



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:08 am GMT

PDB ID : 2RON  
Title : The external thioesterase of the Surfactin-Synthetase  
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Deposited on : 2008-04-04

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 : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

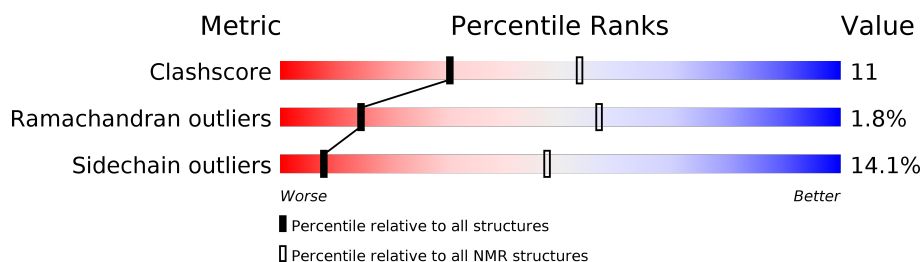
# 1 Overall quality at a glance

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	242	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:2-A:46, A:56-A:238 (228)	0.55	7

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 and 5 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3850 atoms, of which 1902 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Surfactin synthetase thioesterase subunit.

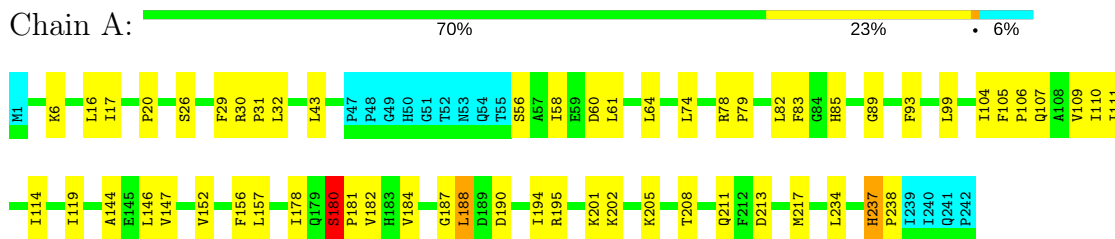
Mol	Chain	Residues	Atoms						Trace
1	A	242	Total	C	H	N	O	S	0
			3850	1253	1902	329	356	10	

## 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: Surfactin synthetase thioesterase subunit

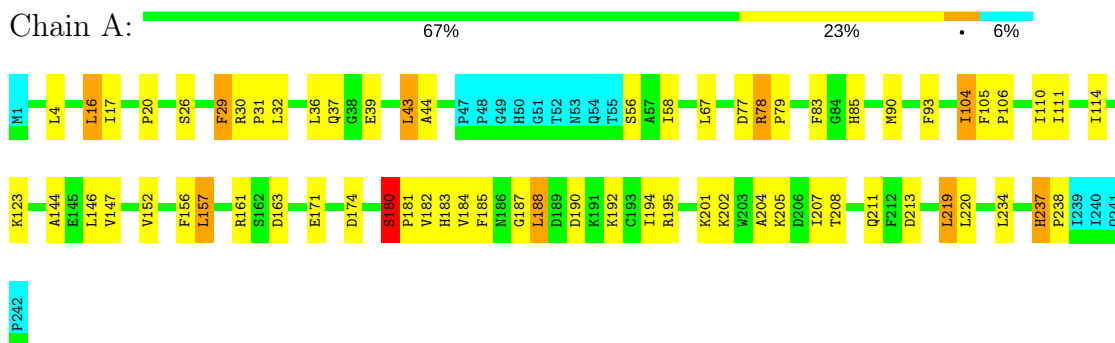


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

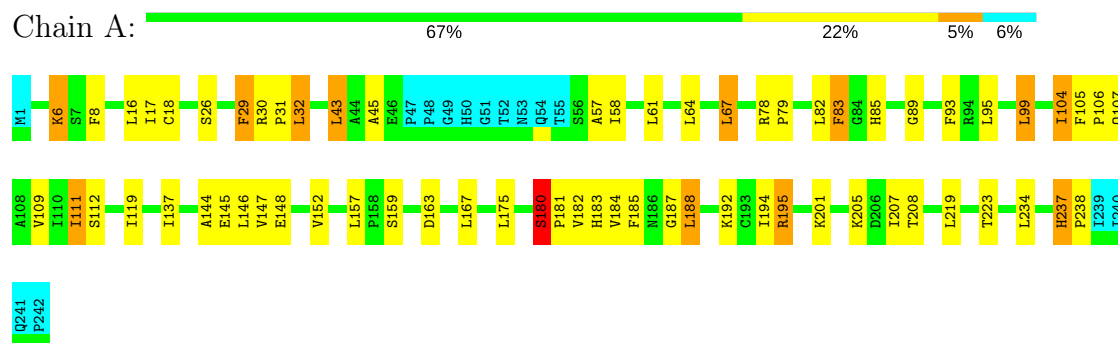
#### 4.2.1 Score per residue for model 1

- Molecule 1: Surfactin synthetase thioesterase subunit



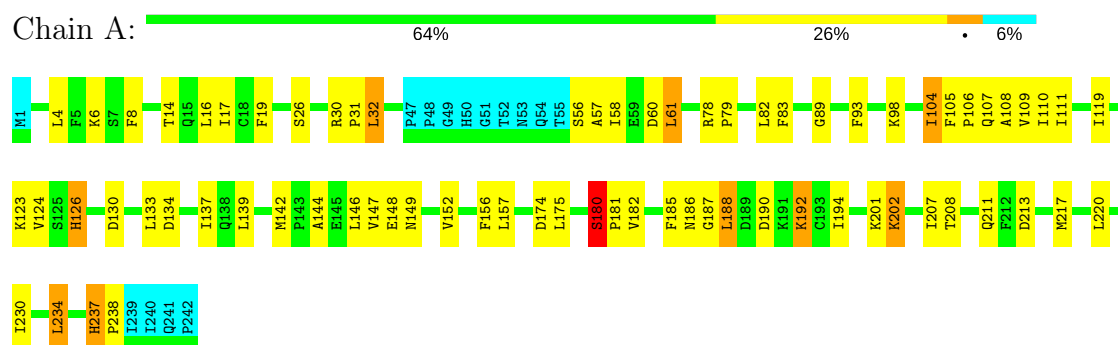
#### 4.2.2 Score per residue for model 2

- Molecule 1: Surfactin synthetase thioesterase subunit



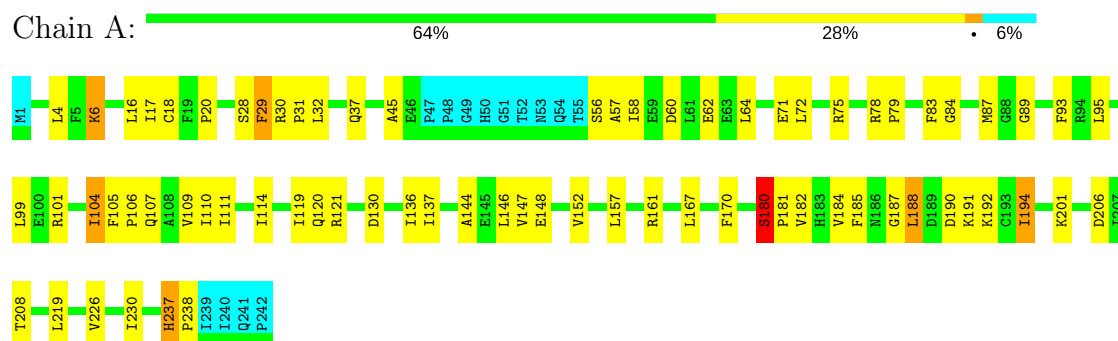
### 4.2.3 Score per residue for model 3

- Molecule 1: Surfactin synthetase thioesterase subunit



### 4.2.4 Score per residue for model 4

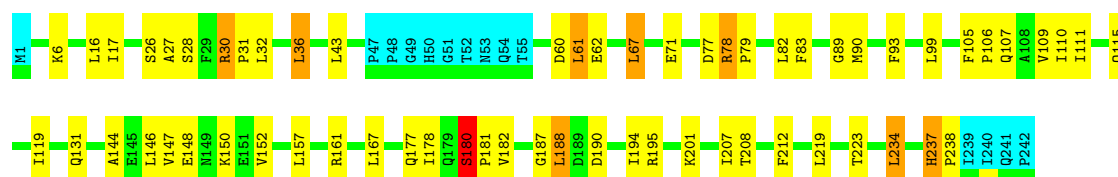
- Molecule 1: Surfactin synthetase thioesterase subunit



### 4.2.5 Score per residue for model 5

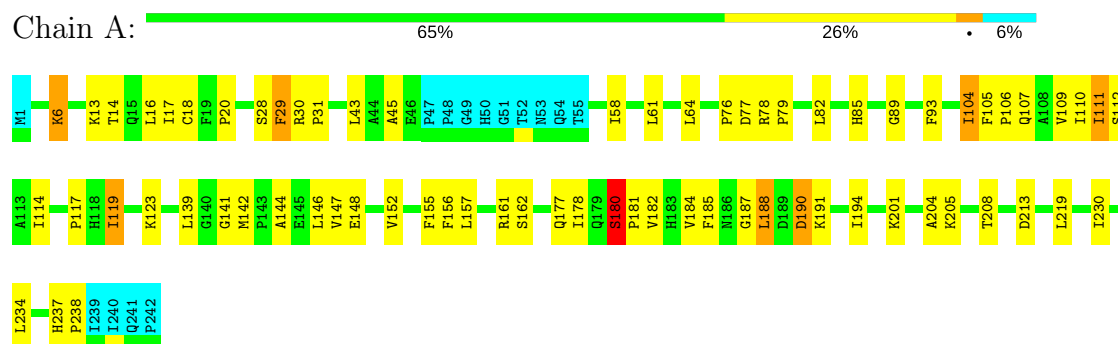
- Molecule 1: Surfactin synthetase thioesterase subunit





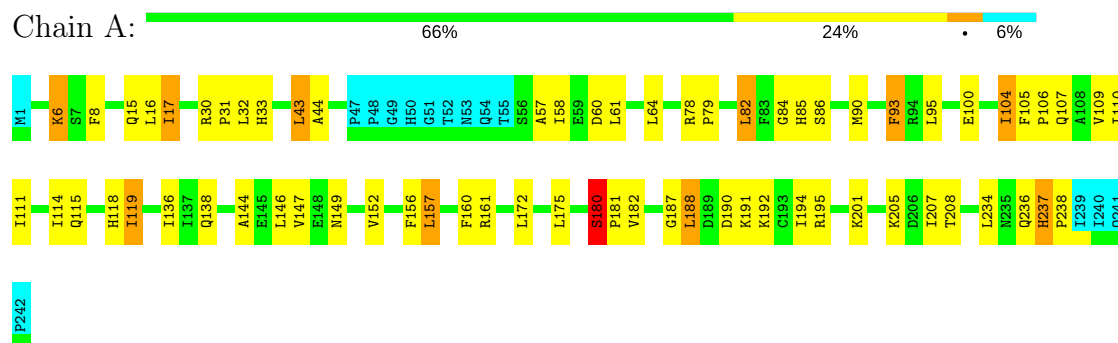
#### 4.2.6 Score per residue for model 6

- Molecule 1: Surfactin synthetase thioesterase subunit



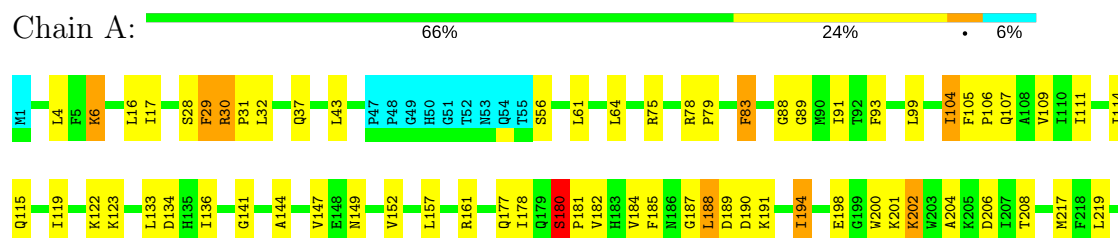
#### 4.2.7 Score per residue for model 7 (medoid)

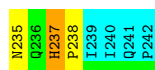
- Molecule 1: Surfactin synthetase thioesterase subunit



#### 4.2.8 Score per residue for model 8

- Molecule 1: Surfactin synthetase thioesterase subunit

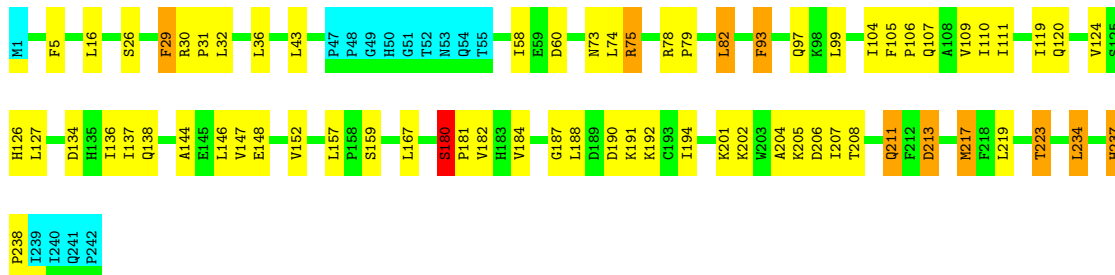




#### 4.2.9 Score per residue for model 9

- Molecule 1: Surfactin synthetase thioesterase subunit

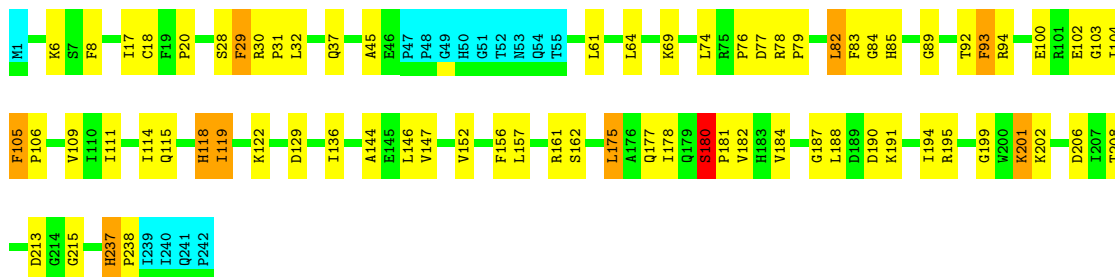
Chain A: 66% 24% 6%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Surfactin synthetase thioesterase subunit

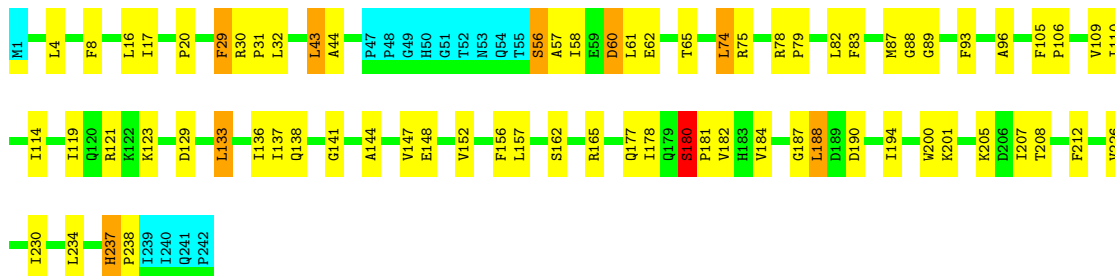
Chain A: 64% 26% 6%



#### 4.2.11 Score per residue for model 11

- Molecule 1: Surfactin synthetase thioesterase subunit

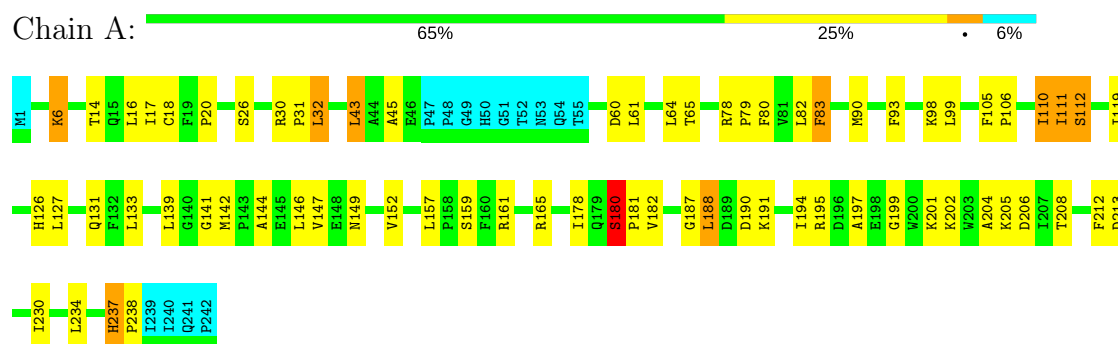
Chain A: 64% 26% 6%





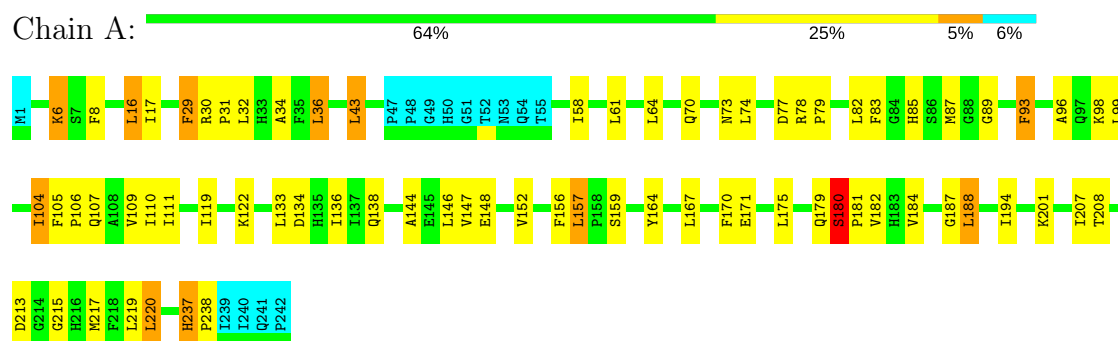
### 4.2.12 Score per residue for model 12

- Molecule 1: Surfactin synthetase thioesterase subunit



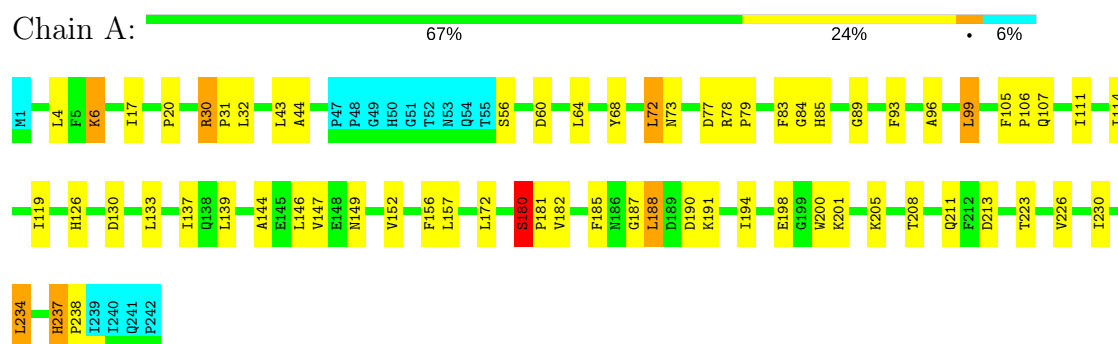
### 4.2.13 Score per residue for model 13

- Molecule 1: Surfactin synthetase thioesterase subunit



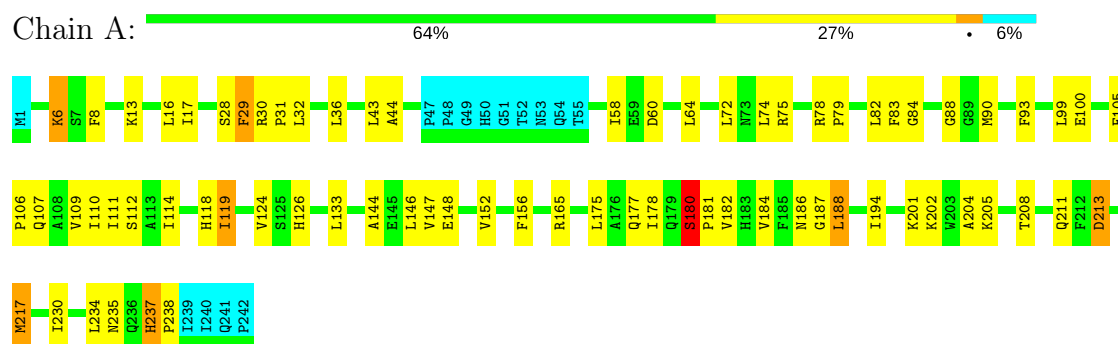
### 4.2.14 Score per residue for model 14

- Molecule 1: Surfactin synthetase thioesterase subunit



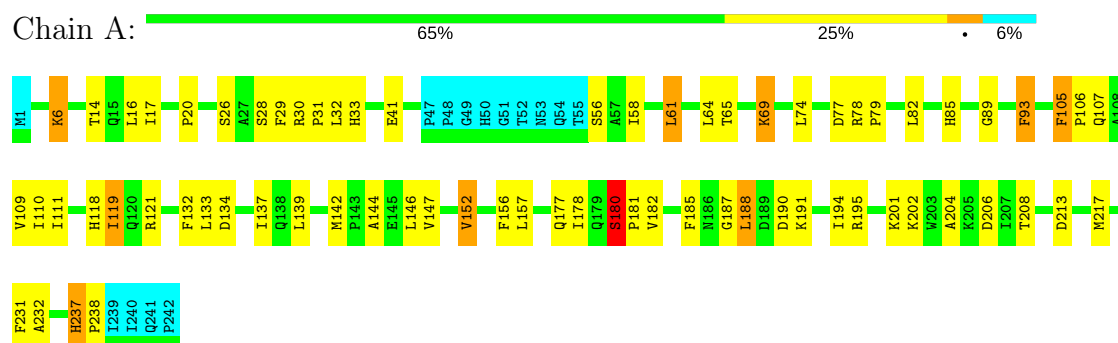
### 4.2.15 Score per residue for model 15

- Molecule 1: Surfactin synthetase thioesterase subunit



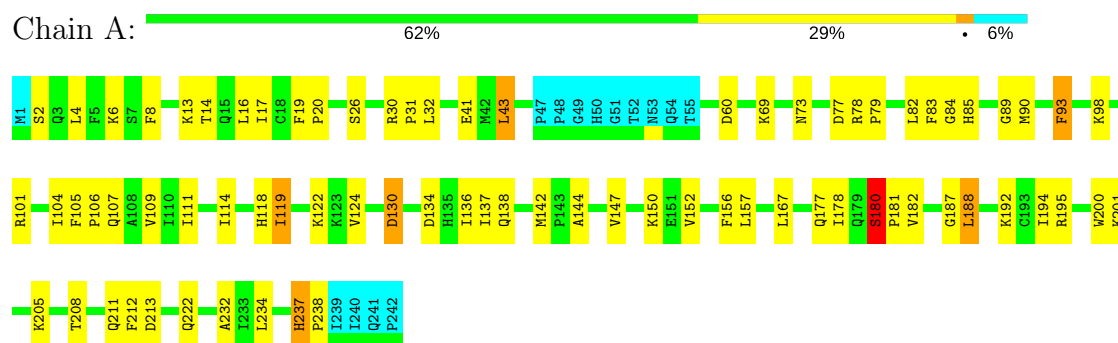
### 4.2.16 Score per residue for model 16

- Molecule 1: Surfactin synthetase thioesterase subunit



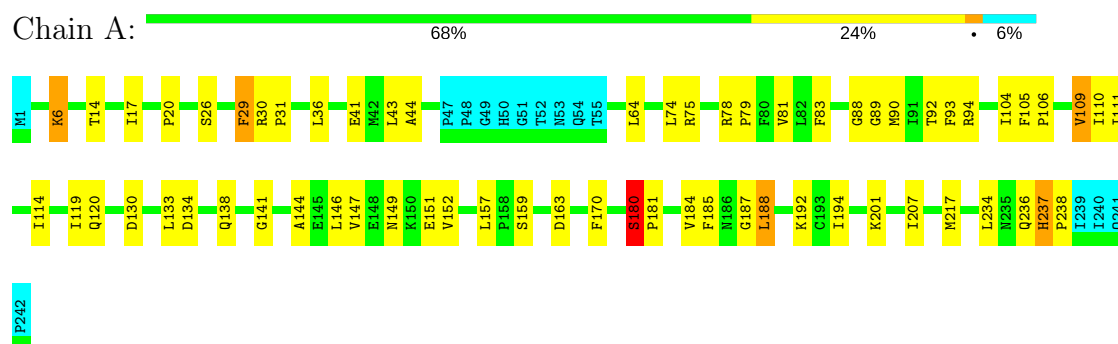
### 4.2.17 Score per residue for model 17

- Molecule 1: Surfactin synthetase thioesterase subunit



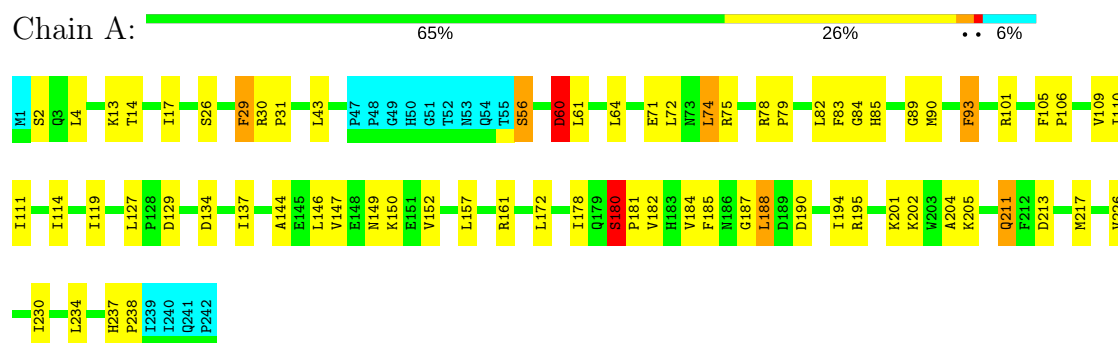
### 4.2.18 Score per residue for model 18

- Molecule 1: Surfactin synthetase thioesterase subunit



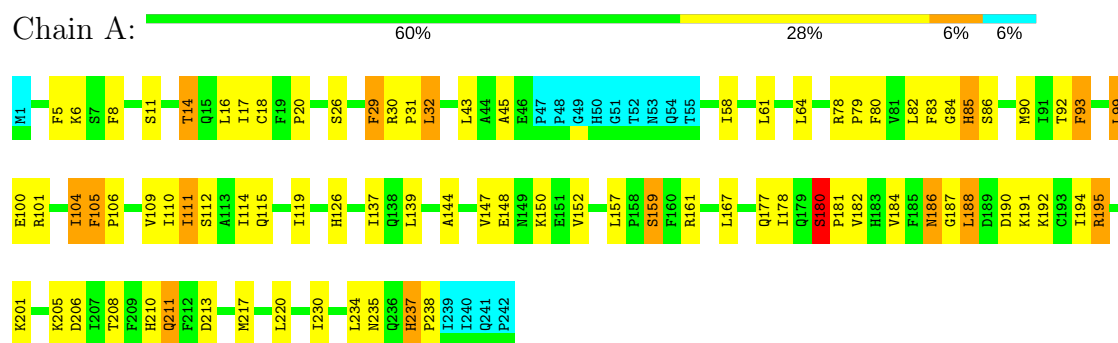
### 4.2.19 Score per residue for model 19

- Molecule 1: Surfactin synthetase thioesterase subunit



### 4.2.20 Score per residue for model 20

- Molecule 1: Surfactin synthetase thioesterase subunit



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics*.

Of the 150 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
CYANA	refinement	2.1

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

### 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	1845	1801	1801	41±5
All	All	36900	36020	36020	822

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:VAL:HG23	1:A:157:LEU:HD22	0.94	1.36	12	5
1:A:16:LEU:HD11	1:A:58:ILE:HD12	0.90	1.39	20	4
1:A:152:VAL:HG22	1:A:157:LEU:HD13	0.82	1.52	13	6
1:A:152:VAL:HG12	1:A:157:LEU:HD22	0.81	1.52	8	1
1:A:144:ALA:HB1	1:A:147:VAL:HG22	0.78	1.53	17	20
1:A:14:THR:HG21	1:A:61:LEU:HD21	0.77	1.56	16	2
1:A:32:LEU:HD12	1:A:208:THR:HG23	0.76	1.57	15	4
1:A:36:LEU:HD11	1:A:182:VAL:HG21	0.73	1.59	13	1
1:A:29:PHE:CE2	1:A:184:VAL:HG21	0.69	2.22	9	12
1:A:16:LEU:HD11	1:A:58:ILE:HG23	0.69	1.64	1	3
1:A:152:VAL:HG13	1:A:157:LEU:HD22	0.67	1.65	20	8
1:A:82:LEU:HD22	1:A:93:PHE:CZ	0.66	2.26	13	5
1:A:217:MET:HB2	1:A:220:LEU:HD23	0.66	1.66	13	1
1:A:133:LEU:HD13	1:A:139:LEU:HD21	0.65	1.67	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HD12	1:A:99:LEU:HD12	0.65	1.69	12	1
1:A:16:LEU:HD12	1:A:43:LEU:HD21	0.65	1.68	17	3
1:A:29:PHE:CZ	1:A:184:VAL:HG21	0.65	2.26	4	7
1:A:69:LYS:HB3	1:A:74:LEU:HD12	0.64	1.68	16	1
1:A:4:LEU:HD22	1:A:56:SER:OG	0.64	1.93	19	2
1:A:107:GLN:HB2	1:A:110:ILE:HD11	0.63	1.68	4	8
1:A:148:GLU:O	1:A:152:VAL:HG23	0.63	1.94	9	9
1:A:107:GLN:CB	1:A:110:ILE:HD11	0.63	2.23	15	4
1:A:57:ALA:O	1:A:95:LEU:HD23	0.63	1.93	2	1
1:A:107:GLN:HB3	1:A:110:ILE:HD11	0.62	1.71	3	2
1:A:144:ALA:HB1	1:A:147:VAL:CG2	0.62	2.24	12	12
1:A:213:ASP:OD1	1:A:230:ILE:HG21	0.62	1.94	14	4
1:A:17:ILE:HG22	1:A:83:PHE:HB2	0.62	1.71	13	16
1:A:82:LEU:HD22	1:A:93:PHE:CE2	0.62	2.29	16	8
1:A:17:ILE:HD12	1:A:20:PRO:HG3	0.62	1.72	10	11
1:A:6:LYS:HB3	1:A:43:LEU:HD13	0.61	1.72	18	3
1:A:58:ILE:HD13	1:A:95:LEU:CB	0.61	2.24	7	2
1:A:111:ILE:HD11	1:A:186:ASN:OD1	0.61	1.95	20	1
1:A:69:LYS:CD	1:A:74:LEU:HD12	0.61	2.25	10	1
1:A:109:VAL:O	1:A:110:ILE:HD13	0.61	1.96	18	2
1:A:119:ILE:HA	1:A:157:LEU:HD12	0.61	1.71	17	5
1:A:4:LEU:HD21	1:A:60:ASP:HB3	0.61	1.72	19	1
1:A:152:VAL:HG12	1:A:157:LEU:HD13	0.60	1.74	3	1
1:A:84:GLY:HA3	1:A:114:ILE:HD11	0.60	1.73	4	8
1:A:202:LYS:HD2	1:A:204:ALA:HB3	0.60	1.72	8	5
1:A:71:GLU:O	1:A:72:LEU:HD22	0.60	1.96	19	1
1:A:78:ARG:HA	1:A:104:ILE:HG21	0.60	1.72	20	8
1:A:14:THR:HG23	1:A:41:GLU:OE2	0.60	1.96	18	1
1:A:152:VAL:HG23	1:A:157:LEU:CD2	0.60	2.27	14	6
1:A:58:ILE:HD13	1:A:95:LEU:HB2	0.60	1.72	7	2
1:A:88:GLY:O	1:A:114:ILE:HD13	0.59	1.97	15	3
1:A:16:LEU:HD13	1:A:82:LEU:CD1	0.59	2.28	11	1
1:A:14:THR:HG21	1:A:61:LEU:HD11	0.59	1.75	19	3
1:A:78:ARG:N	1:A:79:PRO:HD2	0.59	2.13	19	20
1:A:109:VAL:HG12	1:A:182:VAL:HB	0.59	1.74	4	13
1:A:6:LYS:CG	1:A:64:LEU:HD11	0.59	2.28	15	5
1:A:215:GLY:CA	1:A:220:LEU:HD11	0.59	2.28	13	1
1:A:126:HIS:CD2	1:A:197:ALA:HB2	0.58	2.33	12	1
1:A:4:LEU:HD11	1:A:43:LEU:HD13	0.58	1.75	1	1
1:A:188:LEU:HD12	1:A:191:LYS:O	0.58	1.99	10	7
1:A:192:LYS:HE2	1:A:220:LEU:HD13	0.58	1.75	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:LYS:CE	1:A:204:ALA:HB3	0.58	2.29	15	2
1:A:182:VAL:HG13	1:A:208:THR:HB	0.57	1.75	5	17
1:A:16:LEU:CD1	1:A:58:ILE:HG23	0.57	2.29	4	8
1:A:137:ILE:HD11	1:A:144:ALA:O	0.57	1.99	17	5
1:A:14:THR:CG2	1:A:61:LEU:HD21	0.57	2.30	20	1
1:A:13:LYS:CE	1:A:109:VAL:HG21	0.57	2.29	15	1
1:A:202:LYS:HE3	1:A:204:ALA:HB3	0.57	1.75	15	2
1:A:188:LEU:HD13	1:A:195:ARG:HB2	0.57	1.75	2	4
1:A:188:LEU:HD11	1:A:213:ASP:OD1	0.57	2.00	9	3
1:A:129:ASP:O	1:A:133:LEU:HD23	0.56	1.99	11	1
1:A:133:LEU:HB2	1:A:139:LEU:HD21	0.56	1.76	14	2
1:A:61:LEU:HD12	1:A:99:LEU:CD1	0.56	2.29	12	1
1:A:4:LEU:HD13	1:A:56:SER:CB	0.56	2.31	4	2
1:A:226:VAL:O	1:A:230:ILE:HD12	0.56	1.99	4	3
1:A:211:GLN:O	1:A:234:LEU:HD11	0.56	2.01	17	6
1:A:105:PHE:N	1:A:106:PRO:HD2	0.55	2.16	18	20
1:A:16:LEU:HG	1:A:43:LEU:HD11	0.55	1.77	2	6
1:A:188:LEU:HD11	1:A:213:ASP:CG	0.55	2.21	20	1
1:A:78:ARG:HG2	1:A:104:ILE:HG21	0.55	1.77	17	2
1:A:181:PRO:O	1:A:207:ILE:HG22	0.55	2.02	7	5
1:A:14:THR:HG23	1:A:61:LEU:HD21	0.55	1.78	20	1
1:A:32:LEU:HD12	1:A:208:THR:OG1	0.55	2.01	5	2
1:A:187:GLY:C	1:A:188:LEU:HD23	0.54	2.23	10	16
1:A:101:ARG:HD2	1:A:167:LEU:HD12	0.54	1.78	20	1
1:A:78:ARG:CG	1:A:104:ILE:HG21	0.54	2.32	18	2
1:A:220:LEU:HD12	1:A:220:LEU:O	0.54	2.01	13	1
1:A:6:LYS:HB2	1:A:64:LEU:HD11	0.54	1.78	7	4
1:A:16:LEU:HB3	1:A:82:LEU:HD12	0.54	1.79	11	2
1:A:149:ASN:O	1:A:152:VAL:HG12	0.54	2.02	18	4
1:A:6:LYS:CB	1:A:64:LEU:HD11	0.54	2.32	2	2
1:A:99:LEU:O	1:A:99:LEU:HD13	0.54	2.02	12	3
1:A:101:ARG:CD	1:A:167:LEU:HD11	0.54	2.32	4	1
1:A:136:ILE:C	1:A:137:ILE:HG13	0.54	2.23	9	1
1:A:230:ILE:HG22	1:A:234:LEU:CD1	0.54	2.33	12	2
1:A:180:SER:CB	1:A:181:PRO:CD	0.54	2.86	19	20
1:A:137:ILE:HD11	1:A:144:ALA:HB3	0.53	1.79	20	1
1:A:188:LEU:HD12	1:A:192:LYS:HA	0.53	1.80	1	8
1:A:37:GLN:OE1	1:A:109:VAL:HG11	0.53	2.03	10	1
1:A:28:SER:O	1:A:32:LEU:HD23	0.53	2.03	5	4
1:A:117:PRO:CB	1:A:139:LEU:HD12	0.53	2.33	6	1
1:A:175:LEU:HD21	1:A:201:LYS:NZ	0.53	2.18	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:212:PHE:HA	1:A:234:LEU:HD21	0.53	1.79	17	1
1:A:109:VAL:HG12	1:A:182:VAL:CG2	0.53	2.33	19	1
1:A:62:GLU:HG3	1:A:99:LEU:HD11	0.53	1.80	5	1
1:A:133:LEU:CD1	1:A:139:LEU:HD21	0.53	2.34	12	1
1:A:152:VAL:HG13	1:A:157:LEU:CD2	0.52	2.34	4	2
1:A:4:LEU:HD12	1:A:44:ALA:O	0.52	2.03	1	1
1:A:111:ILE:HD13	1:A:112:SER:N	0.52	2.19	20	3
1:A:43:LEU:HD12	1:A:44:ALA:N	0.52	2.19	15	5
1:A:134:ASP:O	1:A:137:ILE:HG23	0.52	2.04	9	3
1:A:152:VAL:CG1	1:A:157:LEU:HD22	0.52	2.30	8	1
1:A:6:LYS:HD3	1:A:64:LEU:HD21	0.52	1.81	13	1
1:A:211:GLN:O	1:A:234:LEU:HD21	0.52	2.05	14	5
1:A:32:LEU:HD12	1:A:208:THR:CG2	0.52	2.34	10	2
1:A:43:LEU:HD22	1:A:60:ASP:CG	0.52	2.25	17	1
1:A:213:ASP:OD2	1:A:230:ILE:HG21	0.52	2.04	19	1
1:A:188:LEU:HD11	1:A:213:ASP:HB3	0.51	1.82	16	2
1:A:67:LEU:O	1:A:67:LEU:HD13	0.51	2.06	5	2
1:A:237:HIS:N	1:A:238:PRO:HD2	0.51	2.21	6	20
1:A:4:LEU:HD12	1:A:43:LEU:CD1	0.51	2.36	17	1
1:A:17:ILE:CD1	1:A:44:ALA:HB2	0.51	2.36	7	1
1:A:192:LYS:NZ	1:A:220:LEU:HD13	0.51	2.21	3	1
1:A:188:LEU:HD21	1:A:213:ASP:OD1	0.50	2.06	20	1
1:A:82:LEU:HD23	1:A:82:LEU:O	0.50	2.06	17	5
1:A:142:MET:CE	1:A:144:ALA:HB3	0.50	2.36	12	1
1:A:82:LEU:O	1:A:82:LEU:HD23	0.50	2.06	15	2
1:A:69:LYS:CB	1:A:74:LEU:HD12	0.50	2.36	16	1
1:A:109:VAL:HG23	1:A:109:VAL:O	0.50	2.06	19	1
1:A:101:ARG:HD2	1:A:167:LEU:HD11	0.50	1.84	4	1
1:A:16:LEU:HD12	1:A:43:LEU:CD2	0.50	2.36	8	1
1:A:30:ARG:CB	1:A:31:PRO:CD	0.49	2.90	18	20
1:A:74:LEU:HD13	1:A:75:ARG:N	0.49	2.23	19	2
1:A:36:LEU:HD23	1:A:37:GLN:OE1	0.49	2.06	1	1
1:A:124:VAL:HG21	1:A:130:ASP:OD2	0.49	2.06	17	1
1:A:215:GLY:HA2	1:A:220:LEU:HD21	0.49	1.83	13	1
1:A:234:LEU:HD13	1:A:234:LEU:O	0.49	2.08	7	2
1:A:114:ILE:HG22	1:A:155:PHE:CD2	0.49	2.43	6	1
1:A:61:LEU:HD21	1:A:76:PRO:HB3	0.49	1.84	6	2
1:A:30:ARG:N	1:A:31:PRO:HD2	0.49	2.23	20	18
1:A:213:ASP:OD2	1:A:234:LEU:HD11	0.49	2.07	1	1
1:A:119:ILE:HD13	1:A:194:ILE:HG13	0.49	1.82	8	1
1:A:4:LEU:HD12	1:A:43:LEU:HD13	0.49	1.84	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:PRO:HB2	1:A:109:VAL:HG22	0.48	1.84	8	7
1:A:74:LEU:HD23	1:A:75:ARG:N	0.48	2.23	9	3
1:A:14:THR:HG23	1:A:41:GLU:OE1	0.48	2.08	17	2
1:A:105:PHE:CB	1:A:106:PRO:CD	0.48	2.91	16	5
1:A:17:ILE:HD11	1:A:44:ALA:HB2	0.48	1.84	7	1
1:A:97:GLN:NE2	1:A:167:LEU:HD21	0.48	2.23	9	1
1:A:178:ILE:O	1:A:204:ALA:HB1	0.48	2.08	12	3
1:A:78:ARG:N	1:A:79:PRO:CD	0.48	2.77	19	6
1:A:133:LEU:HD12	1:A:134:ASP:N	0.48	2.23	8	4
1:A:175:LEU:HD11	1:A:202:LYS:NZ	0.48	2.23	3	1
1:A:8:PHE:CE1	1:A:64:LEU:HD12	0.48	2.44	10	1
1:A:57:ALA:C	1:A:58:ILE:HD12	0.48	2.29	7	4
1:A:177:GLN:O	1:A:178:ILE:HD13	0.48	2.09	16	9
1:A:146:LEU:O	1:A:146:LEU:HD12	0.47	2.09	7	5
1:A:62:GLU:OE2	1:A:99:LEU:HD21	0.47	2.09	4	1
1:A:188:LEU:HD13	1:A:195:ARG:CB	0.47	2.39	2	1
1:A:4:LEU:HD22	1:A:56:SER:HB3	0.47	1.86	14	1
1:A:32:LEU:CD1	1:A:208:THR:HG23	0.47	2.38	10	5
1:A:109:VAL:C	1:A:110:ILE:HD12	0.47	2.30	13	1
1:A:61:LEU:HD21	1:A:76:PRO:CB	0.47	2.40	10	1
1:A:124:VAL:HG12	1:A:126:HIS:H	0.47	1.70	15	1
1:A:119:ILE:HD11	1:A:133:LEU:CD1	0.47	2.40	15	1
1:A:192:LYS:HE2	1:A:220:LEU:HD11	0.47	1.86	1	1
1:A:18:CYS:SG	1:A:45:ALA:HB3	0.47	2.50	12	1
1:A:78:ARG:CB	1:A:79:PRO:CD	0.47	2.92	5	14
1:A:187:GLY:O	1:A:188:LEU:C	0.47	2.53	15	6
1:A:148:GLU:O	1:A:152:VAL:HG13	0.47	2.09	3	1
1:A:118:HIS:O	1:A:119:ILE:HG23	0.47	2.10	16	2
1:A:36:LEU:HD11	1:A:182:VAL:CG2	0.47	2.37	13	1
1:A:126:HIS:CE1	1:A:127:LEU:HD12	0.47	2.45	9	1
1:A:32:LEU:CD2	1:A:208:THR:HG23	0.47	2.40	8	1
1:A:139:LEU:HD11	1:A:191:LYS:HD2	0.47	1.86	20	1
1:A:146:LEU:HD12	1:A:146:LEU:O	0.47	2.09	4	2
1:A:67:LEU:HD23	1:A:67:LEU:O	0.47	2.09	1	1
1:A:69:LYS:HD3	1:A:74:LEU:HD12	0.46	1.86	10	1
1:A:180:SER:O	1:A:207:ILE:HD12	0.46	2.09	9	1
1:A:32:LEU:HG	1:A:208:THR:HG23	0.46	1.87	11	1
1:A:82:LEU:HD13	1:A:96:ALA:CB	0.46	2.39	11	1
1:A:79:PRO:CB	1:A:109:VAL:HG22	0.46	2.41	5	6
1:A:71:GLU:C	1:A:72:LEU:HD22	0.46	2.31	19	1
1:A:14:THR:HG23	1:A:41:GLU:CD	0.46	2.31	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LYS:HG3	1:A:64:LEU:HD11	0.46	1.87	15	3
1:A:18:CYS:HB3	1:A:45:ALA:HB3	0.46	1.88	2	5
1:A:195:ARG:O	1:A:199:GLY:N	0.46	2.49	12	2
1:A:109:VAL:HG13	1:A:182:VAL:CG1	0.46	2.41	3	1
1:A:149:ASN:O	1:A:152:VAL:HG22	0.46	2.11	8	2
1:A:99:LEU:HD23	1:A:99:LEU:O	0.46	2.11	9	1
1:A:78:ARG:CB	1:A:104:ILE:HD13	0.45	2.41	20	1
1:A:8:PHE:CD1	1:A:64:LEU:HD12	0.45	2.46	20	1
1:A:212:PHE:HA	1:A:234:LEU:HD11	0.45	1.87	11	1
1:A:152:VAL:CG2	1:A:157:LEU:HD22	0.45	2.34	18	2
1:A:58:ILE:HG21	1:A:96:ALA:HA	0.45	1.88	13	1
1:A:85:HIS:O	1:A:114:ILE:HG23	0.45	2.10	20	1
1:A:88:GLY:C	1:A:114:ILE:HD13	0.45	2.32	18	1
1:A:17:ILE:HD12	1:A:20:PRO:CG	0.45	2.40	17	1
1:A:105:PHE:N	1:A:106:PRO:CD	0.45	2.80	4	5
1:A:36:LEU:O	1:A:36:LEU:HD13	0.45	2.12	5	1
1:A:215:GLY:HA3	1:A:220:LEU:HD11	0.45	1.87	13	1
1:A:61:LEU:O	1:A:65:THR:HG23	0.45	2.12	11	2
1:A:157:LEU:O	1:A:157:LEU:HD23	0.45	2.12	1	2
1:A:43:LEU:HD22	1:A:60:ASP:OD1	0.44	2.12	11	1
1:A:126:HIS:O	1:A:127:LEU:HD12	0.44	2.13	12	1
1:A:212:PHE:HA	1:A:234:LEU:HD22	0.44	1.88	12	1
1:A:188:LEU:HD13	1:A:195:ARG:HD3	0.44	1.87	1	1
1:A:30:ARG:O	1:A:34:ALA:HB2	0.44	2.12	13	1
1:A:14:THR:HG21	1:A:61:LEU:CD2	0.44	2.37	16	1
1:A:119:ILE:HD11	1:A:134:ASP:HA	0.44	1.89	17	1
1:A:43:LEU:HD12	1:A:44:ALA:H	0.44	1.73	14	2
1:A:13:LYS:HE2	1:A:109:VAL:HG21	0.44	1.89	15	1
1:A:5:PHE:O	1:A:43:LEU:HD12	0.44	2.13	20	2
1:A:234:LEU:O	1:A:234:LEU:HD13	0.43	2.13	5	2
1:A:136:ILE:HG22	1:A:138:GLN:CB	0.43	2.43	7	4
1:A:219:LEU:HD13	1:A:219:LEU:O	0.43	2.13	1	1
1:A:180:SER:N	1:A:181:PRO:HD2	0.43	2.28	10	17
1:A:104:ILE:HG23	1:A:104:ILE:O	0.43	2.13	4	2
1:A:4:LEU:HD13	1:A:56:SER:HB3	0.43	1.90	4	2
1:A:159:SER:OG	1:A:159:SER:O	0.43	2.33	20	1
1:A:6:LYS:HD2	1:A:64:LEU:HD23	0.43	1.90	10	1
1:A:69:LYS:HD2	1:A:74:LEU:HD12	0.43	1.90	10	1
1:A:188:LEU:HD13	1:A:195:ARG:HG3	0.43	1.91	19	1
1:A:124:VAL:HG22	1:A:126:HIS:H	0.43	1.73	9	2
1:A:160:PHE:O	1:A:161:ARG:C	0.43	2.57	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:ILE:HD13	1:A:119:ILE:H	0.43	1.74	17	1
1:A:136:ILE:O	1:A:137:ILE:C	0.43	2.56	9	2
1:A:237:HIS:CB	1:A:238:PRO:CD	0.43	2.96	5	18
1:A:118:HIS:CE1	1:A:157:LEU:HD13	0.43	2.48	10	1
1:A:61:LEU:HD23	1:A:62:GLU:N	0.43	2.28	11	1
1:A:152:VAL:HB	1:A:157:LEU:HD22	0.42	1.90	19	1
1:A:81:VAL:HG13	1:A:109:VAL:HG22	0.42	1.90	18	1
1:A:230:ILE:HG22	1:A:234:LEU:HD12	0.42	1.89	20	1
1:A:180:SER:CB	1:A:181:PRO:HD3	0.42	2.44	19	1
1:A:136:ILE:HG22	1:A:138:GLN:HB2	0.42	1.91	11	2
1:A:80:PHE:O	1:A:110:ILE:HD13	0.42	2.15	20	1
1:A:103:GLY:C	1:A:104:ILE:HD12	0.42	2.35	10	1
1:A:142:MET:HE3	1:A:144:ALA:HB3	0.42	1.91	12	1
1:A:211:GLN:O	1:A:234:LEU:HD22	0.42	2.14	20	1
1:A:4:LEU:HD11	1:A:43:LEU:CD1	0.42	2.44	1	1
1:A:99:LEU:HD13	1:A:99:LEU:O	0.42	2.15	2	1
1:A:4:LEU:HD11	1:A:60:ASP:HB3	0.42	1.92	3	1
1:A:108:ALA:C	1:A:110:ILE:HD12	0.41	2.35	3	1
1:A:234:LEU:C	1:A:234:LEU:HD13	0.41	2.35	7	1
1:A:133:LEU:HD21	1:A:191:LYS:NZ	0.41	2.30	12	1
1:A:36:LEU:HD21	1:A:207:ILE:CG2	0.41	2.45	9	1
1:A:72:LEU:HD13	1:A:73:ASN:N	0.41	2.31	14	1
1:A:58:ILE:O	1:A:99:LEU:HD12	0.41	2.14	15	1
1:A:104:ILE:O	1:A:104:ILE:HG23	0.41	2.16	13	1
1:A:80:PHE:O	1:A:110:ILE:HG22	0.41	2.14	12	1
1:A:219:LEU:O	1:A:223:THR:HG22	0.41	2.16	9	1
1:A:61:LEU:HB2	1:A:99:LEU:HD21	0.41	1.92	8	1
1:A:184:VAL:HG13	1:A:210:HIS:HB3	0.41	1.91	20	1
1:A:119:ILE:HD13	1:A:119:ILE:N	0.41	2.30	17	1
1:A:16:LEU:CD1	1:A:58:ILE:HD12	0.41	2.39	6	1
1:A:18:CYS:CB	1:A:45:ALA:HB3	0.41	2.46	20	1
1:A:182:VAL:HG22	1:A:208:THR:HB	0.41	1.92	15	1
1:A:119:ILE:HG21	1:A:194:ILE:HD11	0.41	1.93	4	1
1:A:237:HIS:N	1:A:238:PRO:CD	0.41	2.84	6	1
1:A:14:THR:HG1	1:A:77:ASP:CG	0.41	2.18	6	1
1:A:105:PHE:HB3	1:A:106:PRO:HD3	0.41	1.92	2	1
1:A:16:LEU:HD12	1:A:43:LEU:HD23	0.41	1.93	15	1
1:A:101:ARG:HE	1:A:167:LEU:HD22	0.41	1.76	17	1
1:A:97:GLN:HE21	1:A:167:LEU:HD21	0.41	1.76	9	1
1:A:4:LEU:HD13	1:A:56:SER:HB2	0.41	1.93	4	1
1:A:234:LEU:HD13	1:A:234:LEU:C	0.41	2.36	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:213:ASP:OD1	1:A:230:ILE:HD12	0.41	2.16	15	1
1:A:163:ASP:O	1:A:167:LEU:N	0.41	2.54	2	1
1:A:217:MET:HB2	1:A:220:LEU:HD12	0.41	1.93	20	1
1:A:175:LEU:HD23	1:A:175:LEU:H	0.41	1.76	15	3
1:A:104:ILE:HD11	1:A:106:PRO:HG2	0.41	1.93	4	2
1:A:111:ILE:HD13	1:A:112:SER:O	0.41	2.16	12	1
1:A:119:ILE:HD12	1:A:119:ILE:O	0.40	2.15	14	1
1:A:223:THR:CG2	1:A:226:VAL:HG23	0.40	2.46	14	1
1:A:202:LYS:CD	1:A:204:ALA:HB3	0.40	2.42	8	1
1:A:82:LEU:HD13	1:A:93:PHE:CD1	0.40	2.52	19	1
1:A:73:ASN:O	1:A:74:LEU:HD12	0.40	2.16	13	1
1:A:82:LEU:HD13	1:A:96:ALA:HB1	0.40	1.93	11	1
1:A:99:LEU:O	1:A:99:LEU:HD23	0.40	2.16	5	1
1:A:182:VAL:HG22	1:A:207:ILE:CG2	0.40	2.47	2	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	228/242 (94%)	178±4 (78±2%)	46±5 (20±2%)	4±1 (2±1%)	14	57
All	All	4560/4840 (94%)	3553 (78%)	926 (20%)	81 (2%)	14	57

All 23 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	180	SER	20
1	A	89	GLY	14
1	A	104	ILE	9
1	A	159	SER	5
1	A	141	GLY	5
1	A	61	LEU	3
1	A	217	MET	3
1	A	190	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	121	ARG	2
1	A	232	ALA	2
1	A	56	SER	2
1	A	71	GLU	2
1	A	114	ILE	1
1	A	92	THR	1
1	A	60	ASP	1
1	A	215	GLY	1
1	A	90	MET	1
1	A	94	ARG	1
1	A	132	PHE	1
1	A	96	ALA	1
1	A	149	ASN	1
1	A	72	LEU	1
1	A	65	THR	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	198/210 (94%)	170±4 (86±2%)	28±4 (14±2%)	8	47
All	All	3960/4200 (94%)	3403 (86%)	557 (14%)	8	47

All 122 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	180	SER	20
1	A	194	ILE	20
1	A	201	LYS	20
1	A	93	PHE	19
1	A	111	ILE	19
1	A	188	LEU	18
1	A	237	HIS	18
1	A	119	ILE	16
1	A	6	LYS	15
1	A	29	PHE	14

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Mol	Chain	Res	Type	Models (Total)
1	A	190	ASP	13
1	A	205	LYS	12
1	A	85	HIS	11
1	A	26	SER	11
1	A	32	LEU	11
1	A	156	PHE	11
1	A	185	PHE	10
1	A	146	LEU	9
1	A	161	ARG	9
1	A	60	ASP	9
1	A	43	LEU	8
1	A	90	MET	8
1	A	8	PHE	7
1	A	219	LEU	7
1	A	206	ASP	7
1	A	77	ASP	7
1	A	234	LEU	6
1	A	217	MET	6
1	A	115	GLN	5
1	A	123	LYS	5
1	A	130	ASP	5
1	A	107	GLN	4
1	A	213	ASP	4
1	A	211	GLN	4
1	A	36	LEU	4
1	A	200	TRP	4
1	A	142	MET	4
1	A	98	LYS	4
1	A	100	GLU	4
1	A	122	LYS	4
1	A	99	LEU	4
1	A	150	LYS	4
1	A	61	LEU	4
1	A	195	ARG	4
1	A	126	HIS	3
1	A	207	ILE	3
1	A	170	PHE	3
1	A	87	MET	3
1	A	186	ASN	3
1	A	136	ILE	3
1	A	223	THR	3
1	A	120	GLN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	28	SER	3
1	A	13	LYS	3
1	A	157	LEU	3
1	A	165	ARG	3
1	A	172	LEU	3
1	A	56	SER	3
1	A	30	ARG	3
1	A	83	PHE	3
1	A	118	HIS	3
1	A	235	ASN	3
1	A	82	LEU	3
1	A	162	SER	3
1	A	202	LYS	3
1	A	75	ARG	3
1	A	110	ILE	3
1	A	105	PHE	3
1	A	174	ASP	2
1	A	92	THR	2
1	A	69	LYS	2
1	A	16	LEU	2
1	A	131	GLN	2
1	A	37	GLN	2
1	A	73	ASN	2
1	A	72	LEU	2
1	A	183	HIS	2
1	A	192	LYS	2
1	A	67	LEU	2
1	A	163	ASP	2
1	A	167	LEU	2
1	A	129	ASP	2
1	A	198	GLU	2
1	A	112	SER	2
1	A	175	LEU	2
1	A	19	PHE	2
1	A	74	LEU	2
1	A	171	GLU	2
1	A	78	ARG	2
1	A	86	SER	2
1	A	33	HIS	2
1	A	91	ILE	1
1	A	152	VAL	1
1	A	212	PHE	1

*Continued on next page...*

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Mol	Chain	Res	Type	Models (Total)
1	A	220	LEU	1
1	A	151	GLU	1
1	A	109	VAL	1
1	A	11	SER	1
1	A	64	LEU	1
1	A	231	PHE	1
1	A	121	ARG	1
1	A	145	GLU	1
1	A	236	GLN	1
1	A	70	GLN	1
1	A	159	SER	1
1	A	2	SER	1
1	A	101	ARG	1
1	A	68	TYR	1
1	A	189	ASP	1
1	A	15	GLN	1
1	A	39	GLU	1
1	A	179	GLN	1
1	A	14	THR	1
1	A	164	TYR	1
1	A	133	LEU	1
1	A	17	ILE	1
1	A	127	LEU	1
1	A	94	ARG	1
1	A	191	LYS	1
1	A	102	GLU	1
1	A	222	GLN	1
1	A	138	GLN	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