



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 06:32 am BST

PDB ID : 5A3G
Title : Structure of herpesvirus nuclear egress complex subunit M50
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This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

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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 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	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

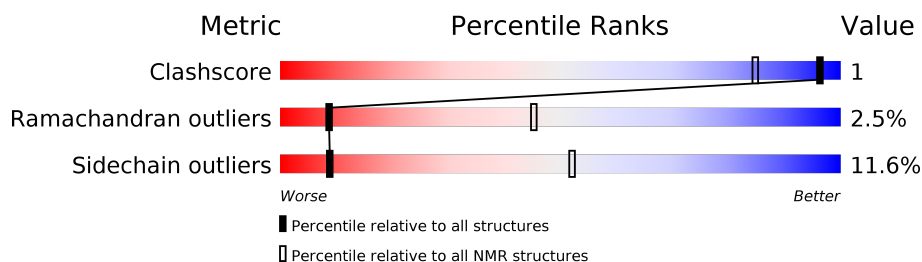
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 7%.

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	171	 79% 16% . .

2 Ensemble composition and analysis

This entry contains 15 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:171 (165)	0.93	12

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 2 clusters and 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2711 atoms, of which 1356 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called M50.

Mol	Chain	Residues	Atoms						Trace
1	A	171	Total	C	H	N	O	S	0
			2711	851	1356	234	258	12	

There are 3 discrepancies between the modelled and reference sequences:

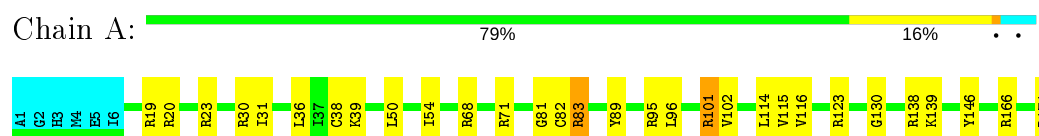
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP H2A365
A	2	GLY	-	expression tag	UNP H2A365
A	3	HIS	-	expression tag	UNP H2A365

4 Residue-property plots

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: M50

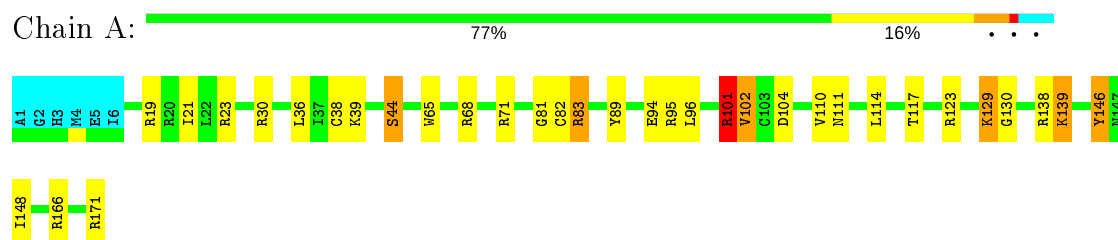


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

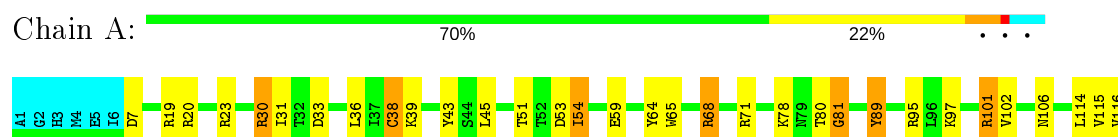
4.2.1 Score per residue for model 1

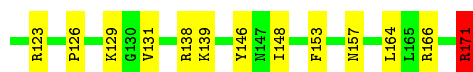
- Molecule 1: M50



4.2.2 Score per residue for model 2

- Molecule 1: M50





4.2.3 Score per residue for model 3

- Molecule 1: M50

Chain A: 75% 19% . .



4.2.4 Score per residue for model 4

- Molecule 1: M50

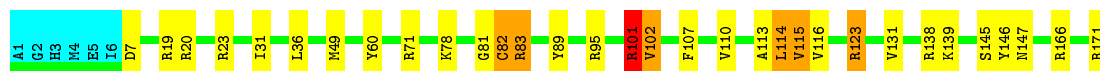
Chain A: 74% 17% 5% .



4.2.5 Score per residue for model 5

- Molecule 1: M50

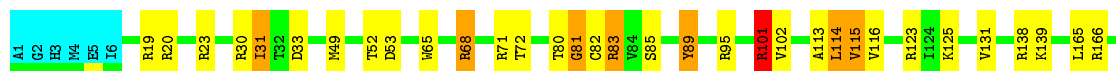
Chain A: 78% 15% . . .



4.2.6 Score per residue for model 6

- Molecule 1: M50

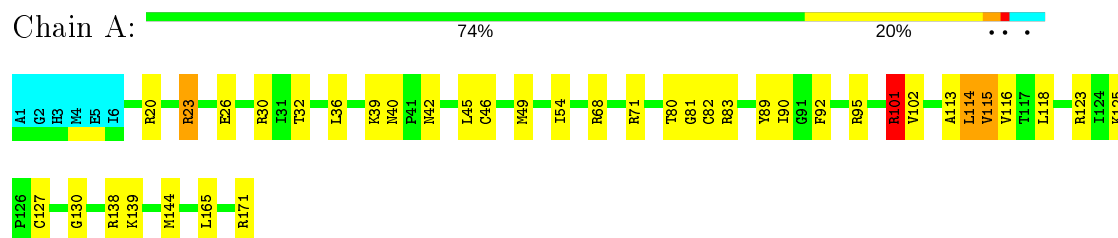
Chain A: 77% 15% . . .



R171

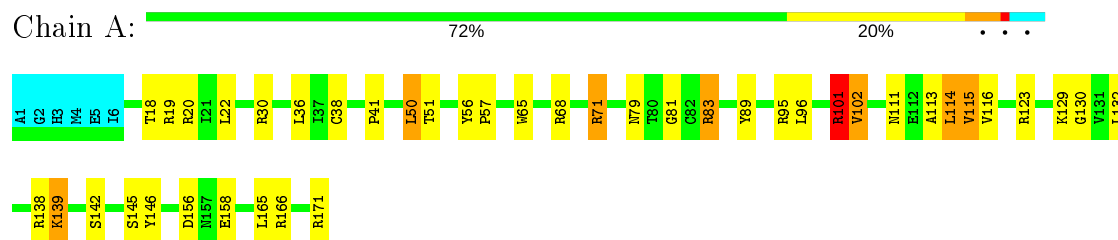
4.2.7 Score per residue for model 7

- Molecule 1: M50



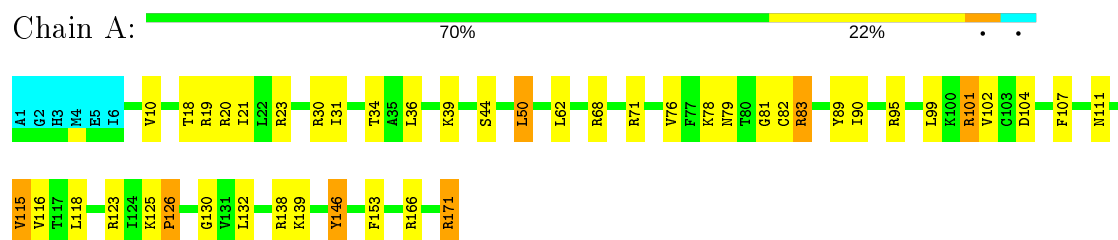
4.2.8 Score per residue for model 8

- Molecule 1: M50



4.2.9 Score per residue for model 9

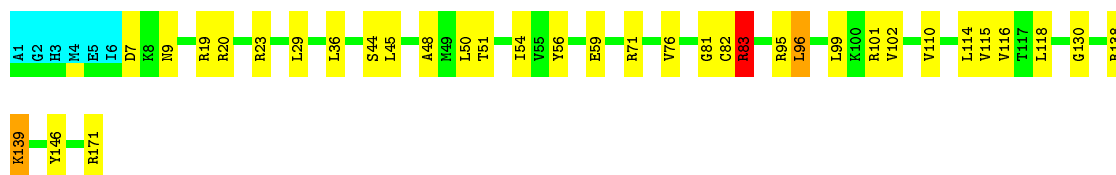
- Molecule 1: M50



4.2.10 Score per residue for model 10

- Molecule 1: M50

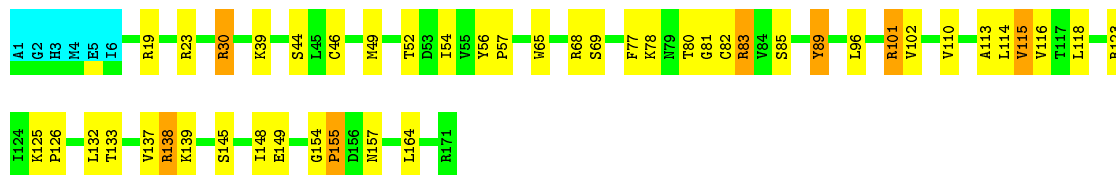




4.2.11 Score per residue for model 11

- Molecule 1: M50

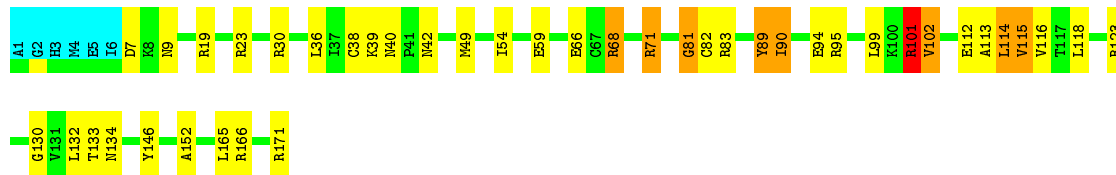
Chain A: 70% 23%



4.2.12 Score per residue for model 12 (medoid)

- Molecule 1: M50

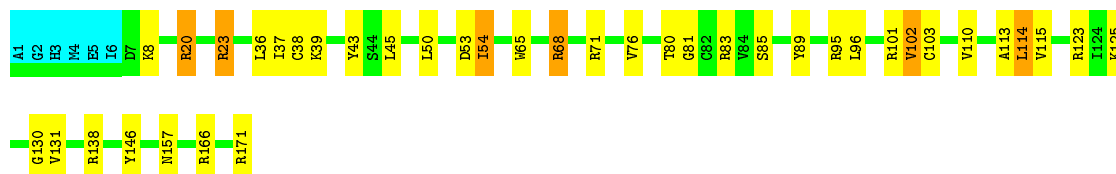
Chain A: 72% 19% 5%



4.2.13 Score per residue for model 13

- Molecule 1: M50

Chain A: 74% 19%



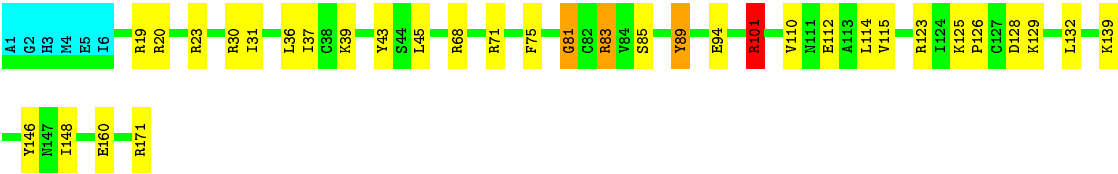
4.2.14 Score per residue for model 14

- Molecule 1: M50

Chain A:

77%

18%



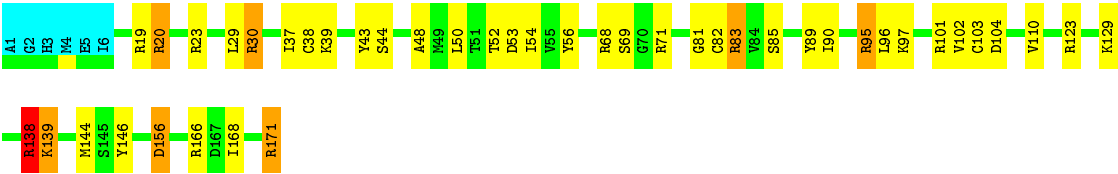
4.2.15 Score per residue for model 15

- Molecule 1: M50

Chain A:

71%

20%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING WITH TORSION ANGLE DYNAMICS SIMULATION FOLLOWED BY RDC AND WATERBOX REFINEMENT*.

Of the 50 calculated structures, 15 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure solution	3.0
NMRDraw	structure solution	11
TALOS+	structure solution	1.2009.0605.17
CcpNmr Analysis	structure solution	2.4
NMRPipe	structure solution	11
hmsIST	structure solution	2.11
CARA	structure solution	1.8.4

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	300
Number of shifts mapped to atoms	300
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	7%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1311	1313	1313	2±2
All	All	19665	19695	19695	31

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:VAL:HG22	1:A:115:VAL:HG22	0.86	1.48	10	3
1:A:113:ALA:C	1:A:114:LEU:HD23	0.62	2.15	13	6
1:A:29:LEU:HD11	1:A:48:ALA:HB1	0.58	1.76	15	2
1:A:139:LYS:HE2	1:A:146:TYR:CD1	0.55	2.36	15	3
1:A:101:ARG:CD	1:A:102:VAL:H	0.53	2.17	5	1
1:A:139:LYS:HE2	1:A:146:TYR:CG	0.52	2.40	8	2
1:A:99:LEU:HD11	1:A:115:VAL:HG23	0.51	1.82	10	1
1:A:53:ASP:C	1:A:54:ILE:HD13	0.50	2.27	4	2
1:A:52:THR:HG22	1:A:137:VAL:HG23	0.49	1.84	11	1
1:A:31:ILE:HD12	1:A:31:ILE:H	0.46	1.70	3	1
1:A:154:GLY:H	1:A:155:PRO:CD	0.44	2.25	11	1
1:A:101:ARG:CZ	1:A:102:VAL:H	0.44	2.24	1	1
1:A:99:LEU:CD1	1:A:115:VAL:HG23	0.44	2.43	10	1
1:A:133:THR:HG22	1:A:152:ALA:HA	0.43	1.89	12	1
1:A:78:LYS:HE3	1:A:113:ALA:HB2	0.43	1.91	11	1
1:A:99:LEU:HD12	1:A:99:LEU:C	0.42	2.34	12	1
1:A:139:LYS:HD2	1:A:146:TYR:CE1	0.42	2.50	1	1
1:A:96:LEU:HD11	1:A:115:VAL:HG21	0.42	1.92	10	1
1:A:90:ILE:H	1:A:90:ILE:HD13	0.42	1.74	12	1

5.2 Torsion angles ⓘ

5.2.1 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	164/171 (96%)	145±2 (88±2%)	15±2 (9±1%)	4±2 (3±1%)	9	45
All	All	2460/2565 (96%)	2176 (88%)	222 (9%)	62 (3%)	9	45

All 21 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	81	GLY	15
1	A	130	GLY	8
1	A	38	CYS	7
1	A	125	LYS	4
1	A	126	PRO	4
1	A	104	ASP	3
1	A	102	VAL	2
1	A	157	ASN	2
1	A	44	SER	2
1	A	144	MET	2
1	A	69	SER	2
1	A	142	SER	2
1	A	57	PRO	1
1	A	94	GLU	1
1	A	33	ASP	1
1	A	155	PRO	1
1	A	156	ASP	1
1	A	111	ASN	1
1	A	129	LYS	1
1	A	82	CYS	1
1	A	41	PRO	1

5.2.2 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	148/152 (97%)	131±3 (88±2%)	17±3 (12±2%)	9	52
All	All	2220/2280 (97%)	1963 (88%)	257 (12%)	9	52

All 83 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	139	LYS	13
1	A	114	LEU	12
1	A	36	LEU	12

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Mol	Chain	Res	Type	Models (Total)
1	A	101	ARG	11
1	A	116	VAL	9
1	A	54	ILE	9
1	A	96	LEU	8
1	A	132	LEU	7
1	A	110	VAL	7
1	A	115	VAL	6
1	A	118	LEU	6
1	A	65	TRP	6
1	A	85	SER	6
1	A	171	ARG	6
1	A	83	ARG	5
1	A	31	ILE	5
1	A	148	ILE	5
1	A	45	LEU	5
1	A	50	LEU	5
1	A	129	LYS	4
1	A	78	LYS	4
1	A	39	LYS	4
1	A	59	GLU	4
1	A	30	ARG	4
1	A	89	TYR	3
1	A	131	VAL	3
1	A	94	GLU	3
1	A	37	ILE	3
1	A	146	TYR	3
1	A	21	ILE	3
1	A	97	LYS	3
1	A	68	ARG	3
1	A	46	CYS	3
1	A	53	ASP	3
1	A	95	ARG	2
1	A	56	TYR	2
1	A	51	THR	2
1	A	128	ASP	2
1	A	125	LYS	2
1	A	23	ARG	2
1	A	164	LEU	2
1	A	90	ILE	2
1	A	156	ASP	2
1	A	103	CYS	2
1	A	112	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	102	VAL	2
1	A	20	ARG	2
1	A	18	THR	2
1	A	9	ASN	2
1	A	62	LEU	1
1	A	158	GLU	1
1	A	38	CYS	1
1	A	92	PHE	1
1	A	138	ARG	1
1	A	66	GLU	1
1	A	160	GLU	1
1	A	123	ARG	1
1	A	26	GLU	1
1	A	8	LYS	1
1	A	134	ASN	1
1	A	153	PHE	1
1	A	72	THR	1
1	A	168	ILE	1
1	A	145	SER	1
1	A	19	ARG	1
1	A	22	LEU	1
1	A	77	PHE	1
1	A	7	ASP	1
1	A	111	ASN	1
1	A	80	THR	1
1	A	107	PHE	1
1	A	136	VAL	1
1	A	106	ASN	1
1	A	133	THR	1
1	A	64	TYR	1
1	A	32	THR	1
1	A	157	ASN	1
1	A	117	THR	1
1	A	79	ASN	1
1	A	10	VAL	1
1	A	75	PHE	1
1	A	99	LEU	1
1	A	40	ASN	1

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 7% for the well-defined parts and 7% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

6.1.1 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	300
Number of shifts mapped to atoms	300
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

6.1.2 Chemical shift referencing

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

6.1.3 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 7%, i.e. 148 atoms were assigned a chemical shift out of a possible 2050. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/815 (0%)	0/325 (0%)	0/330 (0%)	0/160 (0%)
Sidechain	148/1105 (13%)	74/643 (12%)	74/402 (18%)	0/60 (0%)
Aromatic	0/130 (0%)	0/68 (0%)	0/61 (0%)	0/1 (0%)
Overall	148/2050 (7%)	74/1036 (7%)	74/793 (9%)	0/221 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 150 atoms were assigned a chemical shift out of a possible 2116. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	0/845 (0%)	0/337 (0%)	0/342 (0%)	0/166 (0%)
Sidechain	150/1134 (13%)	75/660 (11%)	75/414 (18%)	0/60 (0%)
Aromatic	0/137 (0%)	0/72 (0%)	0/63 (0%)	0/2 (0%)
Overall	150/2116 (7%)	75/1069 (7%)	75/819 (9%)	0/228 (0%)

6.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

6.1.5 Random Coil Index (RCI) plots ⓘ

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list). RCI is only applicable to proteins.