



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 07:06 am BST

PDB ID : 5HVC
Title : Solution structure of the apo state of the acyl carrier protein from the MLSA2 subunit of the mycolactone polyketide synthase
Authors : Vance, S.; Tkachenko, O.; Thomas, B.; Bassuni, M.; Hong, H.; Nietlispach, D.; Broadhurst, R.W.
Deposited on : 2016-01-28

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

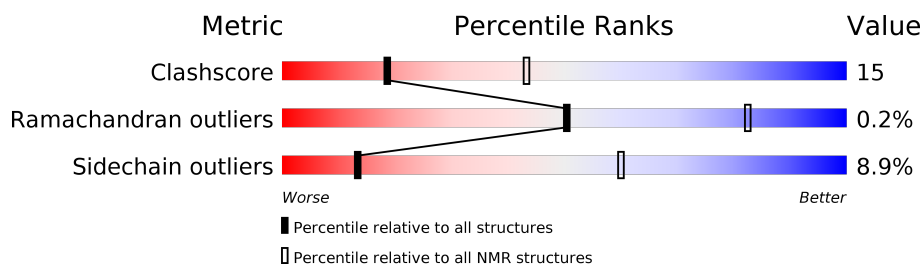
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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	95	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:2056-A:2137 (82)	0.22	13

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. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1447 atoms, of which 726 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Type I modular polyketide synthase.

Mol	Chain	Residues	Atoms						Trace
1	A	95	Total	C	H	N	O	S	0
			1447	448	726	133	139	1	

There are 4 discrepancies between the modelled and reference sequences:

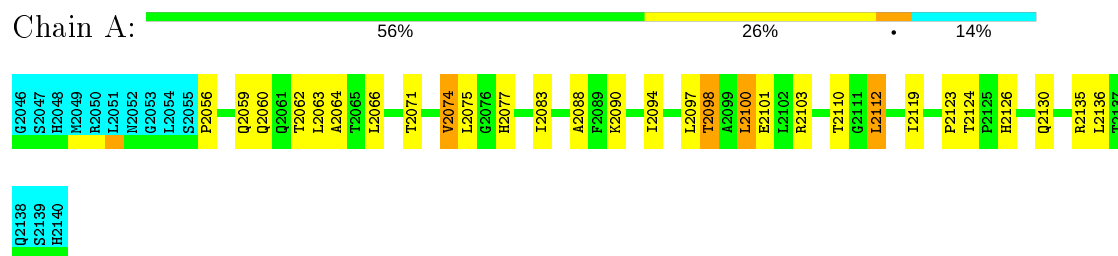
Chain	Residue	Modelled	Actual	Comment	Reference
A	2046	GLY	-	expression tag	UNP Q6MZA5
A	2047	SER	-	expression tag	UNP Q6MZA5
A	2048	HIS	-	expression tag	UNP Q6MZA5
A	2049	MET	-	expression tag	UNP Q6MZA5

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: Type I modular polyketide synthase

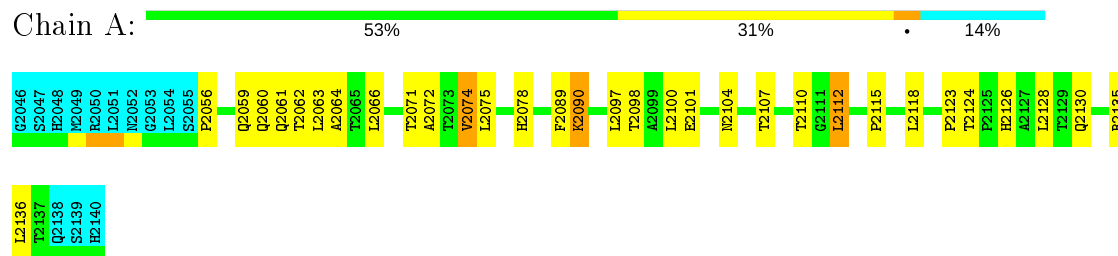


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

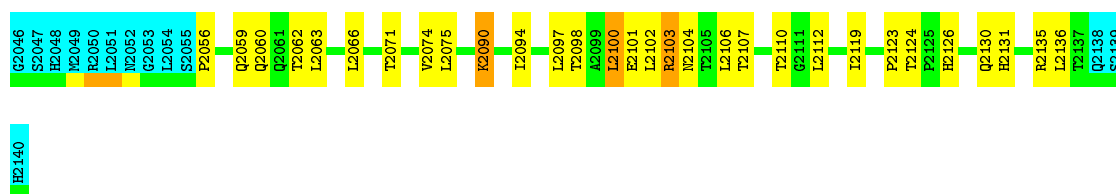
- Molecule 1: Type I modular polyketide synthase



4.2.2 Score per residue for model 2

- Molecule 1: Type I modular polyketide synthase





4.2.3 Score per residue for model 3

- Molecule 1: Type I modular polyketide synthase



4.2.4 Score per residue for model 4

- Molecule 1: Type I modular polyketide synthase



4.2.5 Score per residue for model 5

- Molecule 1: Type I modular polyketide synthase



4.2.6 Score per residue for model 6

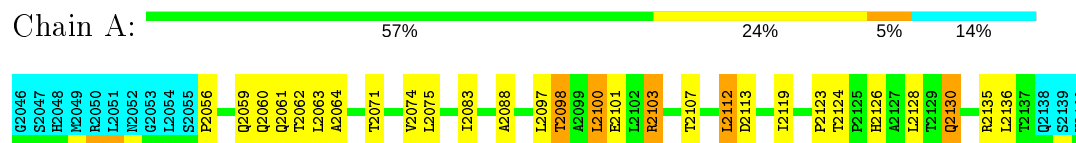
- Molecule 1: Type I modular polyketide synthase



Q2138
S2139
H2140

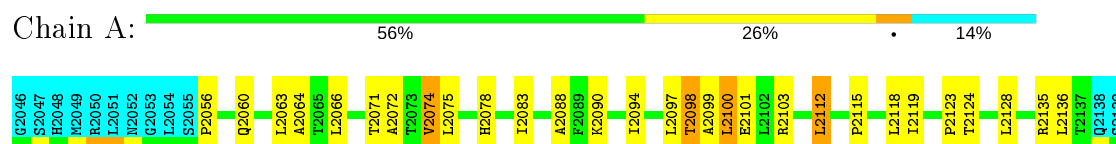
4.2.7 Score per residue for model 7

- Molecule 1: Type I modular polyketide synthase



4.2.8 Score per residue for model 8

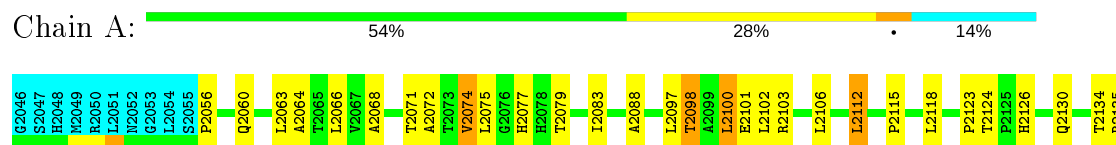
- Molecule 1: Type I modular polyketide synthase



H2140

4.2.9 Score per residue for model 9

- Molecule 1: Type I modular polyketide synthase

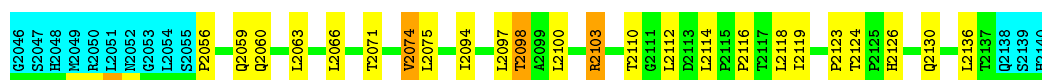


L2136
T2137
Q2138
S2139
H2140

4.2.10 Score per residue for model 10

- Molecule 1: Type I modular polyketide synthase

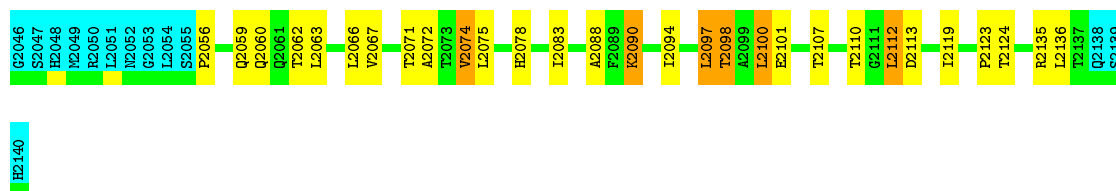




4.2.11 Score per residue for model 11

- Molecule 1: Type I modular polyketide synthase

Chain A: 56% 24% 6% 14%



4.2.12 Score per residue for model 12

- Molecule 1: Type I modular polyketide synthase

Chain A: 59% 22% 5% 14%



4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Type I modular polyketide synthase

Chain A: 58% 24% 14%



4.2.14 Score per residue for model 14

- Molecule 1: Type I modular polyketide synthase

Chain A: 55% 26% 5% 14%



S2139
H2140

4.2.15 Score per residue for model 15

- Molecule 1: Type I modular polyketide synthase

Chain A: 56% 26% 14%

Q2046 S2047 H2048 R2049 R2050 L2051 R2052 Q2053 L2054 S2055 P2056 Q2059 Q2060 Q2061 T2062 L2063 L2066 A2069 A2070 T2071 V2074 L2075 G2076 H2077 P2080 T2083 A2088 L2094 L2097 T2098 A2099 L2100 E2101 L2102 R2103 R2104 T2107 T2110 G2111 L2112 D2113 P2123 T2124 R2135 L2136 T2137 Q2138

S2139
H2140

4.2.16 Score per residue for model 16

- Molecule 1: Type I modular polyketide synthase

Chain A: 56% 26% 14%

Q2046 S2047 H2048 R2049 R2050 L2051 R2052 Q2053 L2054 S2055 P2056 Q2059 Q2060 Q2061 T2062 L2063 A2064 T2065 L2066 T2071 V2074 L2075 A2088 F2089 K2090 T2098 A2099 L2100 R2103 T2110 G2111 L2112 P2115 L2118 L2119 P2123 T2124 P2125 H2126 A2127 L2128 T2129 Q2130 H2131 R2135 L2136 Q2137 S2138

H2140

4.2.17 Score per residue for model 17

- Molecule 1: Type I modular polyketide synthase

Chain A: 57% 25% 14%

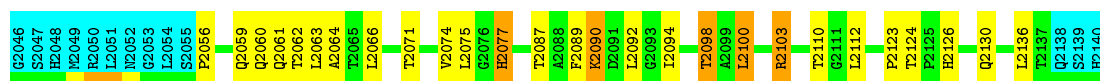
Q2046 S2047 H2048 R2049 R2050 L2051 R2052 Q2053 L2054 S2055 P2056 Q2059 Q2060 Q2061 T2062 L2063 A2064 T2065 L2066 T2071 A2072 T2073 V2074 L2075 G2076 H2077 A2088 F2089 K2090 T2094 L2097 T2098 A2099 L2100 E2101 L2102 R2103 L2112 P2115 I2119 P2123 T2124 P2125 H2126 T2129 Q2130 H2131 R2135 L2136 T2137 Q2138

S2139
H2140

4.2.18 Score per residue for model 18

- Molecule 1: Type I modular polyketide synthase

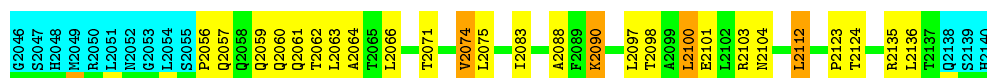
Chain A: 



4.2.19 Score per residue for model 19

- Molecule 1: Type I modular polyketide synthase

Chain A: 



4.2.20 Score per residue for model 20

- Molecule 1: Type I modular polyketide synthase

Chain A: 



5 Refinement protocol and experimental data overview

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

Of the 50 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
ARIA	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	983
Number of shifts mapped to atoms	983
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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	622	629	622	18±2
All	All	12440	12580	12440	362

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2112:LEU:HD21	1:A:2136:LEU:HD23	0.74	1.57	11	17
1:A:2071:THR:O	1:A:2075:LEU:HG	0.74	1.83	19	20
1:A:2123:PRO:O	1:A:2124:THR:HG23	0.69	1.87	17	20
1:A:2100:LEU:HA	1:A:2103:ARG:CZ	0.67	2.18	10	1
1:A:2074:VAL:HG22	1:A:2098:THR:HG22	0.66	1.68	12	16
1:A:2059:GLN:O	1:A:2062:THR:HB	0.64	1.92	7	12
1:A:2097:LEU:O	1:A:2100:LEU:HB3	0.64	1.92	11	6
1:A:2071:THR:HG23	1:A:2083:ILE:HD12	0.63	1.68	12	10
1:A:2100:LEU:O	1:A:2103:ARG:HD3	0.63	1.94	10	1
1:A:2056:PRO:O	1:A:2060:GLN:HG3	0.62	1.94	10	19
1:A:2100:LEU:HA	1:A:2103:ARG:CD	0.62	2.24	10	1
1:A:2112:LEU:HD13	1:A:2135:ARG:HB3	0.60	1.73	14	12
1:A:2059:GLN:O	1:A:2063:LEU:HD22	0.59	1.98	7	1
1:A:2103:ARG:HB2	1:A:2118:LEU:HD12	0.59	1.72	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2100:LEU:O	1:A:2103:ARG:HG3	0.59	1.98	2	8
1:A:2112:LEU:HD21	1:A:2136:LEU:CD2	0.57	2.29	17	10
1:A:2072:ALA:O	1:A:2077:HIS:HB3	0.55	2.01	20	1
1:A:2060:GLN:O	1:A:2063:LEU:HG	0.54	2.01	15	13
1:A:2126:HIS:O	1:A:2130:GLN:HG3	0.54	2.03	14	12
1:A:2132:LEU:O	1:A:2136:LEU:HD23	0.54	2.02	14	1
1:A:2061:GLN:HA	1:A:2064:ALA:HB3	0.54	1.78	7	10
1:A:2071:THR:HA	1:A:2074:VAL:HB	0.54	1.79	12	20
1:A:2100:LEU:HA	1:A:2103:ARG:NE	0.54	2.17	10	1
1:A:2103:ARG:NH2	1:A:2116:PRO:HB2	0.53	2.16	10	1
1:A:2115:PRO:O	1:A:2118:LEU:HG	0.53	2.04	3	9
1:A:2110:THR:HB	1:A:2112:LEU:CD1	0.51	2.36	2	5
1:A:2090:LYS:O	1:A:2090:LYS:HE3	0.50	2.06	11	5
1:A:2110:THR:HB	1:A:2136:LEU:HD21	0.50	1.84	11	4
1:A:2097:LEU:O	1:A:2101:GLU:HG3	0.49	2.07	15	6
1:A:2056:PRO:O	1:A:2059:GLN:HB2	0.49	2.08	16	1
1:A:2100:LEU:HD13	1:A:2101:GLU:N	0.49	2.23	8	5
1:A:2072:ALA:HA	1:A:2077:HIS:CD2	0.48	2.43	14	6
1:A:2112:LEU:HD13	1:A:2135:ARG:CB	0.48	2.38	2	2
1:A:2102:LEU:O	1:A:2106:LEU:HG	0.48	2.08	9	5
1:A:2063:LEU:HA	1:A:2066:LEU:HB3	0.48	1.85	18	3
1:A:2072:ALA:HA	1:A:2077:HIS:NE2	0.47	2.24	4	4
1:A:2131:HIS:O	1:A:2135:ARG:HG2	0.47	2.08	12	5
1:A:2060:GLN:O	1:A:2064:ALA:N	0.46	2.47	12	8
1:A:2101:GLU:O	1:A:2104:ASN:HB2	0.46	2.10	20	5
1:A:2088:ALA:HA	1:A:2124:THR:HG22	0.46	1.88	15	11
1:A:2063:LEU:O	1:A:2067:VAL:HG23	0.46	2.10	4	2
1:A:2103:ARG:HG3	1:A:2115:PRO:O	0.46	2.11	9	4
1:A:2074:VAL:HG22	1:A:2098:THR:CG2	0.45	2.41	20	1
1:A:2094:ILE:HG21	1:A:2119:ILE:HG21	0.45	1.87	17	6
1:A:2072:ALA:HB1	1:A:2078:HIS:C	0.45	2.32	1	5
1:A:2107:THR:OG1	1:A:2113:ASP:HA	0.44	2.12	7	3
1:A:2071:THR:CA	1:A:2102:LEU:HD11	0.44	2.43	20	1
1:A:2074:VAL:HG11	1:A:2094:ILE:CD1	0.44	2.43	15	3
1:A:2074:VAL:HG11	1:A:2094:ILE:HD11	0.43	1.89	11	1
1:A:2063:LEU:N	1:A:2063:LEU:HD13	0.43	2.29	14	1
1:A:2090:LYS:HE3	1:A:2090:LYS:O	0.43	2.13	3	3
1:A:2119:ILE:HD13	1:A:2128:LEU:HD11	0.43	1.90	7	4
1:A:2068:ALA:HB1	1:A:2083:ILE:HG13	0.42	1.91	9	2
1:A:2087:THR:HB	1:A:2092:LEU:HD21	0.42	1.92	18	1
1:A:2099:ALA:HA	1:A:2119:ILE:HG13	0.42	1.92	8	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2069:ALA:N	1:A:2080:PRO:HB3	0.42	2.30	15	2
1:A:2100:LEU:HD13	1:A:2100:LEU:C	0.42	2.35	11	3
1:A:2103:ARG:CB	1:A:2118:LEU:HD12	0.41	2.42	10	1
1:A:2075:LEU:HB2	1:A:2077:HIS:NE2	0.41	2.30	18	1
1:A:2126:HIS:O	1:A:2130:GLN:HG2	0.41	2.15	1	1
1:A:2063:LEU:HD22	1:A:2063:LEU:H	0.41	1.75	7	1
1:A:2112:LEU:HD21	1:A:2136:LEU:HD13	0.41	1.92	2	1
1:A:2089:PHE:CE2	1:A:2128:LEU:HD12	0.41	2.51	1	1
1:A:2114:LEU:HD13	1:A:2118:LEU:HD11	0.41	1.92	10	1
1:A:2119:ILE:O	1:A:2123:PRO:HB3	0.41	2.16	12	2
1:A:2058:GLN:HA	1:A:2058:GLN:HE21	0.41	1.75	14	1
1:A:2063:LEU:CD1	1:A:2129:THR:HA	0.41	2.46	4	2
1:A:2100:LEU:C	1:A:2100:LEU:HD13	0.40	2.36	12	1
1:A:2069:ALA:HB2	1:A:2080:PRO:HG3	0.40	1.94	5	1
1:A:2063:LEU:HG	1:A:2132:LEU:CB	0.40	2.47	14	1
1:A:2057:GLN:HA	1:A:2060:GLN:OE1	0.40	2.16	19	1
1:A:2089:PHE:HB3	1:A:2094:ILE:HG13	0.40	1.94	18	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	82/95 (86%)	74±1 (91±2%)	7±1 (9±2%)	0±0 (0±0%)	50	82
All	All	1640/1900 (86%)	1488 (91%)	148 (9%)	4 (0%)	50	82

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	2079	THR	4

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	70/81 (86%)	64±1 (91±2%)	6±1 (9±2%)	13	60
All	All	1400/1620 (86%)	1276 (91%)	124 (9%)	13	60

All 15 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	2098	THR	20
1	A	2100	LEU	19
1	A	2074	VAL	16
1	A	2066	LEU	15
1	A	2112	LEU	15
1	A	2090	LYS	14
1	A	2103	ARG	12
1	A	2107	THR	3
1	A	2077	HIS	3
1	A	2094	ILE	2
1	A	2130	GLN	1
1	A	2106	LEU	1
1	A	2063	LEU	1
1	A	2058	GLN	1
1	A	2097	LEU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: apo_macp9_160128_2.csdep

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	983
Number of shifts mapped to atoms	983
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
$^{13}\text{C}_\alpha$	92	-0.34 ± 0.30	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	85	0.49 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}'$	77	2.09 ± 0.14	Should be applied
^{15}N	83	-0.26 ± 0.40	None needed (< 0.5 ppm)

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 76%, i.e. 731 atoms were assigned a chemical shift out of a possible 965. 2 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	377/396 (95%)	151/157 (96%)	153/164 (93%)	73/75 (97%)
Sidechain	328/495 (66%)	188/286 (66%)	132/194 (68%)	8/15 (53%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	26/74 (35%)	16/38 (42%)	10/22 (45%)	0/14 (0%)
Overall	731/965 (76%)	355/481 (74%)	295/380 (78%)	81/104 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 839 atoms were assigned a chemical shift out of a possible 1122. 2 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	425/461 (92%)	173/183 (95%)	169/190 (89%)	83/88 (94%)
Sidechain	380/571 (67%)	221/332 (67%)	149/219 (68%)	10/20 (50%)
Aromatic	34/90 (38%)	20/46 (43%)	14/26 (54%)	0/18 (0%)
Overall	839/1122 (75%)	414/561 (74%)	332/435 (76%)	93/126 (74%)

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:

