



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 09:38 am BST

PDB ID : 6C44
Title : Zika virus capsid protein
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Deposited on : 2018-01-11

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 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

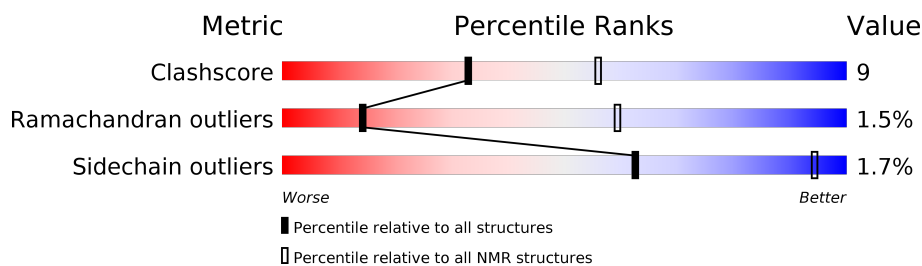
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 41%.

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	104	
1	B	104	

2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:42-A:98, B:42-B:98 (114)	0.32	17

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2374 atoms, of which 1264 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Capsid protein.

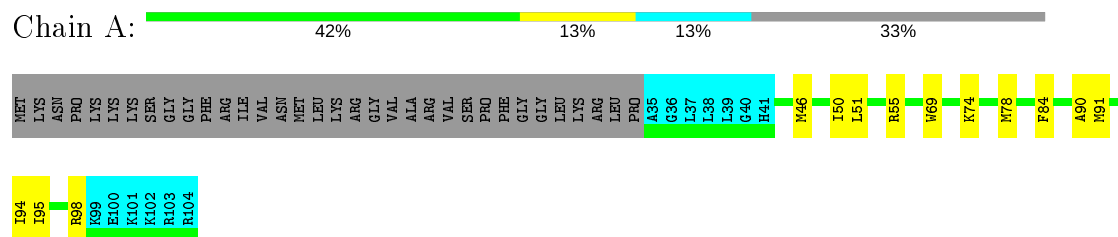
Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1187	362	632	106	84	3	
1	B	70	Total	C	H	N	O	S	0
			1187	362	632	106	84	3	

4 Residue-property plots [i](#)

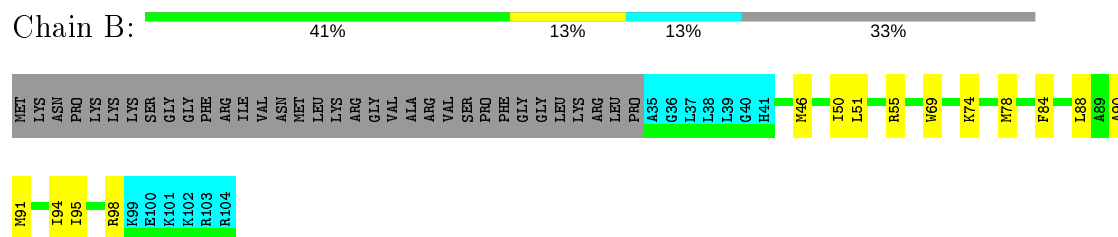
4.1 Average score per residue in the NMR ensemble

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: Capsid protein



- Molecule 1: Capsid protein

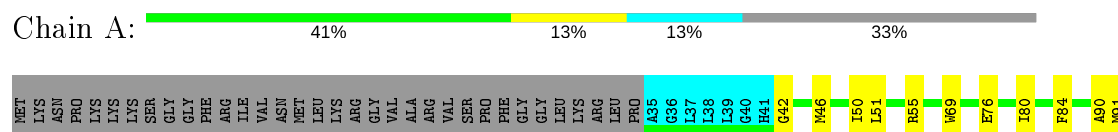


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

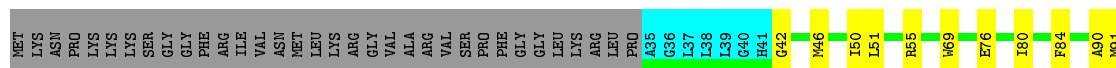
4.2.1 Score per residue for model 1

- Molecule 1: Capsid protein



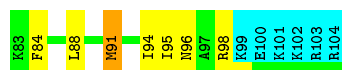
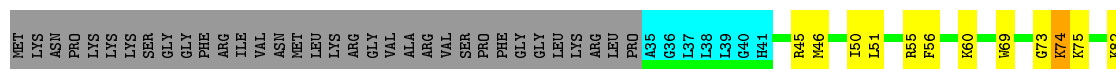
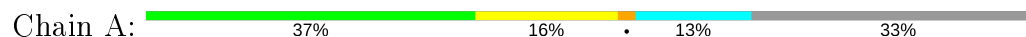


- Molecule 1: Capsid protein

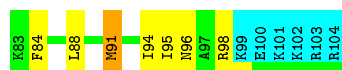
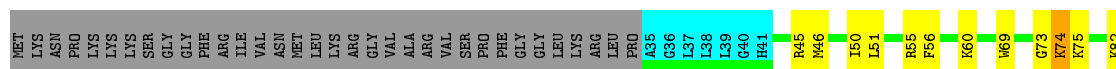
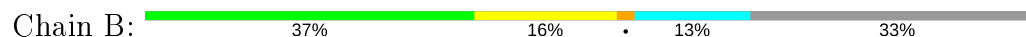


4.2.2 Score per residue for model 2

- Molecule 1: Capsid protein

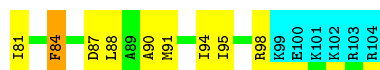
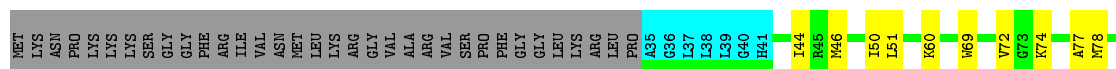


- Molecule 1: Capsid protein

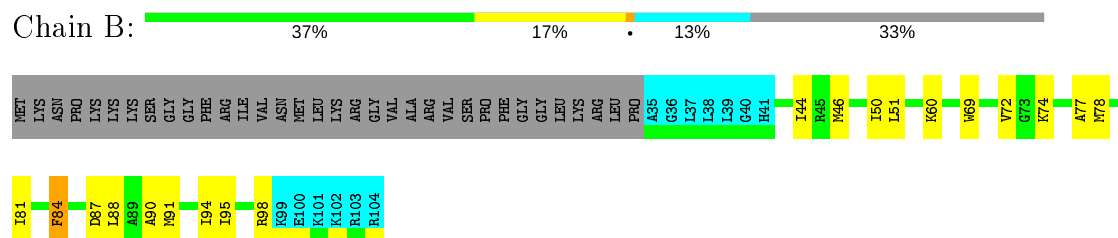


4.2.3 Score per residue for model 3

- Molecule 1: Capsid protein

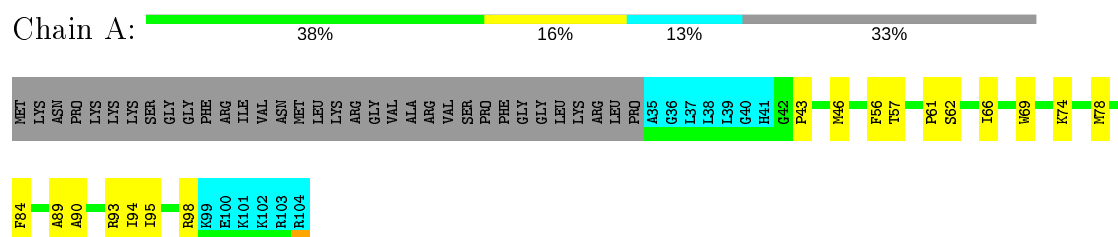


- Molecule 1: Capsid protein

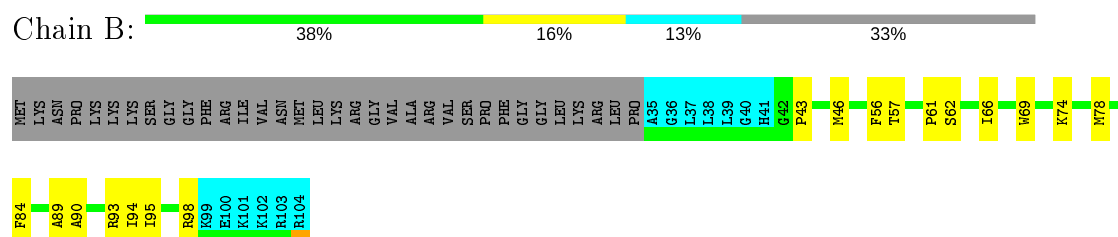


4.2.4 Score per residue for model 4

- Molecule 1: Capsid protein

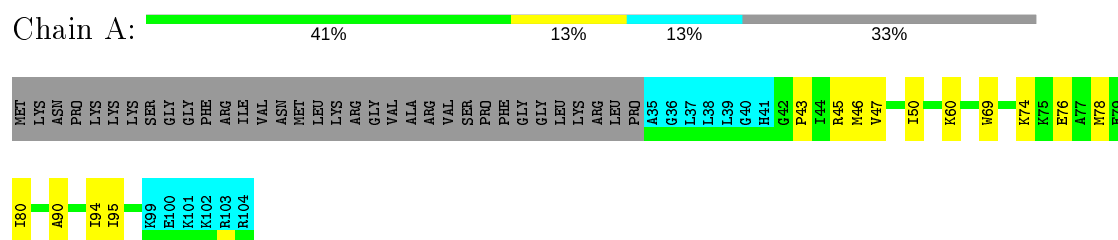


- Molecule 1: Capsid protein

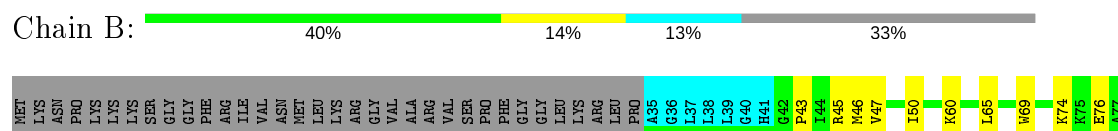


4.2.5 Score per residue for model 5

- Molecule 1: Capsid protein



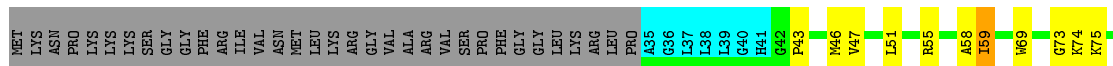
- Molecule 1: Capsid protein



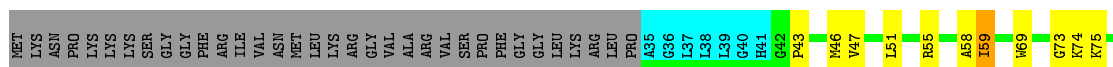


4.2.6 Score per residue for model 6

- Molecule 1: Capsid protein

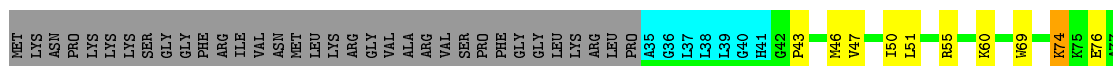


- Molecule 1: Capsid protein

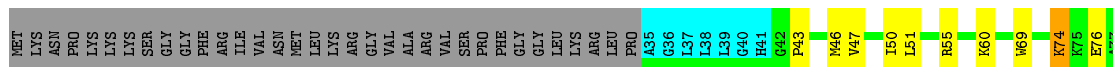


4.2.7 Score per residue for model 7

- Molecule 1: Capsid protein

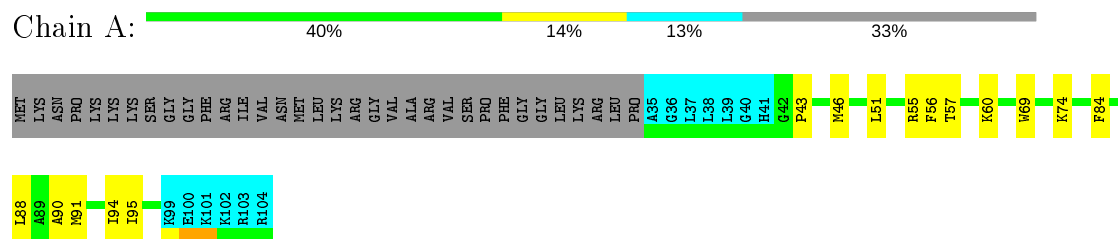


- Molecule 1: Capsid protein

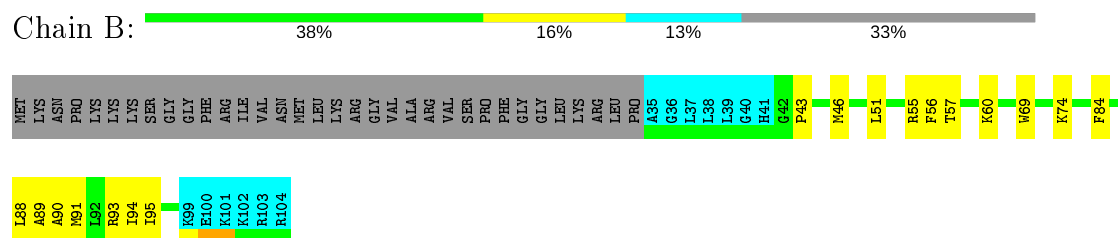


4.2.8 Score per residue for model 8

- Molecule 1: Capsid protein

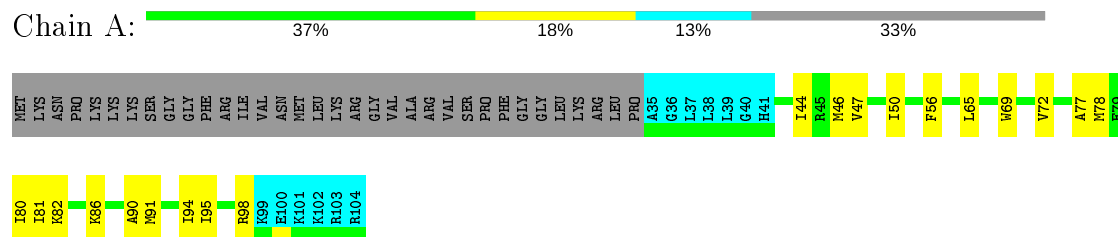


- Molecule 1: Capsid protein

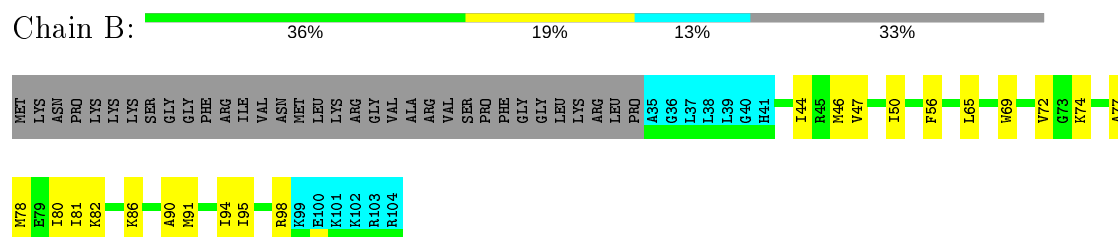


4.2.9 Score per residue for model 9

- Molecule 1: Capsid protein

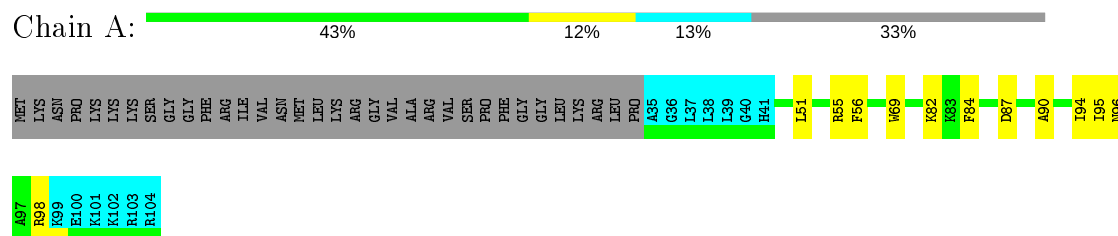


- Molecule 1: Capsid protein

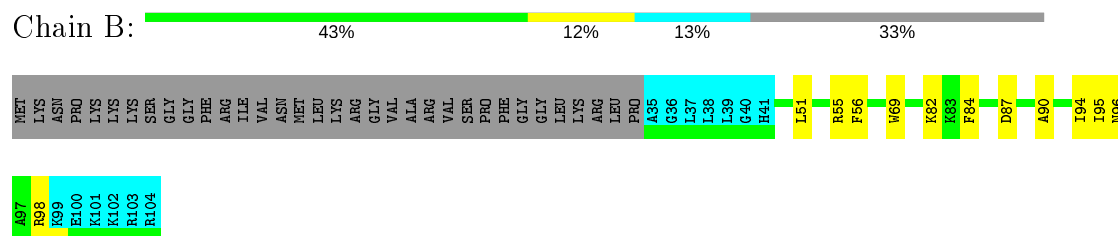


4.2.10 Score per residue for model 10

- Molecule 1: Capsid protein

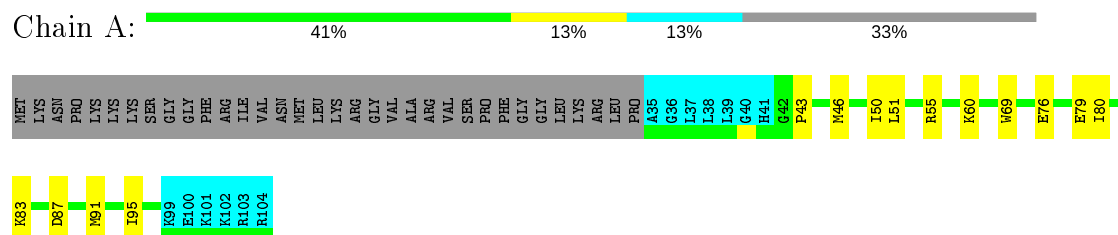


- Molecule 1: Capsid protein

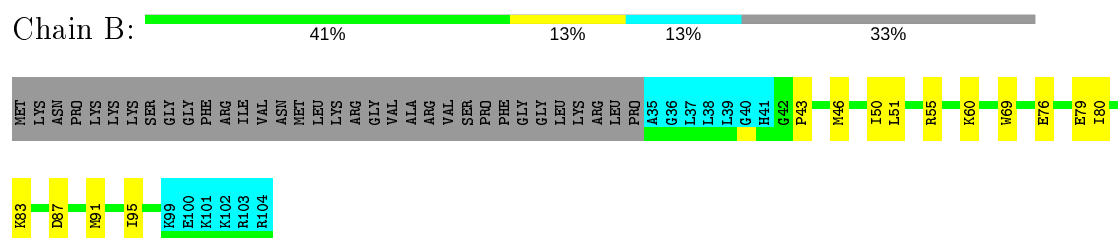


4.2.11 Score per residue for model 11

- Molecule 1: Capsid protein

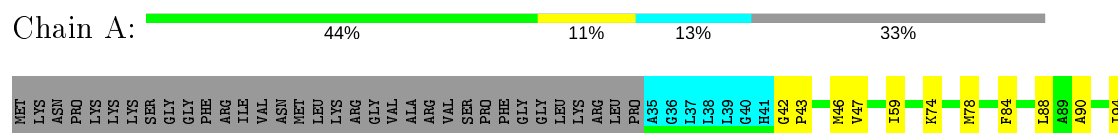


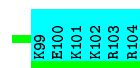
- Molecule 1: Capsid protein



4.2.12 Score per residue for model 12

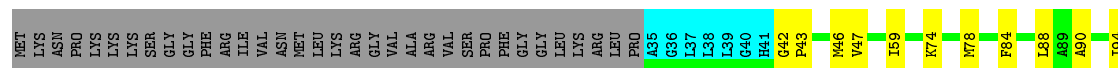
- Molecule 1: Capsid protein





- Molecule 1: Capsid protein

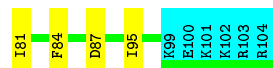
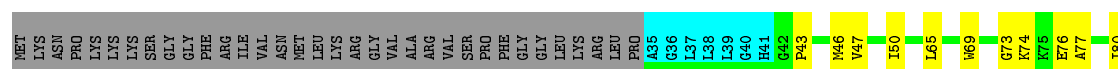
Chain B: 44% 11% 13% 33%



4.2.13 Score per residue for model 13

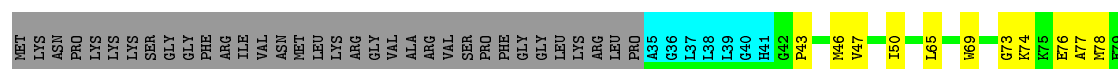
- Molecule 1: Capsid protein

Chain A: 40% 14% 13% 33%



- Molecule 1: Capsid protein

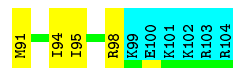
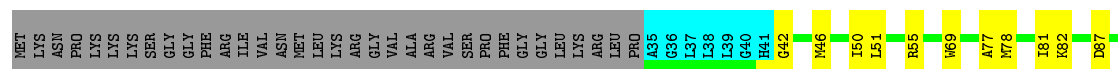
Chain B: 39% 15% 13% 33%



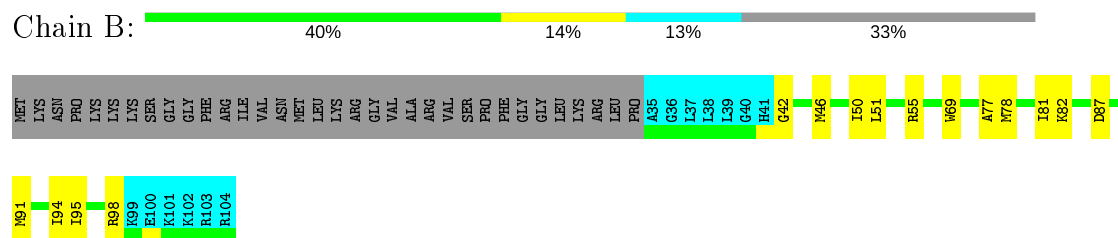
4.2.14 Score per residue for model 14

- Molecule 1: Capsid protein

Chain A: 40% 14% 13% 33%

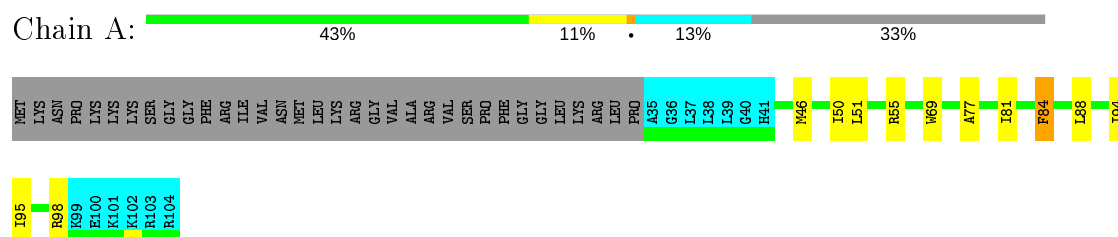


- Molecule 1: Capsid protein

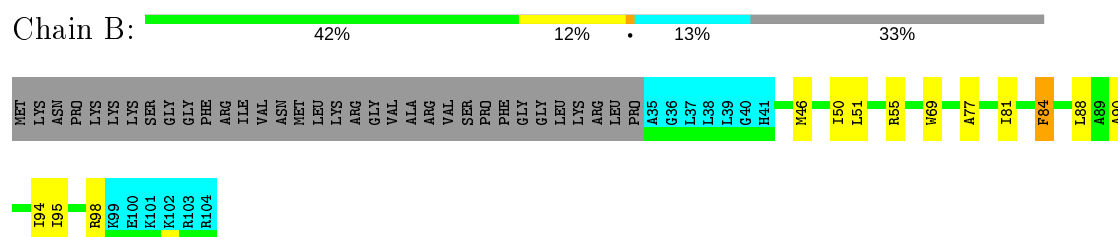


4.2.15 Score per residue for model 15

- Molecule 1: Capsid protein

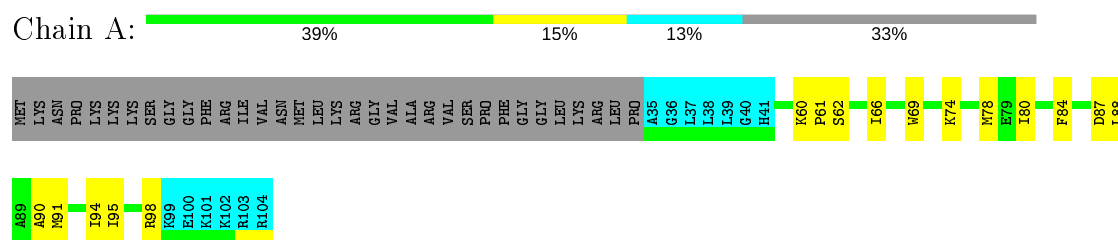


- Molecule 1: Capsid protein

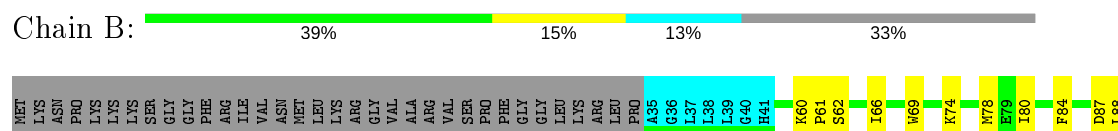


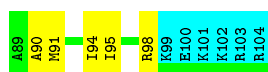
4.2.16 Score per residue for model 16

- Molecule 1: Capsid protein



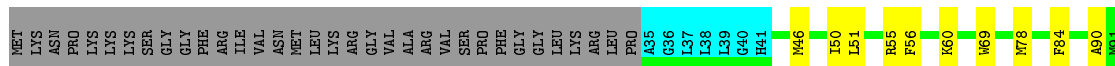
- Molecule 1: Capsid protein



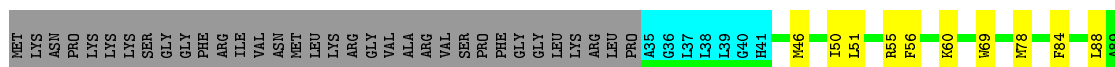


4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Capsid protein

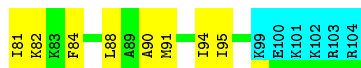
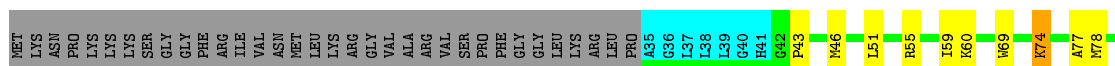


- Molecule 1: Capsid protein

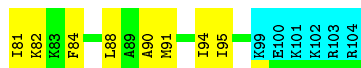
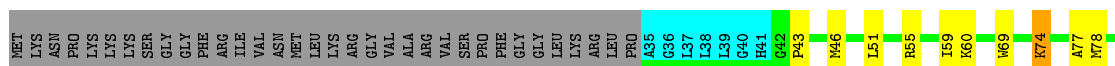


4.2.18 Score per residue for model 18

- Molecule 1: Capsid protein

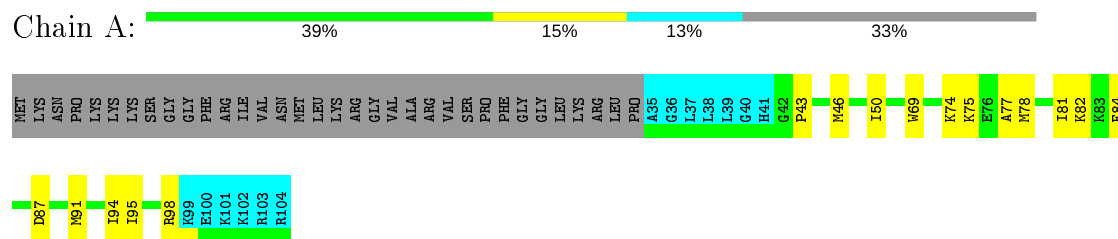


- Molecule 1: Capsid protein

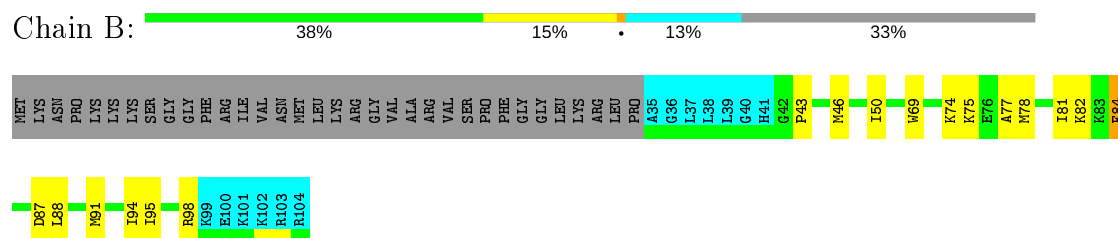


4.2.19 Score per residue for model 19

- Molecule 1: Capsid protein

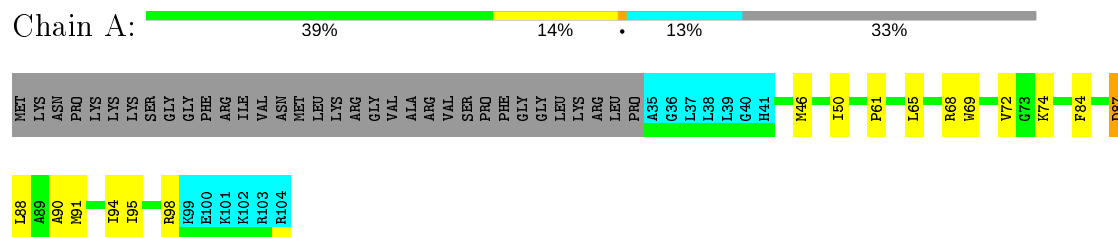


- Molecule 1: Capsid protein

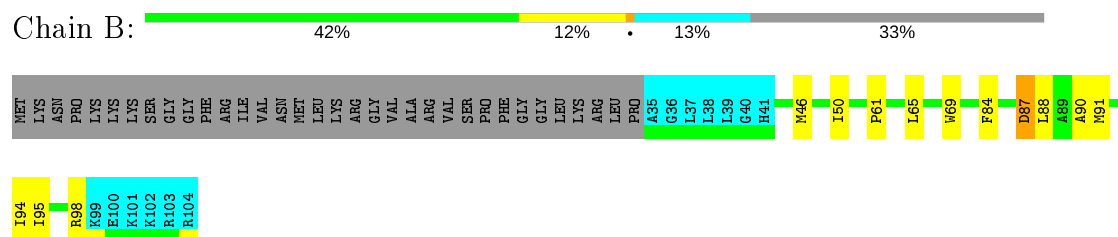


4.2.20 Score per residue for model 20

- Molecule 1: Capsid protein



- Molecule 1: Capsid protein



5 Refinement protocol and experimental data overview

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

Of the 400 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
CNS	refinement	1.21
CNS	structure calculation	

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1307
Number of shifts mapped to atoms	883
Number of unparsed shifts	424
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	41%

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

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	449	509	509	10±2
1	B	449	509	509	11±2
All	All	17960	20360	20360	351

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:GLY:HA3	1:A:46:MET:SD	0.63	2.34	1	2
1:B:42:GLY:HA3	1:B:46:MET:SD	0.62	2.34	1	2
1:A:69:TRP:NE1	1:B:95:ILE:HD11	0.61	2.10	14	17
1:A:95:ILE:HD11	1:B:69:TRP:NE1	0.61	2.10	14	17
1:B:90:ALA:O	1:B:94:ILE:HG13	0.56	2.00	18	15
1:A:78:MET:O	1:A:82:LYS:HG2	0.56	2.00	14	2
1:A:43:PRO:HD2	1:A:46:MET:SD	0.56	2.40	19	7
1:B:51:LEU:O	1:B:55:ARG:HG2	0.56	2.01	10	11
1:A:51:LEU:O	1:A:55:ARG:HG2	0.55	2.01	10	11
1:B:78:MET:O	1:B:82:LYS:HG2	0.55	2.00	14	2
1:B:43:PRO:HD2	1:B:46:MET:SD	0.55	2.41	19	7
1:A:69:TRP:CD1	1:B:95:ILE:HD11	0.55	2.37	14	6
1:A:90:ALA:O	1:A:94:ILE:HG13	0.55	2.01	18	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:MET:O	1:A:95:ILE:HG12	0.54	2.03	19	8
1:A:95:ILE:HD11	1:B:69:TRP:CD1	0.54	2.37	14	7
1:B:91:MET:O	1:B:95:ILE:HG12	0.54	2.03	19	8
1:A:51:LEU:HD23	1:B:91:MET:SD	0.54	2.43	8	2
1:A:46:MET:O	1:A:50:ILE:HG13	0.53	2.03	3	13
1:B:87:ASP:O	1:B:91:MET:HG3	0.53	2.04	11	2
1:B:46:MET:O	1:B:50:ILE:HG13	0.53	2.03	3	13
1:B:94:ILE:O	1:B:98:ARG:HG2	0.52	2.04	4	10
1:A:91:MET:SD	1:B:51:LEU:HD23	0.52	2.44	8	2
1:A:94:ILE:O	1:A:98:ARG:HG2	0.52	2.04	4	10
1:A:84:PHE:HA	1:B:56:PHE:CZ	0.51	2.40	4	5
1:A:98:ARG:NE	1:A:98:ARG:HA	0.51	2.20	14	1
1:B:77:ALA:O	1:B:81:ILE:HG12	0.51	2.06	9	7
1:A:77:ALA:O	1:A:81:ILE:HG12	0.51	2.05	9	7
1:B:84:PHE:O	1:B:88:LEU:HG	0.51	2.06	3	11
1:A:87:ASP:O	1:A:91:MET:HG3	0.51	2.04	11	2
1:B:76:GLU:O	1:B:80:ILE:HG13	0.50	2.06	11	5
1:A:84:PHE:O	1:A:88:LEU:HG	0.50	2.06	3	9
1:A:56:PHE:CZ	1:B:84:PHE:HA	0.50	2.41	4	5
1:A:76:GLU:O	1:A:80:ILE:HG13	0.50	2.07	11	5
1:A:74:LYS:O	1:A:78:MET:HG3	0.50	2.07	3	6
1:B:98:ARG:NE	1:B:98:ARG:HA	0.50	2.20	14	1
1:A:73:GLY:O	1:A:74:LYS:HG2	0.50	2.07	13	1
1:B:73:GLY:O	1:B:74:LYS:HG2	0.49	2.08	13	1
1:B:74:LYS:O	1:B:78:MET:HG2	0.49	2.08	5	2
1:A:74:LYS:O	1:A:78:MET:HG2	0.49	2.08	5	2
1:B:74:LYS:O	1:B:78:MET:HG3	0.48	2.07	3	8
1:B:82:LYS:O	1:B:86:LYS:HG2	0.48	2.08	9	1
1:B:87:ASP:O	1:B:91:MET:HG2	0.48	2.09	14	3
1:A:82:LYS:O	1:A:86:LYS:HG2	0.48	2.08	9	1
1:A:45:ARG:HG3	1:A:46:MET:SD	0.48	2.48	2	1
1:A:87:ASP:O	1:A:91:MET:HG2	0.48	2.09	14	3
1:A:94:ILE:O	1:A:98:ARG:HG3	0.48	2.09	2	2
1:B:45:ARG:HG3	1:B:46:MET:SD	0.47	2.49	2	1
1:A:73:GLY:O	1:A:75:LYS:N	0.47	2.47	2	2
1:B:94:ILE:O	1:B:98:ARG:HG3	0.47	2.09	2	2
1:B:78:MET:O	1:B:82:LYS:HG3	0.47	2.10	19	2
1:A:98:ARG:HA	1:A:98:ARG:CZ	0.47	2.40	14	1
1:B:98:ARG:HA	1:B:98:ARG:CZ	0.47	2.40	14	1
1:A:78:MET:O	1:A:82:LYS:HG3	0.47	2.10	19	2
1:B:62:SER:O	1:B:66:ILE:HG12	0.46	2.11	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:GLY:O	1:B:75:LYS:N	0.46	2.48	2	2
1:A:43:PRO:O	1:A:47:VAL:HG23	0.46	2.10	12	5
1:B:43:PRO:O	1:B:47:VAL:HG23	0.46	2.10	12	5
1:A:62:SER:O	1:A:66:ILE:HG12	0.46	2.11	4	2
1:B:75:LYS:C	1:B:75:LYS:HD3	0.45	2.32	19	1
1:B:58:ALA:O	1:B:59:ILE:HB	0.44	2.12	6	1
1:A:65:LEU:O	1:A:69:TRP:HB2	0.44	2.12	13	2
1:A:92:LEU:HD21	1:B:78:MET:SD	0.44	2.52	17	1
1:A:78:MET:SD	1:B:92:LEU:HD21	0.44	2.52	17	1
1:A:75:LYS:HD3	1:A:75:LYS:C	0.44	2.32	19	1
1:A:58:ALA:O	1:A:59:ILE:HB	0.44	2.12	6	1
1:B:65:LEU:O	1:B:69:TRP:HB2	0.43	2.13	9	3
1:A:98:ARG:HA	1:A:98:ARG:NE	0.43	2.28	1	2
1:B:44:ILE:HB	1:B:72:VAL:HG13	0.43	1.91	3	2
1:B:98:ARG:HA	1:B:98:ARG:NE	0.43	2.29	1	2
1:A:57:THR:HA	1:B:46:MET:HG2	0.43	1.90	4	2
1:A:51:LEU:HD22	1:A:69:TRP:NE1	0.43	2.29	3	2
1:A:46:MET:HG2	1:B:57:THR:HA	0.43	1.90	4	2
1:B:51:LEU:HD22	1:B:69:TRP:NE1	0.43	2.29	3	2
1:A:89:ALA:O	1:A:93:ARG:HG3	0.42	2.15	4	1
1:A:79:GLU:O	1:A:83:LYS:HG2	0.42	2.15	11	1
1:A:80:ILE:HG23	1:B:56:PHE:CZ	0.42	2.50	9	1
1:B:80:ILE:O	1:B:84:PHE:HB2	0.42	2.14	16	1
1:A:80:ILE:O	1:A:84:PHE:HB2	0.42	2.15	16	1
1:A:44:ILE:HB	1:A:72:VAL:HG13	0.41	1.90	3	2
1:B:89:ALA:O	1:B:93:ARG:HG3	0.41	2.16	8	2
1:B:79:GLU:O	1:B:83:LYS:HG2	0.41	2.15	11	1
1:B:75:LYS:HD3	1:B:75:LYS:C	0.41	2.36	6	1
1:A:44:ILE:O	1:A:47:VAL:HB	0.41	2.16	9	1
1:B:44:ILE:O	1:B:47:VAL:HB	0.41	2.15	9	1
1:A:73:GLY:C	1:A:74:LYS:HG2	0.41	2.36	2	1
1:A:61:PRO:O	1:A:65:LEU:HB2	0.41	2.16	20	1
1:A:59:ILE:HG22	1:A:59:ILE:O	0.41	2.15	18	1
1:A:56:PHE:CZ	1:B:80:ILE:HG23	0.40	2.51	9	1
1:B:59:ILE:O	1:B:59:ILE:HG22	0.40	2.16	18	1
1:B:61:PRO:O	1:B:65:LEU:HB2	0.40	2.16	20	1
1:A:75:LYS:C	1:A:75:LYS:HD3	0.40	2.36	6	1
1:B:73:GLY:C	1:B:74:LYS:HG2	0.40	2.37	2	1
1:A:68:ARG:O	1:A:72:VAL:HG23	0.40	2.17	20	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	57/104 (55%)	55±1 (96±2%)	1±1 (3±2%)	1±1 (1±1%)	14	59
1	B	57/104 (55%)	55±1 (96±2%)	1±1 (3±2%)	1±1 (1±1%)	14	59
All	All	2280/4160 (55%)	2188 (96%)	58 (3%)	34 (1%)	14	59

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	B	60	LYS	9
1	A	60	LYS	9
1	B	74	LYS	3
1	A	74	LYS	3
1	A	59	ILE	2
1	A	61	PRO	2
1	B	59	ILE	2
1	B	61	PRO	2
1	A	42	GLY	1
1	B	42	GLY	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	46/84 (55%)	45±1 (98±2%)	1±1 (2±2%)	62	94
1	B	46/84 (55%)	45±1 (98±2%)	1±1 (2±2%)	62	94
All	All	1840/3360 (55%)	1808 (98%)	32 (2%)	62	94

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)
1	B	84	PHE	5
1	A	84	PHE	5
1	B	87	ASP	4
1	A	87	ASP	4
1	B	74	LYS	2
1	B	82	LYS	2
1	A	74	LYS	2
1	A	82	LYS	2
1	A	96	ASN	1
1	B	96	ASN	1
1	B	45	ARG	1
1	B	91	MET	1
1	A	91	MET	1
1	A	45	ARG	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 41% for the well-defined parts and 41% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *data.str*

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	1307
Number of shifts mapped to atoms	883
Number of unparsed shifts	424
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.

- Entity instance (chain) must be specified. All 424 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	1	MET	C	175.530	0.000	1
2	?	1	MET	CA	57.870	0.006	1
3	?	1	MET	CB	32.540	0.000	1
4	?	1	MET	CE	16.212	0.019	1
5	?	1	MET	CG	29.485	0.006	1
6	?	1	MET	HA	4.330	0.004	1
7	?	1	MET	HB2	1.822	0.001	1
8	?	1	MET	HB3	1.822	0.001	1
9	?	1	MET	HE1	1.756	0.001	1
10	?	1	MET	HE2	1.756	0.001	1
11	?	1	MET	HE3	1.756	0.001	1
12	?	1	MET	HG2	1.648	0.001	1
13	?	1	MET	HG3	1.648	0.001	1
14	?	2	LYS	C	175.608	0.000	1
15	?	2	LYS	CA	56.489	0.001	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	2	LYS	CB	32.842	0.002	1
17	?	2	LYS	CD	29.329	0.002	1
18	?	2	LYS	CE	42.140	0.002	1
19	?	2	LYS	CG	24.901	0.002	1
20	?	2	LYS	H	8.169	0.001	1
21	?	2	LYS	HA	4.416	0.002	1
22	?	2	LYS	HB2	1.831	0.001	1
23	?	2	LYS	HB3	1.831	0.001	1
24	?	2	LYS	HD2	1.726	0.000	1
25	?	2	LYS	HD3	1.726	0.000	1
26	?	2	LYS	HE2	3.050	0.001	1
27	?	2	LYS	HE3	3.050	0.001	1
28	?	2	LYS	HG2	1.481	0.000	1
29	?	2	LYS	HG3	1.481	0.000	1
30	?	2	LYS	N	122.667	0.002	1
31	?	3	ASN	C	173.334	0.000	1
32	?	3	ASN	CA	51.363	0.063	1
33	?	3	ASN	CB	39.156	0.025	1
34	?	3	ASN	H	8.583	0.003	1
35	?	3	ASN	HA	5.019	0.002	1
36	?	3	ASN	HB2	2.880	0.002	2
37	?	3	ASN	HB3	2.745	0.000	2
38	?	3	ASN	N	121.313	0.005	1
39	?	4	PRO	C	176.843	0.000	1
40	?	4	PRO	CA	63.475	0.002	1
41	?	4	PRO	CB	32.089	0.167	1
42	?	4	PRO	CD	50.830	0.028	1
43	?	4	PRO	CG	27.413	0.134	1
44	?	4	PRO	HA	4.495	0.003	1
45	?	4	PRO	HB2	2.347	0.006	2
46	?	4	PRO	HB3	1.988	0.009	2
47	?	4	PRO	HD2	3.841	0.015	2
48	?	4	PRO	HD3	3.808	0.010	2
49	?	4	PRO	HG2	2.068	0.010	1
50	?	4	PRO	HG3	2.068	0.010	1
51	?	5	LYS	C	176.612	0.000	1
52	?	5	LYS	CA	56.401	0.032	1
53	?	5	LYS	CB	32.527	0.009	1
54	?	5	LYS	CD	29.031	0.001	1
55	?	5	LYS	CE	42.318	0.002	1
56	?	5	LYS	CG	24.629	0.001	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	5	LYS	H	8.257	0.002	1
58	?	5	LYS	HA	4.330	0.000	1
59	?	5	LYS	HB2	1.843	0.000	1
60	?	5	LYS	HB3	1.843	0.000	1
61	?	5	LYS	HD2	1.738	0.001	1
62	?	5	LYS	HD3	1.738	0.001	1
63	?	5	LYS	HE2	3.053	0.000	1
64	?	5	LYS	HE3	3.053	0.000	1
65	?	5	LYS	HG2	1.481	0.000	1
66	?	5	LYS	HG3	1.481	0.000	1
67	?	5	LYS	N	120.812	0.015	1
68	?	6	LYS	C	176.599	0.000	1
69	?	6	LYS	CA	56.380	0.000	1
70	?	6	LYS	CB	32.537	0.004	1
71	?	6	LYS	CD	29.292	0.002	1
72	?	6	LYS	CE	42.318	0.002	1
73	?	6	LYS	CG	24.898	0.002	1
74	?	6	LYS	H	8.151	0.001	1
75	?	6	LYS	HA	4.329	0.001	1
76	?	6	LYS	HB2	1.839	0.000	1
77	?	6	LYS	HB3	1.839	0.000	1
78	?	6	LYS	HD2	1.738	0.000	1
79	?	6	LYS	HD3	1.738	0.000	1
80	?	6	LYS	HE2	3.053	0.000	1
81	?	6	LYS	HE3	3.053	0.000	1
82	?	6	LYS	HG2	1.480	0.000	1
83	?	6	LYS	HG3	1.480	0.000	1
84	?	6	LYS	N	122.491	0.000	1
85	?	7	LYS	C	176.582	0.000	1
86	?	7	LYS	CA	56.497	0.000	1
87	?	7	LYS	CB	32.771	0.001	1
88	?	7	LYS	CD	29.255	0.005	1
89	?	7	LYS	CE	42.440	0.002	1
90	?	7	LYS	CG	24.571	0.001	1
91	?	7	LYS	H	8.152	0.001	1
92	?	7	LYS	HA	4.392	0.001	1
93	?	7	LYS	HB2	1.854	0.003	1
94	?	7	LYS	HB3	1.854	0.003	1
95	?	7	LYS	HD2	1.731	0.000	1
96	?	7	LYS	HD3	1.731	0.000	1
97	?	7	LYS	HE2	3.053	0.000	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	7	LYS	HE3	3.053	0.000	1
99	?	7	LYS	HG2	1.483	0.000	1
100	?	7	LYS	HG3	1.483	0.000	1
101	?	7	LYS	N	122.495	0.002	1
102	?	8	SER	C	174.940	0.000	1
103	?	8	SER	CA	58.394	0.011	1
104	?	8	SER	CB	64.158	0.001	1
105	?	8	SER	H	8.348	0.001	1
106	?	8	SER	HA	4.535	0.005	1
107	?	8	SER	HB2	3.947	0.001	1
108	?	8	SER	HB3	3.947	0.001	1
109	?	8	SER	N	117.231	0.002	1
110	?	9	GLY	C	174.494	0.000	1
111	?	9	GLY	CA	45.348	0.123	1
112	?	9	GLY	H	8.425	0.001	1
113	?	9	GLY	HA2	4.024	0.010	1
114	?	9	GLY	HA3	4.026	0.010	1
115	?	9	GLY	N	110.803	0.002	1
116	?	10	GLY	C	173.838	0.000	1
117	?	10	GLY	CA	45.334	0.112	1
118	?	10	GLY	H	8.230	0.001	1
119	?	10	GLY	HA2	3.955	0.007	1
120	?	10	GLY	HA3	3.955	0.006	1
121	?	10	GLY	N	108.573	0.003	1
122	?	11	PHE	C	175.501	0.000	1
123	?	11	PHE	CA	57.867	0.034	1
124	?	11	PHE	CB	39.902	0.002	1
125	?	11	PHE	H	8.062	0.006	1
126	?	11	PHE	HA	4.665	0.007	1
127	?	11	PHE	HB2	3.124	0.002	1
128	?	11	PHE	HB3	3.124	0.002	1
129	?	11	PHE	N	120.054	0.029	1
130	?	12	ARG	C	175.669	0.000	1
131	?	12	ARG	CA	56.229	0.004	1
132	?	12	ARG	CB	31.067	0.000	1
133	?	12	ARG	CD	43.640	0.000	1
134	?	12	ARG	CG	26.923	0.077	1
135	?	12	ARG	H	8.171	0.002	1
136	?	12	ARG	HA	4.329	0.005	1
137	?	12	ARG	HB2	1.815	0.001	1
138	?	12	ARG	HB3	1.815	0.001	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	12	ARG	HD2	3.217	0.001	1
140	?	12	ARG	HD3	3.217	0.001	1
141	?	12	ARG	HG2	1.738	0.001	1
142	?	12	ARG	HG3	1.738	0.001	1
143	?	12	ARG	N	123.059	0.186	1
144	?	13	ILE	C	176.222	0.000	1
145	?	13	ILE	CA	61.325	0.022	1
146	?	13	ILE	CB	38.578	0.027	1
147	?	13	ILE	CD1	13.385	0.017	1
148	?	13	ILE	CG1	28.021	0.141	1
149	?	13	ILE	CG2	17.761	0.015	1
150	?	13	ILE	H	8.145	0.001	1
151	?	13	ILE	HA	4.176	0.017	1
152	?	13	ILE	HB	1.904	0.007	1
153	?	13	ILE	HD11	0.878	0.015	1
154	?	13	ILE	HD12	0.878	0.015	1
155	?	13	ILE	HD13	0.878	0.015	1
156	?	13	ILE	HG12	1.259	0.025	2
157	?	13	ILE	HG13	1.538	0.004	2
158	?	13	ILE	HG21	0.931	0.008	1
159	?	13	ILE	HG22	0.931	0.008	1
160	?	13	ILE	HG23	0.931	0.008	1
161	?	13	ILE	N	122.502	0.000	1
162	?	14	VAL	C	175.738	0.000	1
163	?	14	VAL	CA	62.568	0.072	1
164	?	14	VAL	CB	32.467	0.014	1
165	?	14	VAL	CG1	20.769	0.001	1
166	?	14	VAL	CG2	20.769	0.001	1
167	?	14	VAL	H	8.130	0.002	1
168	?	14	VAL	HA	4.121	0.006	1
169	?	14	VAL	HB	2.108	0.001	1
170	?	14	VAL	HG11	0.963	0.001	1
171	?	14	VAL	HG12	0.963	0.001	1
172	?	14	VAL	HG13	0.963	0.001	1
173	?	14	VAL	HG21	0.963	0.001	1
174	?	14	VAL	HG22	0.963	0.001	1
175	?	14	VAL	HG23	0.963	0.001	1
176	?	14	VAL	N	123.812	0.001	1
177	?	15	ASN	C	175.269	0.000	1
178	?	15	ASN	CA	53.375	0.086	1
179	?	15	ASN	CB	38.874	0.175	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	15	ASN	H	8.387	0.013	1
181	?	15	ASN	HA	4.743	0.015	1
182	?	15	ASN	HB2	2.875	0.004	2
183	?	15	ASN	HB3	2.817	0.047	2
184	?	15	ASN	N	122.027	0.117	1
185	?	16	MET	C	176.205	0.000	1
186	?	16	MET	CA	56.024	0.105	1
187	?	16	MET	CB	32.838	0.003	1
188	?	16	MET	CE	17.097	0.001	1
189	?	16	MET	CG	31.017	0.117	1
190	?	16	MET	H	8.295	0.010	1
191	?	16	MET	HA	4.161	0.003	1
192	?	16	MET	HB2	2.211	0.006	1
193	?	16	MET	HB3	2.211	0.006	1
194	?	16	MET	HE1	2.180	0.005	1
195	?	16	MET	HE2	2.180	0.005	1
196	?	16	MET	HE3	2.180	0.005	1
197	?	16	MET	HG2	2.647	0.001	1
198	?	16	MET	HG3	2.647	0.001	1
199	?	16	MET	N	121.200	0.098	1
200	?	17	LEU	C	177.353	0.000	1
201	?	17	LEU	CA	55.437	0.002	1
202	?	17	LEU	CB	42.203	0.046	1
203	?	17	LEU	CD1	24.941	0.002	1
204	?	17	LEU	CD2	24.941	0.002	1
205	?	17	LEU	CG	27.091	0.066	1
206	?	17	LEU	H	8.137	0.002	1
207	?	17	LEU	HA	4.340	0.001	1
208	?	17	LEU	HB2	1.732	0.016	1
209	?	17	LEU	HB3	1.732	0.016	1
210	?	17	LEU	HD11	0.964	0.000	2
211	?	17	LEU	HD12	0.964	0.000	2
212	?	17	LEU	HD13	0.964	0.000	2
213	?	17	LEU	HD21	0.909	0.001	2
214	?	17	LEU	HD22	0.909	0.001	2
215	?	17	LEU	HD23	0.909	0.001	2
216	?	17	LEU	HG	1.610	0.003	1
217	?	17	LEU	N	122.490	0.000	1
218	?	18	LYS	C	176.452	0.000	1
219	?	18	LYS	CA	56.400	0.000	1
220	?	18	LYS	CB	32.640	0.000	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	18	LYS	CD	29.110	0.113	1
222	?	18	LYS	CE	42.301	0.001	1
223	?	18	LYS	CG	24.731	0.001	1
224	?	18	LYS	H	8.125	0.001	1
225	?	18	LYS	HA	4.340	0.000	1
226	?	18	LYS	HB2	1.847	0.000	1
227	?	18	LYS	HB3	1.847	0.000	1
228	?	18	LYS	HD2	1.605	0.004	1
229	?	18	LYS	HD3	1.605	0.004	1
230	?	18	LYS	HE2	3.052	0.000	1
231	?	18	LYS	HE3	3.052	0.000	1
232	?	18	LYS	HG2	1.483	0.000	1
233	?	18	LYS	HG3	1.483	0.000	1
234	?	18	LYS	N	121.649	0.002	1
235	?	19	ARG	C	176.766	0.000	1
236	?	19	ARG	CA	56.435	0.002	1
237	?	19	ARG	CB	30.919	0.001	1
238	?	19	ARG	CD	43.545	0.008	1
239	?	19	ARG	CG	28.258	0.009	1
240	?	19	ARG	H	8.239	0.010	1
241	?	19	ARG	HA	4.384	0.002	1
242	?	19	ARG	HB2	1.889	0.001	1
243	?	19	ARG	HB3	1.889	0.001	1
244	?	19	ARG	HD2	3.266	0.003	1
245	?	19	ARG	HD3	3.266	0.003	1
246	?	19	ARG	HG2	1.731	0.003	1
247	?	19	ARG	HG3	1.731	0.003	1
248	?	19	ARG	N	121.877	0.093	1
249	?	20	GLY	C	174.015	0.000	1
250	?	20	GLY	CA	45.404	0.105	1
251	?	20	GLY	H	8.386	0.001	1
252	?	20	GLY	HA2	4.030	0.011	1
253	?	20	GLY	HA3	4.030	0.011	1
254	?	20	GLY	N	110.025	0.009	1
255	?	21	VAL	C	175.765	0.000	1
256	?	21	VAL	CA	62.128	0.129	1
257	?	21	VAL	CB	32.605	0.005	1
258	?	21	VAL	CG1	21.179	0.001	1
259	?	21	VAL	CG2	21.179	0.001	1
260	?	21	VAL	H	7.907	0.002	1
261	?	21	VAL	HA	4.184	0.013	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	21	VAL	HB	2.136	0.001	1
263	?	21	VAL	HG11	0.968	0.001	1
264	?	21	VAL	HG12	0.968	0.001	1
265	?	21	VAL	HG13	0.968	0.001	1
266	?	21	VAL	HG21	0.968	0.001	1
267	?	21	VAL	HG22	0.968	0.001	1
268	?	21	VAL	HG23	0.968	0.001	1
269	?	21	VAL	N	118.963	0.028	1
270	?	22	ALA	C	177.387	0.000	1
271	?	22	ALA	CA	52.516	0.055	1
272	?	22	ALA	CB	19.316	0.066	1
273	?	22	ALA	H	8.318	0.002	1
274	?	22	ALA	HA	4.399	0.006	1
275	?	22	ALA	HB1	1.436	0.002	1
276	?	22	ALA	HB2	1.436	0.002	1
277	?	22	ALA	HB3	1.436	0.002	1
278	?	22	ALA	N	127.437	0.007	1
279	?	23	ARG	C	176.081	0.000	1
280	?	23	ARG	CA	56.082	0.009	1
281	?	23	ARG	CB	30.656	0.007	1
282	?	23	ARG	CD	44.047	0.026	1
283	?	23	ARG	CG	27.109	0.075	1
284	?	23	ARG	H	8.256	0.002	1
285	?	23	ARG	HA	4.389	0.006	1
286	?	23	ARG	HB2	1.826	0.001	1
287	?	23	ARG	HB3	1.826	0.001	1
288	?	23	ARG	HD2	3.263	0.001	1
289	?	23	ARG	HD3	3.263	0.001	1
290	?	23	ARG	HG2	1.619	0.004	1
291	?	23	ARG	HG3	1.618	0.004	1
292	?	23	ARG	N	120.778	0.001	1
293	?	24	VAL	C	175.679	0.000	1
294	?	24	VAL	CA	61.975	0.133	1
295	?	24	VAL	CB	32.853	0.003	1
296	?	24	VAL	CG1	21.142	0.002	1
297	?	24	VAL	CG2	21.142	0.002	1
298	?	24	VAL	H	8.124	0.007	1
299	?	24	VAL	HA	4.216	0.005	1
300	?	24	VAL	HB	2.101	0.001	1
301	?	24	VAL	HG11	0.963	0.000	1
302	?	24	VAL	HG12	0.963	0.000	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	24	VAL	HG13	0.963	0.000	1
304	?	24	VAL	HG21	0.963	0.000	1
305	?	24	VAL	HG22	0.963	0.000	1
306	?	24	VAL	HG23	0.963	0.000	1
307	?	24	VAL	N	121.120	0.063	1
308	?	25	SER	C	173.495	0.000	1
309	?	25	SER	CA	55.967	0.017	1
310	?	25	SER	CB	63.924	0.028	1
311	?	25	SER	H	8.427	0.004	1
312	?	25	SER	HA	4.831	0.002	1
313	?	25	SER	HB2	3.950	0.006	2
314	?	25	SER	HB3	3.885	0.014	2
315	?	25	SER	N	120.452	0.001	1
316	?	26	PRO	CA	63.636	0.070	1
317	?	26	PRO	CB	31.882	0.095	1
318	?	26	PRO	CD	50.789	0.020	1
319	?	26	PRO	CG	27.374	0.079	1
320	?	26	PRO	HA	4.458	0.005	1
321	?	26	PRO	HB2	1.692	0.001	2
322	?	26	PRO	HB3	2.227	0.012	2
323	?	26	PRO	HD2	3.843	0.012	2
324	?	26	PRO	HD3	3.803	0.003	2
325	?	26	PRO	HG2	2.065	0.010	1
326	?	26	PRO	HG3	2.026	0.048	1
327	?	27	PHE	C	176.368	0.000	1
328	?	27	PHE	CA	57.958	0.003	1
329	?	27	PHE	CB	39.625	0.147	1
330	?	27	PHE	H	8.073	0.001	1
331	?	27	PHE	HA	4.648	0.010	1
332	?	27	PHE	HB2	3.266	0.006	2
333	?	27	PHE	HB3	3.060	0.002	2
334	?	27	PHE	N	118.782	0.000	1
335	?	28	GLY	C	174.330	0.000	1
336	?	28	GLY	CA	45.395	0.088	1
337	?	28	GLY	H	8.182	0.001	1
338	?	28	GLY	HA2	3.950	0.006	1
339	?	28	GLY	HA3	3.950	0.006	1
340	?	28	GLY	N	109.753	0.004	1
341	?	29	GLY	C	173.780	0.000	1
342	?	29	GLY	CA	44.975	0.042	1
343	?	29	GLY	H	7.928	0.003	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	29	GLY	HA2	3.845	0.004	1
345	?	29	GLY	HA3	3.845	0.004	1
346	?	29	GLY	N	107.860	0.004	1
347	?	30	LEU	C	176.993	0.000	1
348	?	30	LEU	CA	55.899	0.001	1
349	?	30	LEU	CB	42.943	0.055	1
350	?	30	LEU	CD1	24.691	0.001	1
351	?	30	LEU	CD2	24.691	0.001	1
352	?	30	LEU	CG	27.310	0.003	1
353	?	30	LEU	H	7.968	0.001	1
354	?	30	LEU	HA	4.362	0.001	1
355	?	30	LEU	HB2	1.814	0.007	1
356	?	30	LEU	HB3	1.814	0.007	1
357	?	30	LEU	HD11	0.967	0.000	2
358	?	30	LEU	HD12	0.967	0.000	2
359	?	30	LEU	HD13	0.967	0.000	2
360	?	30	LEU	HD21	0.904	0.000	2
361	?	30	LEU	HD22	0.904	0.000	2
362	?	30	LEU	HD23	0.904	0.000	2
363	?	30	LEU	HG	1.482	0.000	1
364	?	30	LEU	N	121.181	0.027	1
365	?	31	LYS	C	176.201	0.000	1
366	?	31	LYS	CA	57.057	0.068	1
367	?	31	LYS	CB	33.188	0.002	1
368	?	31	LYS	CD	29.124	0.108	1
369	?	31	LYS	CE	41.791	0.001	1
370	?	31	LYS	CG	24.988	0.002	1
371	?	31	LYS	H	8.674	0.010	1
372	?	31	LYS	HA	4.330	0.009	1
373	?	31	LYS	HB2	1.801	0.001	1
374	?	31	LYS	HB3	1.801	0.001	1
375	?	31	LYS	HD2	1.698	0.003	1
376	?	31	LYS	HD3	1.698	0.003	1
377	?	31	LYS	HE2	3.052	0.001	1
378	?	31	LYS	HE3	3.052	0.001	1
379	?	31	LYS	HG2	1.489	0.000	1
380	?	31	LYS	HG3	1.489	0.000	1
381	?	31	LYS	N	122.645	0.009	1
382	?	32	ARG	C	175.146	0.000	1
383	?	32	ARG	CA	54.853	0.029	1
384	?	32	ARG	CB	32.196	0.022	1

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Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	32	ARG	CD	42.412	0.002	1
386	?	32	ARG	CG	27.244	0.001	1
387	?	32	ARG	H	7.607	0.003	1
388	?	32	ARG	HA	4.261	0.002	1
389	?	32	ARG	HB2	1.729	0.017	1
390	?	32	ARG	HB3	1.729	0.017	1
391	?	32	ARG	HD2	3.041	0.001	1
392	?	32	ARG	HD3	3.041	0.001	1
393	?	32	ARG	HG2	1.446	0.001	1
394	?	32	ARG	HG3	1.446	0.001	1
395	?	32	ARG	N	116.258	0.001	1
396	?	33	LEU	C	176.501	0.000	1
397	?	33	LEU	CA	53.537	0.159	1
398	?	33	LEU	CB	41.434	0.055	1
399	?	33	LEU	CD1	25.233	0.194	1
400	?	33	LEU	CD2	25.233	0.194	1
401	?	33	LEU	H	8.547	0.004	1
402	?	33	LEU	HA	4.435	0.014	1
403	?	33	LEU	HB2	1.795	0.010	1
404	?	33	LEU	HB3	1.795	0.010	1
405	?	33	LEU	HD11	0.711	0.010	1
406	?	33	LEU	HD12	0.711	0.010	1
407	?	33	LEU	HD13	0.711	0.010	1
408	?	33	LEU	HD21	0.707	0.013	1
409	?	33	LEU	HD22	0.707	0.013	1
410	?	33	LEU	HD23	0.707	0.013	1
411	?	33	LEU	HG	1.333	0.000	1
412	?	33	LEU	N	122.179	0.026	1
413	?	34	PRO	C	176.885	0.000	1
414	?	34	PRO	CA	63.031	0.030	1
415	?	34	PRO	CB	31.675	0.232	1
416	?	34	PRO	CD	50.800	0.071	1
417	?	34	PRO	CG	27.356	0.206	1
418	?	34	PRO	HA	4.460	0.009	1
419	?	34	PRO	HB2	2.342	0.006	1
420	?	34	PRO	HB3	2.342	0.006	1
421	?	34	PRO	HD2	3.832	0.040	2
422	?	34	PRO	HD3	3.802	0.004	2
423	?	34	PRO	HG2	2.046	0.043	1
424	?	34	PRO	HG3	2.061	0.023	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	70	-0.45 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	63	0.40 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	68	-0.60 ± 0.28	Should be applied
^{15}N	67	-0.35 ± 0.34	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 41%, i.e. 623 atoms were assigned a chemical shift out of a possible 1516. 9 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	274/562 (49%)	108/224 (48%)	112/228 (49%)	54/110 (49%)
Sidechain	337/876 (38%)	203/516 (39%)	134/312 (43%)	0/48 (0%)
Aromatic	12/78 (15%)	6/42 (14%)	5/34 (15%)	1/2 (50%)
Overall	623/1516 (41%)	317/782 (41%)	251/574 (44%)	55/160 (34%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 41%, i.e. 773 atoms were assigned a chemical shift out of a possible 1890. 12 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	339/692 (49%)	134/276 (49%)	138/280 (49%)	67/136 (49%)
Sidechain	418/1104 (38%)	254/652 (39%)	164/386 (42%)	0/66 (0%)
Aromatic	16/94 (17%)	8/50 (16%)	7/38 (18%)	1/6 (17%)
Overall	773/1890 (41%)	396/978 (40%)	309/704 (44%)	68/208 (33%)

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.

Random coil index (RCI) for chain A:

