



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 03:38 PM UTC

PDB ID : 2L38 / pdb_00002l38
Title : R29Q Sticholysin II mutant
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Deposited on : 2010-09-10

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

We welcome your comments at validation@mail.wwpdb.org

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

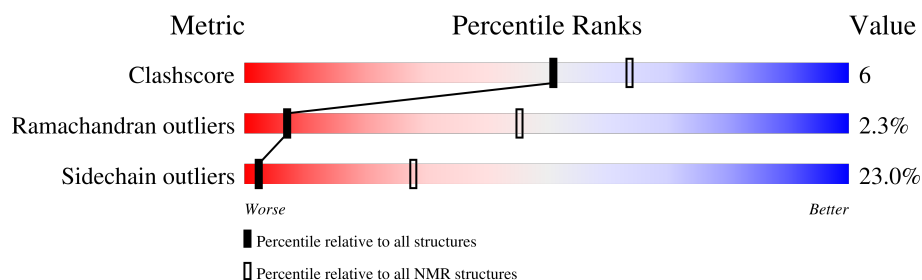
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	175	

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:24, A:30-A:74, A:84-A:105, A:113-A:175 (153)	0.86	15

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2689 atoms, of which 1330 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sticholysin-2.

Mol	Chain	Residues	Atoms						Trace
1	A	175	Total	C	H	N	O	S	0
			2689	870	1330	227	256	6	

There is a discrepancy between the modelled and reference sequences:

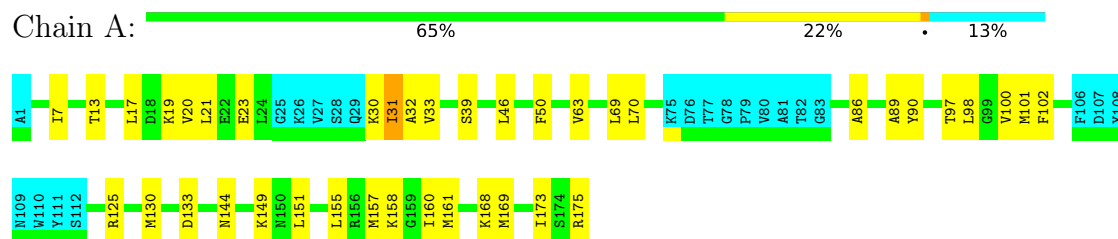
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLN	ARG	engineered mutation	UNP P07845

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: Sticholysin-2

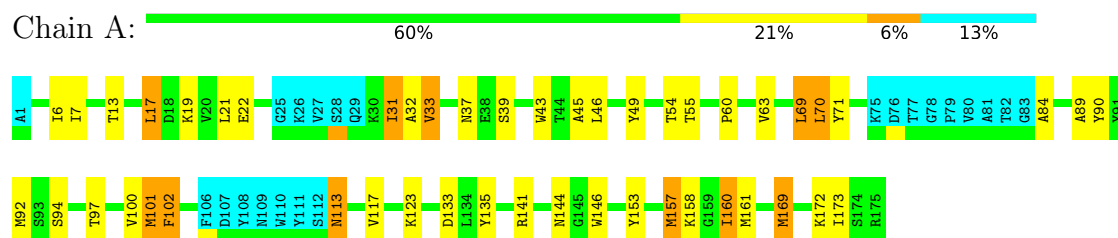


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

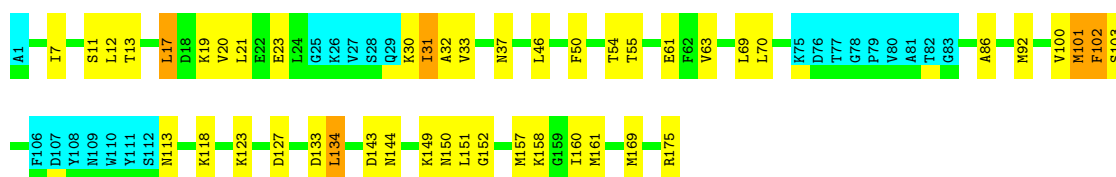
- Molecule 1: Sticholysin-2



4.2.2 Score per residue for model 2

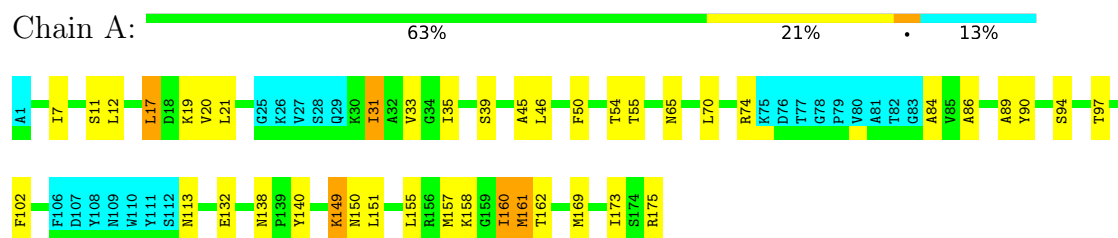
- Molecule 1: Sticholysin-2





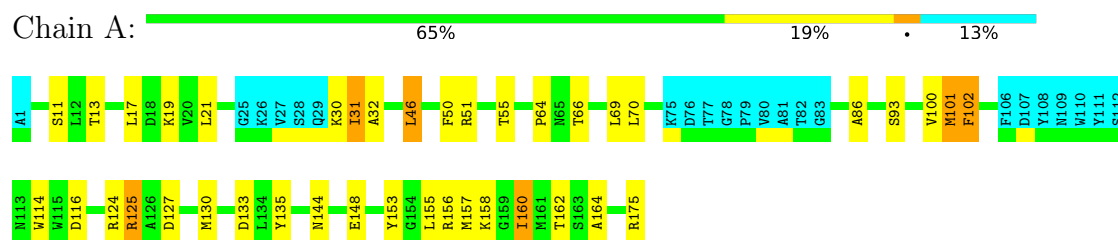
4.2.3 Score per residue for model 3

- Molecule 1: Sticholysin-2



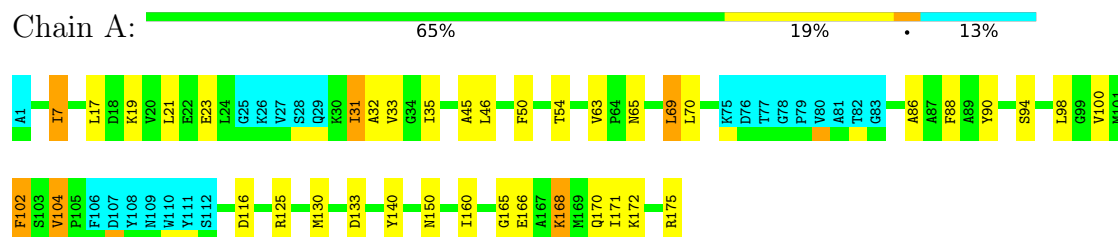
4.2.4 Score per residue for model 4

- Molecule 1: Sticholysin-2



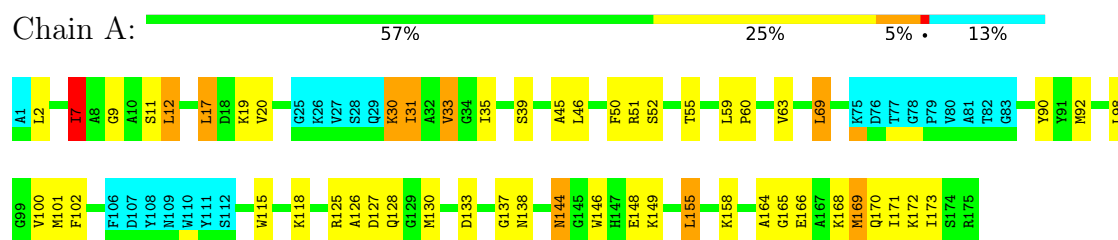
4.2.5 Score per residue for model 5

- Molecule 1: Sticholysin-2



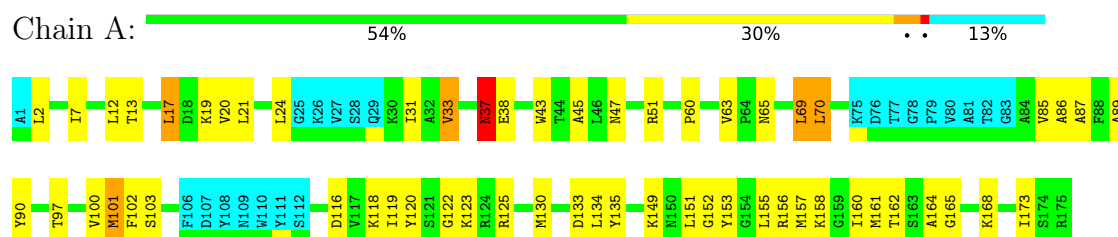
4.2.6 Score per residue for model 6

- Molecule 1: Sticholysin-2



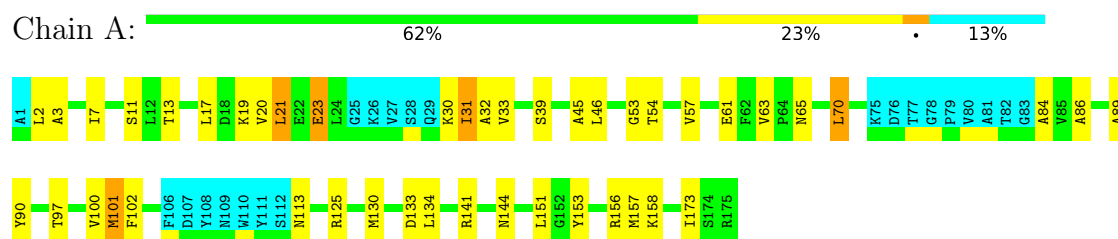
4.2.7 Score per residue for model 7

- Molecule 1: Sticholysin-2



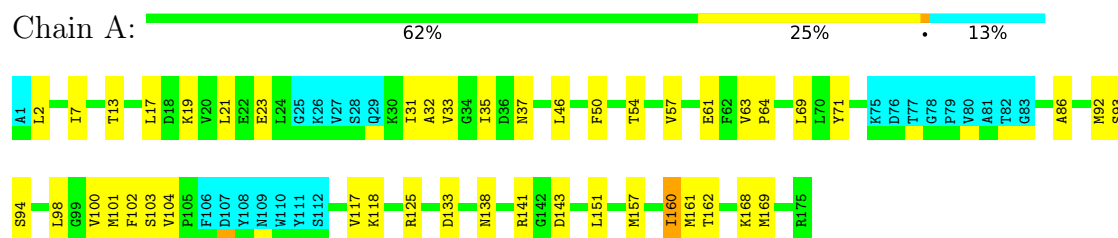
4.2.8 Score per residue for model 8

- Molecule 1: Sticholysin-2



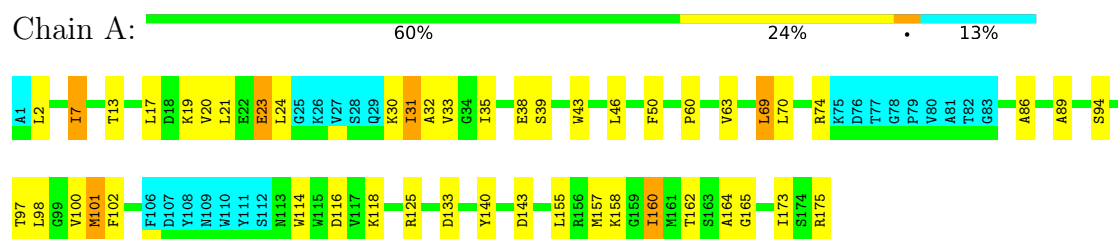
4.2.9 Score per residue for model 9

- Molecule 1: Sticholysin-2



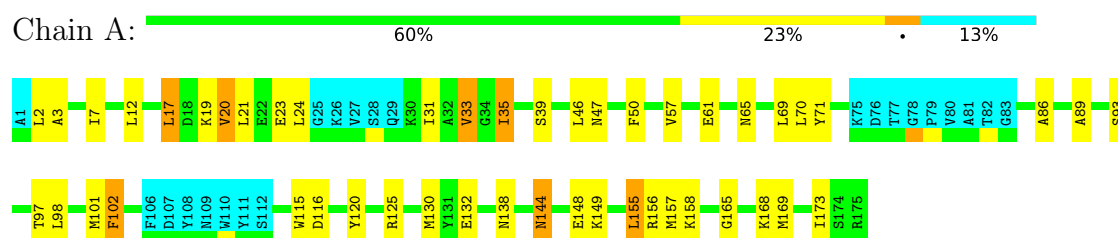
4.2.10 Score per residue for model 10

- Molecule 1: Sticholysin-2



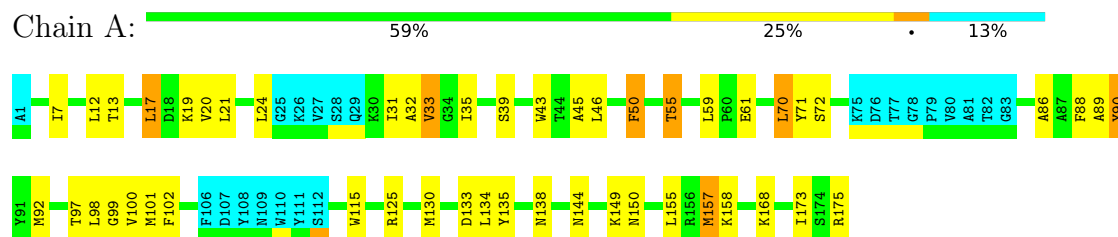
4.2.11 Score per residue for model 11

- Molecule 1: Sticholysin-2



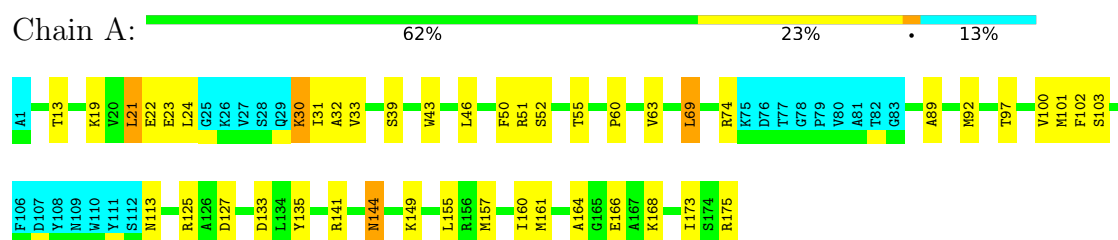
4.2.12 Score per residue for model 12

- Molecule 1: Sticholysin-2



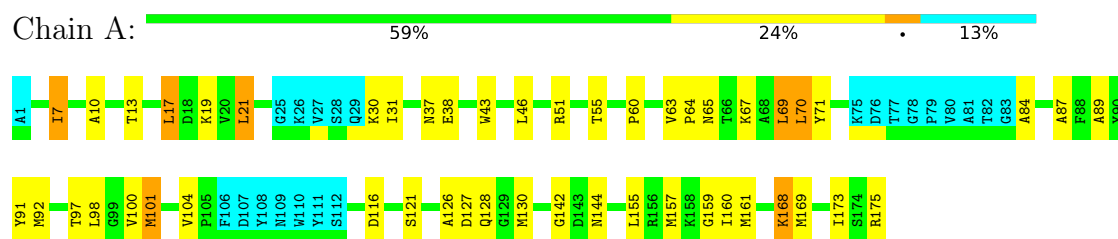
4.2.13 Score per residue for model 13

- Molecule 1: Sticholysin-2



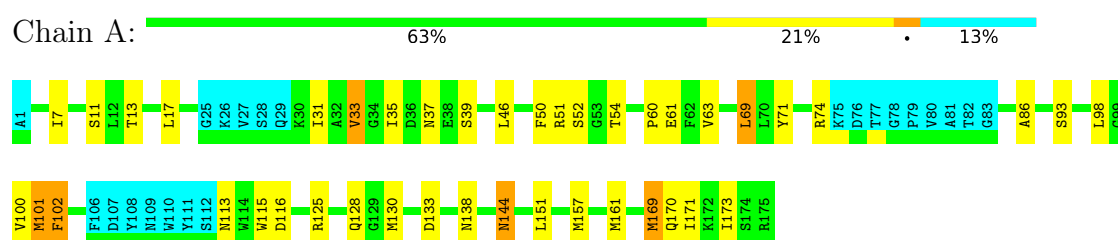
4.2.14 Score per residue for model 14

- Molecule 1: Sticholysin-2



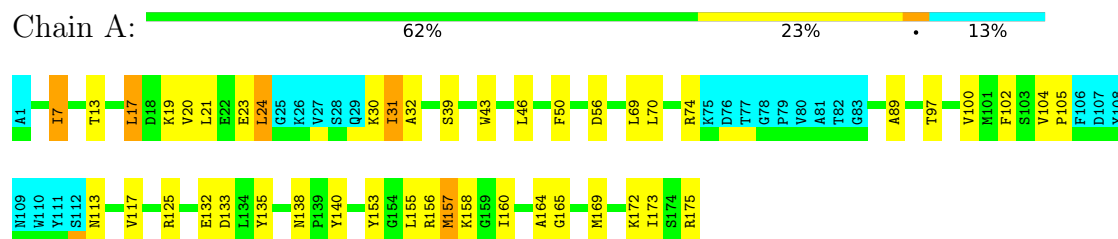
4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Sticholysin-2



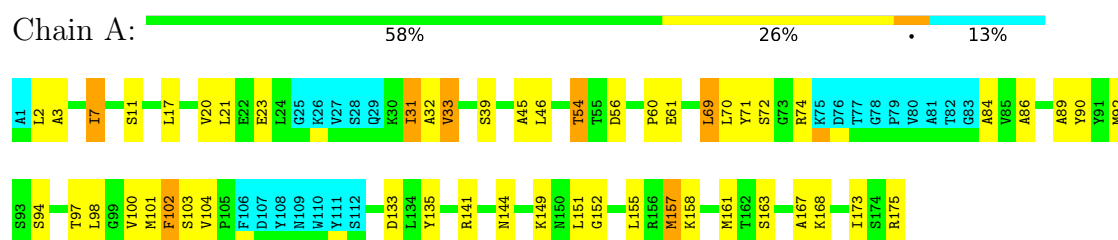
4.2.16 Score per residue for model 16

- Molecule 1: Sticholysin-2



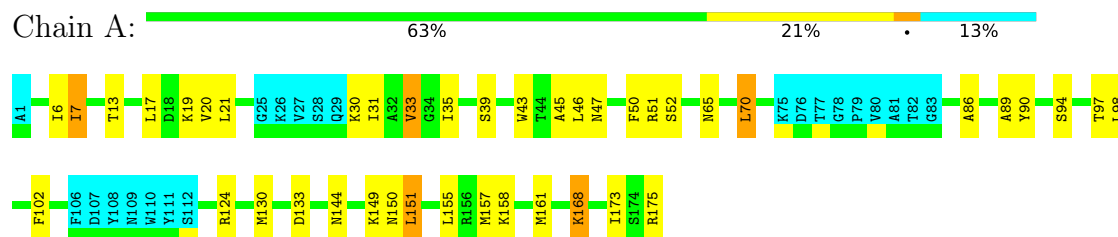
4.2.17 Score per residue for model 17

- Molecule 1: Sticholysin-2



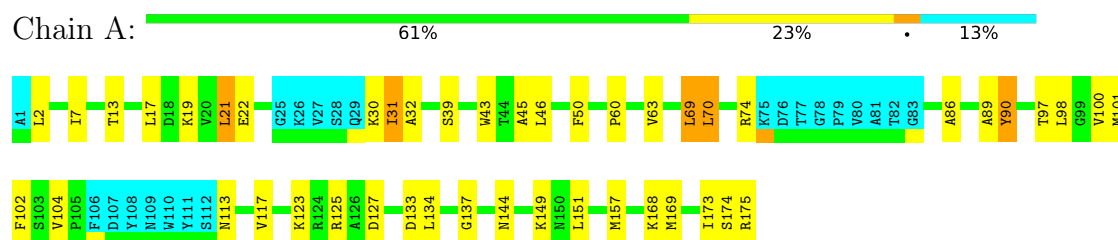
4.2.18 Score per residue for model 18

- Molecule 1: Sticholysin-2



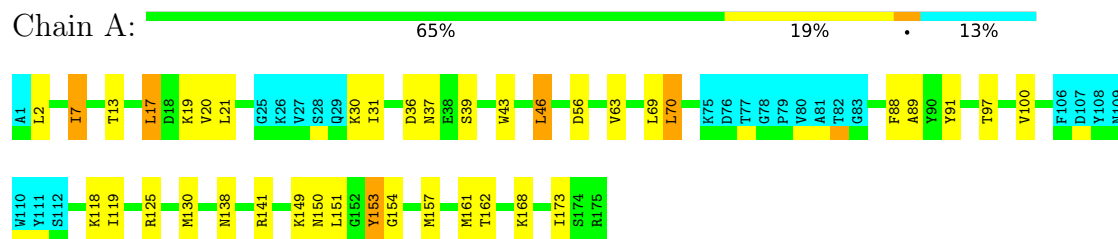
4.2.19 Score per residue for model 19

- Molecule 1: Sticholysin-2



4.2.20 Score per residue for model 20

- Molecule 1: Sticholysin-2



5 Refinement protocol and experimental data overview

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

Of the 100 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
Amber	refinement	
CYANA	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.86±0.10	1±3/1217 (0.1± 0.2%)	1.38±0.03	1±1/1644 (0.1± 0.0%)
All	All	0.87	13/24340 (0.1%)	1.38	23/32880 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.1±0.8
All	All	0	21

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	159	GLY	CA-C	12.46	1.62	1.52	14	1
1	A	126	ALA	N-CA	-9.85	1.34	1.46	14	1
1	A	160	ILE	CA-C	8.96	1.63	1.52	14	1
1	A	128	GLN	CA-C	8.19	1.63	1.52	14	1
1	A	126	ALA	CA-CB	7.54	1.63	1.53	14	1
1	A	92	MET	CA-C	7.40	1.63	1.53	14	1
1	A	127	ASP	CA-C	6.49	1.60	1.52	14	1
1	A	91	TYR	CA-CB	6.43	1.61	1.53	14	1
1	A	91	TYR	N-CA	-6.02	1.38	1.46	14	1
1	A	121	SER	N-CA	5.60	1.53	1.46	14	1
1	A	127	ASP	N-CA	5.27	1.52	1.46	14	1
1	A	126	ALA	CA-C	5.07	1.59	1.52	14	1
1	A	10	ALA	CA-C	5.01	1.59	1.52	14	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	37	ASN	CA-CB-CG	6.73	119.33	112.60	7	2
1	A	113	ASN	CA-CB-CG	6.05	118.65	112.60	1	1
1	A	126	ALA	N-CA-C	5.83	118.23	108.96	14	1
1	A	22	GLU	CA-C-N	5.71	128.71	120.38	19	1
1	A	22	GLU	C-N-CA	5.71	128.71	120.38	19	1
1	A	17	LEU	CA-C-N	5.68	127.83	120.44	16	1
1	A	17	LEU	C-N-CA	5.68	127.83	120.44	16	1
1	A	168	LYS	N-CA-C	5.59	115.67	108.34	18	1
1	A	88	PHE	CA-CB-CG	5.38	119.18	113.80	12	1
1	A	144	ASN	CA-CB-CG	5.27	117.87	112.60	13	1
1	A	23	GLU	CA-C-N	5.17	127.46	120.38	8	3
1	A	23	GLU	C-N-CA	5.17	127.46	120.38	8	3
1	A	54	THR	CA-CB-CG2	5.14	119.25	110.50	17	1
1	A	84	ALA	N-CA-CB	-5.13	103.56	111.46	14	1
1	A	36	ASP	CA-CB-CG	5.09	117.69	112.60	20	1
1	A	137	GLY	CA-C-N	5.06	127.46	122.00	6	1
1	A	137	GLY	C-N-CA	5.06	127.46	122.00	6	1
1	A	20	VAL	CA-CB-CG1	5.01	118.92	110.40	11	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	102	PHE	Sidechain	7
1	A	153	TYR	Sidechain	5
1	A	135	TYR	Sidechain	3
1	A	120	TYR	Sidechain	2
1	A	49	TYR	Sidechain	1
1	A	140	TYR	Sidechain	1
1	A	74	ARG	Sidechain	1
1	A	90	TYR	Sidechain	1

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	1190	1175	1174	13±4
All	All	23800	23500	23480	261

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:12:LEU:HD11	1:A:17:LEU:HD23	0.76	1.56	11	2
1:A:130:MET:HE3	1:A:134:LEU:HD11	0.75	1.57	12	1
1:A:101:MET:CE	1:A:169:MET:HE1	0.74	2.12	2	2
1:A:35:ILE:HG21	1:A:98:LEU:HD21	0.74	1.59	15	5
1:A:63:VAL:HG21	1:A:69:LEU:HD13	0.74	1.58	5	1
1:A:21:LEU:HD11	1:A:32:ALA:HB2	0.74	1.59	17	4
1:A:33:VAL:HG11	1:A:102:PHE:CG	0.68	2.23	18	2
1:A:86:ALA:HB3	1:A:102:PHE:CZ	0.67	2.24	18	12
1:A:21:LEU:HD22	1:A:32:ALA:HB2	0.67	1.65	9	4
1:A:45:ALA:HB2	1:A:90:TYR:CZ	0.63	2.28	6	2
1:A:104:VAL:HG22	1:A:168:LYS:HE2	0.63	1.70	5	2
1:A:17:LEU:HD21	1:A:70:LEU:CD1	0.63	2.24	11	5
1:A:43:TRP:CZ2	1:A:173:ILE:HD11	0.62	2.29	20	10
1:A:33:VAL:HG11	1:A:102:PHE:CD1	0.62	2.29	7	2
1:A:45:ALA:HB2	1:A:90:TYR:CE1	0.61	2.29	18	2
1:A:99:GLY:CA	1:A:130:MET:HE1	0.59	2.27	12	1
1:A:45:ALA:HB2	1:A:90:TYR:CE2	0.59	2.33	19	6
1:A:126:ALA:HA	1:A:130:MET:HE2	0.58	1.73	6	1
1:A:119:ILE:HD12	1:A:153:TYR:CZ	0.58	2.33	7	1
1:A:69:LEU:HD11	1:A:90:TYR:CE2	0.57	2.34	6	1
1:A:89:ALA:HB2	1:A:124:ARG:HH22	0.57	1.59	18	1
1:A:151:LEU:HD13	1:A:157:MET:SD	0.57	2.39	19	3
1:A:55:THR:HG21	1:A:71:TYR:CZ	0.56	2.35	14	1
1:A:60:PRO:CG	1:A:69:LEU:HD12	0.56	2.31	10	7
1:A:60:PRO:HG2	1:A:69:LEU:HD12	0.56	1.77	15	7
1:A:74:ARG:NH1	1:A:104:VAL:HG11	0.55	2.16	16	1
1:A:89:ALA:HB1	1:A:97:THR:HG22	0.55	1.78	20	6
1:A:157:MET:CB	1:A:173:ILE:HG22	0.55	2.31	17	7
1:A:157:MET:HB3	1:A:173:ILE:HG22	0.55	1.77	8	8
1:A:31:ILE:HG21	1:A:84:ALA:HB3	0.55	1.77	1	2
1:A:101:MET:HB3	1:A:134:LEU:HD13	0.55	1.79	2	2
1:A:21:LEU:CB	1:A:32:ALA:HB2	0.55	2.32	19	1
1:A:21:LEU:HD11	1:A:30:LYS:CB	0.53	2.34	14	1
1:A:54:THR:HG22	1:A:74:ARG:O	0.53	2.04	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:86:ALA:HB3	1:A:102:PHE:CE2	0.53	2.39	12	5
1:A:46:LEU:HD12	1:A:125:ARG:HA	0.53	1.80	4	1
1:A:160:ILE:HD11	1:A:162:THR:HG23	0.52	1.80	10	3
1:A:33:VAL:HG11	1:A:102:PHE:CE2	0.52	2.40	12	2
1:A:12:LEU:HD13	1:A:17:LEU:HD23	0.52	1.80	6	1
1:A:33:VAL:C	1:A:70:LEU:HD23	0.52	2.30	5	2
1:A:17:LEU:HD13	1:A:21:LEU:HD23	0.52	1.81	9	1
1:A:33:VAL:HG11	1:A:102:PHE:CE1	0.52	2.40	6	2
1:A:35:ILE:HD11	1:A:100:VAL:HB	0.52	1.82	6	1
1:A:31:ILE:HD11	1:A:102:PHE:CD2	0.51	2.41	6	2
1:A:35:ILE:HG23	1:A:171:ILE:O	0.51	2.06	5	1
1:A:35:ILE:HG21	1:A:98:LEU:CD2	0.51	2.36	11	4
1:A:31:ILE:HD11	1:A:102:PHE:CD1	0.50	2.41	16	3
1:A:63:VAL:HG21	1:A:69:LEU:HD22	0.50	1.83	2	1
1:A:157:MET:HB2	1:A:173:ILE:HG22	0.49	1.84	7	2
1:A:74:ARG:CZ	1:A:104:VAL:HG11	0.49	2.37	16	1
1:A:6:ILE:HD11	1:A:70:LEU:HG	0.49	1.84	1	1
1:A:89:ALA:HB1	1:A:97:THR:CG2	0.49	2.38	13	9
1:A:155:LEU:HD11	1:A:173:ILE:HB	0.49	1.84	6	1
1:A:24:LEU:C	1:A:24:LEU:HD12	0.49	2.33	16	1
1:A:31:ILE:HD13	1:A:32:ALA:N	0.49	2.23	5	4
1:A:98:LEU:HD22	1:A:173:ILE:HD13	0.49	1.85	19	2
1:A:21:LEU:HB2	1:A:32:ALA:HB2	0.48	1.84	19	1
1:A:101:MET:HB2	1:A:134:LEU:HD13	0.48	1.85	12	2
1:A:17:LEU:HD11	1:A:70:LEU:HD13	0.48	1.85	14	1
1:A:87:ALA:HB1	1:A:130:MET:HE2	0.48	1.85	7	2
1:A:170:GLN:C	1:A:171:ILE:HD12	0.48	2.33	6	3
1:A:33:VAL:HG13	1:A:71:TYR:HB3	0.48	1.85	1	5
1:A:7:ILE:HD13	1:A:11:SER:OG	0.48	2.09	6	1
1:A:118:LYS:HA	1:A:151:LEU:HD21	0.47	1.85	20	1
1:A:24:LEU:HD11	1:A:30:LYS:HD2	0.47	1.86	13	1
1:A:12:LEU:CD1	1:A:17:LEU:HD23	0.47	2.39	7	3
1:A:115:TRP:CZ3	1:A:157:MET:HE1	0.47	2.44	12	1
1:A:155:LEU:HD12	1:A:156:ARG:N	0.47	2.25	11	1
1:A:101:MET:HE2	1:A:102:PHE:CA	0.47	2.39	1	1
1:A:98:LEU:HD13	1:A:173:ILE:HG21	0.47	1.87	11	2
1:A:32:ALA:HB1	1:A:70:LEU:HD21	0.47	1.86	12	1
1:A:169:MET:HE3	1:A:171:ILE:CD1	0.46	2.40	15	1
1:A:160:ILE:HD13	1:A:161:MET:N	0.46	2.26	9	2
1:A:21:LEU:C	1:A:21:LEU:HD12	0.46	2.35	14	1
1:A:6:ILE:HD11	1:A:70:LEU:CG	0.46	2.41	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:117:VAL:HG11	1:A:157:MET:SD	0.45	2.51	1	1
1:A:30:LYS:HZ3	1:A:166:GLU:HG2	0.45	1.70	6	1
1:A:85:VAL:HG22	1:A:103:SER:HA	0.45	1.87	7	1
1:A:37:ASN:HB3	1:A:43:TRP:CZ2	0.45	2.46	7	2
1:A:88:PHE:C	1:A:130:MET:HE1	0.45	2.36	20	1
1:A:32:ALA:HB3	1:A:168:LYS:HG2	0.45	1.87	19	2
1:A:33:VAL:HG21	1:A:102:PHE:CD2	0.45	2.47	3	1
1:A:101:MET:HE2	1:A:102:PHE:HA	0.45	1.88	1	1
1:A:101:MET:CB	1:A:134:LEU:HD13	0.45	2.42	2	2
1:A:114:TRP:CZ2	1:A:135:TYR:CE2	0.45	3.04	4	1
1:A:117:VAL:O	1:A:151:LEU:HD11	0.45	2.11	19	1
1:A:101:MET:SD	1:A:114:TRP:CZ3	0.45	3.10	10	1
1:A:101:MET:O	1:A:169:MET:HE1	0.44	2.12	1	2
1:A:149:LYS:CE	1:A:151:LEU:HD12	0.44	2.42	3	1
1:A:32:ALA:HB1	1:A:70:LEU:HD11	0.44	1.90	8	1
1:A:57:VAL:HG23	1:A:71:TYR:CE1	0.44	2.48	11	2
1:A:46:LEU:HD11	1:A:91:TYR:HB2	0.44	1.88	20	1
1:A:101:MET:SD	1:A:114:TRP:CH2	0.44	3.11	4	1
1:A:37:ASN:HB3	1:A:43:TRP:CH2	0.43	2.47	7	1
1:A:146:TRP:CE3	1:A:158:LYS:CG	0.43	3.02	1	1
1:A:101:MET:HE2	1:A:169:MET:HE1	0.43	1.89	2	1
1:A:119:ILE:HD12	1:A:151:LEU:HD22	0.43	1.91	20	1
1:A:146:TRP:CE3	1:A:158:LYS:HG3	0.43	2.49	1	2
1:A:32:ALA:HB1	1:A:70:LEU:CD2	0.43	2.44	19	1
1:A:31:ILE:CD1	1:A:102:PHE:CD2	0.43	3.02	6	1
1:A:21:LEU:HD13	1:A:31:ILE:C	0.43	2.39	8	1
1:A:50:PHE:CZ	1:A:55:THR:HG23	0.43	2.49	12	1
1:A:17:LEU:HD11	1:A:70:LEU:HD11	0.42	1.90	1	2
1:A:21:LEU:HD11	1:A:30:LYS:HB2	0.42	1.91	14	1
1:A:31:ILE:CD1	1:A:102:PHE:CD1	0.42	3.01	16	1
1:A:99:GLY:HA3	1:A:130:MET:HE1	0.42	1.89	12	1
1:A:149:LYS:HE3	1:A:151:LEU:HD12	0.42	1.92	18	2
1:A:151:LEU:HD22	1:A:153:TYR:CE2	0.42	2.49	7	1
1:A:35:ILE:HG12	1:A:98:LEU:HD21	0.42	1.92	6	1
1:A:115:TRP:CE3	1:A:171:ILE:HD11	0.42	2.50	6	1
1:A:84:ALA:H	1:A:104:VAL:CG2	0.42	2.27	17	1
1:A:101:MET:SD	1:A:115:TRP:HA	0.42	2.54	15	2
1:A:89:ALA:HB2	1:A:130:MET:CE	0.41	2.44	8	1
1:A:33:VAL:HG21	1:A:102:PHE:CD1	0.41	2.50	10	1
1:A:160:ILE:CD1	1:A:162:THR:HG23	0.41	2.45	10	1
1:A:21:LEU:CD2	1:A:32:ALA:HB2	0.41	2.44	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:TRP:CE3	1:A:160:ILE:HB	0.41	2.50	1	1
1:A:102:PHE:CD1	1:A:102:PHE:C	0.41	2.98	13	1
1:A:7:ILE:HD12	1:A:9:GLY:H	0.41	1.75	6	1
1:A:24:LEU:CD1	1:A:72:SER:HB2	0.41	2.44	12	1
1:A:31:ILE:CG2	1:A:84:ALA:HB3	0.41	2.46	3	1
1:A:3:ALA:HB3	1:A:57:VAL:HG11	0.41	1.91	8	1
1:A:31:ILE:HD13	1:A:31:ILE:C	0.41	2.41	17	1
1:A:6:ILE:HD11	1:A:70:LEU:HD12	0.41	1.93	18	1
1:A:17:LEU:HD21	1:A:70:LEU:HD11	0.41	1.93	3	1
1:A:88:PHE:O	1:A:130:MET:HE1	0.41	2.16	5	1
1:A:12:LEU:HD21	1:A:17:LEU:HD23	0.41	1.93	12	1
1:A:89:ALA:HB2	1:A:130:MET:HE1	0.40	1.92	8	1
1:A:105:PRO:CG	1:A:164:ALA:HB2	0.40	2.46	16	1
1:A:21:LEU:HD22	1:A:31:ILE:O	0.40	2.16	1	1
1:A:117:VAL:HG11	1:A:157:MET:HE3	0.40	1.94	9	1
1:A:86:ALA:HB3	1:A:102:PHE:CE1	0.40	2.50	11	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	152/175 (87%)	132±4 (87±3%)	17±4 (11±3%)	4±2 (2±1%)	7	45
All	All	3040/3500 (87%)	2639 (87%)	331 (11%)	70 (2%)	7	45

All 22 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	7	ILE	15
1	A	144	ASN	11
1	A	165	GLY	6
1	A	116	ASP	5
1	A	164	ALA	5
1	A	152	GLY	3

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Mol	Chain	Res	Type	Models (Total)
1	A	65	ASN	3
1	A	64	PRO	3
1	A	54	THR	3
1	A	123	LYS	2
1	A	3	ALA	2
1	A	138	ASN	2
1	A	143	ASP	1
1	A	52	SER	1
1	A	122	GLY	1
1	A	53	GLY	1
1	A	142	GLY	1
1	A	56	ASP	1
1	A	167	ALA	1
1	A	137	GLY	1
1	A	153	TYR	1
1	A	154	GLY	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	121/138 (88%)	93±3 (77±3%)	28±3 (23±3%)	2	28
All	All	2420/2760 (88%)	1863 (77%)	557 (23%)	2	28

All 82 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	31	ILE	20
1	A	46	LEU	19
1	A	17	LEU	18
1	A	19	LYS	18
1	A	100	VAL	16
1	A	133	ASP	16
1	A	13	THR	15
1	A	69	LEU	15
1	A	39	SER	14

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Mol	Chain	Res	Type	Models (Total)
1	A	50	PHE	14
1	A	125	ARG	14
1	A	70	LEU	12
1	A	20	VAL	12
1	A	175	ARG	12
1	A	155	LEU	12
1	A	7	ILE	11
1	A	33	VAL	11
1	A	63	VAL	11
1	A	101	MET	11
1	A	158	LYS	11
1	A	21	LEU	11
1	A	160	ILE	10
1	A	161	MET	10
1	A	30	LYS	10
1	A	149	LYS	10
1	A	168	LYS	10
1	A	2	LEU	9
1	A	113	ASN	8
1	A	157	MET	8
1	A	169	MET	8
1	A	23	GLU	8
1	A	55	THR	7
1	A	92	MET	7
1	A	94	SER	7
1	A	61	GLU	7
1	A	51	ARG	7
1	A	141	ARG	6
1	A	11	SER	6
1	A	150	ASN	6
1	A	138	ASN	6
1	A	37	ASN	5
1	A	118	LYS	5
1	A	127	ASP	5
1	A	144	ASN	5
1	A	54	THR	4
1	A	172	LYS	4
1	A	103	SER	4
1	A	151	LEU	4
1	A	74	ARG	4
1	A	93	SER	4
1	A	130	MET	4

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Mol	Chain	Res	Type	Models (Total)
1	A	156	ARG	4
1	A	65	ASN	4
1	A	24	LEU	4
1	A	135	TYR	3
1	A	132	GLU	3
1	A	140	TYR	3
1	A	148	GLU	3
1	A	38	GLU	3
1	A	47	ASN	3
1	A	162	THR	3
1	A	52	SER	3
1	A	22	GLU	2
1	A	123	LYS	2
1	A	35	ILE	2
1	A	104	VAL	2
1	A	166	GLU	2
1	A	59	LEU	2
1	A	128	GLN	2
1	A	143	ASP	2
1	A	116	ASP	2
1	A	56	ASP	2
1	A	134	LEU	1
1	A	66	THR	1
1	A	124	ARG	1
1	A	12	LEU	1
1	A	90	TYR	1
1	A	67	LYS	1
1	A	117	VAL	1
1	A	72	SER	1
1	A	163	SER	1
1	A	174	SER	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 [i](#)

There are no oligosaccharides 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

No chemical shift data were provided