



wwPDB NMR Structure Validation Summary Report ⓘ

Feb 6, 2022 – 02:11 PM JST

PDB ID : 7WKC
Title : A prototype protein nanocage minimized from carboxysomes with gated oxygen permeability
Authors : Tan, H.; Yang, J.
Deposited on : 2022-01-08

This is a wwPDB NMR Structure Validation Summary 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:

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	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

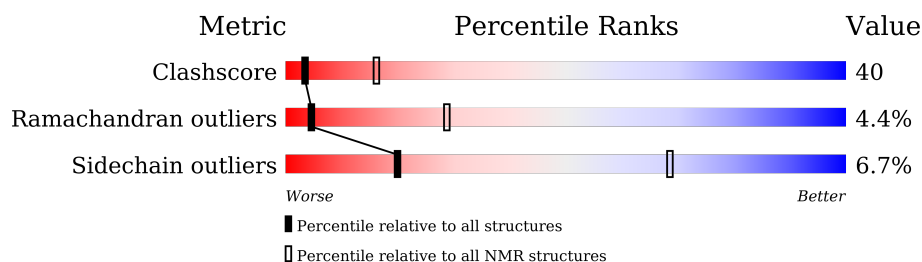
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 6%.

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	<div> <div style="width: 49%; background-color: green;"></div> <div style="width: 36%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 5%; background-color: cyan;"></div> <div style="width: 12%; background-color: grey;"></div> </div> <div>49% 36% • 12%</div>
1	B	104	<div> <div style="width: 49%; background-color: green;"></div> <div style="width: 36%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 5%; background-color: cyan;"></div> <div style="width: 12%; background-color: grey;"></div> </div> <div>49% 36% • 12%</div>
1	C	104	<div> <div style="width: 48%; background-color: green;"></div> <div style="width: 37%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 5%; background-color: cyan;"></div> <div style="width: 12%; background-color: grey;"></div> </div> <div>48% 37% • 12%</div>
1	D	104	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 5%; background-color: cyan;"></div> <div style="width: 12%; background-color: grey;"></div> </div> <div>50% 35% • 12%</div>
1	E	104	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 35%; background-color: yellow;"></div> <div style="width: 12%; background-color: orange;"></div> <div style="width: 5%; background-color: cyan;"></div> <div style="width: 12%; background-color: grey;"></div> </div> <div>50% 35% • 12%</div>

2 Ensemble composition and analysis

This entry contains 5 models. Model 4 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:1-A:92, B:1-B:92, C:1-C:92, D:1-D:92, E:1-E:92 (460)	0.10	4

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 1 single-model cluster was found.

Cluster number	Models
1	2, 4
2	3, 5
Single-model clusters	1

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6960 atoms, of which 3450 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Carboxysome shell vertex protein CcmL.

Mol	Chain	Residues	Atoms						Trace
1	A	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	B	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	C	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	D	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	
1	E	92	Total	C	H	N	O	S	0
			1392	439	690	125	136	2	

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	HIS	-	insertion	UNP Q8DKB4
A	35	HIS	-	insertion	UNP Q8DKB4
A	36	HIS	-	insertion	UNP Q8DKB4
A	37	HIS	-	insertion	UNP Q8DKB4
A	38	HIS	-	insertion	UNP Q8DKB4
B	34	HIS	-	insertion	UNP Q8DKB4
B	35	HIS	-	insertion	UNP Q8DKB4
B	36	HIS	-	insertion	UNP Q8DKB4
B	37	HIS	-	insertion	UNP Q8DKB4
B	38	HIS	-	insertion	UNP Q8DKB4
C	34	HIS	-	insertion	UNP Q8DKB4
C	35	HIS	-	insertion	UNP Q8DKB4
C	36	HIS	-	insertion	UNP Q8DKB4
C	37	HIS	-	insertion	UNP Q8DKB4
C	38	HIS	-	insertion	UNP Q8DKB4
D	34	HIS	-	insertion	UNP Q8DKB4
D	35	HIS	-	insertion	UNP Q8DKB4
D	36	HIS	-	insertion	UNP Q8DKB4
D	37	HIS	-	insertion	UNP Q8DKB4
D	38	HIS	-	insertion	UNP Q8DKB4
E	34	HIS	-	insertion	UNP Q8DKB4
E	35	HIS	-	insertion	UNP Q8DKB4
E	36	HIS	-	insertion	UNP Q8DKB4

Continued on next page...

Continued from previous page...

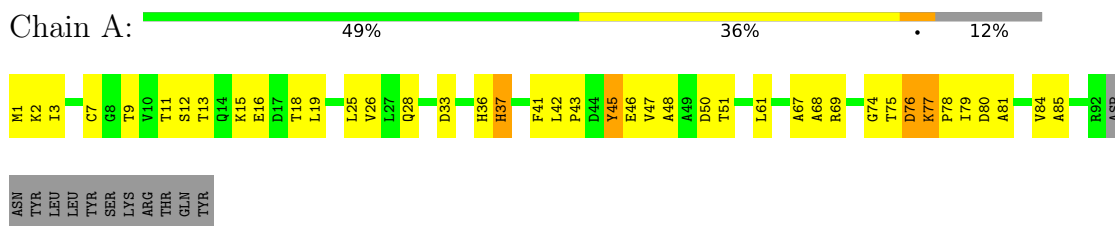
Chain	Residue	Modelled	Actual	Comment	Reference
E	37	HIS	-	insertion	UNP Q8DKB4
E	38	HIS	-	insertion	UNP Q8DKB4

4 Residue-property plots [i](#)

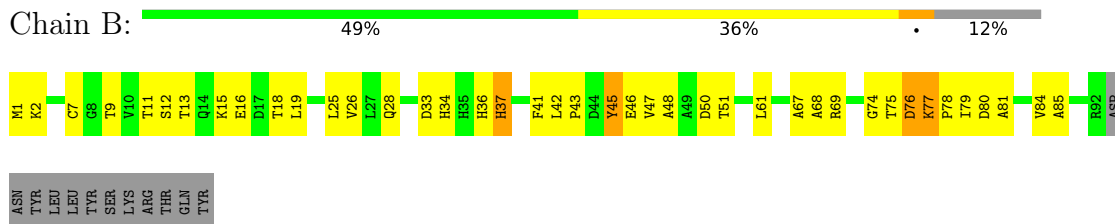
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

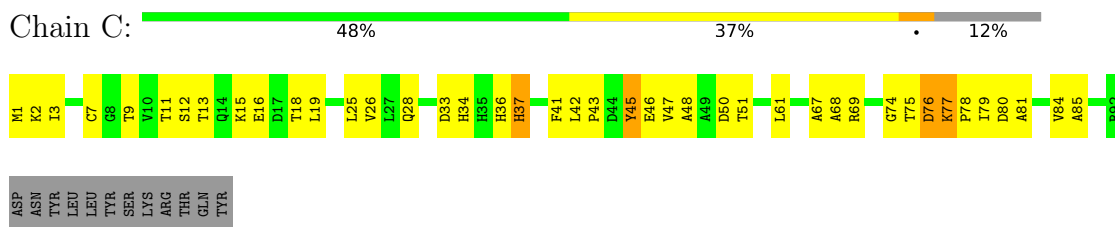
- Molecule 1: Carboxysome shell vertex protein CcmL



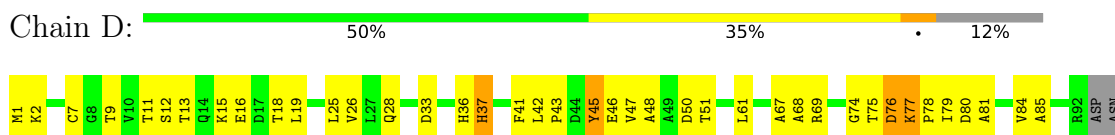
- Molecule 1: Carboxysome shell vertex protein CcmL



- Molecule 1: Carboxysome shell vertex protein CcmL



- Molecule 1: Carboxysome shell vertex protein CcmL



TYR
LEU
LEU
TYR
SER
LYS
ARG
THR
GLN
TYR

- Molecule 1: Carboxysome shell vertex protein CcmL

Chain E:  50% 35% 12%

M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 L25 V26 L27 Q28 D33 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85 R92 ASP ASN

TYR
LEU
LEU
TYR
SER
LYS
ARG
THR
GLN
TYR

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 4. Colouring as in section 4.1 above.

- Molecule 1: Carboxysome shell vertex protein CcmL

Chain A:  45% 38% 12%

M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 F24 L25 V26 L27 Q28 D33 H34 H35 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85 D88

R92 ASP ASN TYR LEU LEU TYR SER ARG THR GLN TYR

- Molecule 1: Carboxysome shell vertex protein CcmL

Chain B:  46% 38% 12%

M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 F24 L25 V26 L27 Q28 D33 H34 H35 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85 D88 R92

ASP ASN TYR LEU LEU TYR SER LYS ARG THR GLN TYR

- Molecule 1: Carboxysome shell vertex protein CcmL

Chain C:  45% 38% 12%

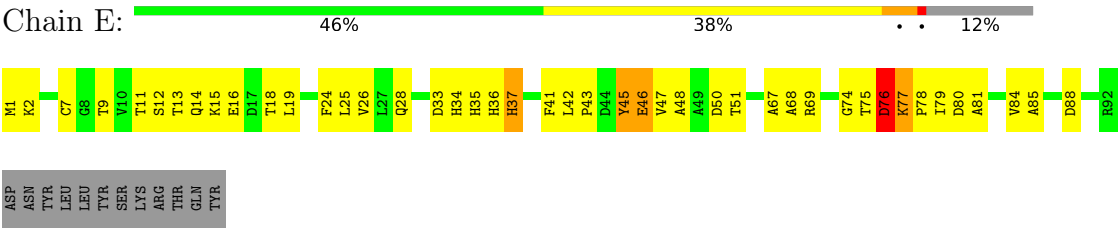
M1 K2 C7 G8 T9 V10 T11 S12 T13 Q14 K15 E16 D17 T18 L19 F24 L25 V26 L27 Q28 D33 H34 H35 H36 H37 F41 L42 P43 D44 Y45 E46 V47 A48 A49 D50 T51 L61 A67 A68 R69 G74 T75 D76 K77 P78 I79 D80 A81 V84 A85 D88

R92 ASP ASN TYR LEU LEU TYR SER LYS ARG THR GLN TYR

- Molecule 1: Carboxysome shell vertex protein CcmL



● Molecule 1: Carboxysome shell vertex protein CcmL



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 500 calculated structures, 5 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
X-PLOR	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	349
Number of shifts mapped to atoms	349
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	6%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [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	702	690	690	83±8
1	B	702	690	690	81±5
1	C	702	690	690	84±8
1	D	702	690	690	81±5
1	E	702	690	690	81±8
All	All	17550	17250	17250	1400

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 40.

5 of 502 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:77:LYS:O	1:E:67:ALA:HB2	1.08	1.47	1	5
1:A:67:ALA:HB2	1:D:77:LYS:O	1.07	1.49	1	5
1:B:77:LYS:O	1:D:67:ALA:HB2	1.06	1.51	1	5
1:A:77:LYS:O	1:C:67:ALA:HB2	1.05	1.51	1	5
1:A:2:LYS:HG2	1:D:47:VAL:HG21	1.04	1.04	1	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	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	4	29
1	B	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	4	29
1	C	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	4	29
1	D	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	4	29
1	E	90/104 (87%)	78±0 (87±0%)	8±0 (9±0%)	4±0 (4±0%)	4	29
All	All	2250/2600 (87%)	1950 (87%)	200 (9%)	100 (4%)	4	29

5 of 20 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	13	THR	5
1	A	37	HIS	5
1	A	76	ASP	5
1	A	77	LYS	5
1	B	13	THR	5

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	75/87 (86%)	70±2 (93±3%)	5±2 (7±3%)	20	68
1	B	75/87 (86%)	70±2 (93±3%)	5±2 (7±3%)	20	68
1	C	75/87 (86%)	70±2 (93±3%)	5±2 (7±3%)	20	68
1	D	75/87 (86%)	70±2 (93±3%)	5±2 (7±3%)	20	68
1	E	75/87 (86%)	70±2 (93±3%)	5±2 (7±3%)	20	68

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1875/2175 (86%)	1750 (93%)	125 (7%)	20 68

5 of 55 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	7	CYS	5
1	B	7	CYS	5
1	C	7	CYS	5
1	D	7	CYS	5
1	E	7	CYS	5

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 monosaccharides 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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 6% for the well-defined parts and 6% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CS_HCcmL@QD.star*

7.1.1 Bookkeeping [i](#)

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	349
Number of shifts mapped to atoms	349
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	70	-0.61 ± 0.29	Should be applied
$^{13}\text{C}_\beta$	61	-0.64 ± 0.21	Should be applied
$^{13}\text{C}'$	69	-0.58 ± 0.12	Should be applied
^{15}N	69	0.83 ± 0.54	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 6%, i.e. 340 atoms were assigned a chemical shift out of a possible 5350. 13 out of 85 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	207/2280 (9%)	0/910 (0%)	139/920 (15%)	68/450 (15%)
Sidechain	133/2630 (5%)	0/1505 (0%)	133/1025 (13%)	0/100 (0%)

Continued on next page...

Continued from previous page...

	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/440 (0%)	0/240 (0%)	0/165 (0%)	0/35 (0%)
Overall	340/5350 (6%)	0/2655 (0%)	272/2110 (13%)	68/585 (12%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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:

