



# Full wwPDB NMR Structure Validation Report ⓘ

Jan 16, 2018 – 03:48 PM EST

PDB ID : 2K2Q  
Title : complex structure of the external thioesterase of the Surfactin-synthetase with a carrier domain  
Authors : Koglin, A.; Lohr, F.; Bernhard, F.; Rogov, V.V.; Frueh, D.P.; Strieter, E.R.; Mofid, M.R.; Guntert, P.; Wagner, G.; Walsh, C.T.; Marahiel, M.A.; Dotsch, V.  
Deposited on : 2008-04-10

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

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20030736
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

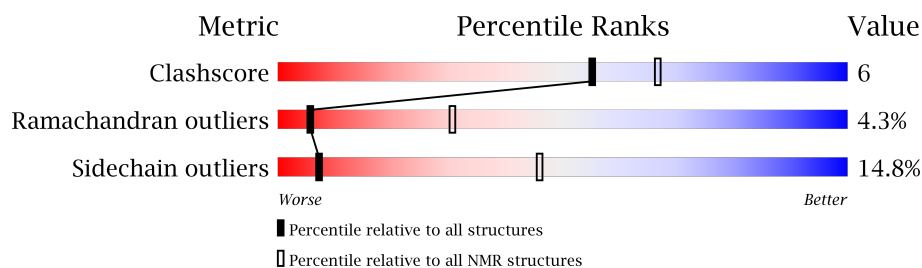
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	82	 82% 18%
2	B	242	 78% 22%

## 2 Ensemble composition and analysis ⓘ

This entry contains 18 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:82, B:1-B:242 (324)	1.09	9

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 3 clusters. No single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5125 atoms, of which 2548 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tyrocidine synthetase 3 (Tyrocidine synthetase III).

Mol	Chain	Residues	Atoms						Trace
1	A	82	Total	C	H	N	O	S	0
			1272	407	644	105	114	2	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP O30409
A	2	GLY	-	EXPRESSION TAG	UNP O30409

- Molecule 2 is a protein called Surfactin synthetase thioesterase subunit.

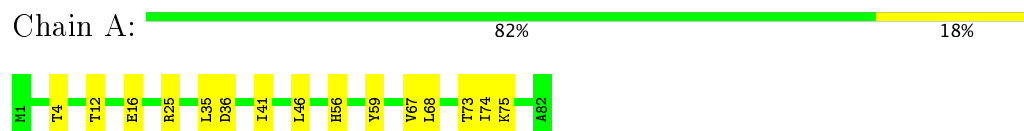
Mol	Chain	Residues	Atoms						Trace
2	B	242	Total	C	H	N	O	S	0
			3853	1253	1904	329	357	10	

## 4 Residue-property plots

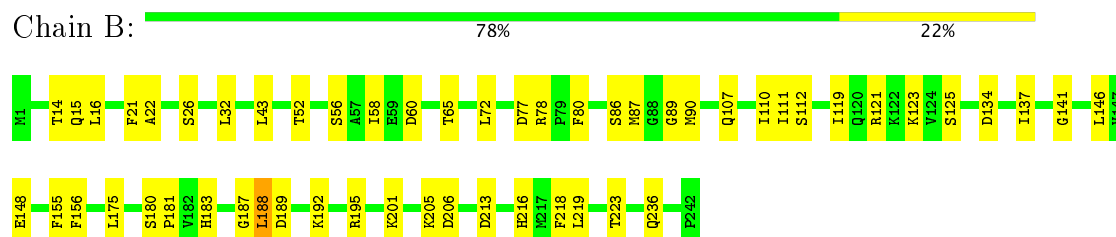
### 4.1 Average score per residue in the NMR ensemble

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: Tyrocidine synthetase 3 (Tyrocidine synthetase III)



- Molecule 2: Surfactin synthetase thioesterase subunit

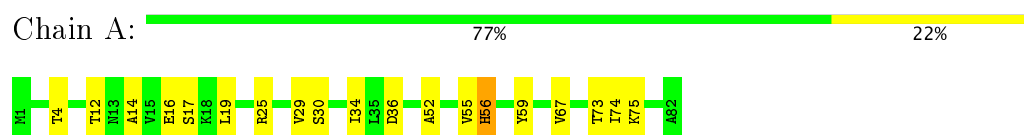


### 4.2 Scores per residue for each member of the ensemble

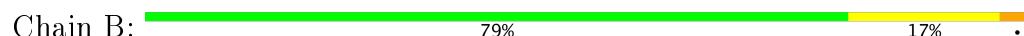
Colouring as in section 4.1 above.

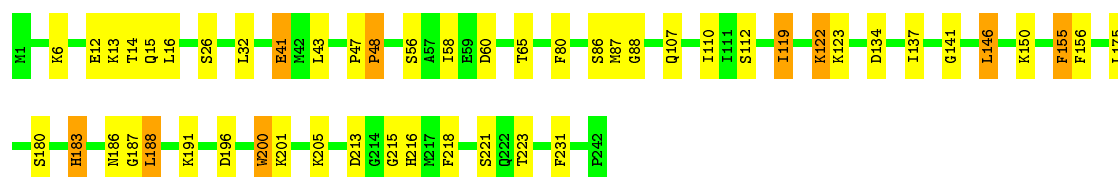
#### 4.2.1 Score per residue for model 1

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)



- Molecule 2: Surfactin synthetase thioesterase subunit



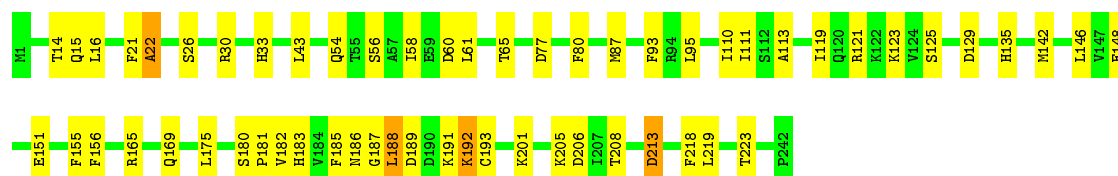


#### 4.2.2 Score per residue for model 2

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

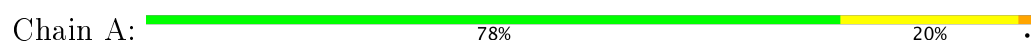


- Molecule 2: Surfactin synthetase thioesterase subunit

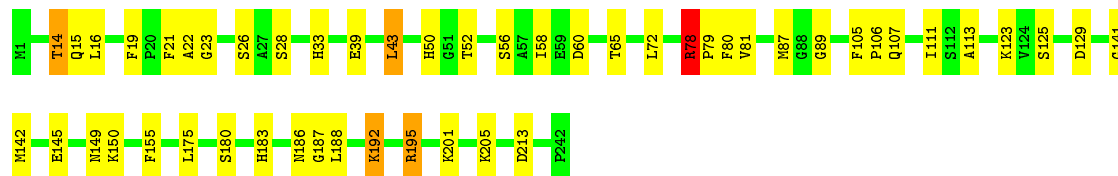
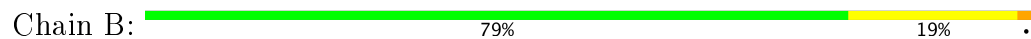


#### 4.2.3 Score per residue for model 3

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)




- Molecule 2: Surfactin synthetase thioesterase subunit




#### 4.2.4 Score per residue for model 4

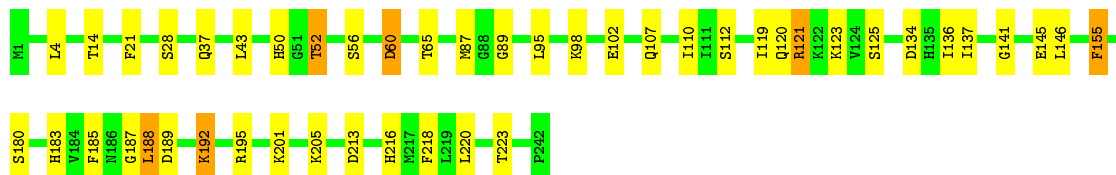
- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

Chain A:  78% 20% .




- Molecule 2: Surfactin synthetase thioesterase subunit

Chain B:  81% 17% .




#### 4.2.5 Score per residue for model 5

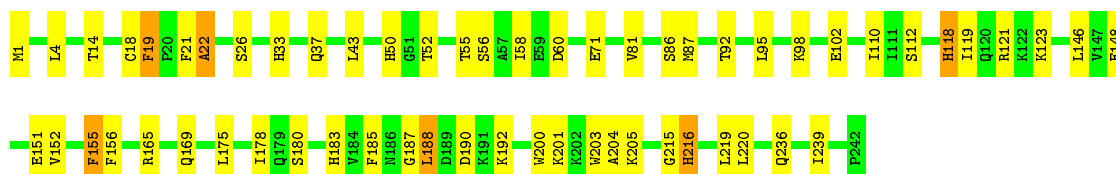
- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

Chain A:  82% 15% .



- Molecule 2: Surfactin synthetase thioesterase subunit

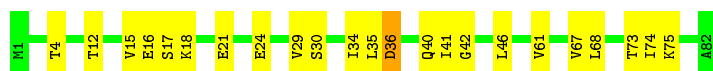
Chain B:  76% 22% .




#### 4.2.6 Score per residue for model 6

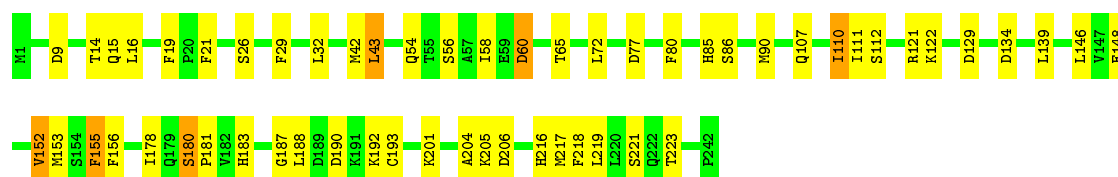
- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

Chain A:  72% 27% .



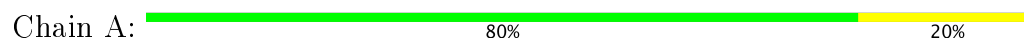
- Molecule 2: Surfactin synthetase thioesterase subunit

Chain B:  77% 21% .

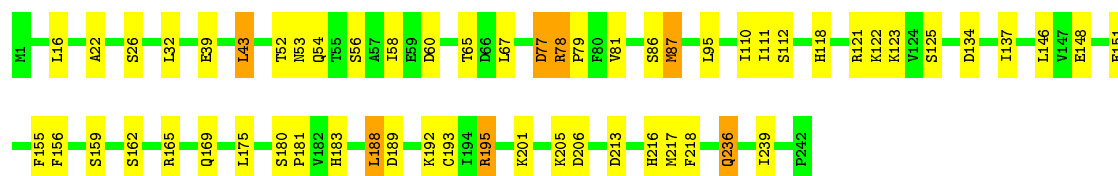
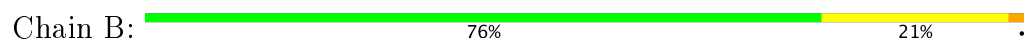


#### 4.2.7 Score per residue for model 7

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

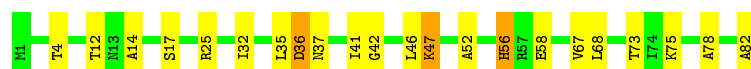


- Molecule 2: Surfactin synthetase thioesterase subunit

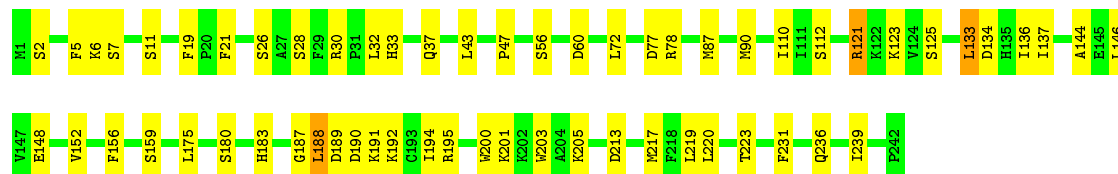
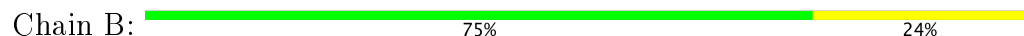


#### 4.2.8 Score per residue for model 8

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)




- Molecule 2: Surfactin synthetase thioesterase subunit



#### 4.2.9 Score per residue for model 9 (medoid)


- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

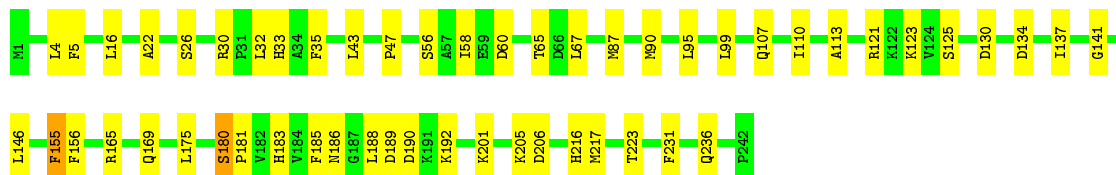


Chain A:  82% 15%




- Molecule 2: Surfactin synthetase thioesterase subunit

Chain B:  78% 21%



#### 4.2.10 Score per residue for model 10

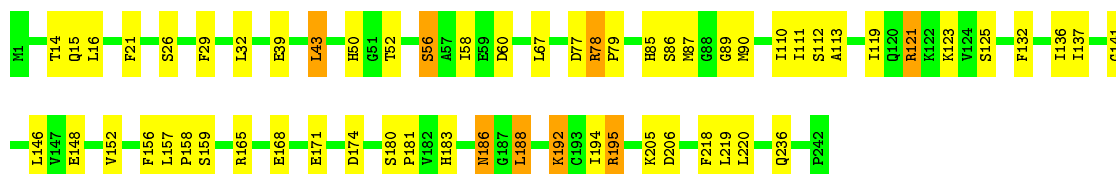
- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

Chain A:  82% 17%




- Molecule 2: Surfactin synthetase thioesterase subunit

Chain B:  75% 21%



#### 4.2.11 Score per residue for model 11

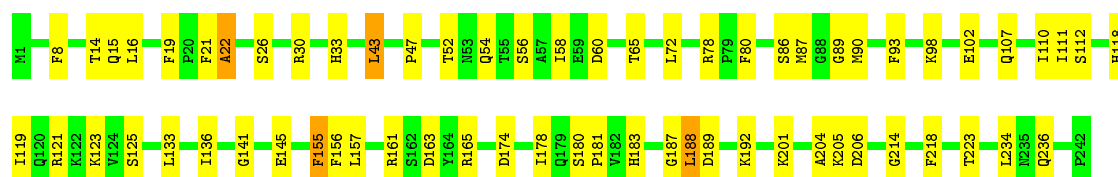
- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

Chain A:  79% 21%



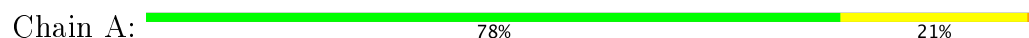
- Molecule 2: Surfactin synthetase thioesterase subunit

Chain B:  73% 25%

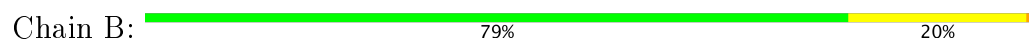


#### 4.2.12 Score per residue for model 12

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

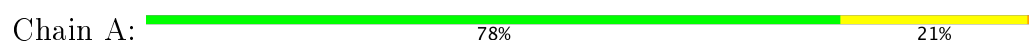


- Molecule 2: Surfactin synthetase thioesterase subunit



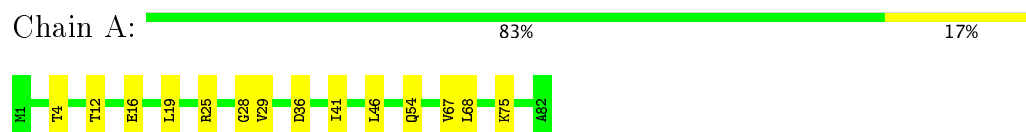
#### 4.2.13 Score per residue for model 13

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

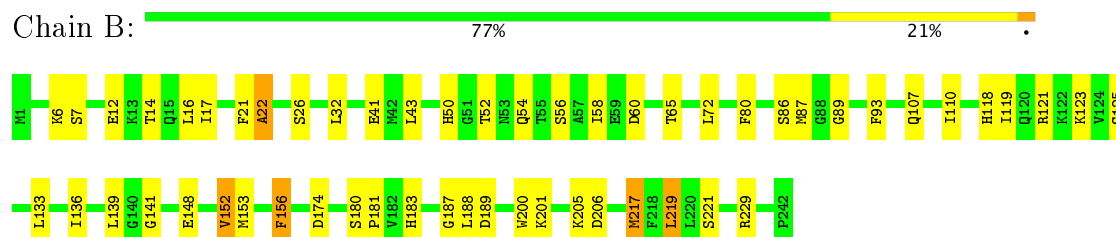


- Molecule 2: Surfactin synthetase thioesterase subunit



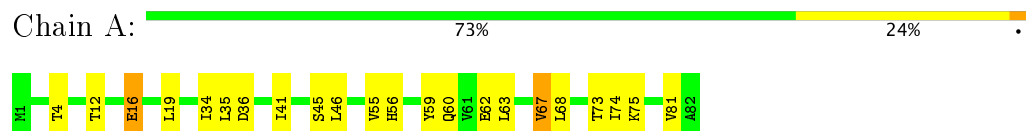


- Molecule 2: Surfactin synthetase thioesterase subunit

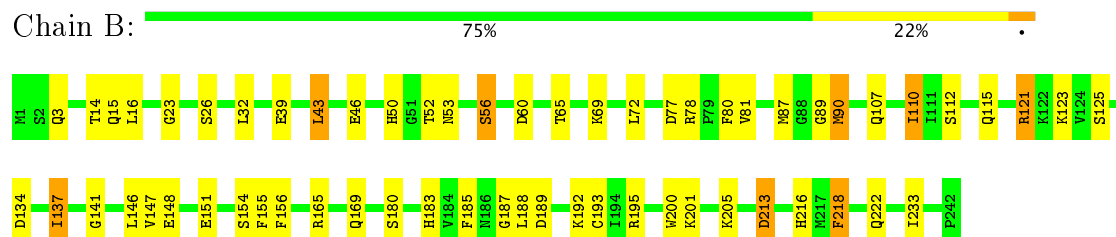


#### 4.2.15 Score per residue for model 15

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

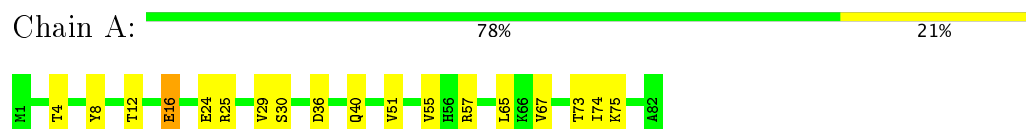


- Molecule 2: Surfactin synthetase thioesterase subunit

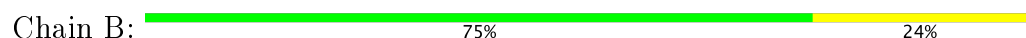


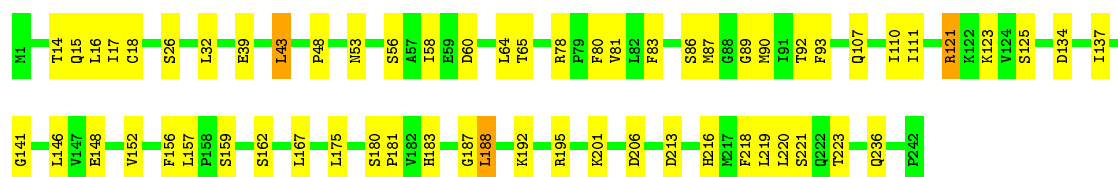
#### 4.2.16 Score per residue for model 16

- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)



- Molecule 2: Surfactin synthetase thioesterase subunit





#### 4.2.17 Score per residue for model 17

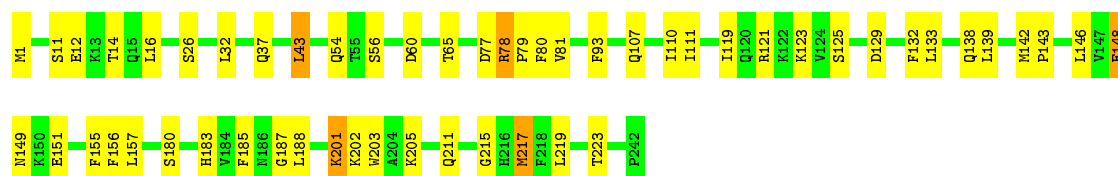
- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

Chain A: 77% 22% .



- Molecule 2: Surfactin synthetase thioesterase subunit

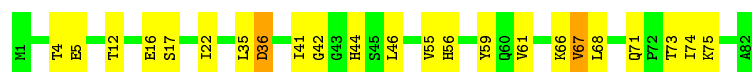
Chain B: 78% 20% .



#### 4.2.18 Score per residue for model 18

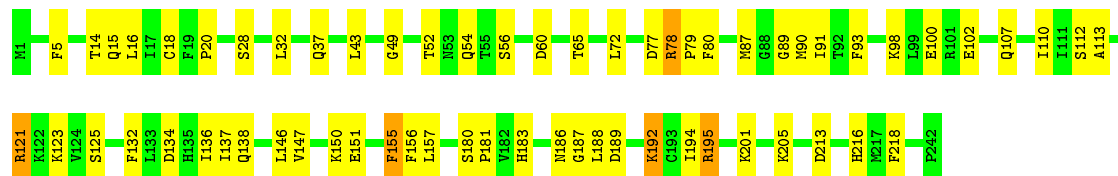
- Molecule 1: Tyrocidine synthetase 3 (Tyrocidine synthetase III)

Chain A: 72% 26% .



- Molecule 2: Surfactin synthetase thioesterase subunit

Chain B: 74% 24% .



## 5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 calculated structures, 18 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
CNS	structure solution	1.2
CNS	refinement	1.2

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 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	628	644	644	10±6
2	B	1949	1904	1904	22±8
All	All	46386	45884	45864	563

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLU:CD	1:A:74:ILE:CD1	1.51	1.79	2	3
2:B:16:LEU:HD22	2:B:80:PHE:CZ	1.40	1.49	6	10
1:A:16:GLU:CD	1:A:74:ILE:HD12	1.40	0.98	2	4
1:A:45:SER:C	1:A:46:LEU:HD12	1.36	1.36	2	2
1:A:16:GLU:OE2	1:A:74:ILE:HB	1.35	1.17	17	1
1:A:16:GLU:OE1	1:A:74:ILE:CD1	1.32	1.77	2	4
1:A:45:SER:O	1:A:46:LEU:HD12	1.31	1.20	15	2
2:B:21:PHE:CE2	2:B:85:HIS:CE1	1.27	2.22	6	1
1:A:16:GLU:CD	1:A:74:ILE:HD13	1.26	1.49	16	4
1:A:16:GLU:OE2	1:A:74:ILE:HD12	1.26	1.12	18	2
1:A:16:GLU:OE2	1:A:74:ILE:CB	1.25	1.83	17	1
1:A:16:GLU:OE2	1:A:34:ILE:CD1	1.25	1.83	4	2
1:A:16:GLU:OE1	1:A:74:ILE:HD13	1.20	1.27	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLU:CD	1:A:74:ILE:HB	1.20	1.57	17	2
2:B:21:PHE:CE2	2:B:85:HIS:NE2	1.17	2.11	6	1
2:B:21:PHE:HE2	2:B:85:HIS:NE2	1.16	1.35	6	1
1:A:16:GLU:OE2	1:A:74:ILE:CD1	1.13	1.97	18	4
1:A:45:SER:O	1:A:46:LEU:CD1	1.12	1.97	2	2
1:A:16:GLU:CG	1:A:74:ILE:HB	1.08	1.77	2	3
2:B:16:LEU:CD2	2:B:80:PHE:HZ	1.08	1.61	13	4
1:A:16:GLU:OE2	1:A:74:ILE:HD13	1.07	1.47	17	2
2:B:14:THR:HG22	2:B:16:LEU:CD1	1.07	1.77	16	9
1:A:16:GLU:CG	1:A:74:ILE:HD13	1.06	1.80	10	4
2:B:14:THR:HG22	2:B:16:LEU:HD11	1.06	1.23	16	10
2:B:14:THR:CG2	2:B:16:LEU:HD11	1.06	1.81	16	8
1:A:16:GLU:OE2	1:A:74:ILE:CG1	1.04	2.06	17	2
1:A:16:GLU:HG2	1:A:74:ILE:HB	1.03	1.27	16	6
1:A:45:SER:C	1:A:46:LEU:CD1	1.02	2.26	2	2
1:A:16:GLU:HG2	1:A:74:ILE:CB	1.02	1.83	2	3
1:A:16:GLU:OE2	1:A:34:ILE:HD12	1.02	1.44	4	2
2:B:16:LEU:CD2	2:B:80:PHE:CZ	1.02	2.42	6	5
2:B:16:LEU:HD13	2:B:80:PHE:CE1	1.01	1.90	6	5
2:B:16:LEU:HD22	2:B:80:PHE:CE1	0.99	1.93	3	9
2:B:16:LEU:HG	2:B:43:LEU:HD21	0.98	1.31	3	8
1:A:16:GLU:OE2	1:A:34:ILE:HD11	0.98	1.58	4	4
2:B:21:PHE:CD2	2:B:22:ALA:N	0.94	2.35	13	7
1:A:16:GLU:OE1	1:A:74:ILE:HD11	0.94	1.63	6	1
2:B:16:LEU:CD1	2:B:80:PHE:CE1	0.93	2.51	6	4
2:B:16:LEU:HD22	2:B:80:PHE:HZ	0.92	1.24	11	7
2:B:16:LEU:CG	2:B:43:LEU:HD21	0.92	1.93	3	6
1:A:16:GLU:CG	1:A:74:ILE:HD12	0.90	1.97	2	2
2:B:16:LEU:HG	2:B:43:LEU:CD2	0.88	1.98	18	6
1:A:16:GLU:OE1	1:A:74:ILE:CG2	0.85	2.23	3	1
2:B:21:PHE:HE2	2:B:85:HIS:HE2	0.84	0.96	6	1
2:B:16:LEU:CD1	2:B:43:LEU:HD21	0.84	2.03	15	8
2:B:16:LEU:CD2	2:B:80:PHE:CE1	0.83	2.60	6	6
1:A:16:GLU:OE1	1:A:19:LEU:CB	0.83	2.27	15	3
1:A:16:GLU:CG	1:A:74:ILE:CD1	0.81	2.57	16	5
1:A:16:GLU:OE1	1:A:19:LEU:HD22	0.81	1.74	4	2
2:B:16:LEU:HG	2:B:43:LEU:HD23	0.81	1.53	13	4
1:A:46:LEU:HD13	1:A:46:LEU:C	0.80	1.96	11	2
2:B:16:LEU:CD1	2:B:43:LEU:HD23	0.78	2.08	14	4
2:B:16:LEU:CD1	2:B:80:PHE:HE1	0.78	1.87	6	2
2:B:21:PHE:CE2	2:B:85:HIS:HE1	0.77	1.90	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:21:PHE:CG	2:B:22:ALA:N	0.77	2.50	5	7
1:A:16:GLU:OE1	1:A:19:LEU:HB3	0.76	1.79	15	2
1:A:16:GLU:OE1	1:A:74:ILE:HD12	0.76	1.79	1	2
1:A:16:GLU:OE1	1:A:74:ILE:HG21	0.73	1.83	3	1
1:A:16:GLU:HG3	1:A:74:ILE:CD1	0.73	2.14	16	3
1:A:16:GLU:OE1	1:A:19:LEU:HD12	0.73	1.83	14	1
1:A:16:GLU:OE1	1:A:19:LEU:HB2	0.72	1.83	10	2
2:B:21:PHE:CD2	2:B:85:HIS:CE1	0.69	2.80	6	1
2:B:21:PHE:HE2	2:B:85:HIS:CE1	0.69	1.74	6	1
1:A:16:GLU:CD	1:A:74:ILE:CB	0.68	2.47	17	1
1:A:16:GLU:HG3	1:A:74:ILE:HD13	0.68	1.66	10	2
2:B:16:LEU:CG	2:B:43:LEU:HD23	0.68	2.18	14	4
2:B:16:LEU:N	2:B:16:LEU:HD12	0.67	2.05	6	6
1:A:63:LEU:HD12	1:A:63:LEU:N	0.67	2.05	15	1
2:B:16:LEU:HD12	2:B:16:LEU:N	0.67	2.05	10	7
2:B:16:LEU:HG	2:B:43:LEU:HD11	0.67	1.67	2	2
1:A:46:LEU:HD12	1:A:46:LEU:N	0.67	2.05	18	1
2:B:16:LEU:HD22	2:B:80:PHE:HE1	0.66	1.50	14	2
1:A:46:LEU:N	1:A:46:LEU:HD12	0.66	2.05	3	2
2:B:4:LEU:HD21	2:B:60:ASP:HB3	0.66	1.68	4	1
2:B:6:LYS:HB3	2:B:43:LEU:HD13	0.66	1.68	8	4
1:A:46:LEU:CD1	1:A:46:LEU:C	0.66	2.64	11	2
2:B:21:PHE:CD2	2:B:85:HIS:NE2	0.65	2.64	6	1
1:A:63:LEU:N	1:A:63:LEU:HD12	0.65	2.05	2	1
1:A:55:VAL:HG13	2:B:218:PHE:CD1	0.65	2.27	1	1
2:B:16:LEU:HD22	2:B:80:PHE:CE2	0.64	2.25	11	1
1:A:16:GLU:OE1	1:A:74:ILE:CG1	0.64	2.45	6	1
2:B:15:GLN:C	2:B:16:LEU:HD12	0.63	2.14	18	10
2:B:16:LEU:CD2	2:B:80:PHE:HE1	0.62	2.05	3	3
1:A:14:ALA:HB2	2:B:47:PRO:HB3	0.62	1.69	1	3
2:B:16:LEU:CD2	2:B:80:PHE:CE2	0.61	2.83	11	1
2:B:21:PHE:CD2	2:B:22:ALA:O	0.60	2.54	3	1
1:A:16:GLU:CG	1:A:74:ILE:CB	0.60	2.61	2	2
2:B:187:GLY:O	2:B:188:LEU:HG	0.60	1.97	11	6
1:A:16:GLU:O	1:A:16:GLU:OE1	0.60	2.20	13	4
2:B:14:THR:CG2	2:B:16:LEU:CD1	0.59	2.59	16	1
1:A:14:ALA:CB	2:B:47:PRO:HB3	0.59	2.27	1	1
2:B:21:PHE:CE2	2:B:22:ALA:HB3	0.59	2.33	5	5
1:A:78:ALA:HA	1:A:82:ALA:HB3	0.59	1.74	8	2
2:B:16:LEU:CD1	2:B:43:LEU:CD2	0.59	2.79	3	3
1:A:15:VAL:HG21	2:B:21:PHE:HZ	0.59	1.58	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:GLU:OE1	1:A:16:GLU:O	0.58	2.21	15	2
2:B:16:LEU:CD1	2:B:16:LEU:N	0.58	2.67	15	8
2:B:16:LEU:N	2:B:16:LEU:CD1	0.58	2.67	12	5
1:A:46:LEU:N	1:A:46:LEU:CD1	0.58	2.67	3	2
2:B:110:ILE:O	2:B:183:HIS:HA	0.57	1.98	15	17
1:A:63:LEU:N	1:A:63:LEU:CD1	0.57	2.67	15	2
1:A:46:LEU:CD1	1:A:46:LEU:N	0.57	2.67	18	2
2:B:16:LEU:CG	2:B:43:LEU:CD2	0.56	2.82	14	3
2:B:133:LEU:HA	2:B:136:ILE:HG22	0.56	1.76	8	4
1:A:55:VAL:HA	2:B:218:PHE:CE1	0.56	2.35	7	2
2:B:217:MET:SD	2:B:219:LEU:HB2	0.56	2.41	14	1
1:A:24:GLU:OE1	1:A:24:GLU:HA	0.56	2.01	3	1
1:A:46:LEU:CD1	1:A:46:LEU:O	0.55	2.54	11	1
2:B:17:ILE:HG22	2:B:83:PHE:HB2	0.55	1.79	16	1
2:B:16:LEU:HD12	2:B:43:LEU:HD21	0.55	1.78	2	2
1:A:24:GLU:OE1	1:A:32:ILE:HG12	0.55	2.02	11	2
2:B:16:LEU:HG	2:B:43:LEU:CD1	0.54	2.32	2	1
1:A:55:VAL:HA	2:B:218:PHE:CE2	0.54	2.38	10	1
1:A:40:GLN:NE2	1:A:72:PRO:HA	0.54	2.17	12	1
1:A:55:VAL:HG22	2:B:218:PHE:CZ	0.54	2.37	7	1
2:B:90:MET:HA	2:B:154:SER:O	0.54	2.03	15	1
1:A:16:GLU:OE1	1:A:74:ILE:HG13	0.53	2.03	6	1
2:B:132:PHE:O	2:B:136:ILE:HB	0.53	2.04	13	3
1:A:17:SER:O	1:A:21:GLU:HG2	0.53	2.02	6	1
2:B:16:LEU:HD11	2:B:43:LEU:HD23	0.53	1.80	14	1
2:B:3:GLN:HB2	2:B:46:GLU:HB2	0.53	1.81	15	1
2:B:217:MET:SD	2:B:219:LEU:HG	0.53	2.43	17	1
2:B:121:ARG:HA	2:B:134:ASP:OD2	0.53	2.03	8	5
2:B:137:ILE:HD11	2:B:144:ALA:HB3	0.53	1.80	8	1
2:B:60:ASP:O	2:B:64:LEU:HG	0.53	2.04	16	2
2:B:119:ILE:HD12	2:B:134:ASP:HA	0.52	1.81	4	1
1:A:16:GLU:HG2	1:A:74:ILE:HD13	0.52	1.77	10	1
2:B:5:PHE:O	2:B:43:LEU:HA	0.52	2.04	9	3
1:A:51:VAL:O	1:A:55:VAL:HG23	0.52	2.04	16	1
1:A:20:ALA:O	1:A:24:GLU:HB3	0.52	2.05	4	1
2:B:21:PHE:CE2	2:B:22:ALA:O	0.51	2.63	3	1
1:A:16:GLU:OE1	1:A:19:LEU:HD11	0.51	2.06	1	1
2:B:122:LYS:HG3	2:B:134:ASP:OD1	0.51	2.05	1	2
2:B:192:LYS:O	2:B:195:ARG:HG3	0.50	2.04	10	4
2:B:16:LEU:HD11	2:B:80:PHE:HE1	0.50	1.65	6	1
2:B:190:ASP:HA	2:B:216:HIS:CB	0.50	2.37	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:107:GLN:HA	2:B:107:GLN:OE1	0.50	2.07	11	1
2:B:165:ARG:O	2:B:169:GLN:HG2	0.50	2.07	7	5
1:A:17:SER:OG	2:B:48:PRO:HD2	0.49	2.07	1	1
2:B:187:GLY:C	2:B:188:LEU:HG	0.49	2.28	1	9
2:B:176:ALA:HA	2:B:202:LYS:O	0.49	2.08	12	1
1:A:25:ARG:NH2	2:B:1:MET:SD	0.49	2.86	17	1
2:B:196:ASP:O	2:B:200:TRP:HB2	0.49	2.08	1	1
1:A:16:GLU:O	1:A:16:GLU:CD	0.49	2.51	10	1
2:B:90:MET:O	2:B:94:ARG:HB2	0.49	2.07	13	1
2:B:178:ILE:O	2:B:204:ALA:HB1	0.49	2.08	5	3
2:B:98:LYS:O	2:B:102:GLU:HG2	0.49	2.08	4	4
1:A:52:ALA:O	1:A:56:HIS:HB2	0.48	2.08	1	5
2:B:16:LEU:HD11	2:B:43:LEU:HD21	0.48	1.84	2	2
2:B:16:LEU:HD21	2:B:60:ASP:OD2	0.48	2.08	6	1
1:A:18:LYS:O	1:A:21:GLU:HG2	0.48	2.08	17	1
2:B:187:GLY:O	2:B:213:ASP:HA	0.48	2.08	3	3
2:B:147:VAL:O	2:B:151:GLU:HB2	0.48	2.09	18	1
2:B:181:PRO:HD2	2:B:206:ASP:OD1	0.48	2.09	10	6
2:B:85:HIS:HB3	2:B:87:MET:SD	0.48	2.49	10	1
1:A:55:VAL:HG11	2:B:216:HIS:O	0.47	2.10	9	1
1:A:18:LYS:HD2	2:B:18:CYS:SG	0.47	2.50	5	1
2:B:188:LEU:HD13	2:B:195:ARG:HG2	0.47	1.86	7	1
2:B:181:PRO:HD2	2:B:206:ASP:OD2	0.47	2.08	16	4
1:A:14:ALA:HA	2:B:47:PRO:HB3	0.47	1.86	11	2
1:A:32:ILE:HB	1:A:37:ASN:OD1	0.47	2.10	2	1
2:B:182:VAL:HG13	2:B:208:THR:HB	0.47	1.85	2	2
2:B:30:ARG:HA	2:B:33:HIS:CD2	0.46	2.46	2	4
2:B:18:CYS:SG	2:B:92:THR:HG21	0.46	2.50	16	1
1:A:22:ILE:HG23	2:B:91:ILE:HD13	0.46	1.86	18	1
1:A:55:VAL:HG11	2:B:218:PHE:HA	0.46	1.87	15	1
2:B:113:ALA:HA	2:B:186:ASN:O	0.46	2.09	3	5
2:B:146:LEU:O	2:B:150:LYS:HE2	0.46	2.11	1	1
1:A:60:GLN:OE1	1:A:67:VAL:HG11	0.46	2.10	9	3
2:B:16:LEU:CG	2:B:43:LEU:HD11	0.46	2.39	2	1
2:B:152:VAL:HG23	2:B:157:LEU:HD22	0.46	1.87	16	2
1:A:62:GLU:C	1:A:63:LEU:HD12	0.45	2.30	15	2
1:A:16:GLU:CD	1:A:16:GLU:O	0.45	2.54	15	3
2:B:16:LEU:HD13	2:B:80:PHE:CZ	0.45	2.46	13	1
2:B:201:LYS:HG3	2:B:202:LYS:N	0.45	2.26	17	1
1:A:46:LEU:HD13	1:A:47:LYS:N	0.45	2.25	8	1
2:B:190:ASP:OD1	2:B:217:MET:HA	0.44	2.12	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:118:HIS:CD2	2:B:151:GLU:HB3	0.44	2.48	7	1
1:A:34:ILE:HG23	1:A:40:GLN:HE22	0.44	1.72	6	1
2:B:122:LYS:HG2	2:B:134:ASP:OD1	0.44	2.12	7	1
1:A:46:LEU:HD13	1:A:46:LEU:O	0.44	2.12	11	1
1:A:16:GLU:OE1	1:A:19:LEU:CD1	0.44	2.65	1	1
2:B:152:VAL:HG13	2:B:153:MET:H	0.44	1.73	6	2
2:B:90:MET:HG2	2:B:91:ILE:HD12	0.44	1.89	13	1
2:B:13:LYS:O	2:B:41:GLU:HB3	0.44	2.12	12	2
2:B:161:ARG:O	2:B:165:ARG:HB2	0.44	2.13	11	1
2:B:180:SER:HB2	2:B:181:PRO:HD3	0.43	1.90	9	3
2:B:21:PHE:CE2	2:B:22:ALA:CB	0.43	3.01	13	1
2:B:78:ARG:N	2:B:79:PRO:HD2	0.43	2.28	17	2
2:B:191:LYS:O	2:B:194:ILE:HG22	0.43	2.13	8	1
1:A:55:VAL:HG13	2:B:218:PHE:CZ	0.43	2.49	11	1
1:A:24:GLU:O	1:A:25:ARG:HD2	0.43	2.13	3	1
2:B:78:ARG:H	2:B:79:PRO:HD2	0.43	1.73	10	3
1:A:60:GLN:CD	1:A:64:PRO:HA	0.43	2.34	2	1
2:B:188:LEU:HD12	2:B:192:LYS:HA	0.43	1.88	2	1
2:B:179:GLN:CB	2:B:206:ASP:HA	0.43	2.43	12	1
2:B:165:ARG:HA	2:B:171:GLU:OE1	0.43	2.14	10	1
2:B:183:HIS:NE2	2:B:206:ASP:OD1	0.43	2.51	9	3
1:A:35:LEU:O	1:A:36:ASP:HB3	0.42	2.14	18	3
2:B:236:GLN:HA	2:B:239:ILE:O	0.42	2.14	7	3
2:B:158:PRO:HB3	2:B:188:LEU:CD2	0.42	2.44	10	1
1:A:16:GLU:HG2	1:A:74:ILE:HD12	0.42	1.91	13	1
2:B:65:THR:O	2:B:69:LYS:HB2	0.42	2.14	15	1
2:B:147:VAL:O	2:B:151:GLU:HG3	0.42	2.15	15	1
2:B:157:LEU:HD23	2:B:157:LEU:H	0.42	1.73	11	1
1:A:55:VAL:CG1	2:B:216:HIS:O	0.42	2.68	1	1
1:A:55:VAL:O	2:B:221:SER:CB	0.42	2.68	1	1
1:A:6:ALA:HB1	1:A:35:LEU:HD12	0.42	1.91	7	1
2:B:183:HIS:NE2	2:B:206:ASP:OD2	0.41	2.53	2	4
2:B:148:GLU:HA	2:B:151:GLU:OE2	0.41	2.15	17	1
2:B:157:LEU:HD21	2:B:163:ASP:HB2	0.41	1.91	11	1
1:A:55:VAL:HG22	2:B:218:PHE:CE2	0.41	2.51	7	1
2:B:93:PHE:CE1	2:B:156:PHE:HB2	0.41	2.51	14	1
1:A:67:VAL:HG13	1:A:68:LEU:H	0.41	1.75	18	1
1:A:37:ASN:ND2	1:A:40:GLN:H	0.41	2.14	2	1
2:B:100:GLU:HB3	2:B:107:GLN:NE2	0.41	2.31	18	1
2:B:54:GLN:OE1	2:B:54:GLN:HA	0.41	2.15	18	1
1:A:51:VAL:HG22	2:B:143:PRO:HD2	0.41	1.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:18:CYS:O	2:B:19:PHE:HB2	0.41	2.16	5	1
2:B:118:HIS:NE2	2:B:151:GLU:HB3	0.41	2.31	5	1
2:B:138:GLN:O	2:B:139:LEU:HB2	0.41	2.16	17	1
2:B:1:MET:HG2	2:B:55:THR:OG1	0.41	2.16	5	1
2:B:130:ASP:O	2:B:134:ASP:HB2	0.41	2.15	9	1
2:B:95:LEU:O	2:B:99:LEU:HG	0.41	2.16	9	1
2:B:157:LEU:H	2:B:157:LEU:HD23	0.41	1.74	17	1
1:A:16:GLU:CG	1:A:74:ILE:CG1	0.40	3.00	2	1
2:B:78:ARG:CB	2:B:79:PRO:HD3	0.40	2.47	3	1
1:A:16:GLU:HG3	1:A:74:ILE:HD12	0.40	1.90	16	1
2:B:148:GLU:HA	2:B:151:GLU:OE1	0.40	2.16	2	1
2:B:77:ASP:OD1	2:B:79:PRO:HD2	0.40	2.15	7	1
2:B:105:PHE:HB3	2:B:106:PRO:HD3	0.40	1.92	3	1
1:A:14:ALA:CA	2:B:47:PRO:HB3	0.40	2.47	1	1
1:A:16:GLU:OE1	1:A:19:LEU:CD2	0.40	2.59	4	1
2:B:136:ILE:O	2:B:138:GLN:HG2	0.40	2.17	18	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	80/82 (98%)	55±2 (69±3%)	19±3 (24±3%)	6±1 (7±2%)	3	17
2	B	240/242 (99%)	193±5 (81±2%)	39±5 (16±2%)	8±2 (3±1%)	8	39
All	All	5760/5832 (99%)	4471 (78%)	1044 (18%)	245 (4%)	6	30

All 48 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	36	ASP	18
1	A	67	VAL	18
2	B	180	SER	18
2	B	87	MET	15
2	B	121	ARG	15

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Mol	Chain	Res	Type	Models (Total)
1	A	68	LEU	12
2	B	58	ILE	12
1	A	41	ILE	11
2	B	141	GLY	10
2	B	89	GLY	9
2	B	137	ILE	9
1	A	59	TYR	9
2	B	22	ALA	8
2	B	155	PHE	8
1	A	66	LYS	7
1	A	42	GLY	6
1	A	29	VAL	5
2	B	19	PHE	5
2	B	53	ASN	4
2	B	215	GLY	3
2	B	78	ARG	3
2	B	12	GLU	3
2	B	152	VAL	3
2	B	56	SER	3
2	B	52	THR	2
1	A	44	HIS	2
2	B	23	GLY	2
2	B	48	PRO	2
2	B	11	SER	2
1	A	61	VAL	2
1	A	34	ILE	2
2	B	181	PRO	1
1	A	70	ALA	1
2	B	149	ASN	1
2	B	20	PRO	1
2	B	139	LEU	1
2	B	88	GLY	1
1	A	45	SER	1
1	A	5	GLU	1
1	A	65	LEU	1
1	A	81	VAL	1
2	B	119	ILE	1
2	B	49	GLY	1
2	B	214	GLY	1
1	A	28	GLY	1
1	A	47	LYS	1
1	A	11	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	32	ILE	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	64/64 (100%)	56±2 (88±3%)	8±2 (12±3%)	10	52
2	B	210/210 (100%)	177±3 (84±2%)	33±3 (16±2%)	6	44
All	All	4932/4932 (100%)	4202 (85%)	730 (15%)	7	46

All 134 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	75	LYS	18
2	B	123	LYS	17
2	B	60	ASP	17
1	A	12	THR	17
1	A	4	THR	17
2	B	205	LYS	17
2	B	201	LYS	17
2	B	26	SER	16
2	B	156	PHE	16
2	B	56	SER	15
1	A	73	THR	15
2	B	125	SER	14
2	B	192	LYS	14
2	B	188	LEU	14
2	B	155	PHE	14
2	B	146	LEU	14
2	B	32	LEU	13
2	B	65	THR	13
2	B	112	SER	12
2	B	148	GLU	11
2	B	107	GLN	11
1	A	56	HIS	11
2	B	43	LEU	11

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Mol	Chain	Res	Type	Models (Total)
2	B	52	THR	10
2	B	90	MET	10
2	B	223	THR	10
2	B	119	ILE	9
2	B	72	LEU	9
2	B	77	ASP	9
2	B	213	ASP	9
2	B	111	ILE	9
2	B	175	LEU	9
2	B	86	SER	9
2	B	189	ASP	9
2	B	78	ARG	8
2	B	216	HIS	8
2	B	219	LEU	8
2	B	195	ARG	8
2	B	81	VAL	8
2	B	54	GLN	7
1	A	25	ARG	7
2	B	185	PHE	7
2	B	50	HIS	7
2	B	236	GLN	7
2	B	14	THR	6
2	B	93	PHE	6
2	B	200	TRP	6
1	A	16	GLU	6
2	B	159	SER	6
2	B	218	PHE	6
1	A	35	LEU	6
2	B	39	GLU	5
2	B	193	CYS	5
2	B	217	MET	5
2	B	28	SER	5
2	B	220	LEU	5
1	A	17	SER	5
2	B	37	GLN	5
1	A	18	LYS	5
2	B	118	HIS	4
2	B	129	ASP	4
2	B	221	SER	4
1	A	46	LEU	4
2	B	174	ASP	4
2	B	95	LEU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	54	GLN	4
1	A	30	SER	4
1	A	24	GLU	3
2	B	7	SER	3
1	A	37	ASN	3
2	B	142	MET	3
2	B	21	PHE	3
1	A	40	GLN	3
2	B	110	ILE	3
2	B	67	LEU	3
2	B	231	PHE	3
2	B	145	GLU	3
2	B	203	TRP	3
1	A	36	ASP	2
2	B	29	PHE	2
2	B	4	LEU	2
2	B	33	HIS	2
2	B	194	ILE	2
2	B	41	GLU	2
2	B	183	HIS	2
2	B	162	SER	2
2	B	191	LYS	2
2	B	229	ARG	2
2	B	133	LEU	2
2	B	150	LYS	2
1	A	47	LYS	2
2	B	186	ASN	2
1	A	8	TYR	2
2	B	190	ASP	2
2	B	211	GLN	1
2	B	87	MET	1
2	B	2	SER	1
2	B	122	LYS	1
1	A	71	GLN	1
2	B	149	ASN	1
2	B	137	ILE	1
2	B	8	PHE	1
2	B	42	MET	1
2	B	17	ILE	1
2	B	121	ARG	1
2	B	157	LEU	1
2	B	139	LEU	1

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Mol	Chain	Res	Type	Models (Total)
2	B	164	TYR	1
2	B	135	HIS	1
2	B	9	ASP	1
1	A	66	LYS	1
1	A	22	ILE	1
2	B	168	GLU	1
2	B	16	LEU	1
1	A	58	GLU	1
1	A	80	TYR	1
2	B	234	LEU	1
1	A	69	PHE	1
2	B	233	ILE	1
2	B	120	GLN	1
2	B	35	PHE	1
2	B	18	CYS	1
1	A	57	ARG	1
2	B	92	THR	1
1	A	60	GLN	1
2	B	132	PHE	1
2	B	115	GLN	1
2	B	136	ILE	1
2	B	61	LEU	1
2	B	167	LEU	1
2	B	152	VAL	1
2	B	71	GLU	1
2	B	222	GLN	1
2	B	224	GLU	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

No chemical shift data were provided