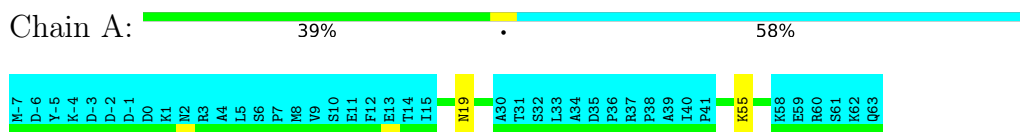
4.2.21 Score per residue for model 21

• Molecule 1: PAAA2

Chain A:
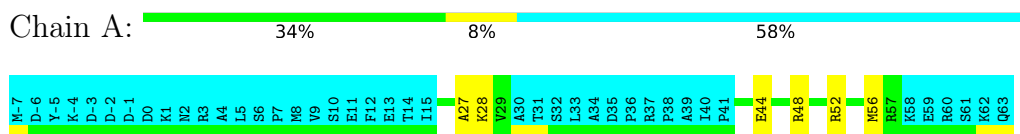
4.2.22 Score per residue for model 22

• Molecule 1: PAAA2

Chain A:
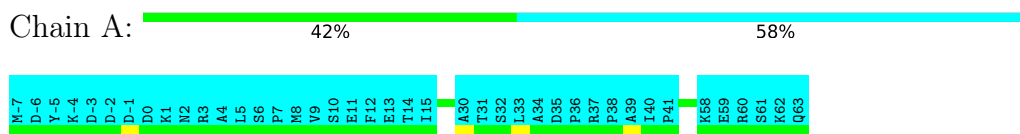
4.2.23 Score per residue for model 23

• Molecule 1: PAAA2

Chain A:
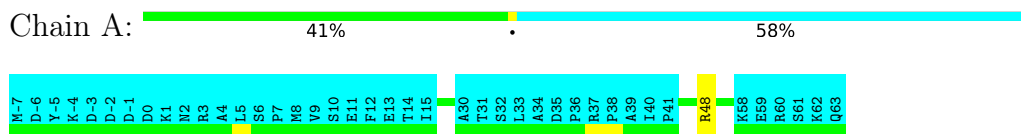
4.2.24 Score per residue for model 24

• Molecule 1: PAAA2

Chain A:
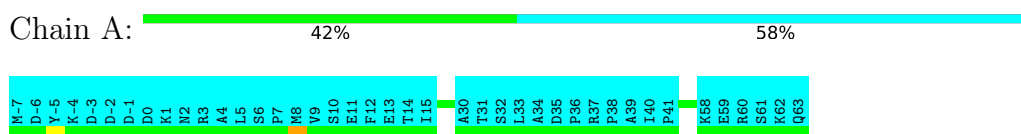
4.2.25 Score per residue for model 25

• Molecule 1: PAAA2

Chain A:
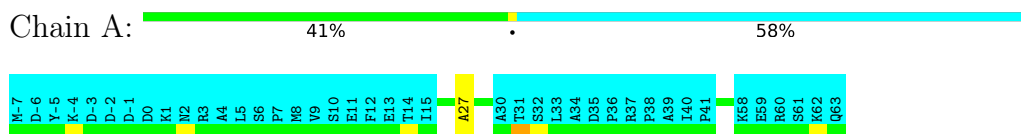
4.2.26 Score per residue for model 26

• Molecule 1: PAAA2

Chain A:
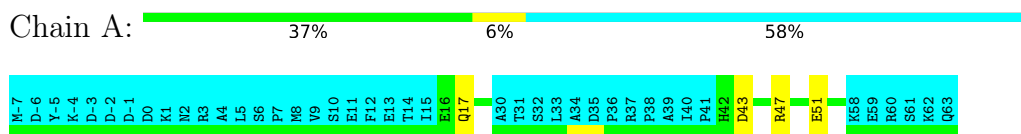
4.2.27 Score per residue for model 27

• Molecule 1: PAAA2

Chain A:
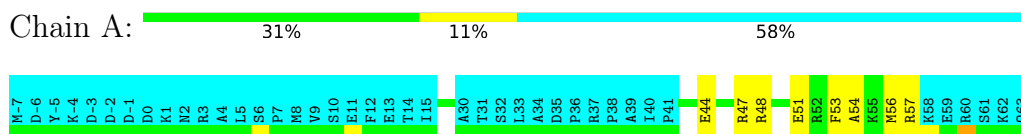
4.2.28 Score per residue for model 28

• Molecule 1: PAAA2

Chain A:
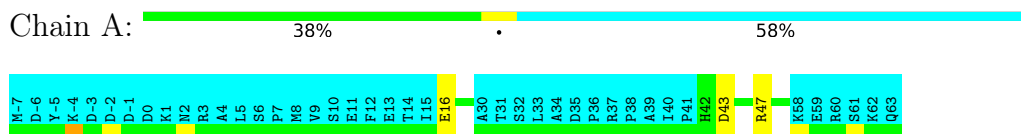
4.2.29 Score per residue for model 29

• Molecule 1: PAAA2

Chain A:
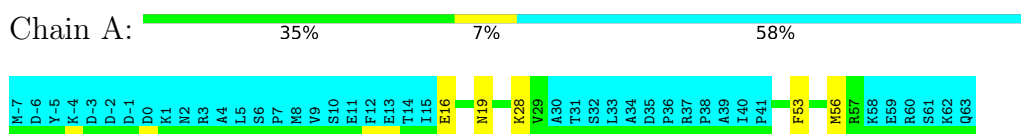
4.2.30 Score per residue for model 30

• Molecule 1: PAAA2

Chain A:
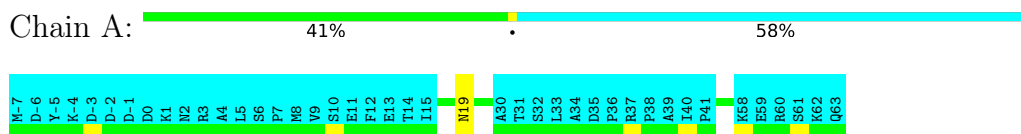
4.2.31 Score per residue for model 31

• Molecule 1: PAAA2

Chain A:
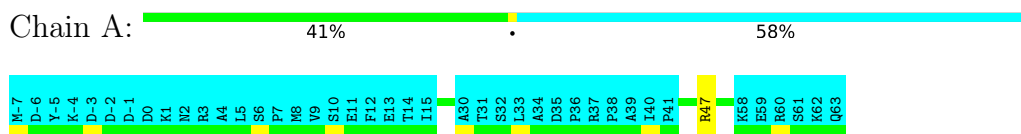
4.2.32 Score per residue for model 32

• Molecule 1: PAAA2

Chain A:
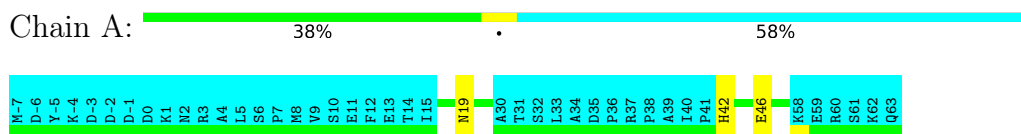
4.2.33　Score per residue for model 33

• Molecule 1: PAAA2

Chain A:
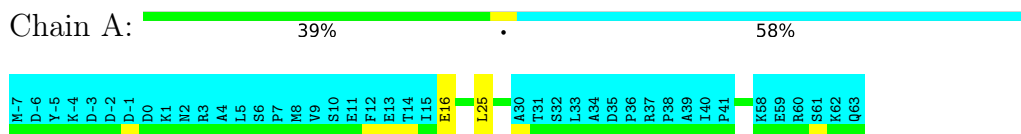
4.2.34　Score per residue for model 34

• Molecule 1: PAAA2

Chain A:
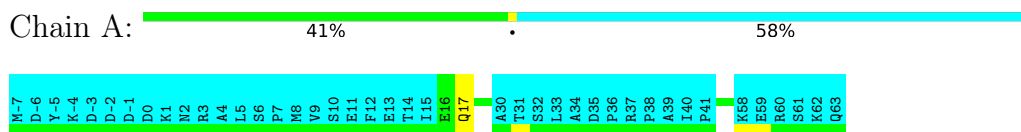
4.2.35　Score per residue for model 35

• Molecule 1: PAAA2

Chain A:
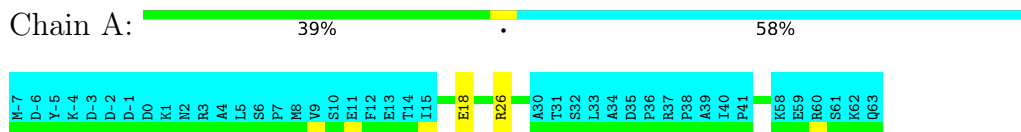
4.2.36　Score per residue for model 36

• Molecule 1: PAAA2

Chain A:
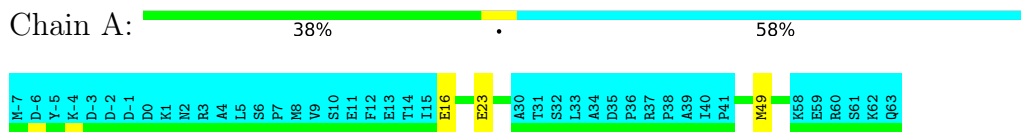
4.2.37　Score per residue for model 37

• Molecule 1: PAAA2

Chain A:
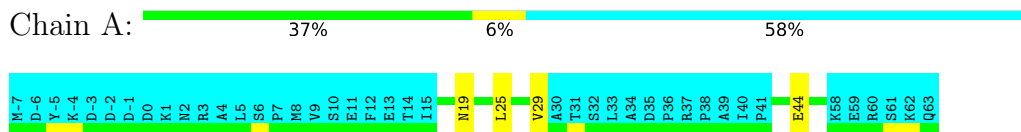
4.2.38 Score per residue for model 38

• Molecule 1: PAAA2

Chain A:
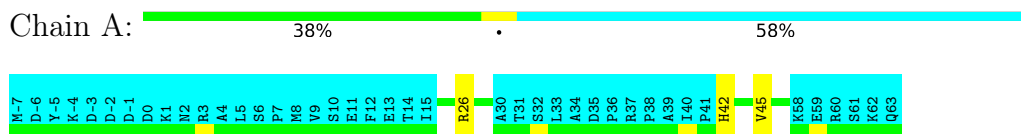
4.2.39 Score per residue for model 39

• Molecule 1: PAAA2

Chain A:
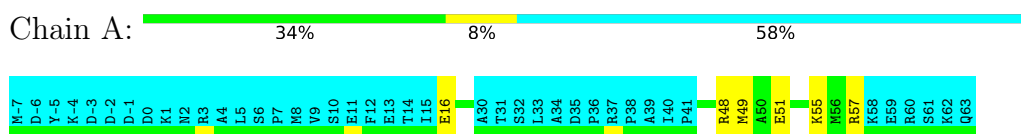
4.2.40 Score per residue for model 40

• Molecule 1: PAAA2

Chain A:
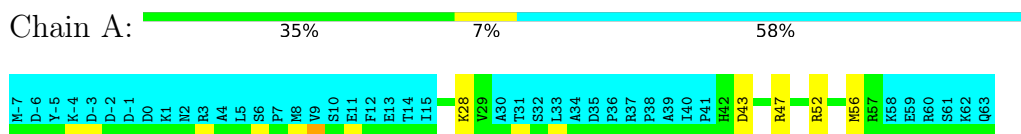
4.2.41 Score per residue for model 41

• Molecule 1: PAAA2

Chain A:
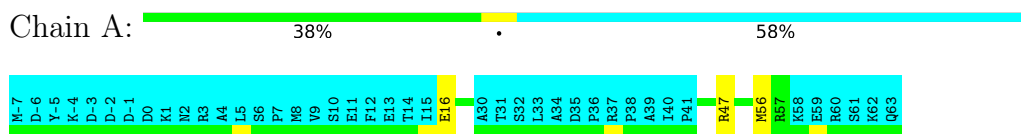
4.2.42 Score per residue for model 42

• Molecule 1: PAAA2

Chain A:
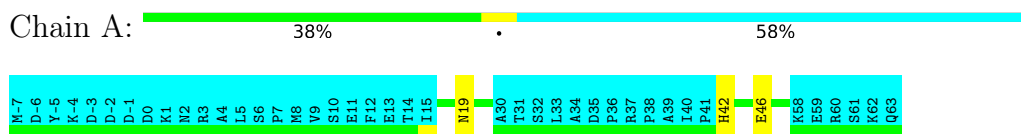
4.2.43 Score per residue for model 43

• Molecule 1: PAAA2

Chain A:
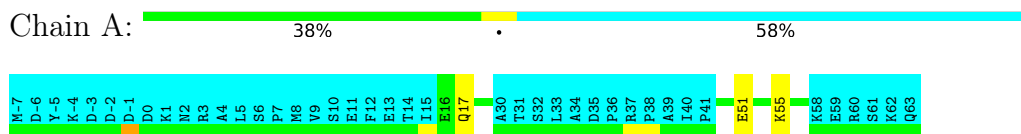
4.2.44 Score per residue for model 44

• Molecule 1: PAAA2

Chain A:
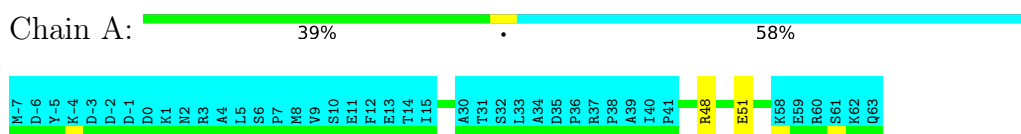
4.2.45 Score per residue for model 45

• Molecule 1: PAAA2

Chain A:
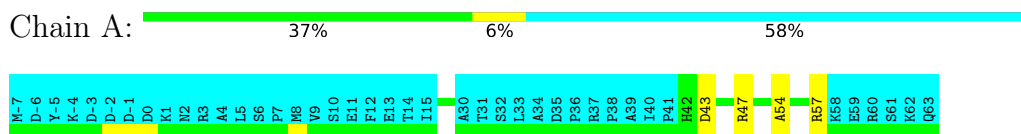
4.2.46 Score per residue for model 46

• Molecule 1: PAAA2

Chain A:
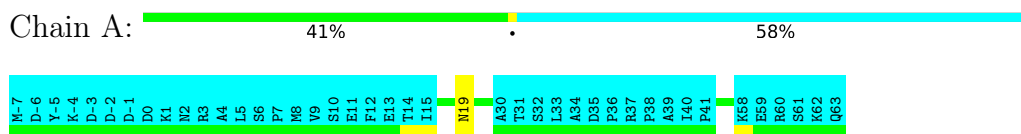
4.2.47 Score per residue for model 47

• Molecule 1: PAAA2

Chain A:
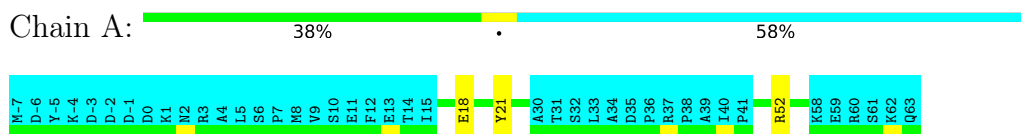
4.2.48 Score per residue for model 48

• Molecule 1: PAAA2

Chain A:
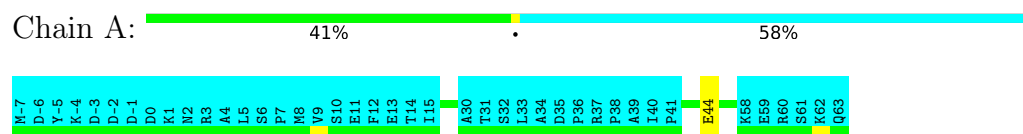
4.2.49 Score per residue for model 49

• Molecule 1: PAAA2

Chain A:
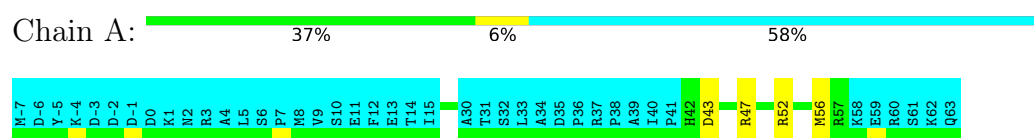
4.2.50 Score per residue for model 50

• Molecule 1: PAAA2

Chain A:
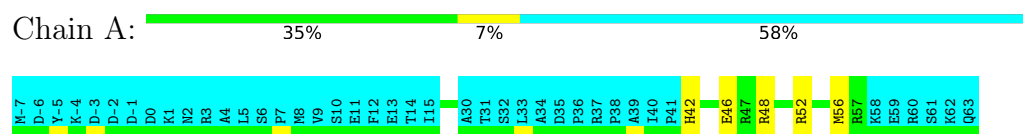
5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *STRUCTURE CALCULATION.*

Of the 5000 calculated structures, 50 were deposited, based on the following criterion: *SAXS DATA.*

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

Software name	Classification	Version
CNS	refinement	
ATSAS	structure solution	2.4.3
TALOS	structure solution	1.0
CNS	structure solution	1.2
CcpNmr Analysis	structure solution	1
CcpNmr Analysis	structure solution	2.2
DANGLE	structure solution	1.1
NMRPipe	structure solution	2.1

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	867
Number of shifts mapped to atoms	867
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	266	254	253	1±1
All	All	13300	12700	12650	65

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 3.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:48:ARG:HA	1:A:48:ARG:NE	0.60	2.12	23	3
1:A:42:HIS:O	1:A:46:GLU:HG2	0.59	1.98	4	3
1:A:48:ARG:O	1:A:51:GLU:HG2	0.58	1.98	44	1
1:A:43:ASP:O	1:A:47:ARG:HG2	0.56	1.99	26	5
1:A:18:GLU:HA	1:A:21:TYR:CD2	0.54	2.36	47	1
1:A:42:HIS:O	1:A:46:GLU:HG3	0.52	2.04	6	3
1:A:47:ARG:O	1:A:51:GLU:HG2	0.52	2.05	17	1
1:A:44:GLU:O	1:A:47:ARG:HG2	0.51	2.05	1	1
1:A:17:GLN:O	1:A:21:TYR:HB2	0.51	2.06	2	1
1:A:53:PHE:O	1:A:57:ARG:HG3	0.50	2.06	27	2
1:A:53:PHE:O	1:A:57:ARG:HB2	0.50	2.07	14	1
1:A:53:PHE:O	1:A:56:MET:HG3	0.50	2.06	27	1
1:A:51:GLU:O	1:A:55:LYS:HG3	0.50	2.07	39	2
1:A:47:ARG:HA	1:A:47:ARG:NE	0.49	2.22	41	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LYS:C	1:A:28:LYS:HD3	0.48	2.29	10	1
1:A:18:GLU:H	1:A:18:GLU:CD	0.48	2.12	11	1
1:A:54:ALA:O	1:A:57:ARG:HG2	0.48	2.09	3	2
1:A:49:MET:SD	1:A:52:ARG:HD3	0.47	2.49	6	1
1:A:42:HIS:O	1:A:45:VAL:HG12	0.47	2.09	38	1
1:A:19:ASN:HD22	1:A:19:ASN:N	0.47	2.08	16	1
1:A:22:ASN:O	1:A:26:ARG:HG3	0.46	2.11	4	1
1:A:47:ARG:O	1:A:51:GLU:HG3	0.46	2.10	18	2
1:A:43:ASP:O	1:A:47:ARG:HG3	0.46	2.10	40	3
1:A:47:ARG:HA	1:A:51:GLU:HB2	0.46	1.86	27	1
1:A:47:ARG:HA	1:A:47:ARG:CZ	0.46	2.40	31	1
1:A:48:ARG:HA	1:A:48:ARG:CZ	0.46	2.40	6	1
1:A:52:ARG:HA	1:A:52:ARG:NE	0.45	2.25	8	2
1:A:22:ASN:C	1:A:22:ASN:HD22	0.45	2.15	16	1
1:A:26:ARG:O	1:A:29:VAL:HG12	0.44	2.12	5	2
1:A:51:GLU:O	1:A:55:LYS:HG2	0.43	2.13	7	1
1:A:22:ASN:O	1:A:26:ARG:HG2	0.43	2.14	2	2
1:A:44:GLU:O	1:A:48:ARG:HG2	0.42	2.14	27	1
1:A:44:GLU:O	1:A:48:ARG:HG3	0.42	2.15	21	1
1:A:52:ARG:O	1:A:56:MET:HG3	0.42	2.15	49	1
1:A:52:ARG:O	1:A:56:MET:HG2	0.41	2.15	18	4
1:A:25:LEU:O	1:A:29:VAL:HG23	0.41	2.15	37	1
1:A:19:ASN:O	1:A:23:GLU:HG2	0.41	2.16	15	1
1:A:48:ARG:O	1:A:52:ARG:HG2	0.41	2.16	50	1
1:A:28:LYS:HA	1:A:28:LYS:CE	0.41	2.46	21	1
1:A:55:LYS:HE2	1:A:55:LYS:HA	0.40	1.94	8	1
1:A:45:VAL:O	1:A:49:MET:HG2	0.40	2.15	19	1
1:A:22:ASN:HB3	1:A:49:MET:SD	0.40	2.56	18	1
1:A:53:PHE:O	1:A:56:MET:HG2	0.40	2.17	29	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	30/71 (42%)	29±1 (98±3%)	1±1 (2±3%)	0±0 (0±0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1500/3550 (42%)	1474 (98%)	26 (2%)	0 (0%)	100 100

There are no Ramachandran outliers.

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	27/64 (42%)	26±1 (97±4%)	1±1 (3±4%)	42 88
All	All	1350/3200 (42%)	1307 (97%)	43 (3%)	42 88

All 15 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	19	ASN	9
1	A	16	GLU	8
1	A	49	MET	3
1	A	55	LYS	3
1	A	17	GLN	3
1	A	28	LYS	3
1	A	22	ASN	2
1	A	23	GLU	2
1	A	48	ARG	2
1	A	25	LEU	2
1	A	44	GLU	2
1	A	18	GLU	1
1	A	26	ARG	1
1	A	57	ARG	1
1	A	52	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7   Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 86% for the entire structure.

7.1   Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	867
Number of shifts mapped to atoms	867
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

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 2 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	24	TRP	HB2	3.477	0.001	2
1	A	38	PRO	HD3	3.772	0.011	2

7.1.2   Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	71	0.10 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_\beta$	71	-0.03 ± 0.03	None needed (< 0.5 ppm)
$^{13}C'$	64	0.01 ± 0.08	None needed (< 0.5 ppm)
^{15}N	64	-0.92 ± 0.14	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 85%, i.e. 389 atoms were assigned a chemical shift out of a possible 455. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	150/150 (100%)	60/60 (100%)	60/60 (100%)	30/30 (100%)
Sidechain	205/266 (77%)	139/167 (83%)	63/79 (80%)	3/20 (15%)
Aromatic	34/39 (87%)	17/19 (89%)	16/17 (94%)	1/3 (33%)
Overall	389/455 (85%)	216/246 (88%)	139/156 (89%)	34/53 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 865 atoms were assigned a chemical shift out of a possible 1003. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	332/347 (96%)	133/138 (96%)	135/142 (95%)	64/67 (96%)
Sidechain	481/598 (80%)	325/379 (86%)	151/184 (82%)	5/35 (14%)
Aromatic	52/58 (90%)	26/28 (93%)	25/27 (93%)	1/3 (33%)
Overall	865/1003 (86%)	484/545 (89%)	311/353 (88%)	70/105 (67%)

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: