



Full wwPDB NMR Structure Validation Report ⓘ

Nov 14, 2017 – 12:52 AM EST

PDB ID : 6B3N
Title : Solution structure of the N-terminal domain of the effector NleG5-1 from Escherichia coli O157:H7 str. Sakai
Authors : Valteau, D.; Houliston, S.; Lemak, A.; Anderson, W.F.; Arrowsmith, C.; Savchenko, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : unknown

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A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20030345
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

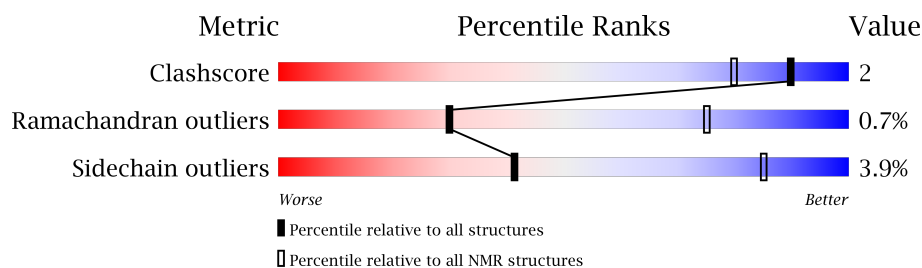
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	137	 62% . 10% 27%

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 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:2-A:49, A:55-A:62, A:66-A:84 (75)	0.43	19
2	A:90-A:100 (11)	0.30	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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1585 atoms, of which 795 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NleG5-1.

Mol	Chain	Residues	Atoms						Trace
1	A	100	Total	C	H	N	O	S	0
			1585	494	795	138	154	4	

There are 21 discrepancies between the modelled and reference sequences:

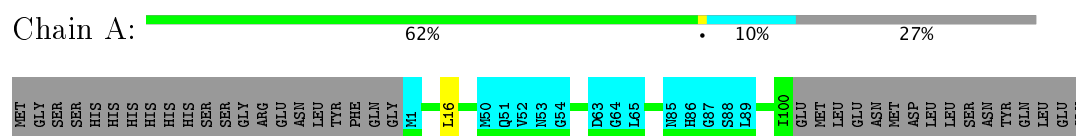
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q8X4X3
A	-19	GLY	-	expression tag	UNP Q8X4X3
A	-18	SER	-	expression tag	UNP Q8X4X3
A	-17	SER	-	expression tag	UNP Q8X4X3
A	-16	HIS	-	expression tag	UNP Q8X4X3
A	-15	HIS	-	expression tag	UNP Q8X4X3
A	-14	HIS	-	expression tag	UNP Q8X4X3
A	-13	HIS	-	expression tag	UNP Q8X4X3
A	-12	HIS	-	expression tag	UNP Q8X4X3
A	-11	HIS	-	expression tag	UNP Q8X4X3
A	-10	SER	-	expression tag	UNP Q8X4X3
A	-9	SER	-	expression tag	UNP Q8X4X3
A	-8	GLY	-	expression tag	UNP Q8X4X3
A	-7	ARG	-	expression tag	UNP Q8X4X3
A	-6	GLU	-	expression tag	UNP Q8X4X3
A	-5	ASN	-	expression tag	UNP Q8X4X3
A	-4	LEU	-	expression tag	UNP Q8X4X3
A	-3	TYR	-	expression tag	UNP Q8X4X3
A	-2	PHE	-	expression tag	UNP Q8X4X3
A	-1	GLN	-	expression tag	UNP Q8X4X3
A	0	GLY	-	expression tag	UNP Q8X4X3

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: NleG5-1

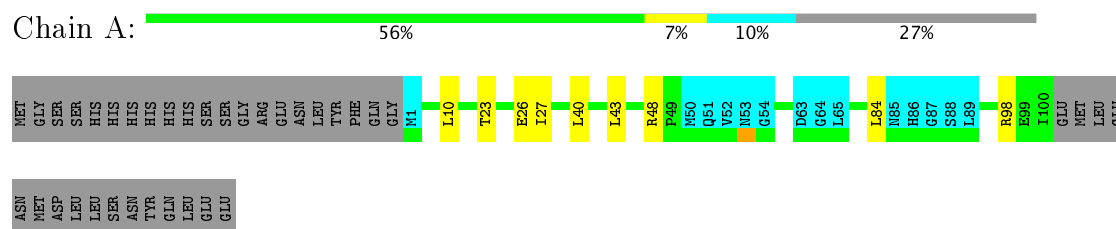


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

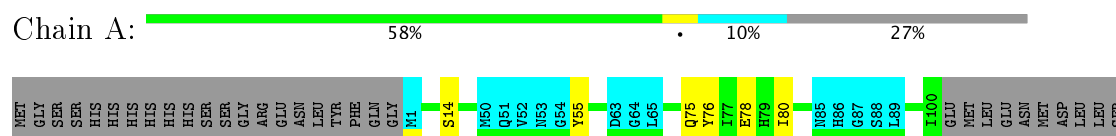
4.2.1 Score per residue for model 1

- Molecule 1: NleG5-1



4.2.2 Score per residue for model 2

- Molecule 1: NleG5-1



ASN
TYR
GLN
LEU
GLU
GLU

4.2.7 Score per residue for model 7

- Molecule 1: NleG5-1

Chain A: 58% 10% 27%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY ARG GLU ASN ASN TYR PHE GLN GLY M1 L16 Q21 E42 M50 Q51 Y52 N53 G54 G58 D63 G64 L65 N85 H86 G87 S88 L89 Y96 I100 GLU MET LEU GLU ASN MET ASP LEU SER

ASN
TYR
GLN
LEU
GLU
GLU

4.2.8 Score per residue for model 8

- Molecule 1: NleG5-1

Chain A: 52% 11% 10% 27%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG ASP GLU ASN LEU TYR PHE GLN GLY M1 L5 T6 P7 L10 L16 T23 E26 N29 R39 M44 M50 Q51 Y52 N53 G54 M57 D63 G64 L65 N69 Y76 I77 T80 E81

M85 H86 G87 S88 L89 I100 GLU MET LEU GLU ASN MET ASP GLU LEU LEU SER ASN TYR PHE GLN GLU LEU GLU

4.2.9 Score per residue for model 9

- Molecule 1: NleG5-1

Chain A: 53% 10% 10% 27%

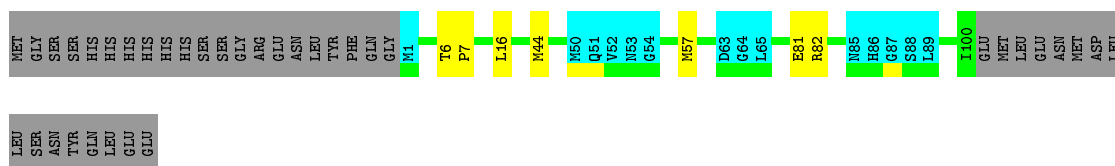
MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY ARG ASP GLU ASN LEU TYR PHE GLN GLY M1 L10 L16 Q21 E22 T23 E26 A36 R39 E42 I47 R48 P49 M50 Q51 Y52 N53 G54 M57 D63 G64 L65 S66 N67 E78 N85 H86

G87 S88 L89 R98 E99 I100 GLU MET LEU GLU ASN MET ASP GLU LEU LEU SER ASN TYR PHE GLN GLU LEU GLU

4.2.10 Score per residue for model 10

- Molecule 1: NleG5-1

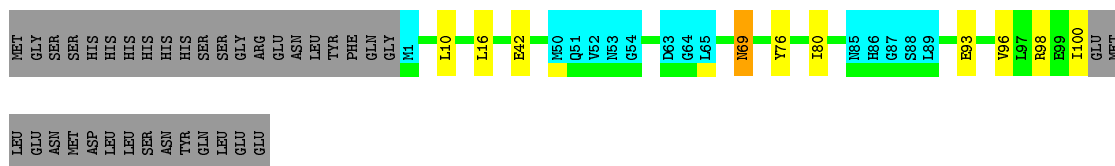
Chain A: 58% 5% 10% 27%



4.2.11 Score per residue for model 11

- Molecule 1: NleG5-1

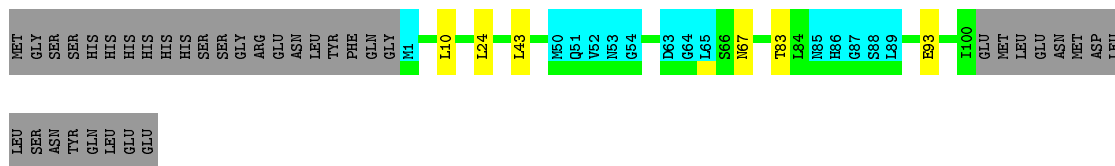
Chain A: 55% 7% 10% 27%



4.2.12 Score per residue for model 12

- Molecule 1: NleG5-1

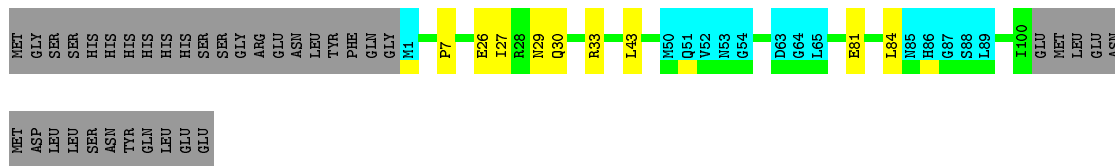
Chain A: 58% 10% 27%



4.2.13 Score per residue for model 13

- Molecule 1: NleG5-1

Chain A: 56% 7% 10% 27%



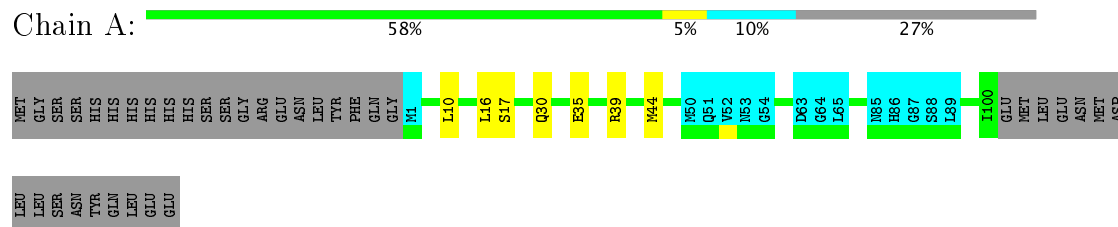
4.2.14 Score per residue for model 14

- Molecule 1: NleG5-1

Chain A: 57% 5% 10% 27%

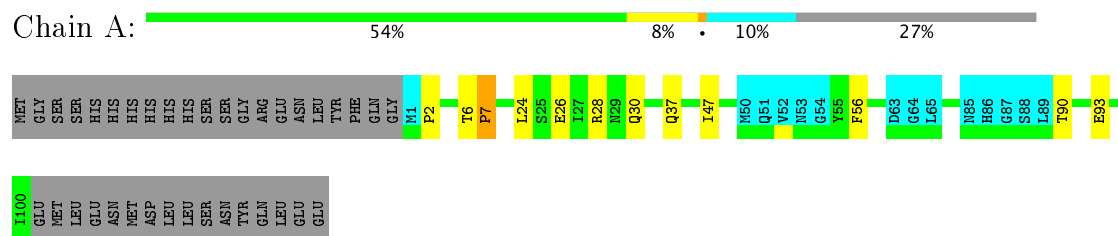
4.2.15 Score per residue for model 15

- Molecule 1: NleG5-1



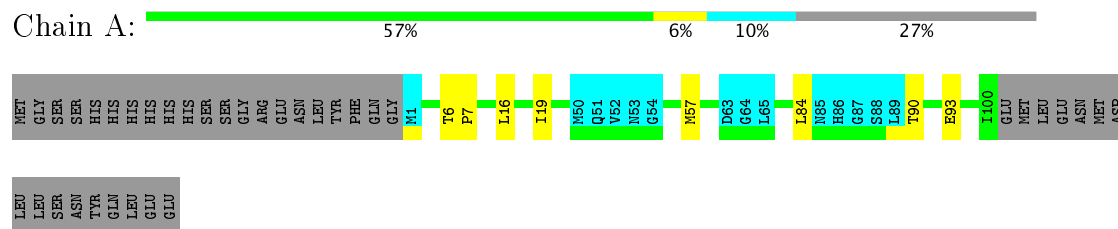
4.2.16 Score per residue for model 16

- Molecule 1: NleG5-1



4.2.17 Score per residue for model 17

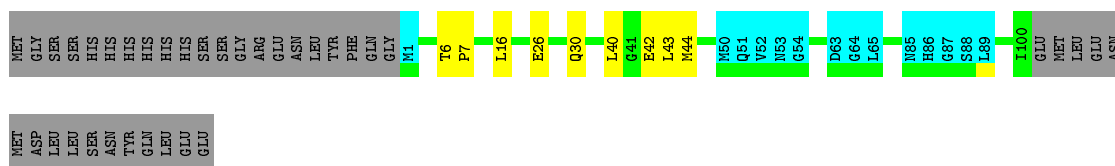
- Molecule 1: NleG5-1



4.2.18 Score per residue for model 18

- Molecule 1: NleG5-1

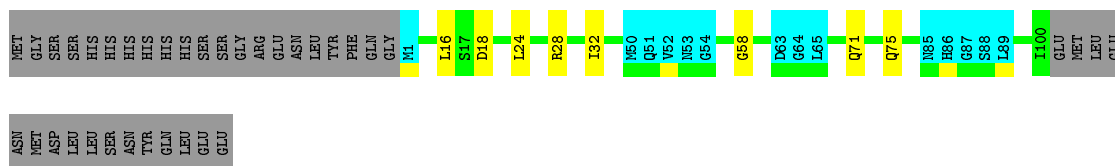




4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: NleG5-1

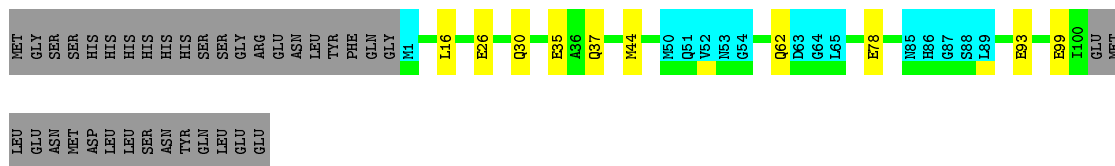
Chain A: 57% 6% 10% 27%



4.2.20 Score per residue for model 20

- Molecule 1: NleG5-1

Chain A: 55% 7% 10% 27%



5 Refinement protocol and experimental data overview

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

Of the 100 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
CYANA	structure calculation	
CNS	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)	6b3n_cs.cif
Number of chemical shift lists	1
Total number of shifts	1253
Number of shifts mapped to atoms	1253
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

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	0.1±0.2
All	All	0	1

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	39	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	690	701	701	3±2
All	All	13800	14020	14020	56

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:39:ARG:HG2	1:A:44:MET:SD	0.61	2.35	8	4
1:A:37:GLN:HB3	1:A:44:MET:SD	0.57	2.37	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:MET:SD	1:A:81:GLU:HB2	0.54	2.42	10	1
1:A:40:LEU:HD11	1:A:80:ILE:HD11	0.52	1.80	5	2
1:A:57:MET:HB3	1:A:81:GLU:HG2	0.49	1.85	8	1
1:A:6:THR:N	1:A:7:PRO:HD3	0.48	2.23	10	6
1:A:14:SER:HA	1:A:75:GLN:HB3	0.48	1.85	2	2
1:A:16:LEU:HD23	1:A:19:ILE:HG12	0.47	1.85	14	2
1:A:26:GLU:O	1:A:30:GLN:HG2	0.47	2.09	18	4
1:A:26:GLU:HA	1:A:29:ASN:ND2	0.47	2.24	8	1
1:A:90:THR:HG22	1:A:93:GLU:HG2	0.44	1.89	17	1
1:A:96:VAL:O	1:A:100:ILE:HG12	0.44	2.13	7	2
1:A:5:LEU:HD13	1:A:23:THR:HG21	0.43	1.89	8	1
1:A:47:ILE:HG22	1:A:56:PHE:HB2	0.43	1.90	16	1
1:A:60:LEU:HG	1:A:73:GLY:HA3	0.43	1.91	3	1
1:A:90:THR:HB	1:A:93:GLU:HG2	0.43	1.90	16	1
1:A:28:ARG:O	1:A:32:ILE:HG12	0.43	2.14	19	1
1:A:36:ALA:HB3	1:A:47:ILE:O	0.42	2.15	9	1
1:A:40:LEU:HB2	1:A:43:LEU:HB2	0.42	1.92	18	2
1:A:76:TYR:O	1:A:80:ILE:HG12	0.42	2.14	2	3
1:A:30:GLN:HB2	1:A:36:ALA:HB2	0.42	1.91	6	1
1:A:77:ILE:O	1:A:81:GLU:HG3	0.42	2.14	8	1
1:A:23:THR:O	1:A:26:GLU:HG2	0.42	2.14	1	2
1:A:26:GLU:O	1:A:30:GLN:HG3	0.42	2.14	13	1
1:A:71:GLN:O	1:A:75:GLN:HG2	0.42	2.14	19	1
1:A:30:GLN:HB3	1:A:35:GLU:O	0.42	2.14	4	2
1:A:2:PRO:HA	1:A:37:GLN:O	0.42	2.15	16	1
1:A:57:MET:HA	1:A:84:LEU:HD23	0.41	1.92	17	1
1:A:24:LEU:O	1:A:28:ARG:HG2	0.41	2.15	19	2
1:A:23:THR:O	1:A:27:ILE:HG12	0.41	2.16	1	1
1:A:16:LEU:HD13	1:A:17:SER:N	0.41	2.30	15	1
1:A:70:ILE:O	1:A:74:LEU:HG	0.41	2.16	3	1
1:A:10:LEU:HB2	1:A:13:VAL:HG22	0.40	1.93	3	1
1:A:27:ILE:HA	1:A:30:GLN:HE21	0.40	1.77	13	1
1:A:24:LEU:HD11	1:A:83:THR:HG22	0.40	1.93	12	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	85/137 (62%)	76±3 (90±3%)	8±3 (10±4%)	1±1 (1±1%)	30	75
All	All	1700/2740 (62%)	1523 (90%)	165 (10%)	12 (1%)	30	75

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	58	GLY	4
1	A	7	PRO	3
1	A	18	ASP	2
1	A	3	VAL	1
1	A	49	PRO	1
1	A	67	ASN	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	80/125 (64%)	77±2 (96±2%)	3±2 (4±2%)	41	85
All	All	1600/2500 (64%)	1538 (96%)	62 (4%)	41	85

All 23 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	16	LEU	10
1	A	10	LEU	8
1	A	42	GLU	6
1	A	93	GLU	6
1	A	98	ARG	4
1	A	44	MET	3
1	A	78	GLU	3
1	A	21	GLN	2
1	A	43	LEU	2
1	A	69	ASN	2
1	A	84	LEU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	57	MET	2
1	A	48	ARG	2
1	A	35	GLU	1
1	A	92	ARG	1
1	A	55	TYR	1
1	A	99	GLU	1
1	A	62	GLN	1
1	A	81	GLU	1
1	A	30	GLN	1
1	A	29	ASN	1
1	A	82	ARG	1
1	A	67	ASN	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates 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 81% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: 6b3n_cs.cif

Chemical shift list name: *ECS1996_cshifts*

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	1253
Number of shifts mapped to atoms	1253
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
$^{13}\text{C}_\alpha$	109	-0.17 ± 0.19	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	97	0.17 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	95	-0.21 ± 0.12	None needed (< 0.5 ppm)
^{15}N	97	0.11 ± 0.32	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 81%, i.e. 883 atoms were assigned a chemical shift out of a possible 1096. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	388/420 (92%)	157/167 (94%)	157/172 (91%)	74/81 (91%)
Sidechain	463/627 (74%)	280/366 (77%)	183/230 (80%)	0/31 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	32/49 (65%)	16/26 (62%)	16/22 (73%)	0/1 (0%)
Overall	883/1096 (81%)	453/559 (81%)	356/424 (84%)	74/113 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 978 atoms were assigned a chemical shift out of a possible 1247. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	441/490 (90%)	179/195 (92%)	177/200 (88%)	85/95 (89%)
Sidechain	505/701 (72%)	305/409 (75%)	200/258 (78%)	0/34 (0%)
Aromatic	32/56 (57%)	16/30 (53%)	16/24 (67%)	0/2 (0%)
Overall	978/1247 (78%)	500/634 (79%)	393/482 (82%)	85/131 (65%)

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.

Random coil index (RCI) for chain A:

