



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 07:15 PM UTC

PDB ID : 2L9Y / pdb_00002l9y
BMRB ID : 17493
Title : Solution structure of the MoCVNH-LysM module from the rice blast fungus
Magnaporthe oryzae protein (MGG_03307)
Authors : Koharudin, L.M.I.; Viscomi, A.R.; Montanini, B.; Kershaw, M.J.; Talbot, N.J.;
Ottonello, S.; Gronenborn, A.M.
Deposited on : 2011-02-26

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

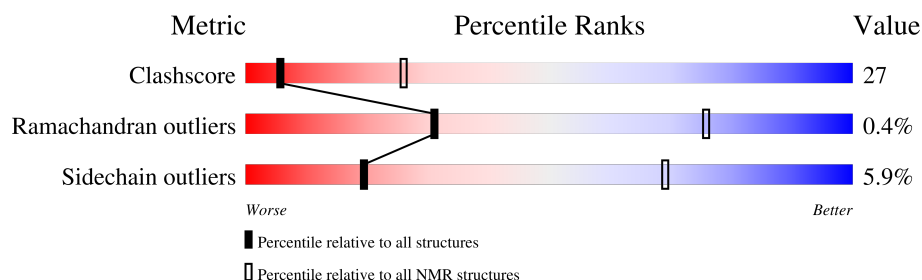
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 62%.

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	167	

2 Ensemble composition and analysis

This entry contains 25 models. Model 24 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:3-A:52, A:118-A:165 (98)	0.32	24
2	A:62-A:109 (48)	0.22	25

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 4 clusters and 1 single-model cluster was found.

Cluster number	Models
1	4, 6, 7, 11, 13, 14, 19, 20, 21, 23
2	2, 5, 9, 16, 18, 24
3	1, 3, 17, 22, 25
4	10, 12, 15
Single-model clusters	8

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2483 atoms, of which 1204 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CVNH-LysM lectin.

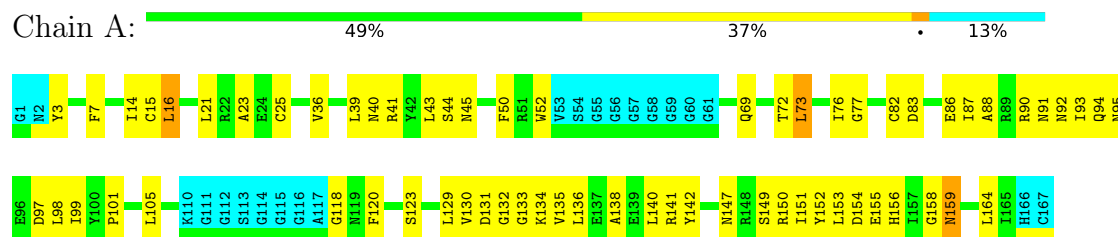
Mol	Chain	Residues	Atoms						Trace
1	A	167	Total	C	H	N	O	S	0
			2483	774	1204	251	250	4	

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: CVNH-LysM lectin

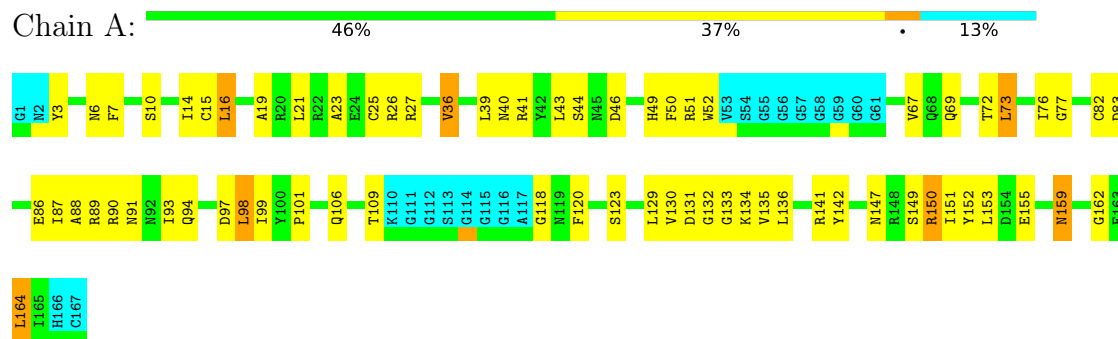


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

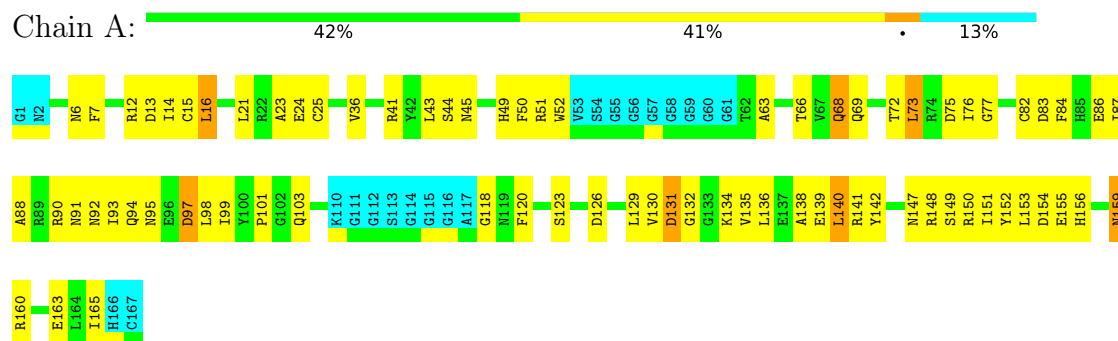
4.2.1 Score per residue for model 1

- Molecule 1: CVNH-LysM lectin



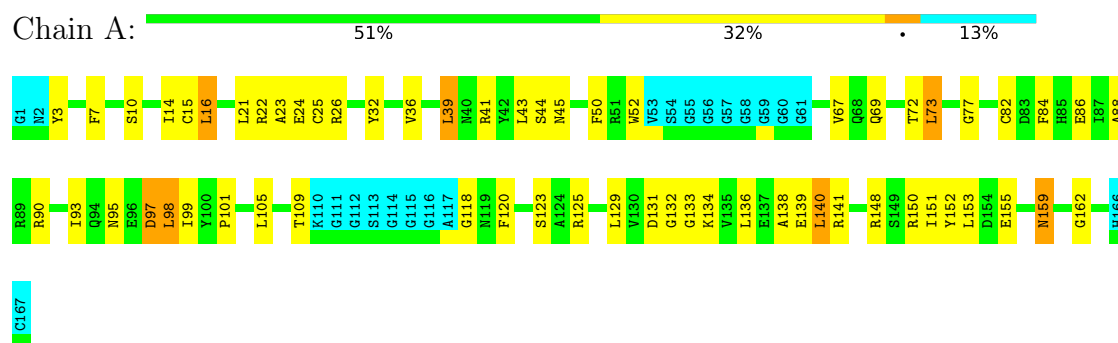
4.2.2 Score per residue for model 2

- Molecule 1: CVNH-LysM lectin



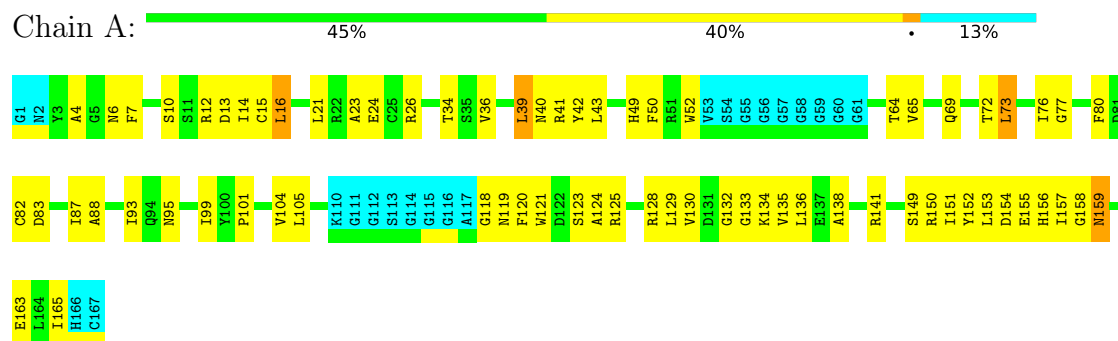
4.2.3 Score per residue for model 3

- Molecule 1: CVNH-LysM lectin



4.2.4 Score per residue for model 4

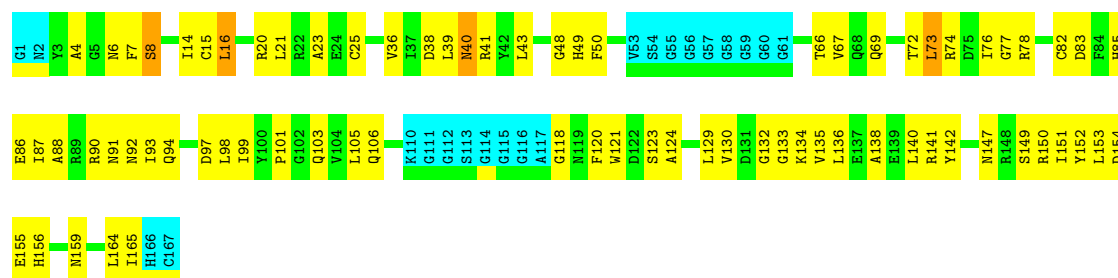
- Molecule 1: CVNH-LysM lectin



4.2.5 Score per residue for model 5

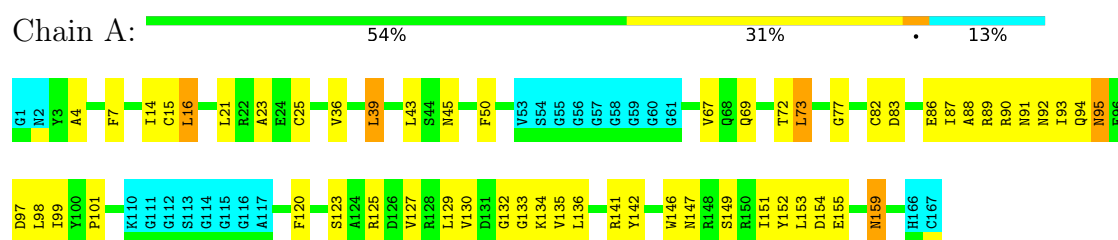
- Molecule 1: CVNH-LysM lectin





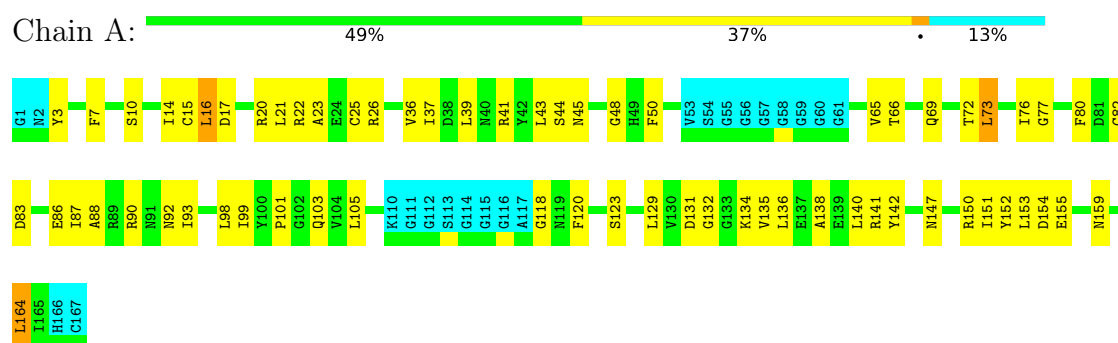
4.2.6 Score per residue for model 6

- Molecule 1: CVNH-LysM lectin



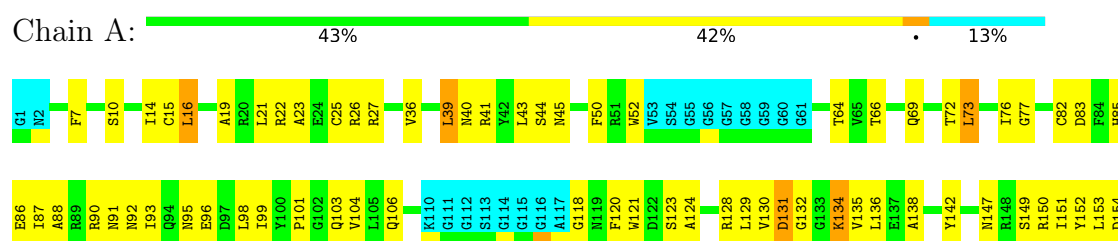
4.2.7 Score per residue for model 7

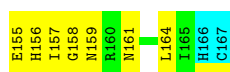
- Molecule 1: CVNH-LysM lectin



4.2.8 Score per residue for model 8

- Molecule 1: CVNH-LysM lectin

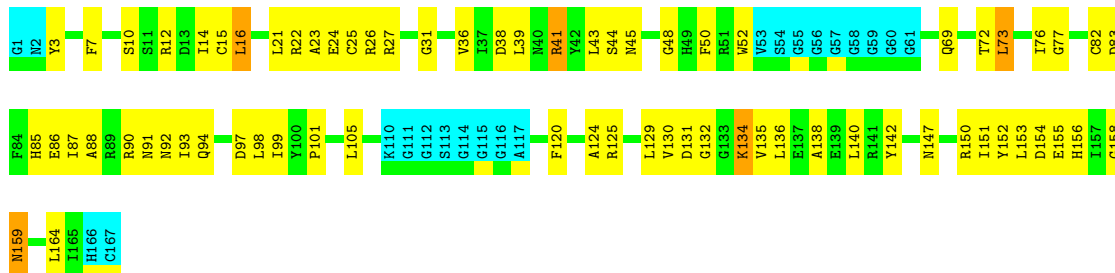




4.2.9 Score per residue for model 9

- Molecule 1: CVNH-LysM lectin

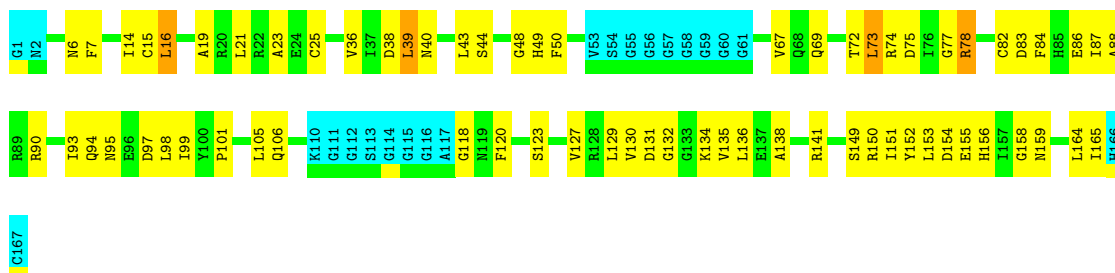
Chain A: 46% 39% 13%



4.2.10 Score per residue for model 10

- Molecule 1: CVNH-LysM lectin

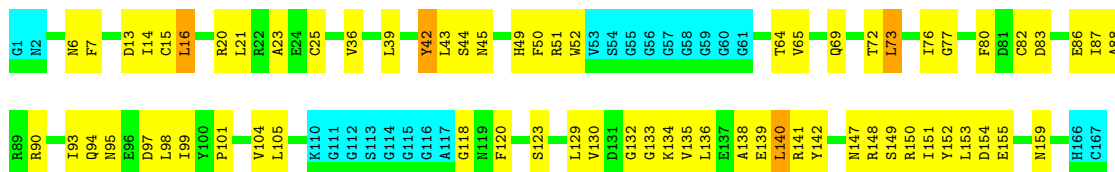
Chain A: 47% 38% 13%



4.2.11 Score per residue for model 11

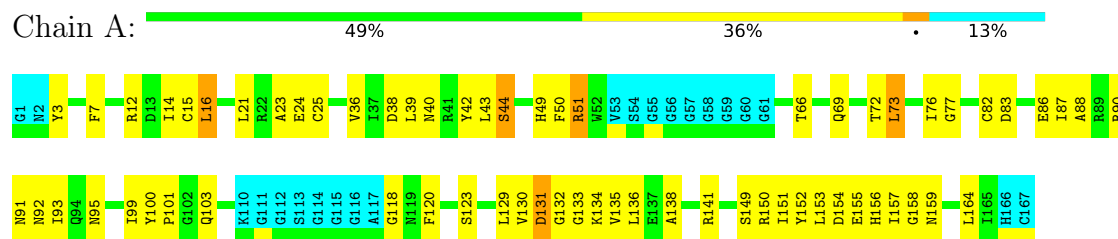
- Molecule 1: CVNH-LysM lectin

Chain A: 47% 38% 13%



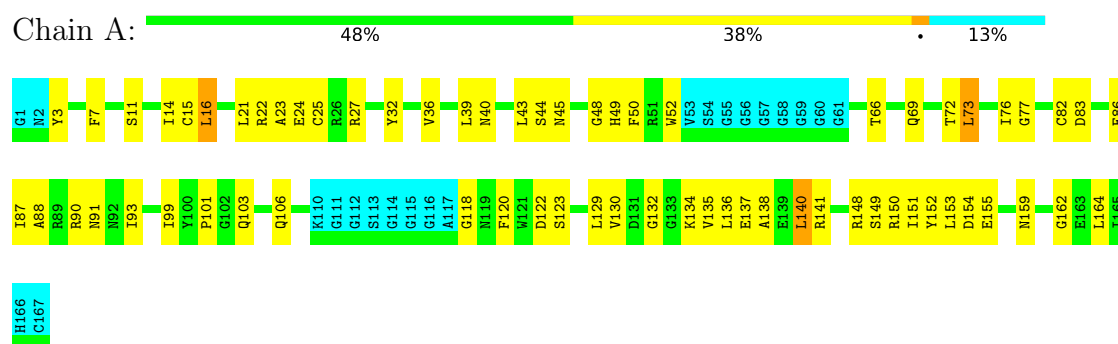
4.2.12 Score per residue for model 12

- Molecule 1: CVNH-LysM lectin



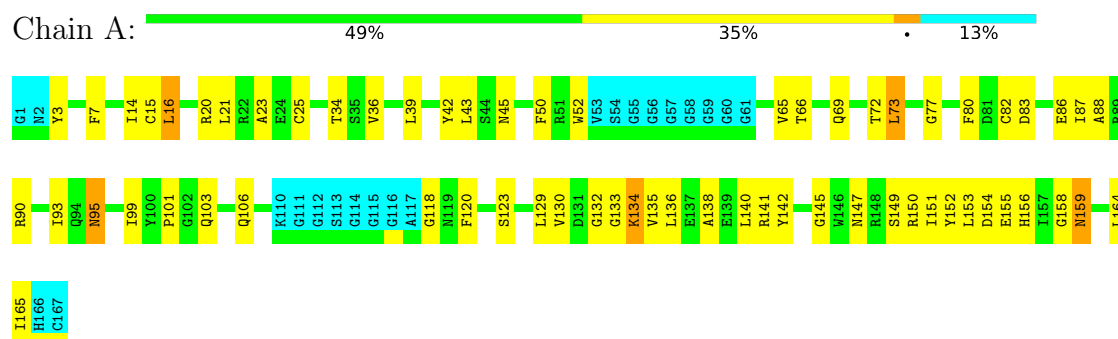
4.2.13 Score per residue for model 13

- Molecule 1: CVNH-LysM lectin



4.2.14 Score per residue for model 14

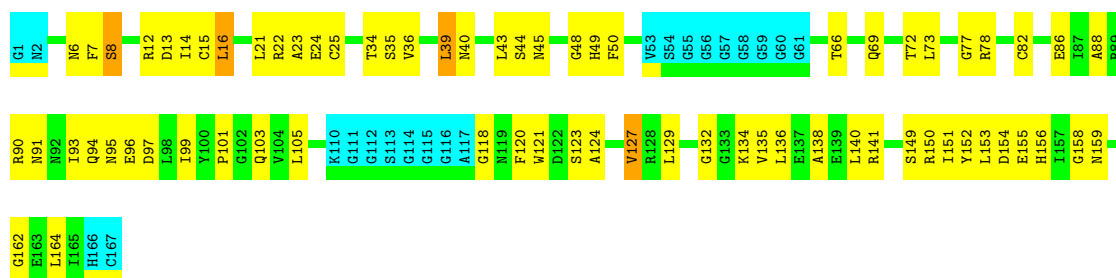
- Molecule 1: CVNH-LysM lectin



4.2.15 Score per residue for model 15

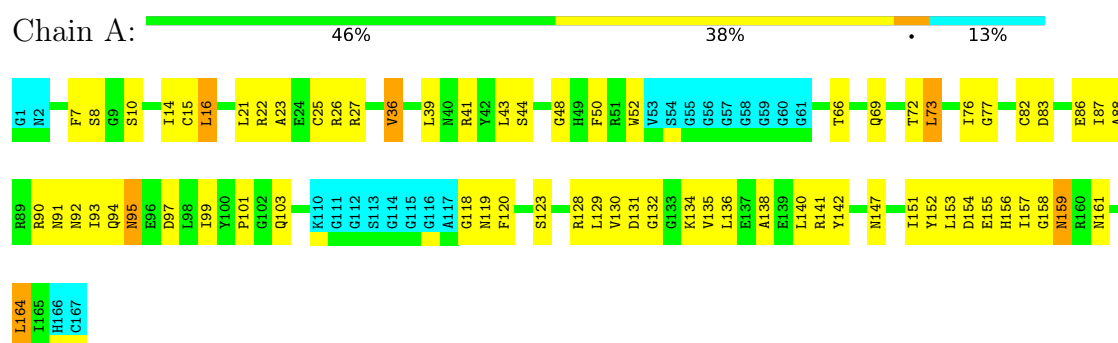
- Molecule 1: CVNH-LysM lectin





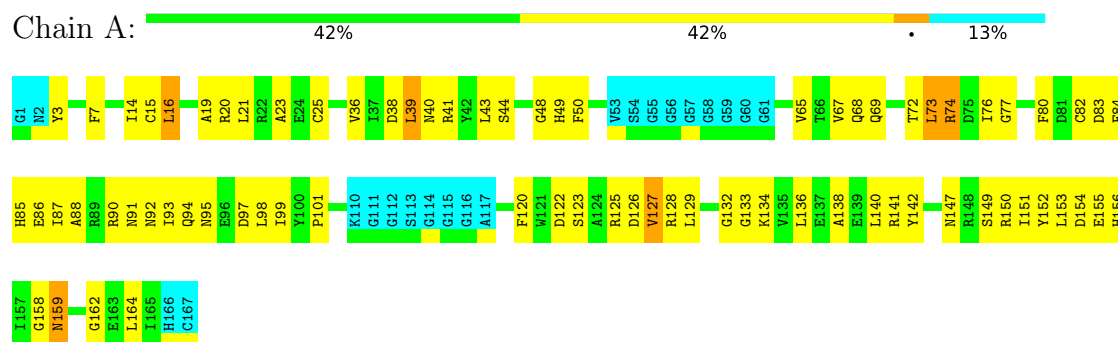
4.2.16 Score per residue for model 16

- Molecule 1: CVNH-LysM lectin



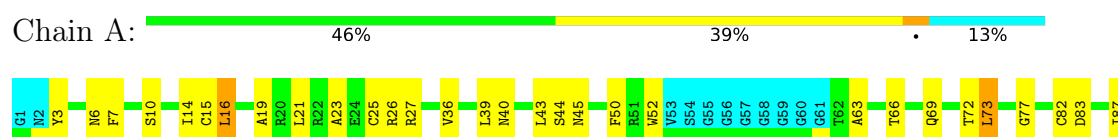
4.2.17 Score per residue for model 17

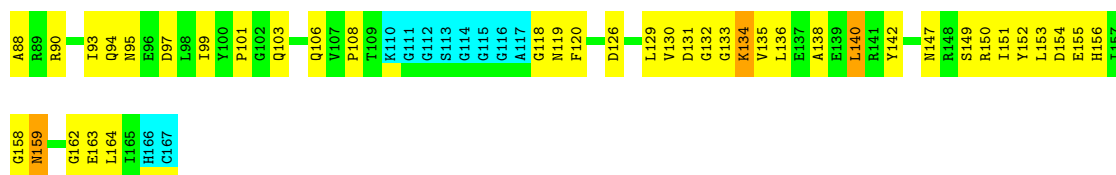
- Molecule 1: CVNH-LysM lectin



4.2.18 Score per residue for model 18

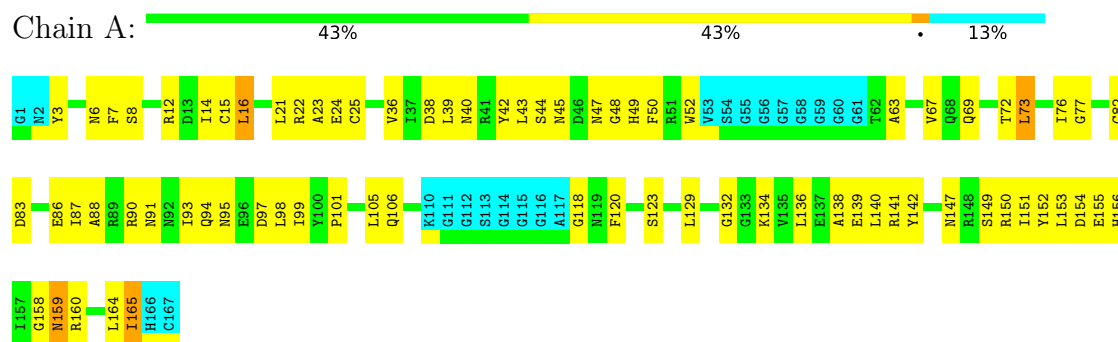
- Molecule 1: CVNH-LysM lectin





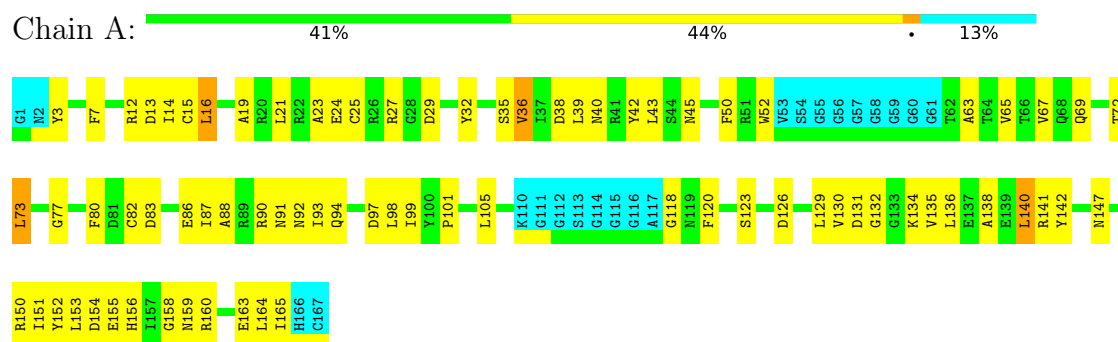
4.2.19 Score per residue for model 19

- Molecule 1: CVNH-LysM lectin



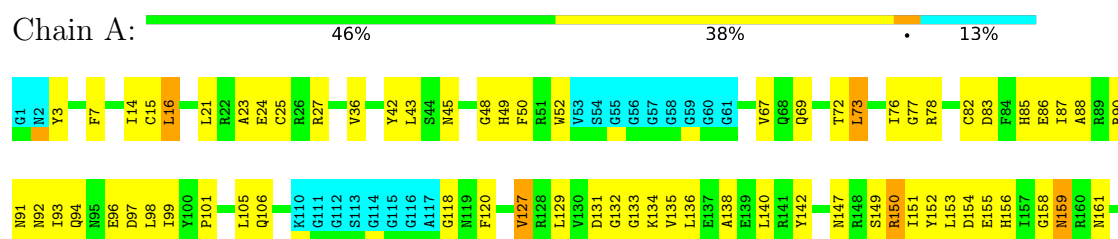
4.2.20 Score per residue for model 20

- Molecule 1: CVNH-LysM lectin



4.2.21 Score per residue for model 21

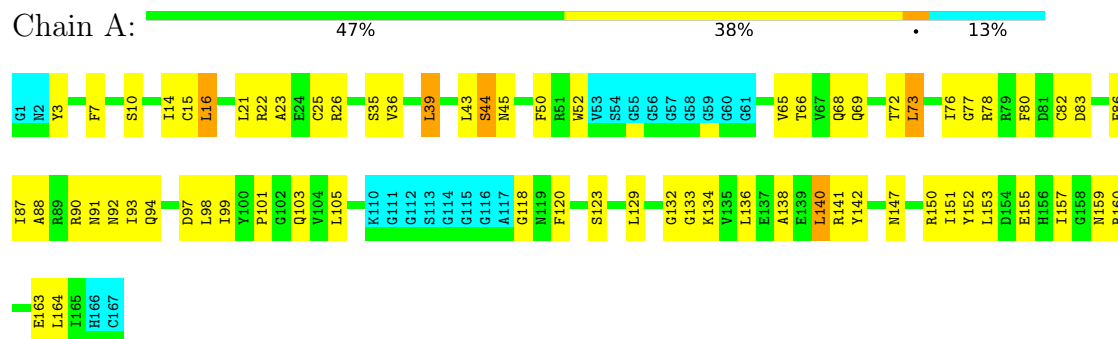
- Molecule 1: CVNH-LysM lectin





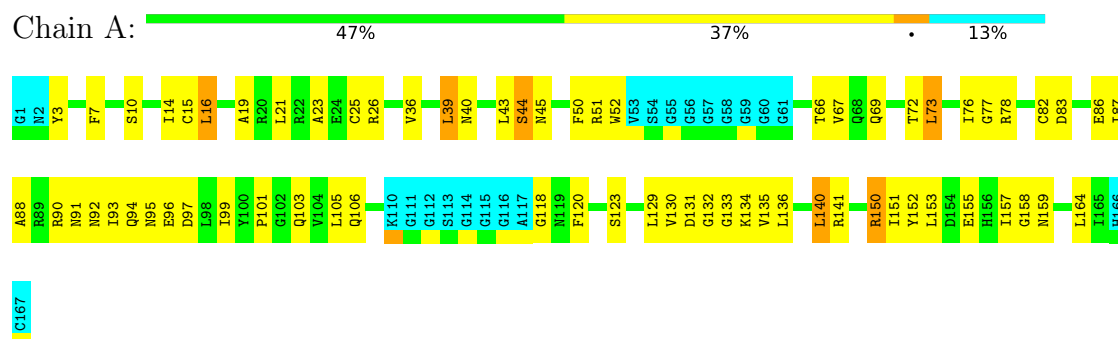
4.2.22 Score per residue for model 22

- Molecule 1: CVNH-LysM lectin



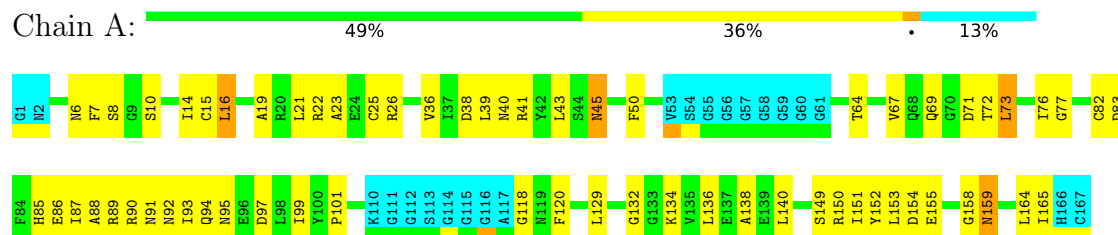
4.2.23 Score per residue for model 23

- Molecule 1: CVNH-LysM lectin



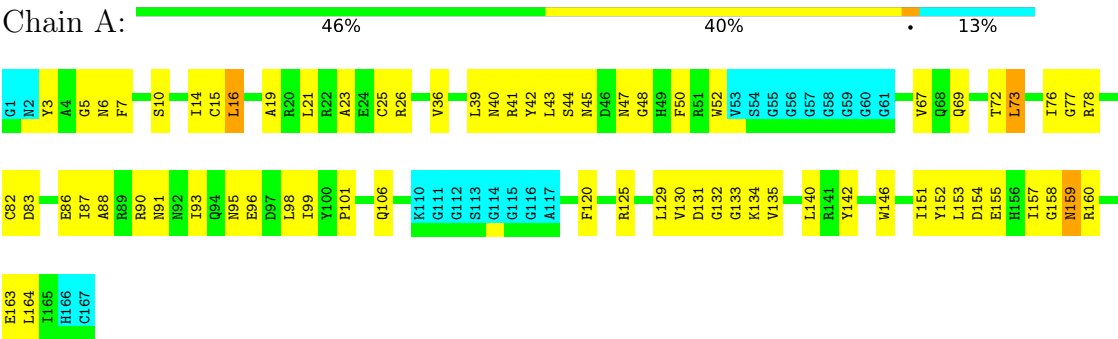
4.2.24 Score per residue for model 24 (medoid)

- Molecule 1: CVNH-LysM lectin



4.2.25 Score per residue for model 25

● Molecule 1: CVNH-LysM lectin



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 25 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CNS	structure calculation	1.1
CNS	refinement	

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	1349
Number of shifts mapped to atoms	1349
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	62%

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	1169	1109	1106	62±4
All	All	29225	27725	27650	1547

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:TYR:HB2	1:A:155:GLU:HA	0.86	1.47	18	13
1:A:14:ILE:HG22	1:A:129:LEU:HD13	0.86	1.46	22	25
1:A:152:TYR:HB2	1:A:155:GLU:HG3	0.83	1.50	16	18
1:A:50:PHE:HB3	1:A:151:ILE:HB	0.83	1.50	1	16
1:A:21:LEU:HD12	1:A:129:LEU:HD11	0.82	1.51	22	3
1:A:45:ASN:CB	1:A:140:LEU:HG	0.79	2.08	3	8
1:A:123:SER:HB3	1:A:141:ARG:HB3	0.78	1.55	23	16
1:A:52:TRP:HZ2	1:A:153:LEU:HA	0.78	1.39	14	5
1:A:130:VAL:HG23	1:A:135:VAL:HB	0.76	1.57	16	16
1:A:131:ASP:HB3	1:A:134:LYS:HE3	0.76	1.57	10	1
1:A:52:TRP:CZ2	1:A:153:LEU:HA	0.76	2.16	14	5
1:A:21:LEU:HB2	1:A:39:LEU:HD22	0.76	1.56	23	11
1:A:43:LEU:HD22	1:A:151:ILE:HD13	0.74	1.57	16	24
1:A:45:ASN:HB3	1:A:140:LEU:HG	0.74	1.58	3	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:PHE:HZ	1:A:138:ALA:HB3	0.74	1.43	3	18
1:A:25:CYS:SG	1:A:164:LEU:HD13	0.74	2.23	1	13
1:A:134:LYS:HA	1:A:154:ASP:HB2	0.73	1.59	6	15
1:A:50:PHE:CB	1:A:151:ILE:HB	0.71	2.15	8	25
1:A:69:GLN:HA	1:A:101:PRO:HB3	0.71	1.61	1	11
1:A:67:VAL:HG21	1:A:99:ILE:HD12	0.70	1.62	3	6
1:A:50:PHE:HB2	1:A:151:ILE:HB	0.69	1.63	14	11
1:A:7:PHE:HD2	1:A:164:LEU:HD11	0.69	1.47	24	10
1:A:7:PHE:CD2	1:A:164:LEU:HD11	0.68	2.23	12	15
1:A:21:LEU:HD22	1:A:153:LEU:HD13	0.67	1.67	7	15
1:A:16:LEU:HD21	1:A:136:LEU:HD12	0.67	1.67	3	1
1:A:152:TYR:HB2	1:A:155:GLU:CG	0.66	2.19	16	14
1:A:133:GLY:O	1:A:153:LEU:HB2	0.66	1.90	14	12
1:A:21:LEU:HD23	1:A:129:LEU:HD11	0.66	1.68	16	1
1:A:77:GLY:HA2	1:A:82:CYS:SG	0.66	2.31	6	25
1:A:129:LEU:HD21	1:A:153:LEU:HD11	0.66	1.65	15	11
1:A:153:LEU:HD12	1:A:157:ILE:HG13	0.66	1.67	25	3
1:A:86:GLU:O	1:A:90:ARG:HG2	0.66	1.91	11	19
1:A:16:LEU:HB3	1:A:21:LEU:HA	0.66	1.68	5	25
1:A:21:LEU:CD2	1:A:129:LEU:HD11	0.65	2.21	16	1
1:A:21:LEU:HD13	1:A:129:LEU:HD11	0.65	1.66	20	14
1:A:90:ARG:HB3	1:A:106:GLN:HB2	0.65	1.68	5	10
1:A:130:VAL:HG23	1:A:135:VAL:HG13	0.65	1.68	10	1
1:A:14:ILE:HG22	1:A:129:LEU:CD1	0.64	2.22	3	25
1:A:123:SER:OG	1:A:141:ARG:HB3	0.64	1.93	6	1
1:A:39:LEU:HD12	1:A:43:LEU:HG	0.64	1.69	22	2
1:A:21:LEU:HD22	1:A:153:LEU:HD23	0.63	1.70	19	3
1:A:44:SER:OG	1:A:118:GLY:HA2	0.62	1.94	12	15
1:A:3:TYR:CD1	1:A:155:GLU:HG2	0.62	2.30	9	9
1:A:21:LEU:CD1	1:A:129:LEU:HD11	0.62	2.24	19	23
1:A:14:ILE:HD12	1:A:132:GLY:O	0.62	1.94	1	25
1:A:99:ILE:HG21	1:A:105:LEU:HD11	0.62	1.71	21	13
1:A:131:ASP:HB3	1:A:134:LYS:HG3	0.62	1.72	12	2
1:A:39:LEU:HG	1:A:153:LEU:HD11	0.62	1.69	12	2
1:A:19:ALA:HB1	1:A:40:ASN:HB3	0.61	1.72	24	8
1:A:46:ASP:HB3	1:A:51:ARG:HD2	0.61	1.71	1	1
1:A:131:ASP:HB3	1:A:134:LYS:HE2	0.61	1.72	25	1
1:A:136:LEU:O	1:A:150:ARG:HA	0.61	1.96	11	22
1:A:69:GLN:CA	1:A:101:PRO:HB3	0.61	2.26	20	23
1:A:48:GLY:HA2	1:A:140:LEU:HB2	0.61	1.73	19	9
1:A:134:LYS:HG3	1:A:135:VAL:HG23	0.61	1.73	21	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ASP:O	1:A:87:ILE:HG13	0.60	1.96	24	23
1:A:50:PHE:CZ	1:A:138:ALA:HB3	0.60	2.30	3	19
1:A:45:ASN:HD22	1:A:120:PHE:HA	0.60	1.57	13	5
1:A:15:CYS:CA	1:A:129:LEU:HD12	0.59	2.27	12	24
1:A:21:LEU:O	1:A:36:VAL:HA	0.59	1.97	21	25
1:A:49:HIS:HA	1:A:149:SER:OG	0.59	1.97	10	12
1:A:139:GLU:HG3	1:A:148:ARG:HH11	0.59	1.57	11	1
1:A:134:LYS:O	1:A:152:TYR:HA	0.58	1.98	11	18
1:A:15:CYS:HA	1:A:129:LEU:HD12	0.58	1.75	12	22
1:A:72:THR:HA	1:A:99:ILE:HG12	0.58	1.75	21	21
1:A:74:ARG:O	1:A:78:ARG:HD3	0.58	1.98	5	1
1:A:7:PHE:CE2	1:A:14:ILE:HD13	0.58	2.34	8	25
1:A:69:GLN:N	1:A:101:PRO:HB3	0.58	2.13	4	19
1:A:152:TYR:CB	1:A:155:GLU:HG3	0.58	2.28	9	24
1:A:25:CYS:HB3	1:A:159:ASN:OD1	0.58	1.99	25	19
1:A:27:ARG:HG2	1:A:162:GLY:HA3	0.58	1.75	13	2
1:A:73:LEU:HD22	1:A:99:ILE:HG23	0.58	1.74	3	24
1:A:45:ASN:ND2	1:A:140:LEU:HD22	0.58	2.14	14	2
1:A:86:GLU:O	1:A:90:ARG:HG3	0.58	1.97	22	4
1:A:91:ASN:HD22	1:A:93:ILE:HD13	0.57	1.58	25	5
1:A:12:ARG:HG2	1:A:24:GLU:HB2	0.57	1.77	12	6
1:A:51:ARG:NE	1:A:51:ARG:HA	0.57	2.15	2	2
1:A:88:ALA:HA	1:A:93:ILE:CG1	0.56	2.31	16	25
1:A:52:TRP:CH2	1:A:153:LEU:HD13	0.56	2.36	25	1
1:A:131:ASP:HB3	1:A:134:LYS:CG	0.56	2.30	2	3
1:A:14:ILE:HA	1:A:22:ARG:O	0.56	2.00	19	6
1:A:123:SER:HB2	1:A:141:ARG:HB3	0.56	1.76	14	2
1:A:43:LEU:HB2	1:A:120:PHE:CD1	0.55	2.35	14	24
1:A:142:TYR:CE1	1:A:147:ASN:HB2	0.55	2.36	2	16
1:A:160:ARG:O	1:A:163:GLU:HG2	0.55	2.01	22	4
1:A:39:LEU:HD21	1:A:153:LEU:HD22	0.55	1.78	24	3
1:A:125:ARG:HD2	1:A:126:ASP:HB2	0.54	1.80	17	1
1:A:43:LEU:CD2	1:A:151:ILE:HD13	0.54	2.33	22	4
1:A:27:ARG:HG2	1:A:162:GLY:CA	0.54	2.33	13	3
1:A:94:GLN:O	1:A:97:ASP:HB2	0.53	2.04	24	16
1:A:73:LEU:CD2	1:A:99:ILE:HG23	0.53	2.34	6	21
1:A:16:LEU:HG	1:A:129:LEU:HG	0.53	1.81	15	17
1:A:38:ASP:HB3	1:A:40:ASN:OD1	0.52	2.04	12	2
1:A:95:ASN:HD22	1:A:96:GLU:HG3	0.52	1.64	23	1
1:A:123:SER:HB3	1:A:141:ARG:CB	0.52	2.31	23	3
1:A:52:TRP:HH2	1:A:153:LEU:HD13	0.52	1.64	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ASN:HD21	1:A:140:LEU:HD22	0.52	1.63	14	1
1:A:14:ILE:HG12	1:A:23:ALA:CB	0.52	2.35	16	25
1:A:73:LEU:HD23	1:A:95:ASN:O	0.52	2.05	12	13
1:A:39:LEU:HD13	1:A:42:TYR:HB2	0.52	1.80	12	2
1:A:78:ARG:O	1:A:78:ARG:HD3	0.52	2.04	10	1
1:A:45:ASN:C	1:A:45:ASN:HD22	0.52	2.13	24	1
1:A:69:GLN:OE1	1:A:101:PRO:HG3	0.52	2.03	7	3
1:A:127:VAL:HB	1:A:138:ALA:CB	0.51	2.35	17	3
1:A:21:LEU:HD22	1:A:22:ARG:N	0.51	2.21	16	1
1:A:25:CYS:HB3	1:A:159:ASN:CG	0.51	2.31	15	12
1:A:24:GLU:HB3	1:A:32:TYR:HB3	0.51	1.83	20	2
1:A:139:GLU:HG2	1:A:148:ARG:HG3	0.50	1.82	2	1
1:A:125:ARG:HB2	1:A:146:TRP:CZ3	0.50	2.42	6	2
1:A:16:LEU:HD23	1:A:39:LEU:HD12	0.50	1.82	16	1
1:A:42:TYR:HD2	1:A:52:TRP:CE3	0.50	2.24	11	1
1:A:152:TYR:HB3	1:A:154:ASP:OD1	0.50	2.06	19	1
1:A:52:TRP:CD1	1:A:151:ILE:HD11	0.50	2.42	13	5
1:A:39:LEU:HD21	1:A:153:LEU:HD11	0.50	1.84	25	1
1:A:45:ASN:ND2	1:A:123:SER:HB2	0.50	2.22	8	2
1:A:19:ALA:CB	1:A:40:ASN:HB3	0.49	2.37	1	4
1:A:134:LYS:HB2	1:A:134:LYS:NZ	0.49	2.23	18	1
1:A:14:ILE:HG12	1:A:23:ALA:HB1	0.49	1.83	24	23
1:A:45:ASN:OD1	1:A:120:PHE:HB2	0.49	2.07	25	1
1:A:16:LEU:HD11	1:A:136:LEU:CD1	0.49	2.38	17	4
1:A:152:TYR:O	1:A:155:GLU:HG3	0.48	2.08	8	14
1:A:15:CYS:O	1:A:22:ARG:HB3	0.48	2.08	3	1
1:A:124:ALA:O	1:A:125:ARG:HD2	0.48	2.08	4	2
1:A:38:ASP:HB3	1:A:41:ARG:CD	0.48	2.37	9	1
1:A:39:LEU:HD13	1:A:43:LEU:HD11	0.48	1.83	16	1
1:A:45:ASN:CG	1:A:140:LEU:HD22	0.48	2.33	25	1
1:A:65:VAL:HG21	1:A:80:PHE:CE2	0.48	2.44	7	7
1:A:45:ASN:ND2	1:A:120:PHE:HB2	0.48	2.24	14	1
1:A:67:VAL:CG2	1:A:99:ILE:HD12	0.48	2.39	21	10
1:A:39:LEU:HD23	1:A:43:LEU:HD11	0.48	1.86	14	2
1:A:21:LEU:HB3	1:A:39:LEU:HD23	0.48	1.84	7	7
1:A:14:ILE:CG2	1:A:21:LEU:HD21	0.48	2.38	16	1
1:A:91:ASN:HD22	1:A:93:ILE:HG23	0.48	1.69	5	1
1:A:14:ILE:CG2	1:A:21:LEU:HD11	0.48	2.39	20	2
1:A:45:ASN:CG	1:A:140:LEU:HB3	0.48	2.33	21	3
1:A:21:LEU:HB2	1:A:39:LEU:CD1	0.47	2.39	16	1
1:A:73:LEU:HD23	1:A:95:ASN:HA	0.47	1.83	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:SER:O	1:A:26:ARG:HB2	0.47	2.09	22	12
1:A:14:ILE:HG23	1:A:23:ALA:HB2	0.47	1.85	18	18
1:A:84:PHE:HD2	1:A:95:ASN:HB2	0.47	1.68	3	3
1:A:21:LEU:HG	1:A:153:LEU:HD13	0.47	1.86	16	1
1:A:131:ASP:O	1:A:134:LYS:HE2	0.47	2.09	8	1
1:A:20:ARG:HG2	1:A:36:VAL:CG2	0.47	2.39	11	1
1:A:50:PHE:HE1	1:A:120:PHE:CD2	0.47	2.28	3	7
1:A:25:CYS:SG	1:A:164:LEU:HG	0.47	2.50	5	5
1:A:20:ARG:HG3	1:A:36:VAL:CG2	0.47	2.40	5	1
1:A:12:ARG:CG	1:A:24:GLU:HB2	0.47	2.40	15	2
1:A:12:ARG:HG2	1:A:13:ASP:N	0.47	2.24	20	1
1:A:66:THR:HA	1:A:103:GLN:O	0.47	2.10	22	12
1:A:160:ARG:HD3	1:A:165:ILE:HD12	0.47	1.86	2	1
1:A:74:ARG:HA	1:A:84:PHE:HB3	0.46	1.86	17	2
1:A:94:GLN:H	1:A:97:ASP:HB2	0.46	1.71	9	1
1:A:27:ARG:HG3	1:A:161:ASN:OD1	0.46	2.10	16	1
1:A:42:TYR:O	1:A:52:TRP:HA	0.46	2.10	4	5
1:A:134:LYS:HA	1:A:154:ASP:HB3	0.46	1.88	18	1
1:A:68:GLN:HE21	1:A:68:GLN:HA	0.46	1.69	2	1
1:A:45:ASN:HB2	1:A:140:LEU:HG	0.46	1.84	18	3
1:A:159:ASN:HA	1:A:163:GLU:O	0.46	2.10	18	2
1:A:14:ILE:HG21	1:A:133:GLY:HA3	0.46	1.88	3	2
1:A:52:TRP:CH2	1:A:157:ILE:HG12	0.46	2.46	23	4
1:A:7:PHE:HB3	1:A:158:GLY:HA2	0.46	1.88	20	5
1:A:131:ASP:HB3	1:A:134:LYS:CE	0.46	2.41	7	1
1:A:21:LEU:HD22	1:A:22:ARG:H	0.45	1.71	16	1
1:A:72:THR:O	1:A:76:ILE:HG12	0.45	2.10	12	18
1:A:91:ASN:O	1:A:92:ASN:HB2	0.45	2.11	24	13
1:A:127:VAL:CG1	1:A:136:LEU:HD11	0.45	2.41	6	2
1:A:88:ALA:HA	1:A:93:ILE:HG13	0.45	1.87	8	13
1:A:129:LEU:HD21	1:A:153:LEU:CD1	0.45	2.39	11	9
1:A:16:LEU:CD2	1:A:39:LEU:HD12	0.45	2.42	16	1
1:A:94:GLN:HB2	1:A:97:ASP:HB2	0.45	1.87	6	1
1:A:137:GLU:OE2	1:A:148:ARG:HD2	0.45	2.11	13	1
1:A:16:LEU:HB3	1:A:21:LEU:CA	0.45	2.40	5	11
1:A:83:ASP:HB3	1:A:86:GLU:HG3	0.45	1.89	14	1
1:A:21:LEU:HD13	1:A:153:LEU:HG	0.44	1.89	25	1
1:A:43:LEU:O	1:A:118:GLY:HA3	0.44	2.12	8	7
1:A:17:ASP:HB3	1:A:20:ARG:HB2	0.44	1.89	7	1
1:A:27:ARG:HD3	1:A:161:ASN:O	0.44	2.13	21	1
1:A:134:LYS:CA	1:A:154:ASP:HB2	0.44	2.39	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:LEU:HD11	1:A:136:LEU:HD13	0.44	1.88	19	3
1:A:43:LEU:HD22	1:A:151:ILE:HG21	0.44	1.88	14	3
1:A:135:VAL:HG22	1:A:152:TYR:CD2	0.44	2.48	16	1
1:A:10:SER:HB3	1:A:26:ARG:HB3	0.44	1.89	18	1
1:A:52:TRP:HZ2	1:A:152:TYR:O	0.44	1.96	25	3
1:A:48:GLY:O	1:A:149:SER:HB2	0.44	2.11	13	3
1:A:38:ASP:OD1	1:A:40:ASN:HB3	0.44	2.13	5	1
1:A:5:GLY:HA3	1:A:157:ILE:O	0.44	2.13	25	1
1:A:21:LEU:CB	1:A:39:LEU:HD23	0.44	2.43	12	4
1:A:73:LEU:HB3	1:A:84:PHE:HB2	0.44	1.89	3	1
1:A:47:ASN:OD1	1:A:142:TYR:HB2	0.44	2.13	25	2
1:A:21:LEU:HD22	1:A:153:LEU:HD12	0.43	1.89	22	1
1:A:25:CYS:HB2	1:A:162:GLY:HA2	0.43	1.89	1	4
1:A:121:TRP:HA	1:A:124:ALA:HB3	0.43	1.89	5	4
1:A:97:ASP:O	1:A:98:LEU:HB2	0.43	2.14	1	5
1:A:68:GLN:HE21	1:A:68:GLN:CA	0.43	2.26	2	1
1:A:139:GLU:HA	1:A:148:ARG:HA	0.43	1.90	3	1
1:A:90:ARG:NE	1:A:90:ARG:HA	0.43	2.29	9	1
1:A:40:ASN:HD22	1:A:121:TRP:HB3	0.43	1.72	15	1
1:A:134:LYS:HB2	1:A:154:ASP:OD2	0.43	2.13	18	1
1:A:21:LEU:HB2	1:A:39:LEU:CD2	0.43	2.42	25	1
1:A:84:PHE:HD1	1:A:95:ASN:HB2	0.43	1.72	2	1
1:A:64:THR:HB	1:A:104:VAL:CG1	0.43	2.44	4	3
1:A:39:LEU:HD12	1:A:43:LEU:CG	0.43	2.41	22	2
1:A:65:VAL:HG21	1:A:80:PHE:CZ	0.43	2.48	17	1
1:A:45:ASN:OD1	1:A:140:LEU:HD22	0.43	2.14	25	1
1:A:27:ARG:HG2	1:A:31:GLY:O	0.43	2.14	9	1
1:A:43:LEU:HD13	1:A:136:LEU:HD23	0.43	1.91	22	2
1:A:43:LEU:CD1	1:A:136:LEU:HD13	0.43	2.43	3	1
1:A:37:ILE:HG22	1:A:164:LEU:HD23	0.42	1.90	7	1
1:A:129:LEU:HD23	1:A:136:LEU:HD13	0.42	1.90	15	2
1:A:40:ASN:HD21	1:A:119:ASN:HA	0.42	1.74	4	1
1:A:96:GLU:HG2	1:A:96:GLU:O	0.42	2.15	21	1
1:A:152:TYR:HB2	1:A:155:GLU:CD	0.42	2.40	24	1
1:A:7:PHE:CE2	1:A:14:ILE:HG21	0.42	2.50	18	4
1:A:95:ASN:ND2	1:A:96:GLU:HG3	0.42	2.30	23	1
1:A:6:ASN:HA	1:A:154:ASP:HB2	0.42	1.92	11	1
1:A:21:LEU:CD2	1:A:153:LEU:HD23	0.42	2.43	14	1
1:A:85:HIS:O	1:A:89:ARG:HG3	0.42	2.14	24	1
1:A:27:ARG:HG3	1:A:161:ASN:CG	0.42	2.39	8	1
1:A:90:ARG:HA	1:A:90:ARG:HE	0.42	1.75	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:LEU:N	1:A:151:ILE:O	0.42	2.53	9	1
1:A:90:ARG:CB	1:A:106:GLN:HB2	0.42	2.45	14	3
1:A:136:LEU:HB2	1:A:153:LEU:HD11	0.42	1.91	19	1
1:A:8:SER:HA	1:A:14:ILE:HD11	0.42	1.90	15	2
1:A:45:ASN:ND2	1:A:123:SER:HB3	0.42	2.30	6	1
1:A:139:GLU:HA	1:A:147:ASN:O	0.42	2.15	19	1
1:A:22:ARG:HA	1:A:35:SER:O	0.42	2.15	15	2
1:A:45:ASN:HB2	1:A:140:LEU:HB3	0.42	1.92	15	1
1:A:40:ASN:HA	1:A:120:PHE:CE1	0.42	2.50	17	2
1:A:25:CYS:SG	1:A:35:SER:HB3	0.42	2.55	20	1
1:A:129:LEU:CD2	1:A:153:LEU:HD11	0.41	2.45	3	1
1:A:78:ARG:HA	1:A:78:ARG:NE	0.41	2.30	25	1
1:A:39:LEU:HD21	1:A:153:LEU:HD13	0.41	1.91	11	1
1:A:27:ARG:HD3	1:A:29:ASP:HB3	0.41	1.91	20	1
1:A:40:ASN:ND2	1:A:119:ASN:HA	0.41	2.30	4	1
1:A:46:ASP:CB	1:A:51:ARG:HD2	0.41	2.42	1	1
1:A:131:ASP:HB3	1:A:134:LYS:HD2	0.41	1.92	21	2
1:A:19:ALA:HB1	1:A:40:ASN:HB2	0.41	1.91	8	1
1:A:100:TYR:HB3	1:A:101:PRO:HD2	0.41	1.91	12	1
1:A:3:TYR:HB2	1:A:155:GLU:CA	0.41	2.40	19	1
1:A:74:ARG:O	1:A:74:ARG:HD3	0.41	2.15	17	1
1:A:39:LEU:HD21	1:A:153:LEU:CD1	0.41	2.45	25	1
1:A:11:SER:OG	1:A:25:CYS:HA	0.41	2.16	13	1
1:A:141:ARG:HA	1:A:145:GLY:O	0.41	2.16	14	1
1:A:50:PHE:CD2	1:A:140:LEU:HD11	0.41	2.51	25	1
1:A:73:LEU:HD12	1:A:87:ILE:HB	0.41	1.93	11	2
1:A:50:PHE:HE2	1:A:120:PHE:CD2	0.41	2.34	7	1
1:A:118:GLY:O	1:A:119:ASN:HB2	0.41	2.16	18	2
1:A:24:GLU:O	1:A:32:TYR:HD2	0.40	1.98	13	1
1:A:71:ASP:HB3	1:A:76:ILE:HD11	0.40	1.93	24	1
1:A:135:VAL:HA	1:A:152:TYR:HA	0.40	1.93	10	1
1:A:12:ARG:CG	1:A:13:ASP:N	0.40	2.85	20	1
1:A:16:LEU:HD23	1:A:39:LEU:HD22	0.40	1.92	25	1
1:A:136:LEU:HD23	1:A:136:LEU:C	0.40	2.41	3	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	146/167 (87%)	134±2 (92±1%)	11±2 (8±1%)	1±1 (0±0%)	31	76
All	All	3650/4175 (87%)	3352 (92%)	284 (8%)	14 (0%)	31	76

All 2 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	98	LEU	13
1	A	165	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	122/129 (95%)	115±2 (94±2%)	7±2 (6±2%)	19	69
All	All	3050/3225 (95%)	2869 (94%)	181 (6%)	19	69

All 41 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	16	LEU	25
1	A	73	LEU	24
1	A	159	ASN	14
1	A	39	LEU	9
1	A	131	ASP	8
1	A	140	LEU	8
1	A	44	SER	6
1	A	8	SER	5
1	A	85	HIS	5
1	A	149	SER	5
1	A	78	ARG	5
1	A	13	ASP	4
1	A	128	ARG	4
1	A	134	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	38	ASP	4
1	A	36	VAL	3
1	A	150	ARG	3
1	A	164	LEU	3
1	A	68	GLN	3
1	A	126	ASP	3
1	A	34	THR	3
1	A	95	ASN	3
1	A	96	GLU	3
1	A	127	VAL	3
1	A	89	ARG	2
1	A	75	ASP	2
1	A	97	ASP	2
1	A	40	ASN	2
1	A	42	TYR	2
1	A	122	ASP	2
1	A	20	ARG	2
1	A	125	ARG	1
1	A	165	ILE	1
1	A	92	ASN	1
1	A	41	ARG	1
1	A	51	ARG	1
1	A	74	ARG	1
1	A	160	ARG	1
1	A	24	GLU	1
1	A	45	ASN	1
1	A	64	THR	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 oligosaccharides 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

The completeness of assignment taking into account all chemical shift lists is 62% for the well-defined parts and 62% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: `mgcvnh2.str`

7.1.1 Bookkeeping

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	1349
Number of shifts mapped to atoms	1349
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	161	-0.24 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	136	0.07 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	164	0.05 ± 0.29	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 62%, i.e. 1244 atoms were assigned a chemical shift out of a possible 1998. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	594/743 (80%)	305/307 (99%)	146/292 (50%)	143/144 (99%)
Sidechain	608/1091 (56%)	371/696 (53%)	236/324 (73%)	1/71 (1%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	42/164 (26%)	39/79 (49%)	0/76 (0%)	3/9 (33%)
Overall	1244/1998 (62%)	715/1082 (66%)	382/692 (55%)	147/224 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 1348 atoms were assigned a chemical shift out of a possible 2170. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	671/861 (78%)	346/362 (96%)	161/334 (48%)	164/165 (99%)
Sidechain	635/1137 (56%)	388/726 (53%)	246/338 (73%)	1/73 (1%)
Aromatic	42/172 (24%)	39/83 (47%)	0/78 (0%)	3/11 (27%)
Overall	1348/2170 (62%)	773/1171 (66%)	407/750 (54%)	168/249 (67%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	89	ARG	CG	36.95	21.24 – 33.19	8.2
1	A	156	HIS	HB3	0.06	1.18 – 4.91	-8.0
1	A	86	GLU	HB2	3.18	1.00 – 3.05	5.7
1	A	86	GLU	HB3	3.18	0.95 – 3.05	5.6
1	A	141	ARG	NE	76.33	76.53 – 92.65	-5.1

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

