



# Full wwPDB NMR Structure Validation Report ⓘ

Jul 7, 2022 – 04:43 PM EDT

PDB ID : 7RY6  
Title : Solution NMR structural bundle of the first cyclization domain from yersini-abactin synthetase (Cy1) impacted by dynamics  
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Deposited on : 2021-08-24

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

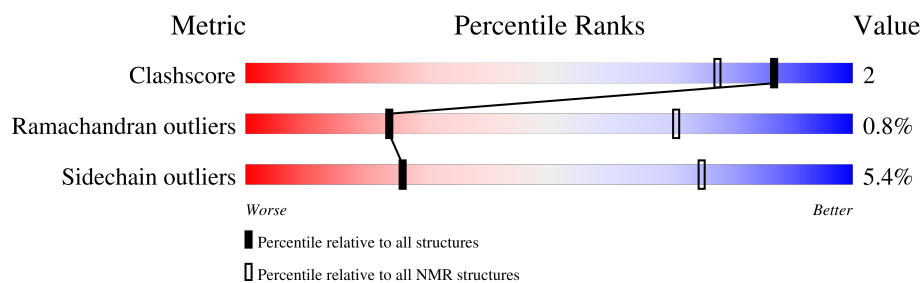
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 51%.

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  $\geq 3$ , 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	453	 90% 8%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:11-A:35, A:41-A:363, A:374-A:382, A:388-A:447 (417)	1.10	1

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 5 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7223 atoms, of which 3560 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HMWP2 nonribosomal peptide synthetase.

Mol	Chain	Residues	Atoms						Trace
1	A	453	Total	C	H	N	O	S	0
			7223	2326	3560	658	663	16	

There are 9 discrepancies between the modelled and reference sequences:

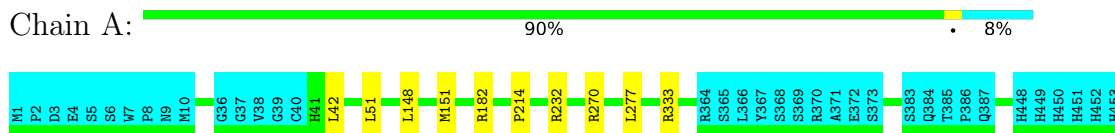
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A5P8YEQ8
A	446	LEU	-	expression tag	UNP A0A5P8YEQ8
A	447	GLU	-	expression tag	UNP A0A5P8YEQ8
A	448	HIS	-	expression tag	UNP A0A5P8YEQ8
A	449	HIS	-	expression tag	UNP A0A5P8YEQ8
A	450	HIS	-	expression tag	UNP A0A5P8YEQ8
A	451	HIS	-	expression tag	UNP A0A5P8YEQ8
A	452	HIS	-	expression tag	UNP A0A5P8YEQ8
A	453	HIS	-	expression tag	UNP A0A5P8YEQ8

## 4 Residue-property plots

### 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: HMWP2 nonribosomal peptide synthetase

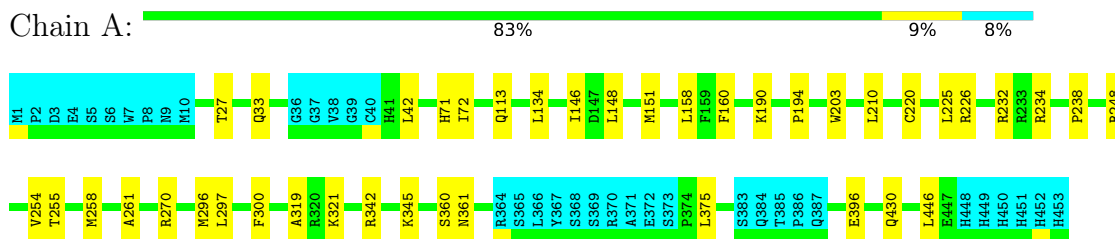


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

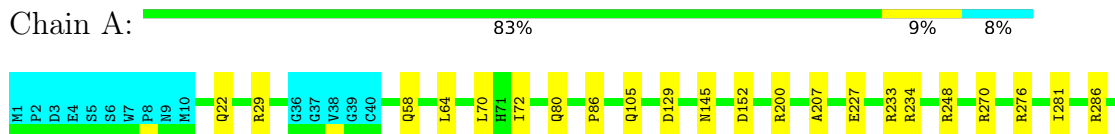
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: HMWP2 nonribosomal peptide synthetase



#### 4.2.2 Score per residue for model 2

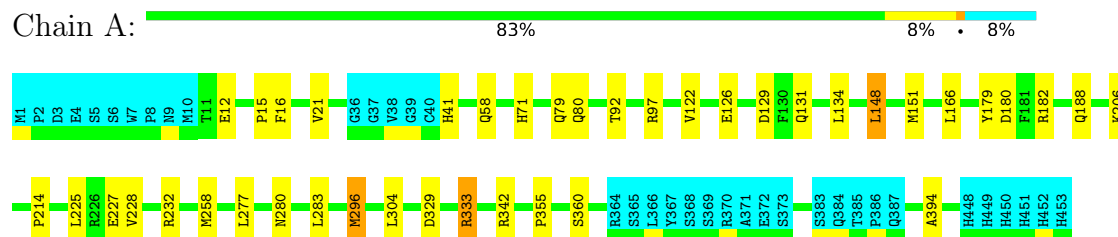
- Molecule 1: HMWP2 nonribosomal peptide synthetase





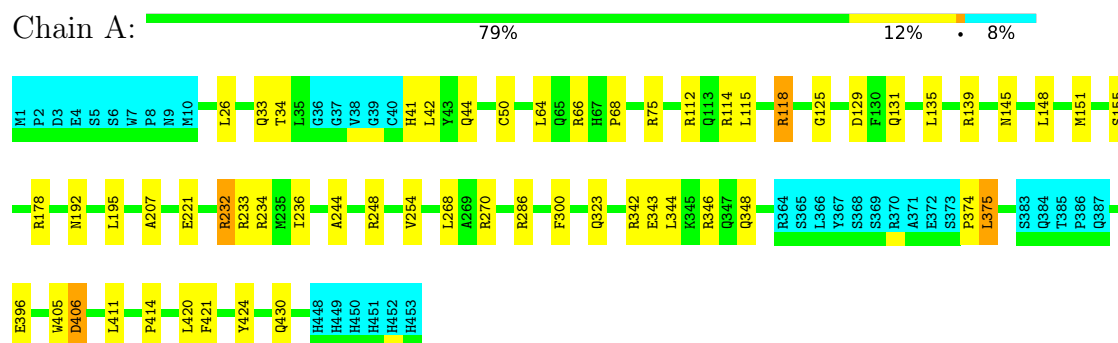
### 4.2.3 Score per residue for model 3

- Molecule 1: HMWP2 nonribosomal peptide synthetase



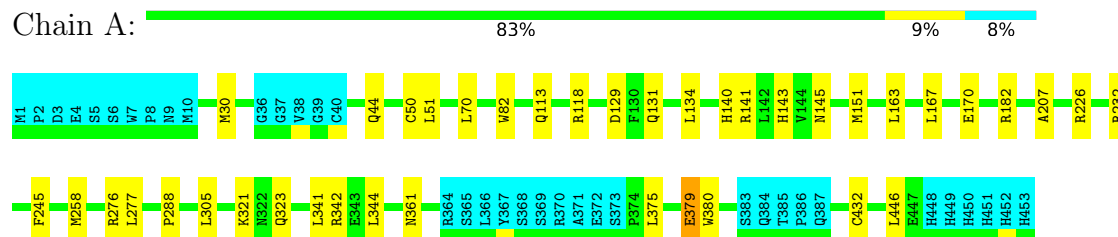
### 4.2.4 Score per residue for model 4

- Molecule 1: HMWP2 nonribosomal peptide synthetase



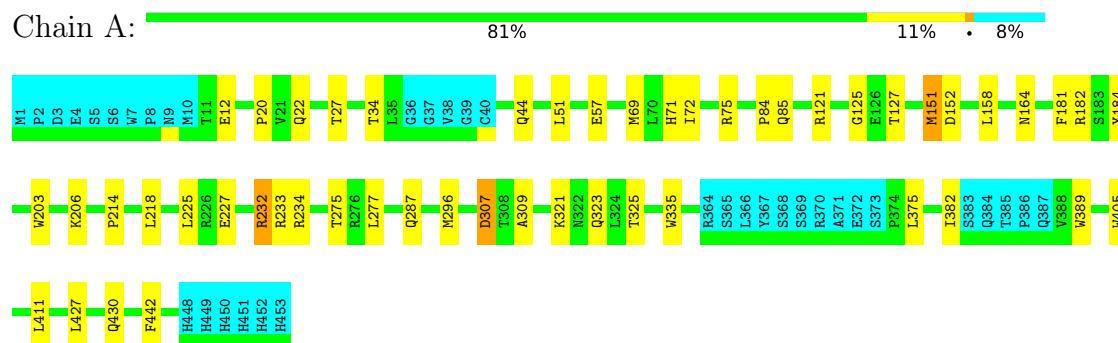
### 4.2.5 Score per residue for model 5

- Molecule 1: HMWP2 nonribosomal peptide synthetase



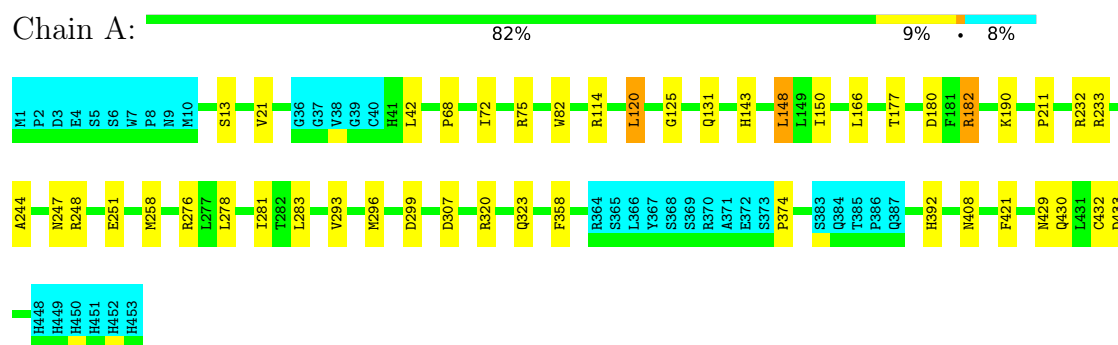
### 4.2.6 Score per residue for model 6

- Molecule 1: HMWP2 nonribosomal peptide synthetase



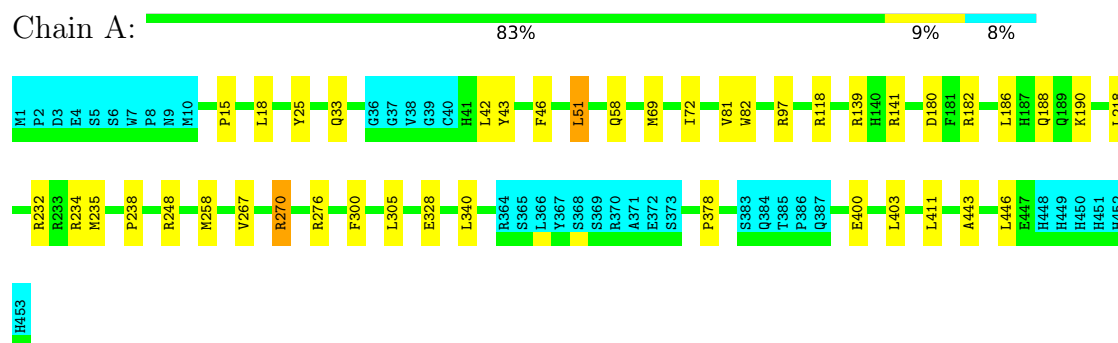
#### 4.2.7 Score per residue for model 7

- Molecule 1: HMWP2 nonribosomal peptide synthetase



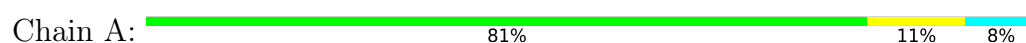
#### 4.2.8 Score per residue for model 8

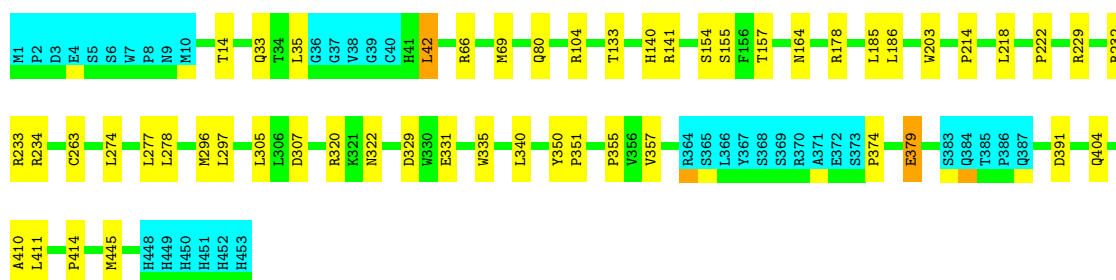
- Molecule 1: HMWP2 nonribosomal peptide synthetase



#### 4.2.9 Score per residue for model 9

- Molecule 1: HMWP2 nonribosomal peptide synthetase

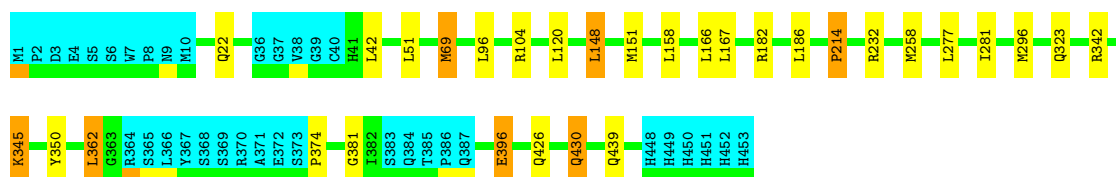




#### 4.2.10 Score per residue for model 10

- Molecule 1: HMWP2 nonribosomal peptide synthetase

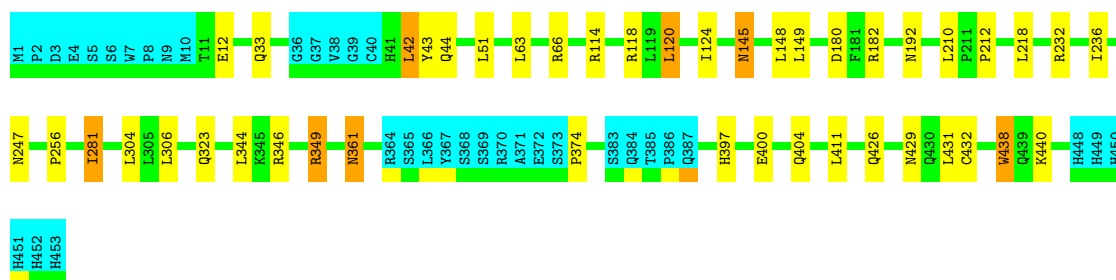
Chain A: 85% 5% 8%



#### 4.2.11 Score per residue for model 11

- Molecule 1: HMWP2 nonribosomal peptide synthetase

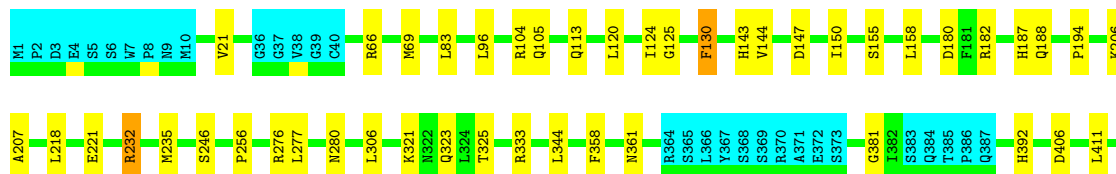
Chain A: 82% 8% 8%



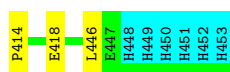
#### 4.2.12 Score per residue for model 12

- Molecule 1: HMWP2 nonribosomal peptide synthetase

Chain A: 81% 10% 8%

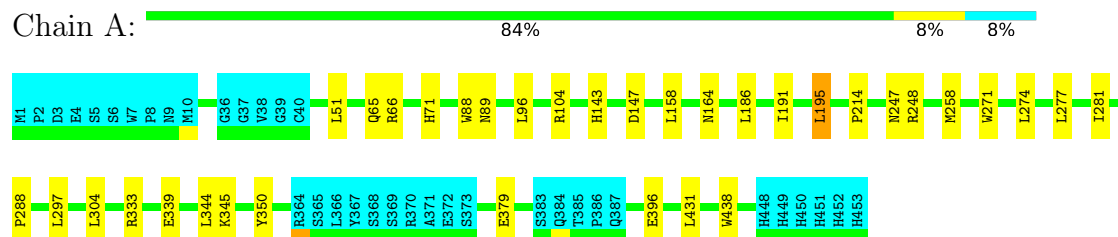






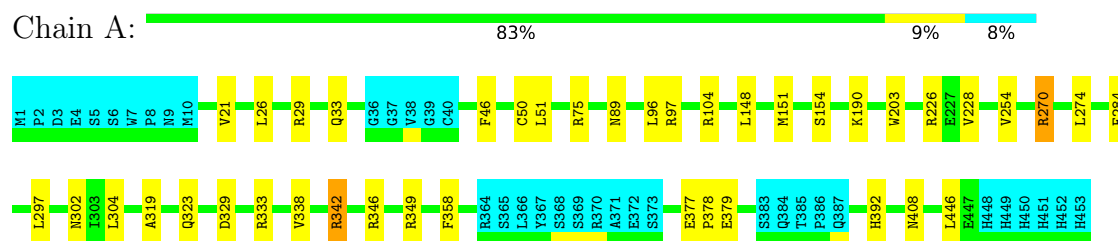
#### 4.2.13 Score per residue for model 13

- Molecule 1: HMWP2 nonribosomal peptide synthetase



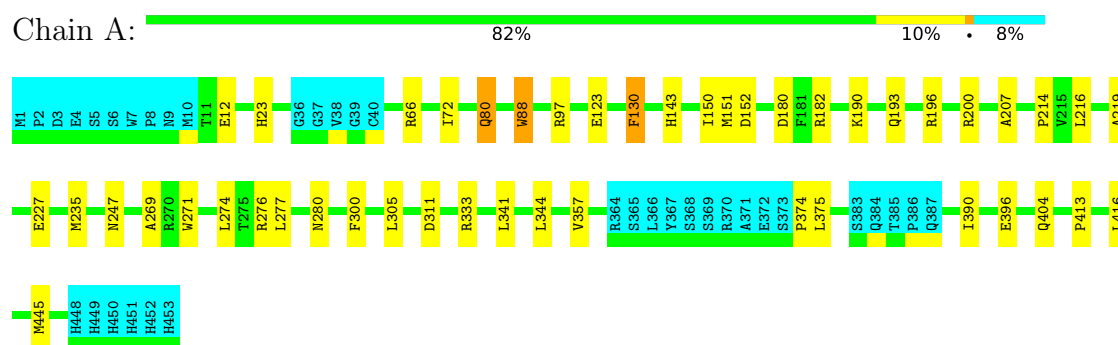
#### 4.2.14 Score per residue for model 14

- Molecule 1: HMWP2 nonribosomal peptide synthetase



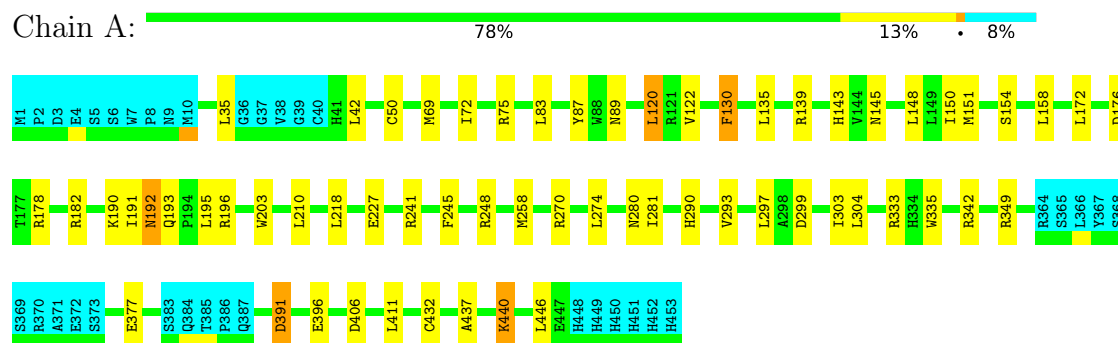
#### 4.2.15 Score per residue for model 15

- Molecule 1: HMWP2 nonribosomal peptide synthetase



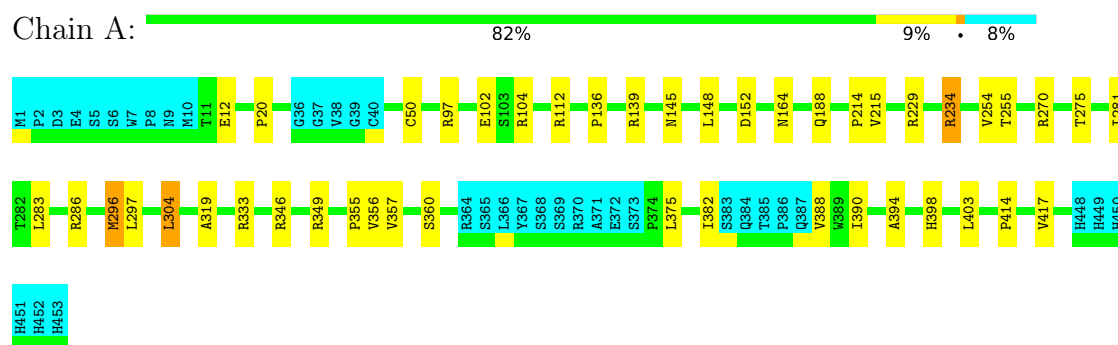
#### 4.2.16 Score per residue for model 16

- Molecule 1: HMWP2 nonribosomal peptide synthetase



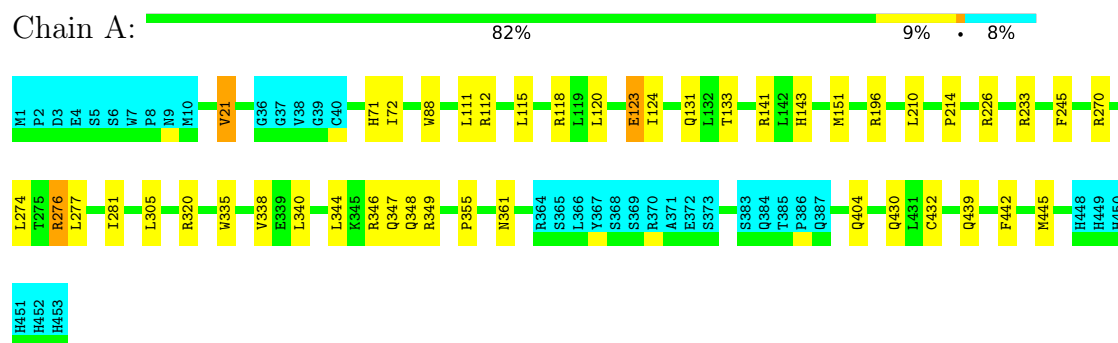
#### 4.2.17 Score per residue for model 17

- Molecule 1: HMWP2 nonribosomal peptide synthetase



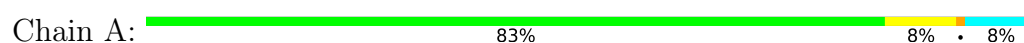
#### 4.2.18 Score per residue for model 18

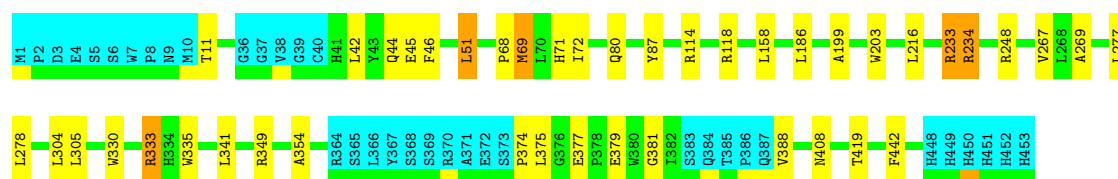
- Molecule 1: HMWP2 nonribosomal peptide synthetase



#### 4.2.19 Score per residue for model 19

- Molecule 1: HMWP2 nonribosomal peptide synthetase

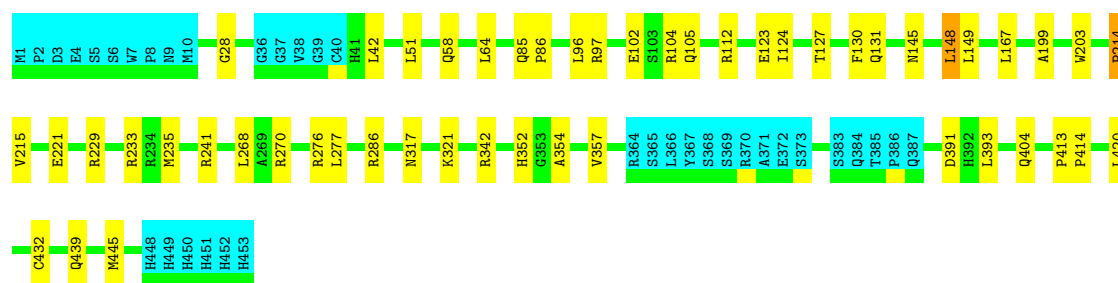




#### 4.2.20 Score per residue for model 20

- Molecule 1: HMWP2 nonribosomal peptide synthetase

Chain A: 81% 11% 8%



## 5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure calculation	3.98.13
CNS	refinement	1.3

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	3188
Number of shifts mapped to atoms	3188
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	51%

## 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	3378	3307	3288	13±4
All	All	67560	66140	65760	268

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:245:PHE:HE2	1:A:432:CYS:HG	0.68	1.31	16	1
1:A:391:ASP:HB3	1:A:406:ASP:HB3	0.62	1.70	16	1
1:A:180:ASP:HB2	1:A:182:ARG:HG2	0.62	1.69	15	5
1:A:245:PHE:HB2	1:A:432:CYS:SG	0.61	2.35	18	2
1:A:293:VAL:HA	1:A:296:MET:HB3	0.57	1.77	7	1
1:A:207:ALA:HB1	1:A:344:LEU:HD11	0.57	1.76	15	2
1:A:268:LEU:HA	1:A:420:LEU:HD13	0.56	1.75	4	2
1:A:225:LEU:HD11	1:A:411:LEU:HD21	0.56	1.76	6	1
1:A:96:LEU:HD23	1:A:104:ARG:HG2	0.56	1.77	20	3
1:A:214:PRO:HB3	1:A:277:LEU:HD11	0.56	1.77	18	1
1:A:258:MET:SD	1:A:281:ILE:HG21	0.55	2.42	10	1
1:A:21:VAL:HA	1:A:338:VAL:HG11	0.54	1.78	14	1
1:A:63:LEU:HG	1:A:66:ARG:HH21	0.54	1.60	11	1
1:A:229:ARG:HG2	1:A:410:ALA:HB2	0.54	1.80	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:358:PHE:HA	1:A:392:HIS:HB2	0.53	1.78	12	1
1:A:228:VAL:HB	1:A:408:ASN:HD21	0.53	1.63	14	1
1:A:72:ILE:HD11	1:A:80:GLN:HB2	0.53	1.81	2	3
1:A:75:ARG:HH21	1:A:83:LEU:HD21	0.53	1.62	16	1
1:A:304:LEU:HD13	1:A:329:ASP:HB3	0.53	1.80	3	1
1:A:360:SER:HA	1:A:394:ALA:HB3	0.52	1.81	2	3
1:A:83:LEU:HD11	1:A:125:GLY:HA3	0.52	1.81	12	1
1:A:72:ILE:HG22	1:A:82:TRP:HA	0.52	1.79	8	1
1:A:421:PHE:HA	1:A:424:TYR:HB3	0.52	1.80	4	1
1:A:212:PRO:HG3	1:A:349:ARG:HH12	0.51	1.64	11	1
1:A:362:LEU:HD12	1:A:396:GLU:HB2	0.51	1.81	10	1
1:A:357:VAL:O	1:A:391:ASP:HA	0.51	2.05	20	2
1:A:214:PRO:HB2	1:A:354:ALA:HB3	0.51	1.83	20	1
1:A:254:VAL:HG12	1:A:323:GLN:HB2	0.50	1.83	4	1
1:A:207:ALA:HB1	1:A:344:LEU:HD13	0.50	1.84	5	2
1:A:296:MET:SD	1:A:297:LEU:N	0.50	2.84	17	1
1:A:443:ALA:HA	1:A:446:LEU:HD23	0.50	1.83	8	1
1:A:358:PHE:HA	1:A:392:HIS:HB3	0.50	1.84	14	3
1:A:35:LEU:HD22	1:A:222:PRO:HB3	0.50	1.82	9	1
1:A:157:THR:HB	1:A:297:LEU:HB2	0.50	1.82	9	1
1:A:270:ARG:HB2	1:A:274:LEU:HB2	0.50	1.84	14	1
1:A:41:HIS:HB2	1:A:118:ARG:HG2	0.50	1.81	4	1
1:A:278:LEU:HA	1:A:307:ASP:HA	0.49	1.84	9	2
1:A:133:THR:HB	1:A:141:ARG:HB2	0.49	1.83	9	1
1:A:258:MET:SD	1:A:283:LEU:HD21	0.49	2.47	7	1
1:A:393:LEU:HB2	1:A:404:GLN:HB2	0.49	1.84	20	1
1:A:120:LEU:H	1:A:120:LEU:HD13	0.49	1.68	7	1
1:A:129:ASP:HB3	1:A:145:ASN:HB3	0.49	1.85	2	2
1:A:309:ALA:HB2	1:A:321:LYS:HG3	0.49	1.84	2	1
1:A:232:ARG:HH21	1:A:406:ASP:HB3	0.49	1.67	12	1
1:A:12:GLU:HB2	1:A:182:ARG:HB2	0.49	1.83	15	1
1:A:241:ARG:NH2	1:A:432:CYS:SG	0.49	2.86	16	1
1:A:304:LEU:HD11	1:A:333:ARG:HG3	0.49	1.83	3	1
1:A:69:MET:SD	1:A:155:SER:HA	0.49	2.47	12	1
1:A:258:MET:SD	1:A:283:LEU:HD11	0.48	2.48	7	2
1:A:405:TRP:O	1:A:406:ASP:HB2	0.48	2.08	4	1
1:A:305:LEU:HD12	1:A:340:LEU:HB3	0.48	1.83	8	3
1:A:46:PHE:HB2	1:A:379:GLU:HB2	0.48	1.86	14	1
1:A:50:CYS:SG	1:A:375:LEU:HD21	0.48	2.49	17	1
1:A:130:PHE:HB2	1:A:144:VAL:HA	0.48	1.85	12	1
1:A:216:LEU:HD21	1:A:269:ALA:HA	0.48	1.85	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:CYS:SG	1:A:134:LEU:HD21	0.48	2.49	5	1
1:A:274:LEU:HB2	1:A:277:LEU:HD12	0.48	1.86	18	1
1:A:46:PHE:HB3	1:A:377:GLU:O	0.48	2.09	14	2
1:A:330:TRP:O	1:A:333:ARG:HD2	0.48	2.08	2	2
1:A:206:LYS:NZ	1:A:325:THR:HG23	0.48	2.23	12	1
1:A:114:ARG:HH11	1:A:131:GLN:NE2	0.48	2.07	7	1
1:A:158:LEU:HG	1:A:297:LEU:HB2	0.48	1.84	16	1
1:A:218:LEU:HD22	1:A:411:LEU:HB3	0.47	1.86	16	5
1:A:69:MET:SD	1:A:69:MET:N	0.47	2.87	10	2
1:A:75:ARG:NH1	1:A:125:GLY:HA3	0.47	2.24	4	2
1:A:233:ARG:NH2	1:A:414:PRO:HB3	0.47	2.25	9	1
1:A:131:GLN:HB2	1:A:143:HIS:HB2	0.47	1.86	7	1
1:A:280:ASN:HD22	1:A:357:VAL:HG22	0.47	1.69	15	1
1:A:28:GLY:HA2	1:A:149:LEU:HD21	0.47	1.87	20	1
1:A:158:LEU:HG	1:A:297:LEU:HD23	0.46	1.86	13	1
1:A:96:LEU:HD22	1:A:104:ARG:HA	0.46	1.87	14	1
1:A:267:VAL:HA	1:A:270:ARG:HG2	0.46	1.86	8	1
1:A:431:LEU:HA	1:A:438:TRP:HB3	0.46	1.87	11	1
1:A:196:ARG:O	1:A:200:ARG:HG2	0.46	2.10	15	1
1:A:192:ASN:HA	1:A:195:LEU:HB3	0.46	1.88	16	2
1:A:118:ARG:HB3	1:A:120:LEU:HD12	0.46	1.87	11	1
1:A:164:ASN:HB3	1:A:375:LEU:HD22	0.46	1.88	6	1
1:A:307:ASP:H	1:A:325:THR:HG21	0.46	1.71	6	1
1:A:92:THR:HB	1:A:131:GLN:HG3	0.46	1.88	3	1
1:A:344:LEU:HA	1:A:347:GLN:HB2	0.46	1.88	18	1
1:A:207:ALA:HB1	1:A:347:GLN:HE22	0.45	1.71	2	1
1:A:254:VAL:HG21	1:A:319:ALA:HB1	0.45	1.88	17	2
1:A:130:PHE:HB3	1:A:143:HIS:O	0.45	2.11	12	3
1:A:354:ALA:HB1	1:A:388:VAL:HG22	0.45	1.88	19	1
1:A:15:PRO:HB3	1:A:81:VAL:HG22	0.45	1.88	8	1
1:A:255:THR:HB	1:A:258:MET:HB3	0.45	1.89	1	1
1:A:122:VAL:HA	1:A:126:GLU:HB2	0.45	1.88	3	1
1:A:114:ARG:HH21	1:A:129:ASP:HB2	0.45	1.71	4	1
1:A:305:LEU:HD11	1:A:341:LEU:HB2	0.45	1.87	19	3
1:A:72:ILE:HG21	1:A:151:MET:HB2	0.45	1.87	6	1
1:A:46:PHE:HB2	1:A:379:GLU:N	0.45	2.27	19	1
1:A:244:ALA:O	1:A:248:ARG:HD3	0.45	2.12	7	2
1:A:123:GLU:HB2	1:A:124:ILE:HD12	0.45	1.88	18	1
1:A:64:LEU:HA	1:A:68:PRO:HG3	0.45	1.89	4	1
1:A:211:PRO:HB3	1:A:276:ARG:HG3	0.45	1.87	7	1
1:A:445:MET:SD	1:A:445:MET:N	0.45	2.90	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:MET:SD	1:A:158:LEU:HD13	0.45	2.52	12	1
1:A:270:ARG:HB3	1:A:275:THR:HA	0.45	1.87	17	1
1:A:290:HIS:HB3	1:A:293:VAL:HG23	0.44	1.89	16	1
1:A:181:PHE:HA	1:A:184:TYR:HB3	0.44	1.88	6	1
1:A:284:PHE:HA	1:A:302:ASN:HB2	0.44	1.89	14	1
1:A:309:ALA:HB2	1:A:321:LYS:HE2	0.44	1.89	6	1
1:A:345:LYS:HG3	1:A:350:TYR:HB3	0.44	1.87	13	1
1:A:280:ASN:HD21	1:A:303:ILE:HB	0.44	1.71	16	1
1:A:11:THR:HG22	1:A:186:LEU:HD12	0.44	1.89	19	1
1:A:68:PRO:HA	1:A:177:THR:OG1	0.44	2.13	7	1
1:A:236:ILE:HD11	1:A:400:GLU:HB2	0.44	1.87	11	1
1:A:135:LEU:HB2	1:A:139:ARG:HB3	0.44	1.88	16	1
1:A:121:ARG:HB2	1:A:127:THR:HB	0.44	1.90	6	1
1:A:50:CYS:SG	1:A:51:LEU:HD23	0.44	2.53	14	1
1:A:158:LEU:HD13	1:A:297:LEU:H	0.43	1.73	1	1
1:A:114:ARG:NH2	1:A:129:ASP:HB2	0.43	2.28	4	1
1:A:238:PRO:HA	1:A:400:GLU:HG2	0.43	1.90	8	1
1:A:210:LEU:HD21	1:A:344:LEU:HD11	0.43	1.89	11	1
1:A:344:LEU:HD23	1:A:345:LYS:NZ	0.43	2.28	13	1
1:A:118:ARG:HG3	1:A:120:LEU:HD13	0.43	1.90	18	1
1:A:96:LEU:HD12	1:A:104:ARG:HA	0.43	1.89	12	1
1:A:214:PRO:HA	1:A:274:LEU:HG	0.43	1.91	15	2
1:A:271:TRP:NE1	1:A:416:LEU:HD11	0.43	2.29	15	1
1:A:232:ARG:HD2	1:A:382:ILE:HG22	0.43	1.91	6	1
1:A:82:TRP:HB3	1:A:182:ARG:HG2	0.43	1.90	7	1
1:A:429:ASN:HA	1:A:432:CYS:SG	0.43	2.54	7	2
1:A:158:LEU:HD13	1:A:296:MET:SD	0.43	2.54	10	1
1:A:69:MET:SD	1:A:158:LEU:HD22	0.43	2.53	16	1
1:A:356:VAL:HG12	1:A:390:ILE:HB	0.43	1.90	17	1
1:A:199:ALA:HB1	1:A:335:TRP:HB2	0.43	1.89	19	1
1:A:278:LEU:HD12	1:A:305:LEU:HD13	0.43	1.90	19	1
1:A:141:ARG:NH1	1:A:379:GLU:HG3	0.43	2.29	5	1
1:A:120:LEU:HD23	1:A:122:VAL:HB	0.43	1.90	16	1
1:A:154:SER:HB2	1:A:299:ASP:HA	0.43	1.91	16	1
1:A:232:ARG:H	1:A:232:ARG:HD3	0.43	1.74	4	1
1:A:228:VAL:HB	1:A:408:ASN:ND2	0.43	2.28	14	1
1:A:280:ASN:HB2	1:A:355:PRO:HG2	0.42	1.89	3	1
1:A:190:LYS:HA	1:A:190:LYS:HE2	0.42	1.90	7	1
1:A:51:LEU:HD11	1:A:167:LEU:HD22	0.42	1.90	10	2
1:A:133:THR:HB	1:A:141:ARG:HB3	0.42	1.90	18	1
1:A:276:ARG:HD3	1:A:276:ARG:H	0.42	1.74	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:GLU:HG3	1:A:124:ILE:HG13	0.42	1.90	20	1
1:A:214:PRO:HA	1:A:277:LEU:HD11	0.42	1.91	6	2
1:A:69:MET:SD	1:A:155:SER:HB2	0.42	2.54	9	1
1:A:342:ARG:O	1:A:346:ARG:HB2	0.42	2.14	14	1
1:A:111:LEU:O	1:A:115:LEU:HB2	0.42	2.14	18	1
1:A:64:LEU:HB3	1:A:86:PRO:HA	0.42	1.89	20	1
1:A:235:MET:HB3	1:A:403:LEU:HB2	0.42	1.89	8	1
1:A:270:ARG:HB2	1:A:274:LEU:O	0.42	2.14	16	1
1:A:241:ARG:HG3	1:A:432:CYS:SG	0.42	2.54	20	1
1:A:431:LEU:HG	1:A:438:TRP:HB3	0.42	1.92	13	1
1:A:232:ARG:HD3	1:A:232:ARG:N	0.42	2.29	4	1
1:A:203:TRP:HA	1:A:206:LYS:HB2	0.42	1.92	6	1
1:A:82:TRP:HB3	1:A:182:ARG:NH1	0.42	2.29	5	1
1:A:154:SER:HB3	1:A:296:MET:SD	0.42	2.55	9	1
1:A:234:ARG:H	1:A:234:ARG:HD3	0.42	1.74	19	1
1:A:220:CYS:HB2	1:A:225:LEU:HD11	0.42	1.92	1	1
1:A:315:VAL:HB	1:A:442:PHE:HZ	0.42	1.75	2	1
1:A:84:PRO:HB2	1:A:85:GLN:NE2	0.42	2.30	6	1
1:A:43:TYR:HA	1:A:145:ASN:HA	0.42	1.92	11	1
1:A:414:PRO:O	1:A:418:GLU:HG2	0.42	2.15	12	1
1:A:127:THR:HG23	1:A:148:LEU:HD12	0.42	1.91	20	1
1:A:70:LEU:H	1:A:70:LEU:HD23	0.41	1.75	5	1
1:A:18:LEU:HD22	1:A:25:TYR:HA	0.41	1.92	8	1
1:A:345:LYS:HE3	1:A:350:TYR:HB2	0.41	1.91	10	1
1:A:72:ILE:HG23	1:A:150:ILE:HB	0.41	1.92	15	1
1:A:219:ALA:HB2	1:A:413:PRO:HG3	0.41	1.91	15	1
1:A:437:ALA:HA	1:A:440:LYS:HB2	0.41	1.91	16	1
1:A:267:VAL:HG11	1:A:442:PHE:CE1	0.41	2.50	19	1
1:A:186:LEU:O	1:A:190:LYS:HG2	0.41	2.16	8	1
1:A:214:PRO:HB3	1:A:277:LEU:HD22	0.41	1.91	9	1
1:A:199:ALA:HA	1:A:203:TRP:CE3	0.41	2.49	20	1
1:A:179:TYR:O	1:A:296:MET:HG3	0.41	2.15	3	1
1:A:135:LEU:HB2	1:A:139:ARG:O	0.41	2.15	4	1
1:A:180:ASP:HB2	1:A:182:ARG:HG3	0.41	1.92	7	1
1:A:225:LEU:HD23	1:A:228:VAL:HG12	0.41	1.93	3	1
1:A:50:CYS:HB3	1:A:375:LEU:HD23	0.41	1.92	4	1
1:A:233:ARG:HH12	1:A:414:PRO:HB2	0.41	1.74	4	1
1:A:191:ILE:HG13	1:A:192:ASN:HD22	0.41	1.74	16	1
1:A:357:VAL:HG23	1:A:388:VAL:HG11	0.41	1.92	17	1
1:A:131:GLN:HB3	1:A:143:HIS:HB3	0.41	1.92	5	1
1:A:218:LEU:HA	1:A:411:LEU:O	0.41	2.15	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:CYS:HA	1:A:375:LEU:HB2	0.41	1.93	5	1
1:A:69:MET:HG2	1:A:158:LEU:HD13	0.41	1.92	6	1
1:A:141:ARG:HH22	1:A:379:GLU:HG3	0.41	1.76	9	1
1:A:12:GLU:HB2	1:A:182:ARG:HB3	0.41	1.91	11	1
1:A:163:LEU:O	1:A:167:LEU:HG	0.41	2.16	5	1
1:A:46:PHE:O	1:A:141:ARG:HA	0.41	2.15	8	1
1:A:64:LEU:HB3	1:A:86:PRO:HB3	0.41	1.92	2	1
1:A:126:GLU:HG3	1:A:148:LEU:HD13	0.41	1.93	3	1
1:A:234:ARG:HA	1:A:403:LEU:O	0.41	2.15	17	1
1:A:21:VAL:HG13	1:A:338:VAL:HG11	0.41	1.91	18	1
1:A:41:HIS:HB3	1:A:115:LEU:HA	0.41	1.91	4	1
1:A:427:LEU:HB2	1:A:442:PHE:HB2	0.41	1.93	6	1
1:A:69:MET:HA	1:A:72:ILE:HG23	0.41	1.93	8	1
1:A:426:GLN:O	1:A:430:GLN:HB2	0.41	2.15	10	1
1:A:281:ILE:HD11	1:A:306:LEU:HD13	0.41	1.93	11	1
1:A:215:VAL:HG22	1:A:270:ARG:HH22	0.41	1.75	17	1
1:A:233:ARG:N	1:A:233:ARG:HD2	0.41	2.31	19	1
1:A:151:MET:SD	1:A:155:SER:HB3	0.41	2.56	4	1
1:A:72:ILE:HD11	1:A:150:ILE:HG12	0.41	1.93	7	1
1:A:306:LEU:HA	1:A:325:THR:HG21	0.41	1.92	12	1
1:A:442:PHE:HA	1:A:445:MET:SD	0.41	2.56	18	1
1:A:215:VAL:HA	1:A:352:HIS:HB3	0.41	1.93	20	1
1:A:261:ALA:HB2	1:A:360:SER:HB2	0.40	1.93	1	1
1:A:278:LEU:H	1:A:278:LEU:HD23	0.40	1.75	7	1
1:A:263:CYS:SG	1:A:322:ASN:ND2	0.40	2.93	9	1
1:A:304:LEU:HD21	1:A:329:ASP:HB3	0.40	1.92	14	1
1:A:97:ARG:HA	1:A:136:PRO:HD3	0.40	1.94	17	1
1:A:283:LEU:HD23	1:A:304:LEU:HB2	0.40	1.92	17	1
1:A:414:PRO:HA	1:A:417:VAL:HB	0.40	1.93	17	1
1:A:131:GLN:HB2	1:A:143:HIS:HB3	0.40	1.92	18	1
1:A:68:PRO:HD2	1:A:71:HIS:HB3	0.40	1.92	19	1
1:A:75:ARG:HH21	1:A:125:GLY:HA3	0.40	1.76	6	1
1:A:151:MET:SD	1:A:152:ASP:N	0.40	2.93	6	1
1:A:233:ARG:HB2	1:A:405:TRP:HB2	0.40	1.93	6	1
1:A:247:ASN:O	1:A:251:GLU:HG2	0.40	2.17	7	1
1:A:355:PRO:HB2	1:A:388:VAL:HG12	0.40	1.92	17	1
1:A:254:VAL:HG11	1:A:319:ALA:HB1	0.40	1.92	1	1
1:A:214:PRO:HG3	1:A:277:LEU:HD21	0.40	1.94	3	1
1:A:246:SER:HA	1:A:256:PRO:HB3	0.40	1.92	12	1
1:A:148:LEU:HD13	1:A:150:ILE:HG13	0.40	1.93	7	1
1:A:191:ILE:O	1:A:195:LEU:HG	0.40	2.17	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:154:SER:HB3	1:A:297:LEU:HG	0.40	1.93	14	1
1:A:445:MET:N	1:A:445:MET:SD	0.40	2.95	15	1
1:A:233:ARG:HG3	1:A:235:MET:SD	0.40	2.56	20	1
1:A:15:PRO:HB3	1:A:79:GLN:HB3	0.40	1.94	3	1
1:A:134:LEU:HA	1:A:140:HIS:HB3	0.40	1.92	5	1
1:A:234:ARG:HB3	1:A:404:GLN:HG3	0.40	1.93	9	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	417/453 (92%)	392±3 (94±1%)	21±3 (5±1%)	3±1 (1±0%)	24	71
All	All	8340/9060 (92%)	7849 (94%)	428 (5%)	63 (1%)	24	71

All 28 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	374	PRO	7
1	A	66	ARG	5
1	A	51	LEU	5
1	A	300	PHE	4
1	A	21	VAL	4
1	A	148	LEU	3
1	A	214	PRO	3
1	A	381	GLY	3
1	A	88	TRP	3
1	A	194	PRO	2
1	A	351	PRO	2
1	A	288	PRO	2
1	A	20	PRO	2
1	A	355	PRO	2
1	A	89	ASN	2
1	A	87	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	238	PRO	1
1	A	152	ASP	1
1	A	406	ASP	1
1	A	13	SER	1
1	A	299	ASP	1
1	A	256	PRO	1
1	A	390	ILE	1
1	A	50	CYS	1
1	A	176	ASP	1
1	A	348	GLN	1
1	A	413	PRO	1
1	A	414	PRO	1

### 6.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	361/393 (92%)	341±4 (95±1%)	20±4 (5±1%)	26	75
All	All	7220/7860 (92%)	6827 (95%)	393 (5%)	26	75

All 141 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	232	ARG	11
1	A	42	LEU	10
1	A	151	MET	9
1	A	342	ARG	9
1	A	333	ARG	9
1	A	148	LEU	8
1	A	234	ARG	7
1	A	270	ARG	7
1	A	276	ARG	7
1	A	281	ILE	7
1	A	323	GLN	7
1	A	33	GLN	6
1	A	248	ARG	6

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Mol	Chain	Res	Type	Models (Total)
1	A	277	LEU	6
1	A	349	ARG	6
1	A	71	HIS	5
1	A	203	TRP	5
1	A	396	GLU	5
1	A	430	GLN	5
1	A	446	LEU	5
1	A	227	GLU	5
1	A	361	ASN	5
1	A	97	ARG	5
1	A	44	GLN	5
1	A	145	ASN	5
1	A	120	LEU	5
1	A	304	LEU	5
1	A	190	LYS	4
1	A	226	ARG	4
1	A	296	MET	4
1	A	321	LYS	4
1	A	375	LEU	4
1	A	58	GLN	4
1	A	233	ARG	4
1	A	286	ARG	4
1	A	188	GLN	4
1	A	112	ARG	4
1	A	118	ARG	4
1	A	346	ARG	4
1	A	258	MET	4
1	A	182	ARG	4
1	A	335	TRP	4
1	A	130	PHE	4
1	A	72	ILE	3
1	A	113	GLN	3
1	A	210	LEU	3
1	A	345	LYS	3
1	A	22	GLN	3
1	A	105	GLN	3
1	A	80	GLN	3
1	A	166	LEU	3
1	A	178	ARG	3
1	A	221	GLU	3
1	A	379	GLU	3
1	A	51	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	320	ARG	3
1	A	164	ASN	3
1	A	439	GLN	3
1	A	247	ASN	3
1	A	404	GLN	3
1	A	134	LEU	2
1	A	29	ARG	2
1	A	26	LEU	2
1	A	131	GLN	2
1	A	12	GLU	2
1	A	408	ASN	2
1	A	139	ARG	2
1	A	104	ARG	2
1	A	69	MET	2
1	A	114	ARG	2
1	A	124	ILE	2
1	A	192	ASN	2
1	A	440	LYS	2
1	A	147	ASP	2
1	A	150	ILE	2
1	A	235	MET	2
1	A	123	GLU	2
1	A	152	ASP	2
1	A	193	GLN	2
1	A	196	ARG	2
1	A	102	GLU	2
1	A	229	ARG	2
1	A	146	ILE	1
1	A	160	PHE	1
1	A	70	LEU	1
1	A	200	ARG	1
1	A	290	HIS	1
1	A	303	ILE	1
1	A	435	GLU	1
1	A	16	PHE	1
1	A	129	ASP	1
1	A	206	LYS	1
1	A	236	ILE	1
1	A	343	GLU	1
1	A	348	GLN	1
1	A	411	LEU	1
1	A	30	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	170	GLU	1
1	A	380	TRP	1
1	A	34	THR	1
1	A	57	GLU	1
1	A	275	THR	1
1	A	287	GLN	1
1	A	307	ASP	1
1	A	389	TRP	1
1	A	421	PHE	1
1	A	433	ASP	1
1	A	43	TYR	1
1	A	328	GLU	1
1	A	14	THR	1
1	A	140	HIS	1
1	A	185	LEU	1
1	A	274	LEU	1
1	A	329	ASP	1
1	A	331	GLU	1
1	A	350	TYR	1
1	A	214	PRO	1
1	A	362	LEU	1
1	A	149	LEU	1
1	A	438	TRP	1
1	A	280	ASN	1
1	A	65	GLN	1
1	A	143	HIS	1
1	A	195	LEU	1
1	A	271	TRP	1
1	A	339	GLU	1
1	A	75	ARG	1
1	A	89	ASN	1
1	A	88	TRP	1
1	A	311	ASP	1
1	A	374	PRO	1
1	A	35	LEU	1
1	A	172	LEU	1
1	A	377	GLU	1
1	A	391	ASP	1
1	A	255	THR	1
1	A	382	ILE	1
1	A	45	GLU	1
1	A	158	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	85	GLN	1
1	A	317	ASN	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no 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 51% for the well-defined parts and 49% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch\_output*

#### 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	3188
Number of shifts mapped to atoms	3188
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 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
$^{13}\text{C}_\alpha$	426	$0.34 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	399	$0.99 \pm 0.10$	Should be applied
$^{13}\text{C}'$	420	$0.07 \pm 0.05$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	381	$0.23 \pm 0.14$	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 51%, i.e. 2709 atoms were assigned a chemical shift out of a possible 5307. 78 out of 81 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	1895/2031 (93%)	726/807 (90%)	805/834 (97%)	364/390 (93%)
Sidechain	772/2729 (28%)	217/1600 (14%)	555/996 (56%)	0/133 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	42/547 (8%)	31/283 (11%)	0/214 (0%)	11/50 (22%)
Overall	2709/5307 (51%)	974/2690 (36%)	1360/2044 (67%)	375/573 (65%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 49%, i.e. 2825 atoms were assigned a chemical shift out of a possible 5742. 79 out of 83 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	1987/2205 (90%)	760/876 (87%)	846/906 (93%)	381/423 (90%)
Sidechain	794/2922 (27%)	219/1719 (13%)	575/1061 (54%)	0/142 (0%)
Aromatic	44/615 (7%)	32/317 (10%)	0/235 (0%)	12/63 (19%)
Overall	2825/5742 (49%)	1011/2912 (35%)	1421/2202 (65%)	393/628 (63%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	292	ALA	H	12.18	11.19 – 5.19	6.7
1	A	10	MET	H	11.73	11.26 – 5.26	5.8
1	A	68	PRO	CA	54.76	71.13 – 55.53	-5.5

#### 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:

