



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 01:29 am GMT

PDB ID : 2MZV  
Title : Resonance assignments and secondary structure of a phytocystatin from Sesamum indicum  
Authors : Chyan, C.  
Deposited on : 2015-02-25

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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

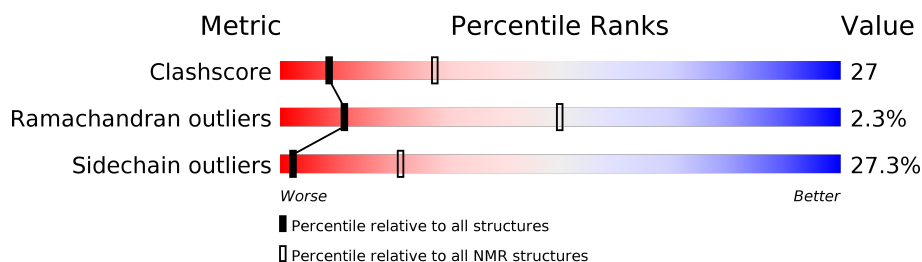
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 85%.

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	199	

## 2 Ensemble composition and analysis

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

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:91 (89)	0.34	1
2	A:112-A:137, A:144-A:183, A:189-A:197 (75)	0.12	13

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

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

There is only 1 type of molecule in this entry. The entry contains 3148 atoms, of which 1571 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cystatin.

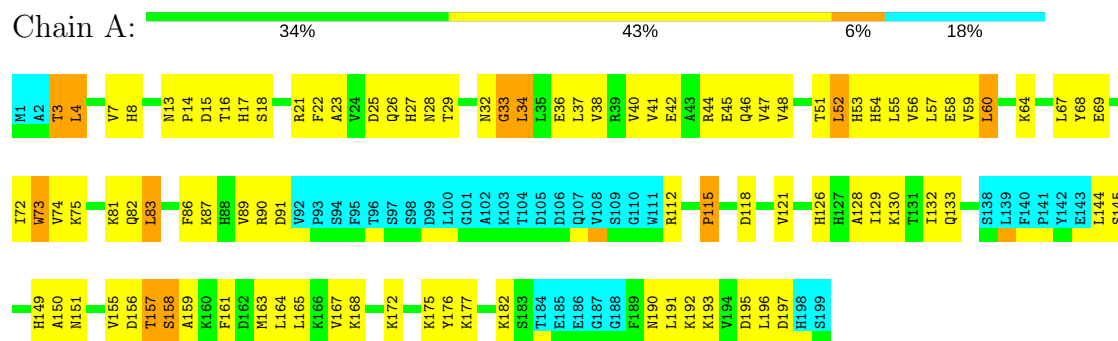
Mol	Chain	Residues	Atoms						Trace
1	A	199	Total	C	H	N	O	S	0
			3148	994	1571	280	300	3	

## 4 Residue-property plots [i](#)

### 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: Cystatin

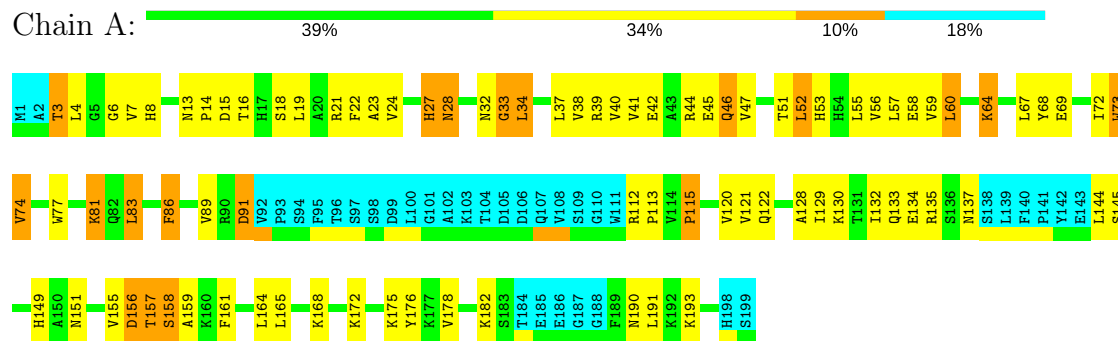


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

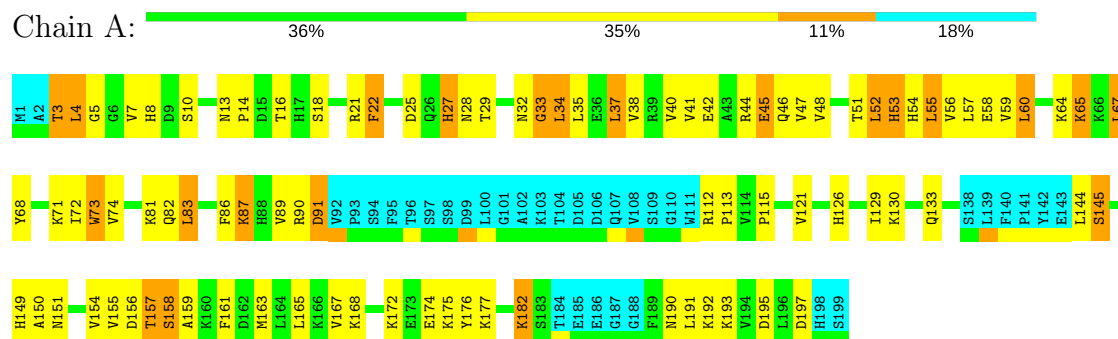
#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Cystatin



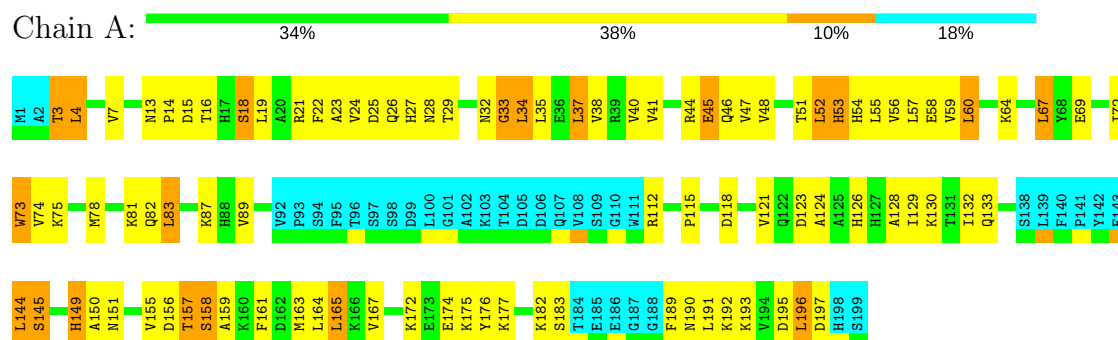
### 4.2.2 Score per residue for model 2

- Molecule 1: Cystatin



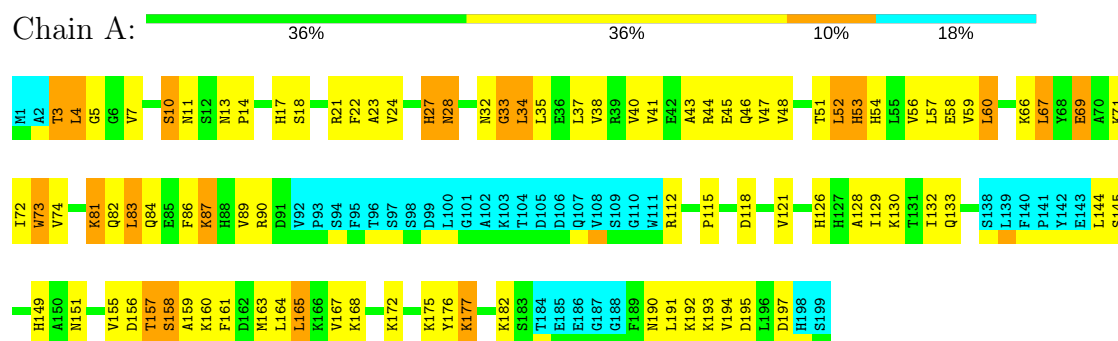
### 4.2.3 Score per residue for model 3

- Molecule 1: Cystatin



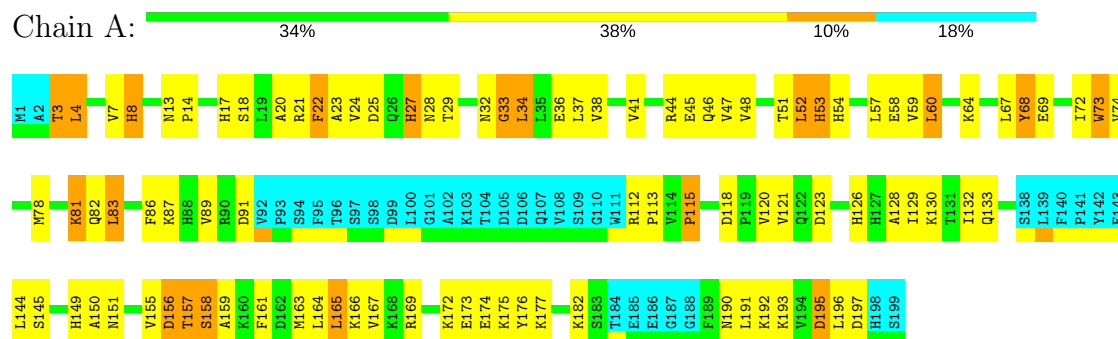
#### 4.2.4 Score per residue for model 4

- Molecule 1: Cystatin



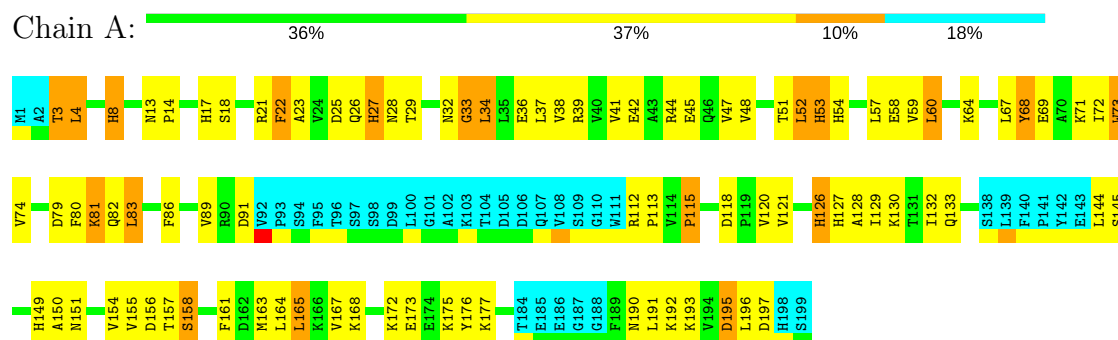
### 4.2.5 Score per residue for model 5

#### • Molecule 1: Cystatin



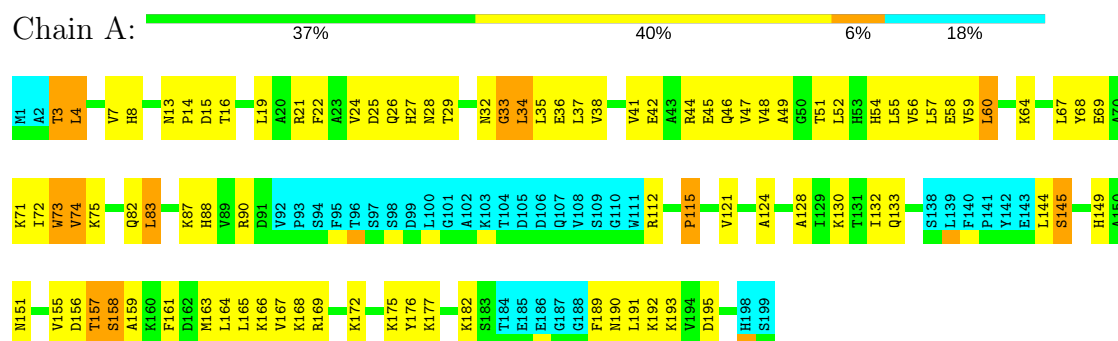
### 4.2.6 Score per residue for model 6

#### • Molecule 1: Cystatin



### 4.2.7 Score per residue for model 7

#### • Molecule 1: Cystatin



- Molecule 1: Cystatin

Chain A:

39% 35% 8% 18%

Nodes in Chain A (177 total):

- Row 1: M1, T3, A2, L4, V7, S10, M13, P14, D15, T16, H17, R21, F22, A23, Q26, H27, N28, T29, N32, G33, L34, L35, E36, L37, V38, R39, V40, V41, E42, A43, R44, E45, Q46, V47, V48, T51, L52, H53, H54, L55, V56, L57, E58, V59, L60, K64, K65, K66, L67, Y68, T72
- Row 2: W73, V74, K75, L83, K87, H88, V89, R90, D91, V92, P93, S94, F95, T96, S97, S98, D99, L100, G101, A102, K103, T104, D105, D106, Q107, V108, S109, G110, W111, R112, P115, D118, V121, H127, A128, L129, K130, T131, L132, Q133, S138, L139, F140, P141, V142, E143, L144, S145, A150, M151, V156

- Molecule 1: Cystatin

Chain A:

Amino Acid	Category 1 (36%)	Category 2 (39%)	Category 3 (8%)	Category 4 (18%)
M1	Yes	No	No	No
A2	Yes	No	No	No
T3	No	Yes	No	No
L4	No	Yes	No	No
V7	Yes	No	No	No
H8	Yes	No	No	No
N13	Yes	No	No	No
P14	Yes	No	No	No
A20	Yes	No	No	No
R21	Yes	No	No	No
F22	Yes	No	No	No
A23	Yes	No	No	No
V24	Yes	No	No	No
D25	Yes	No	No	No
G26	Yes	No	No	No
H27	Yes	No	No	No
N28	Yes	No	No	No
T29	Yes	No	No	No
N32	Yes	No	No	No
G33	Yes	No	No	No
L34	Yes	No	No	No
L35	Yes	No	No	No
E36	Yes	No	No	No
L37	Yes	No	No	No
V38	Yes	No	No	No
R39	Yes	No	No	No
V40	Yes	No	No	No
V41	Yes	No	No	No
E42	Yes	No	No	No
A43	Yes	No	No	No
R44	Yes	No	No	No
E45	Yes	No	No	No
G46	Yes	No	No	No
V47	Yes	No	No	No
V48	Yes	No	No	No
T51	Yes	No	No	No
L52	Yes	No	No	No
H53	Yes	No	No	No
H54	Yes	No	No	No
L55	Yes	No	No	No
V56	Yes	No	No	No
L57	Yes	No	No	No
E58	Yes	No	No	No
V59	Yes	No	No	No
L60	Yes	No	No	No
K64	Yes	No	No	No
K65	Yes	No	No	No
K66	Yes	No	No	No
L67	Yes	No	No	No
V68	Yes	No	No	No
K71	Yes	No	No	No
L72	Yes	No	No	No
V73	Yes	No	No	No
V74	Yes	No	No	No
K75	Yes	No	No	No
P76	Yes	No	No	No
V77	Yes	No	No	No
K78	Yes	No	No	No
D79	Yes	No	No	No
K82	Yes	No	No	No
Q82	Yes	No	No	No
L83	Yes	No	No	No
K87	Yes	No	No	No
R90	Yes	No	No	No
D91	Yes	No	No	No
V92	Yes	No	No	No
P93	Yes	No	No	No
S94	Yes	No	No	No
P95	Yes	No	No	No
T96	Yes	No	No	No
S97	Yes	No	No	No
S98	Yes	No	No	No
D99	Yes	No	No	No
L100	Yes	No	No	No
G101	Yes	No	No	No
A102	Yes	No	No	No
K103	Yes	No	No	No
L104	Yes	No	No	No
D105	Yes	No	No	No
D106	Yes	No	No	No
Q107	Yes	No	No	No
V108	Yes	No	No	No
S109	Yes	No	No	No
G110	Yes	No	No	No
V111	Yes	No	No	No
R112	Yes	No	No	No
P115	Yes	No	No	No
L116	Yes	No	No	No
D118	Yes	No	No	No
V121	Yes	No	No	No
H126	Yes	No	No	No
H127	Yes	No	No	No
A128	Yes	No	No	No
L129	Yes	No	No	No
K130	Yes	No	No	No
V131	Yes	No	No	No
L132	Yes	No	No	No
Q133	Yes	No	No	No
S138	Yes	No	No	No
L139	Yes	No	No	No
F140	Yes	No	No	No
P141	Yes	No	No	No
V142	Yes	No	No	No
E143	Yes	No	No	No
L144	Yes	No	No	No
S145	Yes	No	No	No
H149	Yes	No	No	No
A150	Yes	No	No	No
N151	Yes	No	No	No
V155	Yes	No	No	No
D156	Yes	No	No	No
T157	Yes	No	No	No
S158	Yes	No	No	No
A159	Yes	No	No	No
K160	Yes	No	No	No
F161	Yes	No	No	No
D162	Yes	No	No	No
M163	Yes	No	No	No
L164	Yes	No	No	No
L165	Yes	No	No	No
K166	Yes	No	No	No
V167	Yes</			

- Molecule 1: Cystatin

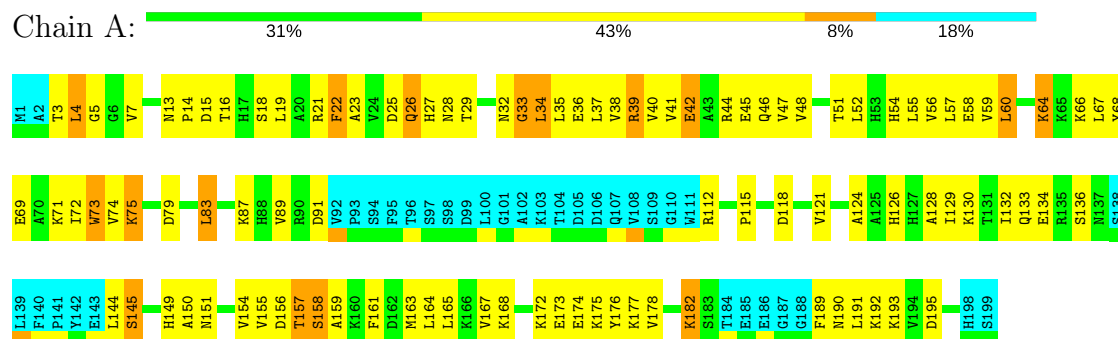
Chain A:

Token	Category	Percentage
M1	Green	32%
A2	Green	32%
T3	Green	32%
L4	Green	32%
G5	Green	32%
G6	Green	32%
V7	Green	32%
M13	Green	32%
P14	Green	32%
D15	Green	32%
S18	Green	32%
L19	Green	32%
A20	Green	32%
R21	Green	32%
F22	Green	32%
A23	Green	32%
V24	Green	32%
D25	Green	32%
Q26	Green	32%
H27	Green	32%
N28	Green	32%
T29	Green	32%
N32	Green	32%
G33	Green	32%
L34	Green	32%
L35	Green	32%
E36	Green	32%
L37	Green	32%
V38	Green	32%
V41	Green	32%
E42	Green	32%
A43	Green	32%
R44	Green	32%
E45	Green	32%
Q46	Green	32%
V47	Green	32%
V48	Green	32%
T51	Green	32%
L52	Green	32%
H53	Green	32%
H54	Green	32%
L55	Green	32%
V56	Green	32%
L57	Green	32%
E58	Green	32%
V59	Green	32%
L60	Green	32%
K64	Green	32%
L67	Green	32%
V68	Green	32%
E69	Green	32%
A70	Green	32%
V71	Green	32%
T72	Green	32%
W73	Green	32%
V74	Green	32%
K75	Green	32%
V76	Green	32%
V77	Green	32%
V78	Green	32%
D79	Green	32%
F80	Green	32%
K81	Green	32%
Q82	Green	32%
L83	Green	32%
K87	Green	32%
H88	Green	32%
V89	Green	32%
F90	Green	32%
D91	Green	32%
V92	Green	32%
P93	Green	32%
S94	Green	32%
F95	Green	32%
T96	Green	32%
S97	Green	32%
S98	Green	32%
D99	Green	32%
L100	Green	32%
G101	Green	32%
A102	Green	32%
K103	Green	32%
T104	Green	32%
D105	Green	32%
V106	Green	32%
Q107	Green	32%
V108	Green	32%
S109	Green	32%
G110	Green	32%
M111	Green	32%
R112	Green	32%
P115	Green	32%
D118	Green	32%
P119	Green	32%
N120	Green	32%
V121	Green	32%
A125	Green	32%
H126	Green	32%
L127	Green	32%
A128	Green	32%
T129	Green	32%
K130	Green	32%
T131	Green	32%
L132	Green	32%
Q133	Green	32%
E134	Green	32%
R135	Green	32%
S136	Green	32%
V137	Green	32%
S138	Green	32%
L139	Green	32%
L140	Green	32%
P141	Green	32%
V142	Green	32%
E143	Green	32%
L144	Green	32%
S145	Green	32%
H149	Green	32%
A150	Green	32%
M151	Green	32%
V154	Green	32%
V155	Green	32%
D156	Green	32%
T157	Green	32%
S158	Green	32%
A159	Green	32%
K160	Green	32%
F161	Green	32%
D162	Green	32%
M163	Green	32%
L164	Green	32%
L165	Green	32%
K168	Green	32%
R169	Green	32%
K172	Green	32%
E173	Green	32%
E174	Green	32%
K175	Green	32%
V176	Green	32%
K177	Green	32%
K182	Green	32%
S183	Green	32%
T184	Green	32%
E185	Green	32%
E186	Green	32%
G187	Green	32%
G188</		



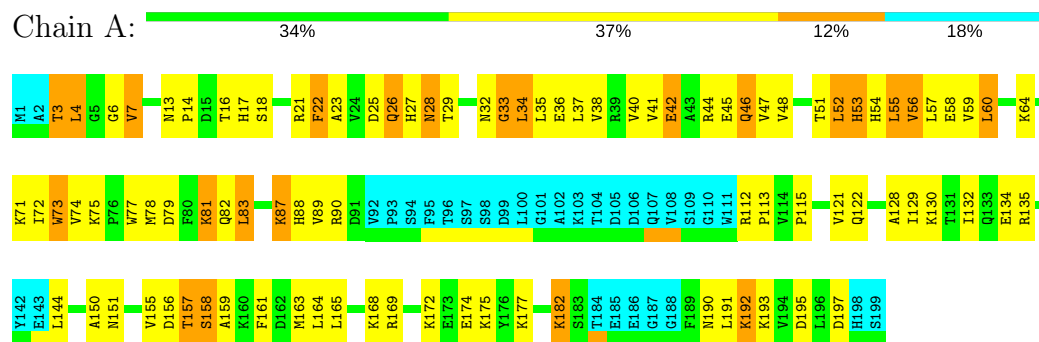
### 4.2.11 Score per residue for model 11

#### • Molecule 1: Cystatin



#### 4.2.14 Score per residue for model 14

- Molecule 1: Cystatin



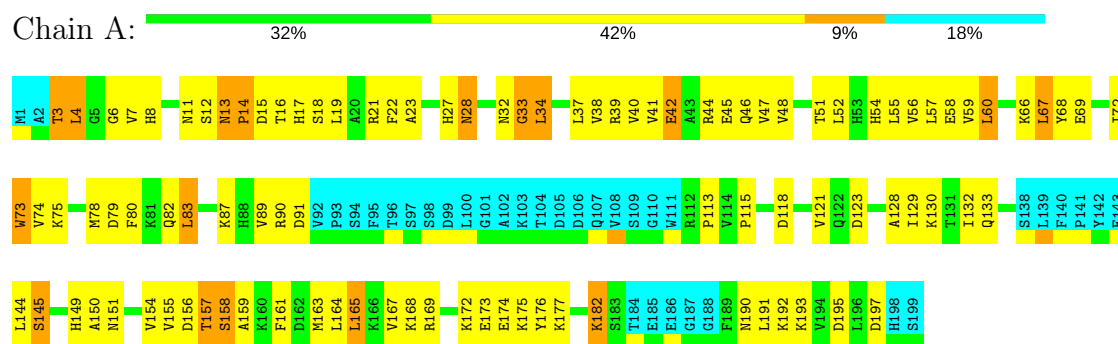
#### 4.2.15 Score per residue for model 15

- Molecule 1: Cystatin



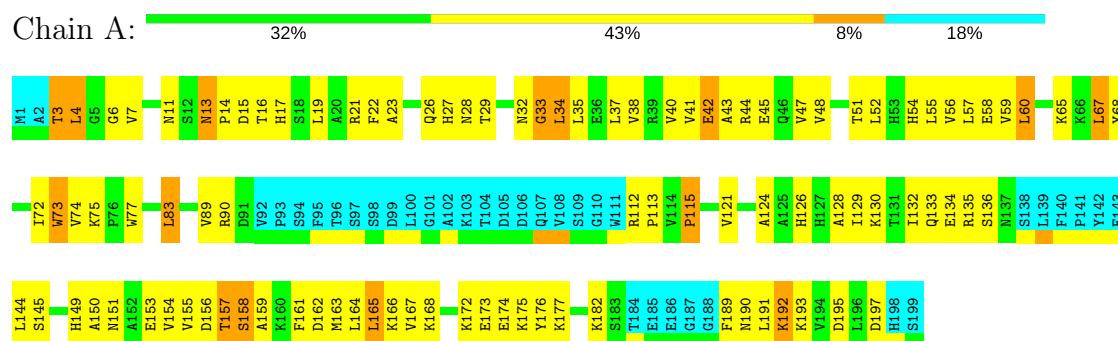
#### 4.2.16 Score per residue for model 16

- Molecule 1: Cystatin



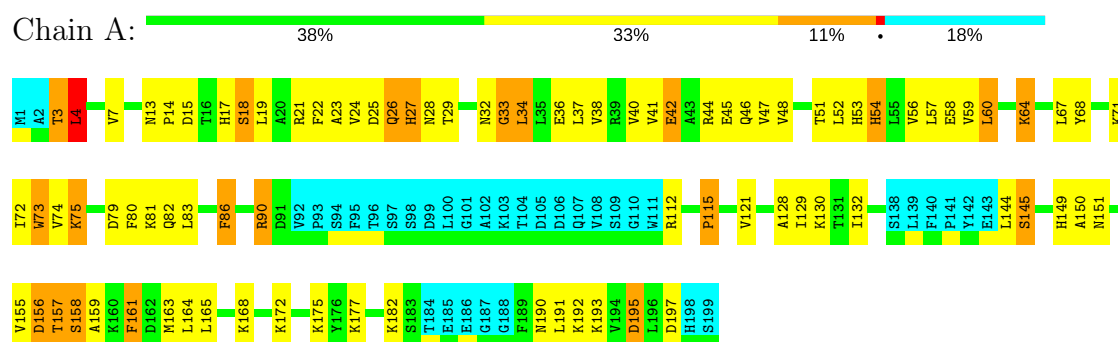
## 4.2.17 Score per residue for model 17

## • Molecule 1: Cystatin



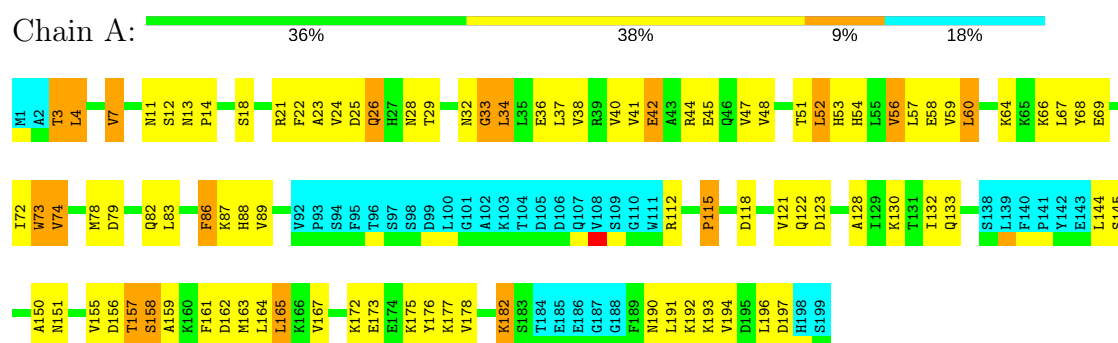
## 4.2.18 Score per residue for model 18

## • Molecule 1: Cystatin



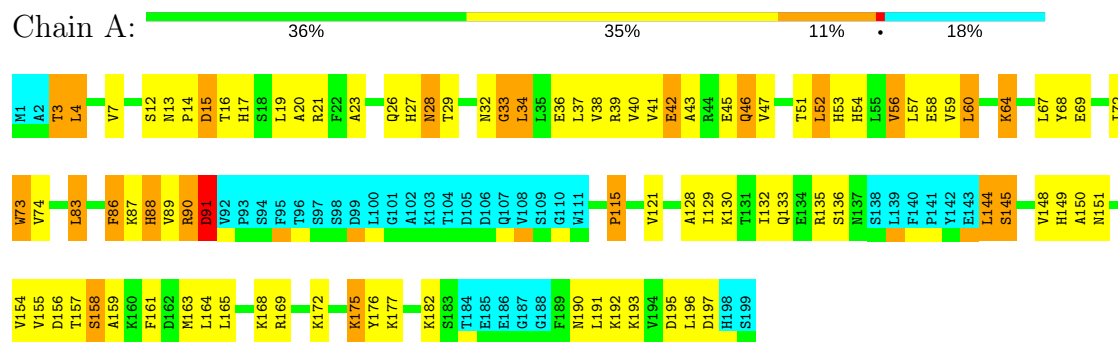
## 4.2.19 Score per residue for model 19

## • Molecule 1: Cystatin



## 4.2.20 Score per residue for model 20

## ● Molecule 1: Cystatin



## 5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 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
CYANA	structure solution	2.1
CNSSOLVE	refinement	1.2
CYANA	refinement	2.1

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)	2mzv_cs.str
Number of chemical shift lists	1
Total number of shifts	2353
Number of shifts mapped to atoms	2353
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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	1315	1339	1328	70±6
All	All	26300	26780	26560	1402

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:129:ILE:HD11	1:A:165:LEU:HD11	1.03	1.27	1	12
1:A:3:THR:HG22	1:A:51:THR:HG21	1.00	1.29	3	8
1:A:52:LEU:HD12	1:A:73:TRP:CH2	0.89	2.01	19	5
1:A:17:HIS:CD2	1:A:40:VAL:HG21	0.88	2.03	14	2
1:A:38:VAL:HG21	1:A:60:LEU:HD23	0.85	1.48	1	6
1:A:4:LEU:HD11	1:A:53:HIS:CE1	0.83	2.08	13	2
1:A:129:ILE:CD1	1:A:165:LEU:HD11	0.83	2.03	1	1
1:A:4:LEU:HD21	1:A:53:HIS:ND1	0.80	1.90	13	3
1:A:46:GLN:CB	1:A:52:LEU:HD12	0.78	2.09	20	2
1:A:56:VAL:HG22	1:A:69:GLU:CG	0.77	2.09	10	1
1:A:17:HIS:CE1	1:A:40:VAL:HG21	0.77	2.14	17	3
1:A:52:LEU:HD23	1:A:73:TRP:CZ3	0.77	2.14	20	3
1:A:52:LEU:HD13	1:A:52:LEU:O	0.76	1.81	20	1
1:A:58:GLU:HG3	1:A:67:LEU:HD22	0.75	1.57	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:THR:HB	1:A:74:VAL:HG13	0.74	1.59	9	11
1:A:52:LEU:HD12	1:A:53:HIS:N	0.74	1.97	2	10
1:A:52:LEU:HD13	1:A:73:TRP:CZ3	0.73	2.18	12	8
1:A:52:LEU:HD22	1:A:53:HIS:N	0.73	1.98	4	3
1:A:46:GLN:HB3	1:A:52:LEU:HD12	0.73	1.60	1	3
1:A:58:GLU:HG2	1:A:67:LEU:HD22	0.73	1.61	17	18
1:A:41:VAL:HG23	1:A:57:LEU:HA	0.72	1.61	4	20
1:A:155:VAL:HG12	1:A:158:SER:O	0.72	1.85	6	19
1:A:164:LEU:HD12	1:A:176:TYR:O	0.71	1.86	15	11
1:A:3:THR:C	1:A:4:LEU:HD13	0.71	2.06	3	10
1:A:3:THR:HG22	1:A:51:THR:OG1	0.71	1.86	9	8
1:A:41:VAL:HG22	1:A:58:GLU:OE2	0.71	1.86	1	2
1:A:52:LEU:O	1:A:52:LEU:HD13	0.70	1.86	1	2
1:A:69:GLU:OE1	1:A:89:VAL:HG11	0.70	1.86	4	7
1:A:38:VAL:CG2	1:A:60:LEU:HD23	0.70	2.17	4	6
1:A:69:GLU:CD	1:A:89:VAL:HG11	0.70	2.07	16	5
1:A:23:ALA:HB2	1:A:83:LEU:HD22	0.70	1.63	1	6
1:A:46:GLN:HB3	1:A:52:LEU:HD22	0.70	1.63	18	2
1:A:7:VAL:HG23	1:A:45:GLU:O	0.69	1.88	8	3
1:A:58:GLU:CG	1:A:67:LEU:HD22	0.69	2.17	4	7
1:A:56:VAL:HG22	1:A:69:GLU:HG2	0.68	1.64	13	3
1:A:167:VAL:HG22	1:A:174:GLU:O	0.68	1.88	9	8
1:A:129:ILE:HD13	1:A:176:TYR:OH	0.68	1.88	9	12
1:A:72:ILE:CD1	1:A:83:LEU:HD23	0.67	2.19	11	17
1:A:4:LEU:HD12	1:A:45:GLU:CD	0.67	2.09	13	3
1:A:41:VAL:HG23	1:A:57:LEU:CA	0.66	2.21	17	20
1:A:144:LEU:HD23	1:A:145:SER:N	0.66	2.05	11	9
1:A:122:GLN:NE2	1:A:144:LEU:HD21	0.65	2.06	1	4
1:A:37:LEU:HA	1:A:59:VAL:HG12	0.65	1.68	3	16
1:A:52:LEU:HD22	1:A:72:ILE:O	0.65	1.91	9	1
1:A:21:ARG:HD3	1:A:37:LEU:HD22	0.65	1.65	19	20
1:A:126:HIS:CD2	1:A:144:LEU:HD23	0.65	2.27	6	4
1:A:51:THR:CG2	1:A:74:VAL:HG13	0.65	2.22	19	11
1:A:74:VAL:HG13	1:A:81:LYS:HA	0.65	1.69	5	8
1:A:72:ILE:HG12	1:A:83:LEU:HD23	0.65	1.67	1	12
1:A:16:THR:HB	1:A:55:LEU:HD21	0.65	1.67	1	5
1:A:67:LEU:N	1:A:67:LEU:HD23	0.64	2.07	17	11
1:A:167:VAL:HG13	1:A:176:TYR:CE1	0.64	2.27	7	3
1:A:155:VAL:HG12	1:A:158:SER:C	0.64	2.13	12	19
1:A:52:LEU:HD12	1:A:73:TRP:CZ3	0.64	2.27	19	5
1:A:10:SER:OG	1:A:43:ALA:HB3	0.64	1.93	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:HIS:CG	1:A:40:VAL:HG21	0.64	2.27	14	1
1:A:4:LEU:HD13	1:A:4:LEU:N	0.63	2.09	14	7
1:A:52:LEU:HD23	1:A:73:TRP:CD1	0.63	2.28	9	2
1:A:52:LEU:C	1:A:52:LEU:HD23	0.63	2.14	17	3
1:A:49:ALA:HB3	1:A:73:TRP:CH2	0.62	2.30	7	1
1:A:60:LEU:HD23	1:A:64:LYS:N	0.62	2.09	14	14
1:A:42:GLU:HG2	1:A:56:VAL:HG13	0.62	1.69	20	6
1:A:4:LEU:N	1:A:4:LEU:HD13	0.62	2.09	6	6
1:A:16:THR:HB	1:A:55:LEU:HD13	0.62	1.70	16	4
1:A:69:GLU:OE2	1:A:89:VAL:HG11	0.62	1.94	13	4
1:A:164:LEU:HD13	1:A:177:LYS:HD2	0.61	1.71	9	14
1:A:48:VAL:HG11	1:A:73:TRP:CZ2	0.61	2.29	13	11
1:A:67:LEU:HD23	1:A:67:LEU:N	0.61	2.10	4	9
1:A:52:LEU:HD23	1:A:52:LEU:C	0.61	2.15	18	2
1:A:25:ASP:O	1:A:29:THR:HG22	0.60	1.97	19	13
1:A:56:VAL:HG22	1:A:69:GLU:HG3	0.60	1.74	10	1
1:A:15:ASP:O	1:A:19:LEU:HD23	0.60	1.97	17	9
1:A:115:PRO:O	1:A:121:VAL:HG21	0.59	1.96	4	14
1:A:23:ALA:HA	1:A:83:LEU:HD22	0.59	1.74	20	3
1:A:24:VAL:HG21	1:A:37:LEU:HD11	0.59	1.71	18	7
1:A:121:VAL:HG13	1:A:163:MET:SD	0.59	2.37	2	11
1:A:42:GLU:HG2	1:A:56:VAL:CG1	0.59	2.27	17	6
1:A:4:LEU:HD23	1:A:51:THR:HG21	0.59	1.73	20	2
1:A:34:LEU:N	1:A:34:LEU:HD13	0.58	2.14	2	7
1:A:3:THR:HG22	1:A:51:THR:CB	0.58	2.29	10	2
1:A:40:VAL:HG22	1:A:57:LEU:HD12	0.58	1.74	9	12
1:A:72:ILE:HG21	1:A:81:LYS:HD2	0.58	1.75	13	1
1:A:165:LEU:HD11	1:A:176:TYR:OH	0.58	1.98	19	2
1:A:34:LEU:HD13	1:A:34:LEU:N	0.57	2.15	18	13
1:A:21:ARG:CD	1:A:37:LEU:HD22	0.57	2.30	5	11
1:A:41:VAL:HG12	1:A:42:GLU:CD	0.57	2.19	16	6
1:A:52:LEU:HD22	1:A:52:LEU:C	0.57	2.19	20	3
1:A:165:LEU:HD23	1:A:165:LEU:N	0.57	2.15	20	1
1:A:72:ILE:CG1	1:A:83:LEU:HD23	0.57	2.29	1	12
1:A:74:VAL:HG13	1:A:81:LYS:CA	0.56	2.30	15	8
1:A:4:LEU:HD22	1:A:51:THR:HG23	0.56	1.76	10	1
1:A:7:VAL:HG22	1:A:46:GLN:HA	0.56	1.77	4	7
1:A:159:ALA:HB3	1:A:182:LYS:HB2	0.56	1.78	12	18
1:A:176:TYR:HB3	1:A:196:LEU:HD13	0.56	1.78	19	2
1:A:48:VAL:HG11	1:A:73:TRP:CH2	0.56	2.35	3	4
1:A:7:VAL:HG13	1:A:7:VAL:O	0.56	2.00	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:GLN:CB	1:A:52:LEU:HD22	0.56	2.31	11	1
1:A:4:LEU:HD22	1:A:4:LEU:N	0.56	2.16	4	2
1:A:51:THR:CB	1:A:74:VAL:HG13	0.56	2.31	9	11
1:A:38:VAL:HG22	1:A:60:LEU:HD12	0.55	1.77	13	14
1:A:4:LEU:N	1:A:4:LEU:HD22	0.55	2.16	2	2
1:A:155:VAL:HG22	1:A:160:LYS:HG3	0.55	1.77	8	1
1:A:46:GLN:HB3	1:A:52:LEU:HD23	0.55	1.77	14	3
1:A:33:GLY:C	1:A:34:LEU:HD13	0.55	2.22	7	20
1:A:7:VAL:HG13	1:A:45:GLU:O	0.55	2.01	3	2
1:A:16:THR:HG21	1:A:43:ALA:HB2	0.55	1.78	20	1
1:A:155:VAL:HG13	1:A:157:THR:H	0.55	1.61	12	19
1:A:52:LEU:HD13	1:A:73:TRP:HZ3	0.55	1.58	13	10
1:A:37:LEU:HD23	1:A:57:LEU:HD13	0.55	1.78	20	11
1:A:4:LEU:HD12	1:A:45:GLU:OE2	0.55	2.02	1	2
1:A:3:THR:CG2	1:A:51:THR:HG21	0.55	2.31	5	2
1:A:26:GLN:O	1:A:29:THR:HG22	0.54	2.03	17	4
1:A:48:VAL:O	1:A:48:VAL:HG13	0.54	2.02	10	3
1:A:12:SER:HG	1:A:40:VAL:HG21	0.54	1.61	12	1
1:A:41:VAL:HG22	1:A:58:GLU:CG	0.54	2.33	2	12
1:A:48:VAL:HG13	1:A:48:VAL:O	0.54	2.02	6	6
1:A:59:VAL:HG13	1:A:68:TYR:CE1	0.54	2.38	19	17
1:A:23:ALA:CA	1:A:83:LEU:HD22	0.54	2.33	20	9
1:A:20:ALA:HB1	1:A:68:TYR:OH	0.54	2.03	9	3
1:A:124:ALA:HB2	1:A:189:PHE:CZ	0.53	2.38	3	4
1:A:3:THR:HG23	1:A:74:VAL:CG1	0.53	2.32	5	4
1:A:72:ILE:HD11	1:A:83:LEU:HD23	0.53	1.80	20	16
1:A:163:MET:O	1:A:178:VAL:HG22	0.53	2.04	11	3
1:A:3:THR:HG22	1:A:51:THR:HB	0.52	1.80	20	2
1:A:7:VAL:O	1:A:7:VAL:HG12	0.52	2.03	16	1
1:A:52:LEU:HD13	1:A:52:LEU:C	0.52	2.25	4	3
1:A:47:VAL:O	1:A:47:VAL:HG13	0.52	2.05	2	13
1:A:47:VAL:HG13	1:A:47:VAL:O	0.52	2.05	16	7
1:A:7:VAL:HG12	1:A:7:VAL:O	0.52	2.03	17	4
1:A:3:THR:HG23	1:A:74:VAL:HG11	0.52	1.80	14	6
1:A:48:VAL:HG12	1:A:73:TRP:CZ2	0.52	2.38	7	1
1:A:3:THR:C	1:A:4:LEU:HD22	0.52	2.24	13	1
1:A:41:VAL:HG22	1:A:58:GLU:HG3	0.51	1.81	10	9
1:A:24:VAL:CG2	1:A:37:LEU:HD11	0.51	2.35	18	5
1:A:52:LEU:HD23	1:A:73:TRP:HZ3	0.51	1.64	20	3
1:A:4:LEU:HD22	1:A:4:LEU:H	0.51	1.64	5	2
1:A:28:ASN:HA	1:A:32:ASN:HB3	0.51	1.83	20	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:164:LEU:HD23	1:A:176:TYR:O	0.51	2.06	13	1
1:A:144:LEU:HD13	1:A:165:LEU:HD22	0.51	1.82	14	1
1:A:38:VAL:HG12	1:A:39:ARG:HD3	0.50	1.81	11	1
1:A:155:VAL:HG22	1:A:156:ASP:H	0.50	1.66	4	19
1:A:4:LEU:HD13	1:A:45:GLU:OE2	0.50	2.06	18	1
1:A:36:GLU:CG	1:A:60:LEU:HB2	0.50	2.36	7	14
1:A:86:PHE:CD1	1:A:86:PHE:N	0.50	2.80	18	3
1:A:176:TYR:CB	1:A:196:LEU:HD13	0.50	2.37	6	7
1:A:32:ASN:ND2	1:A:35:LEU:HD12	0.50	2.22	15	6
1:A:52:LEU:C	1:A:52:LEU:HD13	0.50	2.27	1	2
1:A:52:LEU:O	1:A:52:LEU:HD23	0.50	2.06	17	4
1:A:53:HIS:CE1	1:A:72:ILE:HD12	0.50	2.42	18	3
1:A:4:LEU:CD2	1:A:51:THR:HG23	0.50	2.36	10	1
1:A:129:ILE:HD11	1:A:165:LEU:CD1	0.50	2.18	1	3
1:A:167:VAL:HG13	1:A:176:TYR:HE1	0.50	1.66	19	3
1:A:42:GLU:H	1:A:56:VAL:HG13	0.50	1.66	12	5
1:A:38:VAL:CG2	1:A:60:LEU:HD12	0.50	2.37	7	13
1:A:12:SER:OG	1:A:40:VAL:HG21	0.50	2.07	12	1
1:A:129:ILE:HD13	1:A:144:LEU:N	0.50	2.22	8	3
1:A:155:VAL:HG23	1:A:160:LYS:HE2	0.50	1.83	15	2
1:A:144:LEU:HD12	1:A:165:LEU:HD13	0.49	1.83	19	1
1:A:4:LEU:H	1:A:4:LEU:HD22	0.49	1.67	3	2
1:A:72:ILE:HG23	1:A:82:GLN:C	0.49	2.28	9	11
1:A:23:ALA:HA	1:A:83:LEU:HD13	0.49	1.83	1	1
1:A:12:SER:HA	1:A:16:THR:HG23	0.49	1.85	20	1
1:A:20:ALA:HB3	1:A:37:LEU:HD21	0.49	1.85	12	1
1:A:72:ILE:HG21	1:A:81:LYS:HD3	0.48	1.84	4	1
1:A:23:ALA:CB	1:A:83:LEU:HD22	0.48	2.34	1	2
1:A:41:VAL:HG23	1:A:57:LEU:C	0.48	2.29	17	10
1:A:87:LYS:HE2	1:A:89:VAL:HG13	0.48	1.86	14	3
1:A:4:LEU:HD11	1:A:53:HIS:HB2	0.48	1.84	18	1
1:A:41:VAL:HB	1:A:56:VAL:HG13	0.48	1.84	17	5
1:A:52:LEU:HD13	1:A:53:HIS:N	0.48	2.23	9	1
1:A:125:ALA:HB1	1:A:165:LEU:CD2	0.48	2.38	10	1
1:A:87:LYS:NZ	1:A:89:VAL:HG12	0.48	2.24	8	1
1:A:22:PHE:O	1:A:83:LEU:HD13	0.48	2.08	3	2
1:A:42:GLU:N	1:A:56:VAL:HG13	0.48	2.23	12	4
1:A:59:VAL:CG1	1:A:68:TYR:CE1	0.47	2.97	9	13
1:A:17:HIS:ND1	1:A:40:VAL:HG21	0.47	2.22	17	1
1:A:53:HIS:ND1	1:A:72:ILE:HD12	0.47	2.25	18	2
1:A:4:LEU:O	1:A:51:THR:HG23	0.47	2.09	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LEU:HD13	1:A:64:LYS:N	0.47	2.25	3	3
1:A:51:THR:CG2	1:A:74:VAL:CG1	0.47	2.92	20	11
1:A:41:VAL:HG22	1:A:58:GLU:HG2	0.46	1.87	16	4
1:A:191:LEU:HD13	1:A:192:LYS:N	0.46	2.25	16	19
1:A:14:PRO:HG2	1:A:16:THR:HG23	0.46	1.87	17	2
1:A:148:VAL:HG21	1:A:175:LYS:HD2	0.46	1.88	15	1
1:A:150:ALA:HB1	1:A:163:MET:SD	0.46	2.50	14	15
1:A:72:ILE:HG23	1:A:83:LEU:HA	0.46	1.87	15	8
1:A:40:VAL:HA	1:A:57:LEU:HD12	0.46	1.86	12	8
1:A:51:THR:HG22	1:A:74:VAL:HG13	0.46	1.88	19	2
1:A:10:SER:HB2	1:A:43:ALA:HB3	0.46	1.88	4	1
1:A:22:PHE:N	1:A:22:PHE:CD1	0.46	2.82	12	8
1:A:4:LEU:HD12	1:A:45:GLU:CG	0.45	2.40	1	1
1:A:35:LEU:HD22	1:A:59:VAL:HG21	0.45	1.88	17	1
1:A:17:HIS:CD2	1:A:40:VAL:CG1	0.45	3.00	4	2
1:A:126:HIS:CE1	1:A:144:LEU:CB	0.45	3.00	2	5
1:A:52:LEU:HD23	1:A:52:LEU:O	0.45	2.11	19	1
1:A:161:PHE:CD1	1:A:163:MET:CE	0.45	3.00	15	2
1:A:191:LEU:HD13	1:A:191:LEU:C	0.45	2.32	16	9
1:A:41:VAL:HB	1:A:56:VAL:HG22	0.45	1.87	19	4
1:A:176:TYR:CE2	1:A:178:VAL:CG1	0.45	3.00	9	2
1:A:54:HIS:CE1	1:A:71:LYS:CE	0.45	3.00	18	1
1:A:22:PHE:CD1	1:A:22:PHE:N	0.45	2.83	2	11
1:A:17:HIS:CG	1:A:40:VAL:CG2	0.45	3.00	15	1
1:A:161:PHE:CE1	1:A:163:MET:CE	0.45	3.00	18	2
1:A:128:ALA:O	1:A:132:ILE:HD12	0.45	2.12	12	18
1:A:13:ASN:CB	1:A:14:PRO:HD3	0.45	2.42	10	2
1:A:60:LEU:HD21	1:A:65:LYS:CD	0.45	2.42	2	1
1:A:191:LEU:C	1:A:191:LEU:HD13	0.44	2.32	19	11
1:A:13:ASN:CB	1:A:14:PRO:CD	0.44	2.95	17	16
1:A:17:HIS:NE2	1:A:40:VAL:HG11	0.44	2.27	4	1
1:A:40:VAL:CG2	1:A:57:LEU:HD12	0.44	2.42	3	1
1:A:23:ALA:O	1:A:26:GLN:CG	0.44	2.66	18	8
1:A:49:ALA:CB	1:A:73:TRP:CH2	0.44	3.00	7	1
1:A:161:PHE:CD1	1:A:163:MET:HE2	0.44	2.47	15	1
1:A:177:LYS:O	1:A:194:VAL:HG23	0.44	2.12	4	1
1:A:48:VAL:HG12	1:A:52:LEU:HB3	0.44	1.90	6	4
1:A:144:LEU:CD1	1:A:165:LEU:HD13	0.44	2.42	19	3
1:A:24:VAL:HG21	1:A:37:LEU:CD1	0.44	2.42	18	1
1:A:52:LEU:CD2	1:A:73:TRP:CD1	0.44	2.99	9	1
1:A:155:VAL:HG23	1:A:159:ALA:HA	0.44	1.89	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:CD1	1:A:73:TRP:CH2	0.43	2.95	16	1
1:A:52:LEU:HD12	1:A:52:LEU:C	0.43	2.32	13	1
1:A:52:LEU:CD2	1:A:52:LEU:C	0.43	2.87	18	1
1:A:176:TYR:HB2	1:A:196:LEU:HD13	0.43	1.89	20	4
1:A:51:THR:HG22	1:A:74:VAL:CG1	0.43	2.43	19	5
1:A:13:ASN:N	1:A:14:PRO:CD	0.43	2.81	8	4
1:A:144:LEU:HG	1:A:165:LEU:HD13	0.43	1.89	17	1
1:A:17:HIS:CD2	1:A:57:LEU:CD1	0.43	3.02	5	2
1:A:148:VAL:HG21	1:A:175:LYS:NZ	0.43	2.29	20	1
1:A:16:THR:CB	1:A:55:LEU:HD21	0.43	2.44	15	2
1:A:68:TYR:HA	1:A:89:VAL:HG22	0.43	1.90	5	2
1:A:67:LEU:CD2	1:A:67:LEU:N	0.42	2.82	18	4
1:A:20:ALA:CB	1:A:37:LEU:HD21	0.42	2.44	12	1
1:A:4:LEU:N	1:A:4:LEU:CD1	0.42	2.81	17	3
1:A:67:LEU:N	1:A:67:LEU:CD2	0.42	2.82	20	1
1:A:48:VAL:HG12	1:A:52:LEU:CB	0.42	2.44	6	4
1:A:19:LEU:HB3	1:A:55:LEU:HD12	0.42	1.91	13	1
1:A:72:ILE:HG23	1:A:83:LEU:CA	0.42	2.44	9	1
1:A:52:LEU:C	1:A:52:LEU:CD2	0.42	2.87	16	1
1:A:3:THR:HG22	1:A:51:THR:CG2	0.42	2.38	5	2
1:A:17:HIS:CD2	1:A:40:VAL:HG11	0.42	2.49	8	1
1:A:4:LEU:CD1	1:A:4:LEU:N	0.42	2.81	16	4
1:A:67:LEU:O	1:A:89:VAL:HG22	0.42	2.15	17	1
1:A:27:HIS:CB	1:A:86:PHE:CZ	0.42	3.03	2	2
1:A:74:VAL:CG2	1:A:75:LYS:N	0.42	2.83	11	7
1:A:12:SER:HB3	1:A:40:VAL:HG11	0.42	1.92	19	1
1:A:177:LYS:N	1:A:195:ASP:O	0.42	2.53	14	10
1:A:4:LEU:HD23	1:A:51:THR:CG2	0.41	2.44	12	2
1:A:68:TYR:O	1:A:68:TYR:CD1	0.41	2.72	12	1
1:A:52:LEU:CD1	1:A:73:TRP:CZ3	0.41	3.02	11	2
1:A:18:SER:CB	1:A:22:PHE:CZ	0.41	3.04	3	1
1:A:17:HIS:CE1	1:A:40:VAL:CG2	0.41	3.03	18	1
1:A:3:THR:HG21	1:A:76:PRO:CG	0.41	2.45	10	1
1:A:126:HIS:CD2	1:A:144:LEU:HD13	0.41	2.49	9	1
1:A:35:LEU:HD21	1:A:66:LYS:NZ	0.41	2.30	4	1
1:A:40:VAL:CA	1:A:57:LEU:HD12	0.41	2.45	4	2
1:A:27:HIS:HB2	1:A:86:PHE:CZ	0.41	2.51	12	6
1:A:132:ILE:HG23	1:A:194:VAL:HG11	0.41	1.92	19	1
1:A:120:VAL:HG13	1:A:121:VAL:N	0.41	2.31	10	1
1:A:34:LEU:CD1	1:A:34:LEU:N	0.41	2.84	2	1
1:A:18:SER:O	1:A:22:PHE:CE1	0.41	2.74	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ILE:CD1	1:A:144:LEU:CA	0.41	2.99	8	2
1:A:132:ILE:HD11	1:A:178:VAL:HG23	0.41	1.92	1	1
1:A:150:ALA:HB1	1:A:163:MET:CE	0.41	2.46	15	1
1:A:144:LEU:HD23	1:A:145:SER:H	0.41	1.76	3	3
1:A:34:LEU:N	1:A:34:LEU:CD1	0.41	2.84	7	1
1:A:129:ILE:CD1	1:A:144:LEU:N	0.41	2.84	14	4
1:A:72:ILE:HG23	1:A:83:LEU:N	0.41	2.31	9	2
1:A:7:VAL:O	1:A:8:HIS:CG	0.41	2.74	7	3
1:A:86:PHE:N	1:A:86:PHE:CD1	0.41	2.89	13	1
1:A:17:HIS:ND1	1:A:40:VAL:CG2	0.41	2.84	18	1
1:A:7:VAL:HG23	1:A:46:GLN:HG3	0.40	1.93	14	1
1:A:54:HIS:CE1	1:A:71:LYS:HE2	0.40	2.51	18	1
1:A:52:LEU:C	1:A:52:LEU:HD12	0.40	2.36	8	1
1:A:43:ALA:CB	1:A:55:LEU:CD2	0.40	2.99	17	1
1:A:20:ALA:O	1:A:24:VAL:HG23	0.40	2.16	5	1
1:A:48:VAL:HG12	1:A:52:LEU:HB2	0.40	1.93	19	1
1:A:88:HIS:CD2	1:A:88:HIS:O	0.40	2.74	12	1
1:A:88:HIS:O	1:A:88:HIS:CD2	0.40	2.75	7	1
1:A:32:ASN:ND2	1:A:35:LEU:CD1	0.40	2.85	2	1
1:A:149:HIS:CD2	1:A:149:HIS:O	0.40	2.75	3	1
1:A:87:LYS:NZ	1:A:89:VAL:CG1	0.40	2.84	15	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	164/199 (82%)	137±2 (84±1%)	23±2 (14±1%)	4±1 (2±1%)	11	50
All	All	3280/3980 (82%)	2739 (84%)	464 (14%)	77 (2%)	11	50

All 14 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	33	GLY	20

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Mol	Chain	Res	Type	Models (Total)
1	A	115	PRO	19
1	A	113	PRO	7
1	A	6	GLY	6
1	A	90	ARG	4
1	A	7	VAL	4
1	A	8	HIS	4
1	A	5	GLY	3
1	A	91	ASP	3
1	A	13	ASN	2
1	A	4	LEU	2
1	A	14	PRO	1
1	A	78	MET	1
1	A	10	SER	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	145/174 (83%)	105±4 (73±3%)	40±4 (27±3%)	2	21
All	All	2900/3480 (83%)	2107 (73%)	793 (27%)	2	21

All 87 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	60	LEU	20
1	A	193	LYS	20
1	A	3	THR	20
1	A	190	ASN	20
1	A	158	SER	20
1	A	130	LYS	20
1	A	172	LYS	20
1	A	161	PHE	20
1	A	151	ASN	20
1	A	34	LEU	20
1	A	44	ARG	19
1	A	175	LYS	19

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Mol	Chain	Res	Type	Models (Total)
1	A	73	TRP	19
1	A	27	HIS	19
1	A	145	SER	19
1	A	112	ARG	18
1	A	54	HIS	18
1	A	4	LEU	17
1	A	157	THR	17
1	A	83	LEU	17
1	A	197	ASP	17
1	A	87	LYS	16
1	A	45	GLU	16
1	A	149	HIS	16
1	A	168	LYS	15
1	A	18	SER	15
1	A	42	GLU	14
1	A	52	LEU	14
1	A	118	ASP	12
1	A	165	LEU	12
1	A	195	ASP	11
1	A	53	HIS	11
1	A	90	ARG	10
1	A	67	LEU	9
1	A	26	GLN	9
1	A	71	LYS	9
1	A	79	ASP	8
1	A	78	MET	8
1	A	81	LYS	8
1	A	75	LYS	8
1	A	182	LYS	8
1	A	169	ARG	7
1	A	64	LYS	7
1	A	173	GLU	7
1	A	39	ARG	7
1	A	28	ASN	7
1	A	55	LEU	6
1	A	22	PHE	6
1	A	91	ASP	6
1	A	164	LEU	5
1	A	65	LYS	5
1	A	77	TRP	5
1	A	86	PHE	4
1	A	66	LYS	4

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Mol	Chain	Res	Type	Models (Total)
1	A	11	ASN	4
1	A	82	GLN	4
1	A	135	ARG	4
1	A	56	VAL	4
1	A	80	PHE	4
1	A	177	LYS	4
1	A	136	SER	4
1	A	46	GLN	4
1	A	8	HIS	4
1	A	123	ASP	4
1	A	162	ASP	4
1	A	156	ASP	4
1	A	68	TYR	3
1	A	74	VAL	3
1	A	166	LYS	3
1	A	69	GLU	3
1	A	127	HIS	3
1	A	120	VAL	3
1	A	192	LYS	3
1	A	144	LEU	3
1	A	37	LEU	2
1	A	174	GLU	2
1	A	15	ASP	2
1	A	88	HIS	2
1	A	10	SER	1
1	A	196	LEU	1
1	A	12	SER	1
1	A	126	HIS	1
1	A	17	HIS	1
1	A	134	GLU	1
1	A	84	GLN	1
1	A	183	SER	1
1	A	153	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 [i](#)

There are no carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 85% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mzv\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 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	2353
Number of shifts mapped to atoms	2353
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	194	$-0.15 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	184	$-0.00 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	194	$0.10 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	190	$-0.53 \pm 0.19$	Should be applied

#### 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 85%, i.e. 1782 atoms were assigned a chemical shift out of a possible 2090. 38 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	802/810 (99%)	320/323 (99%)	324/328 (99%)	158/159 (99%)
Sidechain	927/1107 (84%)	572/643 (89%)	345/412 (84%)	10/52 (19%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	53/173 (31%)	51/89 (57%)	0/60 (0%)	2/24 (8%)
Overall	1782/2090 (85%)	943/1055 (89%)	669/800 (84%)	170/235 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 2095 atoms were assigned a chemical shift out of a possible 2468. 42 out of 43 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	963/981 (98%)	385/391 (98%)	388/398 (97%)	190/192 (99%)
Sidechain	1060/1268 (84%)	655/738 (89%)	394/476 (83%)	11/54 (20%)
Aromatic	72/219 (33%)	69/113 (61%)	0/79 (0%)	3/27 (11%)
Overall	2095/2468 (85%)	1109/1242 (89%)	782/953 (82%)	204/273 (75%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	153	GLU	HB3	0.27	3.10 – 0.90	-7.9
1	A	153	GLU	HB2	0.71	3.08 – 0.98	-6.3

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

