



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:32 pm GMT

PDB ID : 1Q8G  
Title : NMR structure of human Cofilin  
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Deposited on : 2003-08-21

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk28760  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

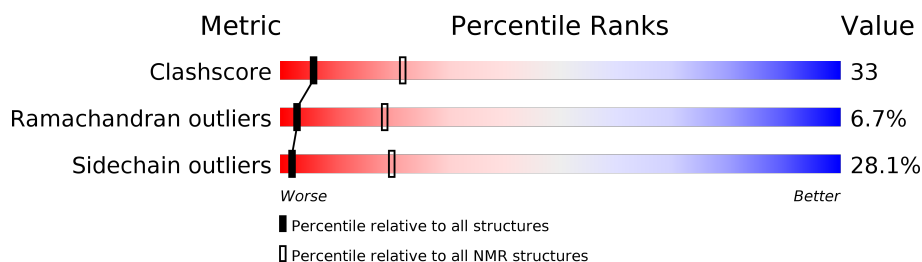
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

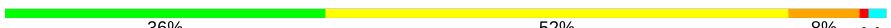
The overall completeness of chemical shifts assignment is 82%.

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	166	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:5-A:166 (162)	0.47	14

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

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

There is only 1 type of molecule in this entry. The entry contains 2642 atoms, of which 1346 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cofilin, non-muscle isoform.

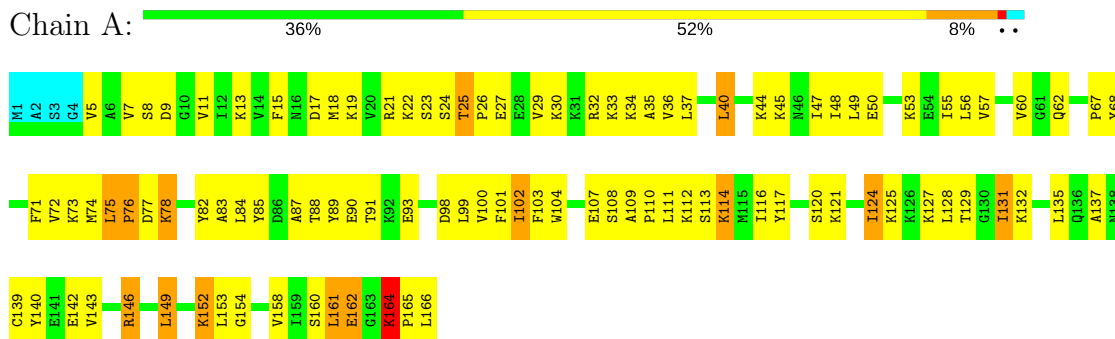
Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2642	826	1346	211	251	8	

## 4 Residue-property plots

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

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Cofilin, non-muscle isoform

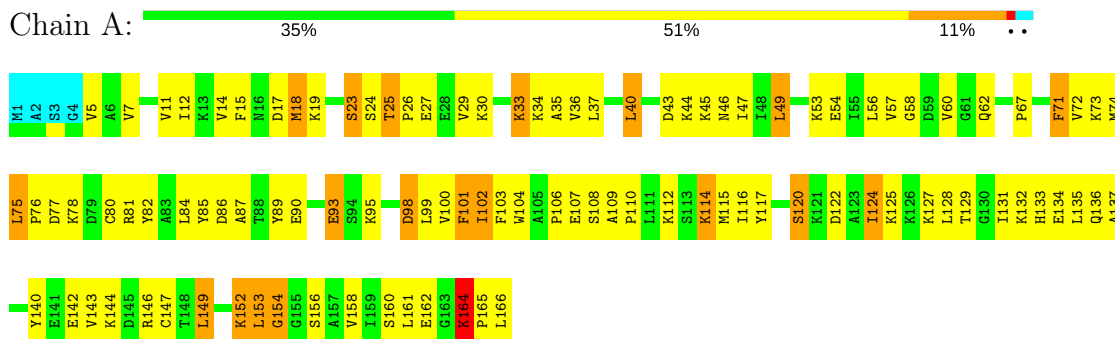


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

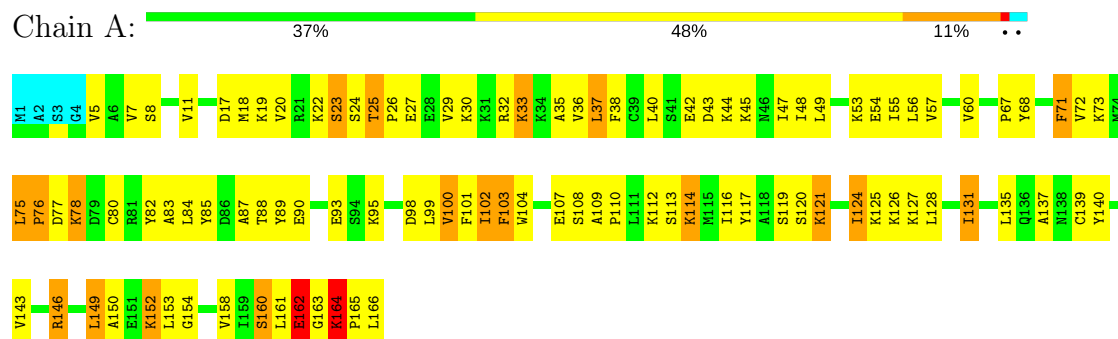
#### 4.2.1 Score per residue for model 1

- Molecule 1: Cofilin, non-muscle isoform



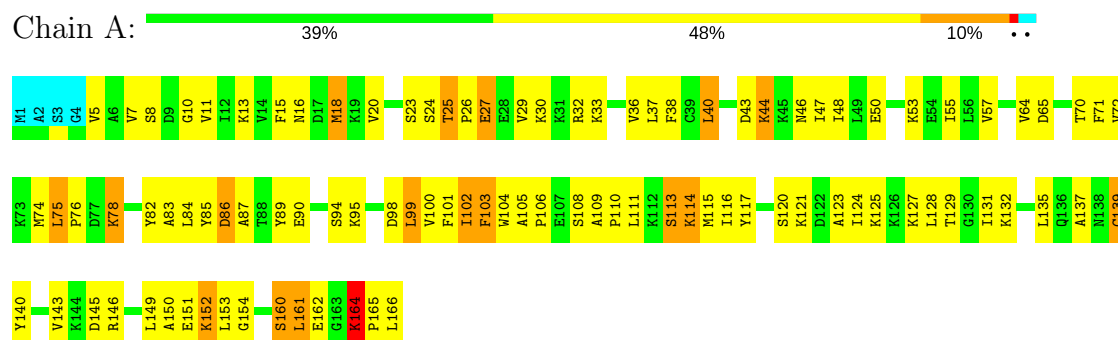
### 4.2.2 Score per residue for model 2

- Molecule 1: Cofilin, non-muscle isoform



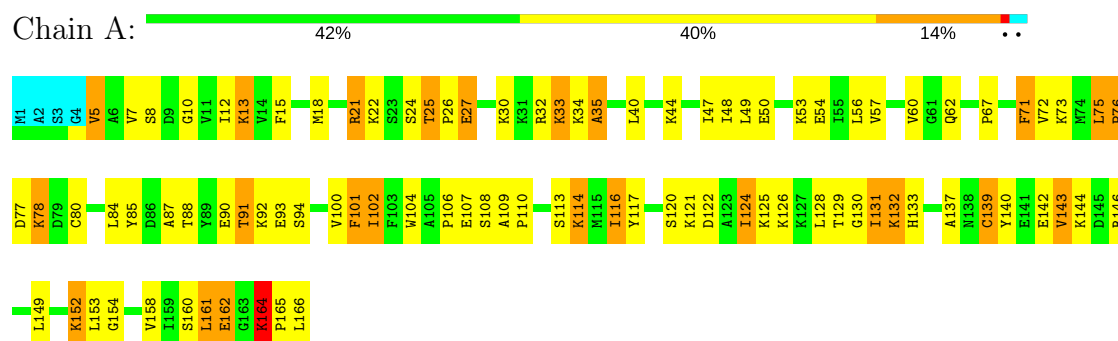
### 4.2.3 Score per residue for model 3

- Molecule 1: Cofilin, non-muscle isoform



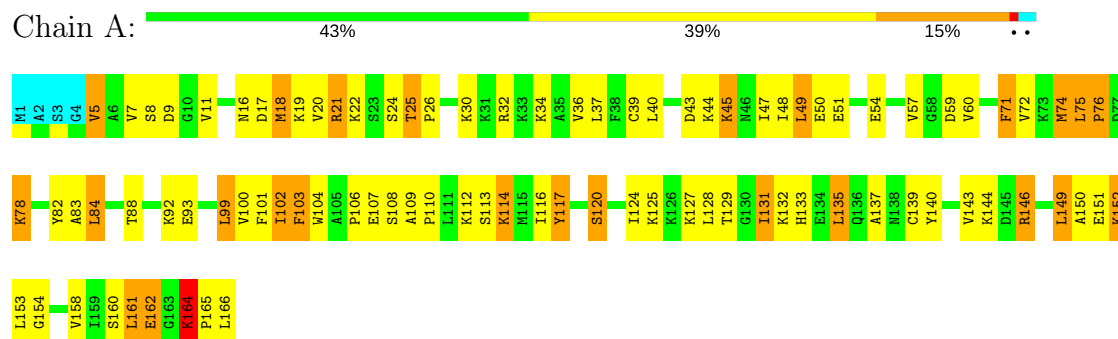
### 4.2.4 Score per residue for model 4

- Molecule 1: Cofilin, non-muscle isoform



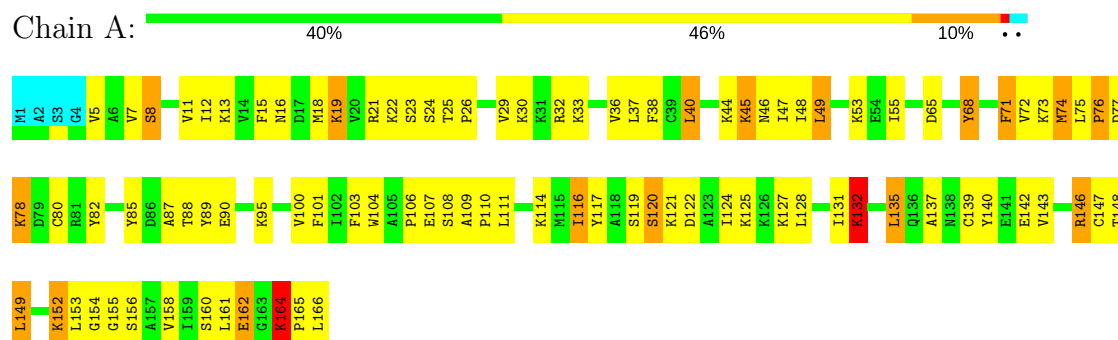
### 4.2.5 Score per residue for model 5

- Molecule 1: Cofilin, non-muscle isoform



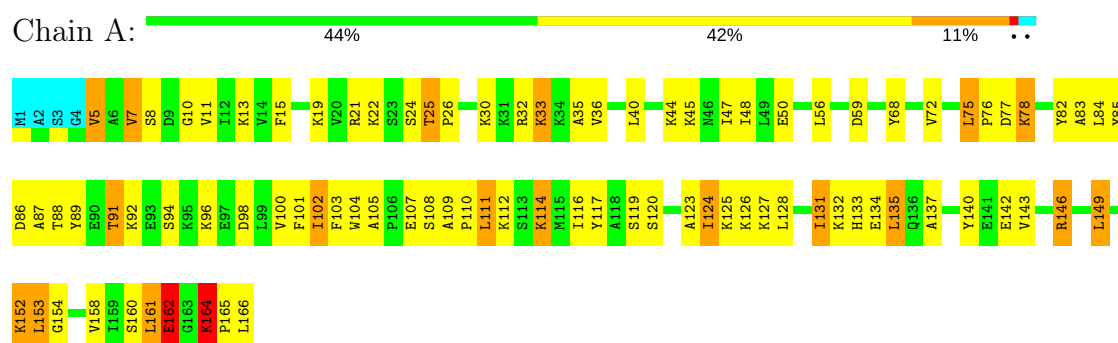
### 4.2.6 Score per residue for model 6

- Molecule 1: Cofilin, non-muscle isoform



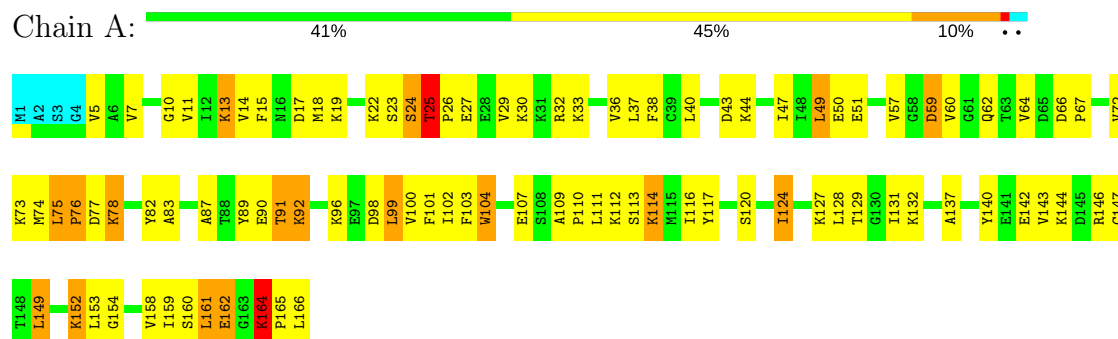
### 4.2.7 Score per residue for model 7

- Molecule 1: Cofilin, non-muscle isoform



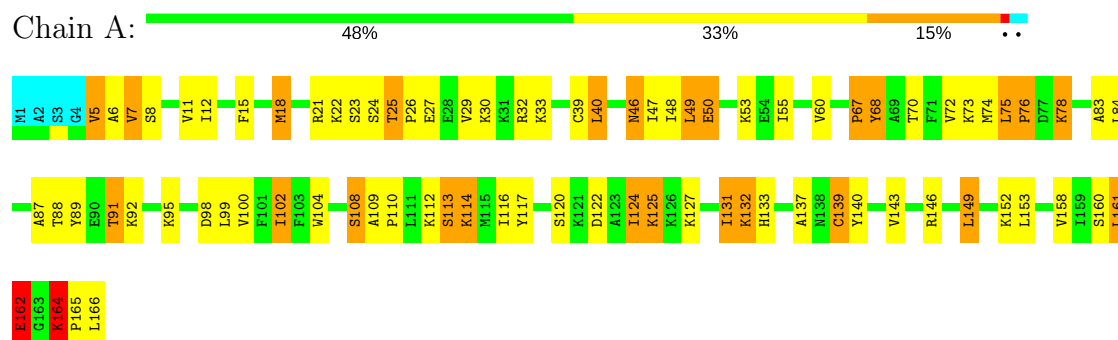
### 4.2.8 Score per residue for model 8

- Molecule 1: Cofilin, non-muscle isoform



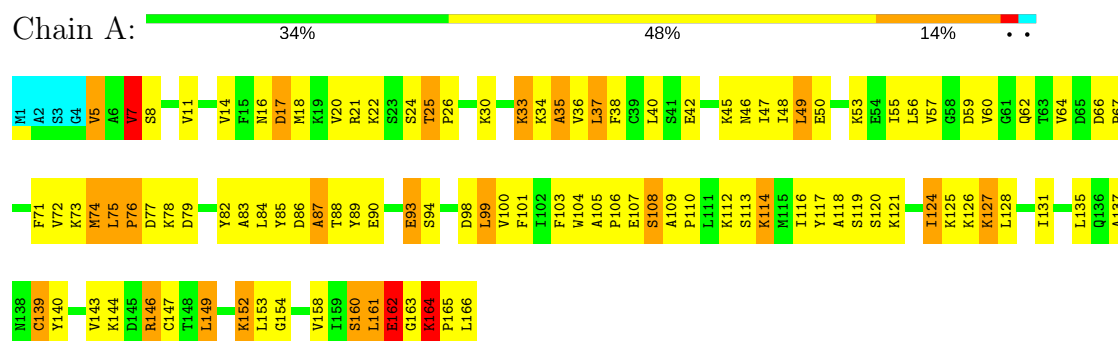
### 4.2.9 Score per residue for model 9

- Molecule 1: Cofilin, non-muscle isoform



### 4.2.10 Score per residue for model 10

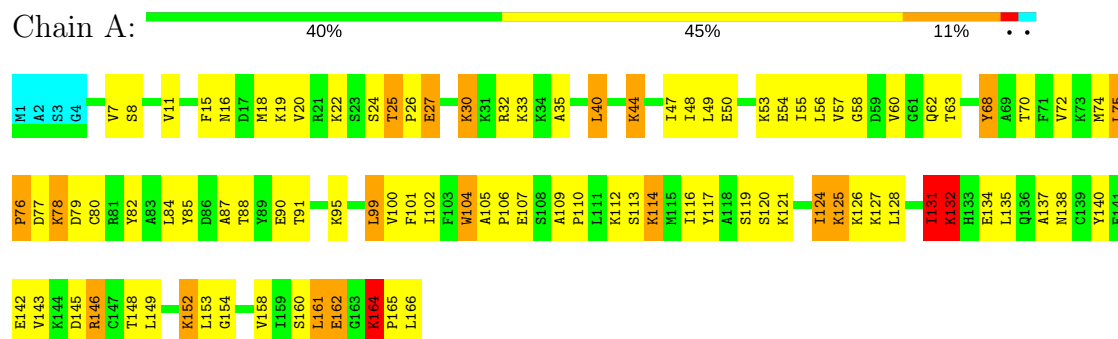
- Molecule 1: Cofilin, non-muscle isoform





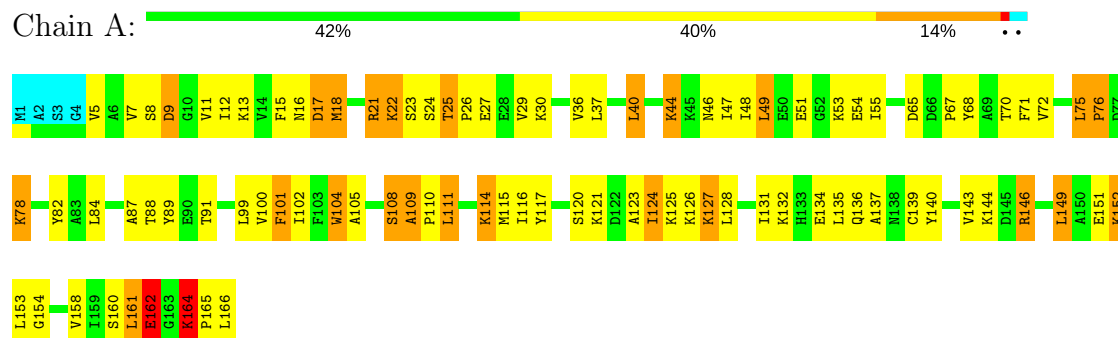
### 4.2.11 Score per residue for model 11

- Molecule 1: Cofilin, non-muscle isoform



### 4.2.12 Score per residue for model 12

- Molecule 1: Cofilin, non-muscle isoform



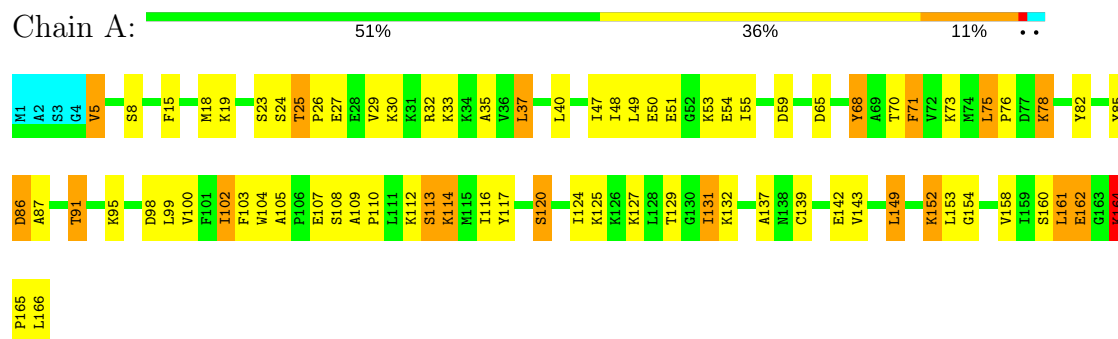
### 4.2.13 Score per residue for model 13

- Molecule 1: Cofilin, non-muscle isoform



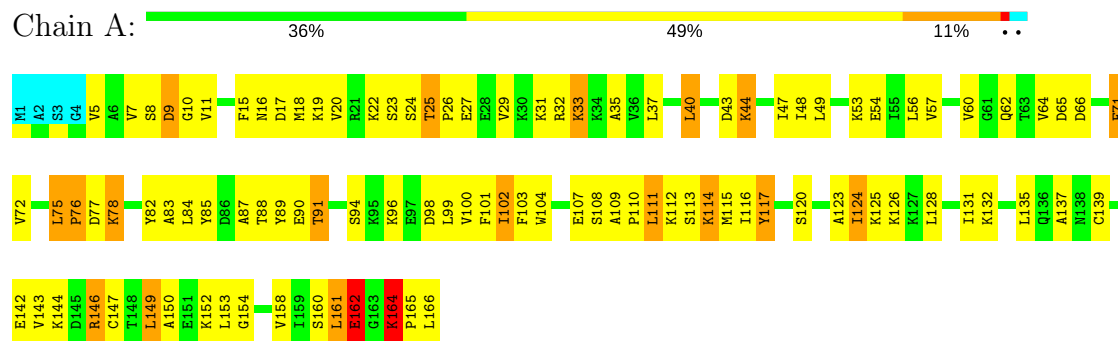
### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Cofilin, non-muscle isoform



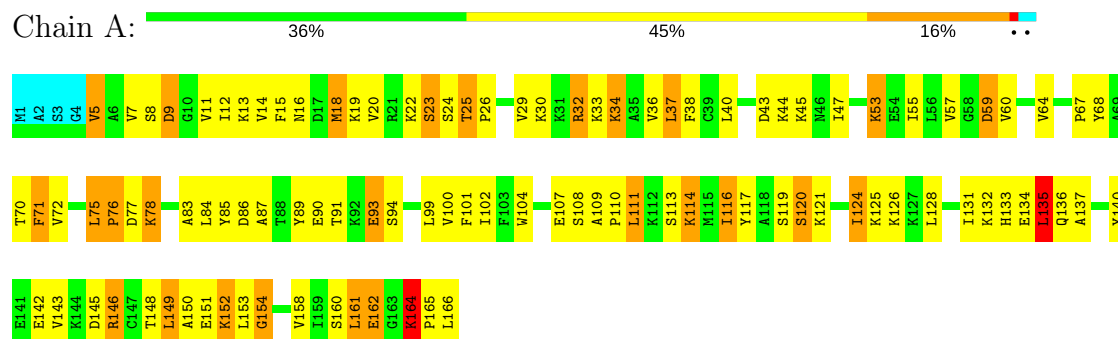
### 4.2.15 Score per residue for model 15

- Molecule 1: Cofilin, non-muscle isoform



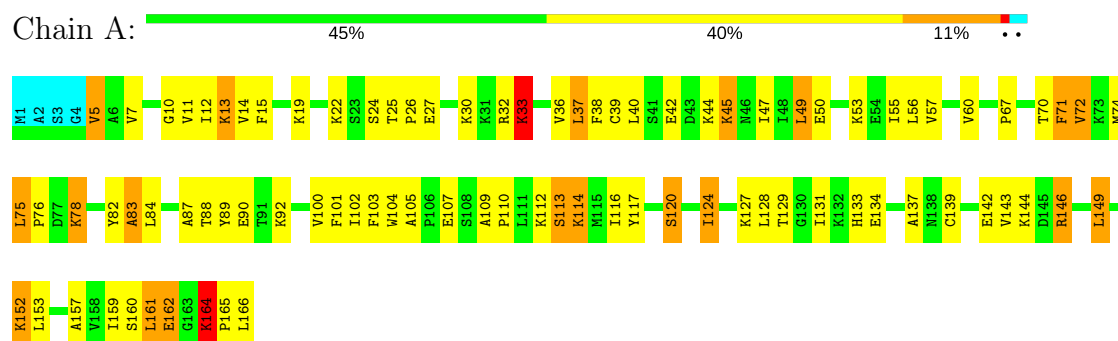
### 4.2.16 Score per residue for model 16

- Molecule 1: Cofilin, non-muscle isoform



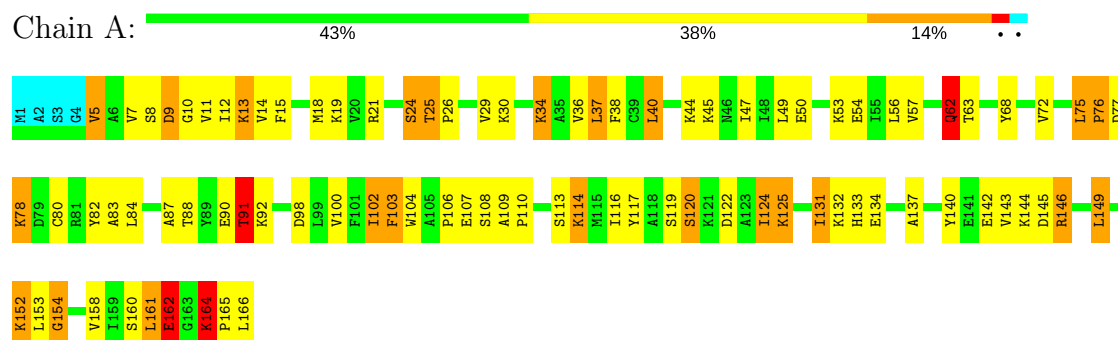
### 4.2.17 Score per residue for model 17

- Molecule 1: Cofilin, non-muscle isoform



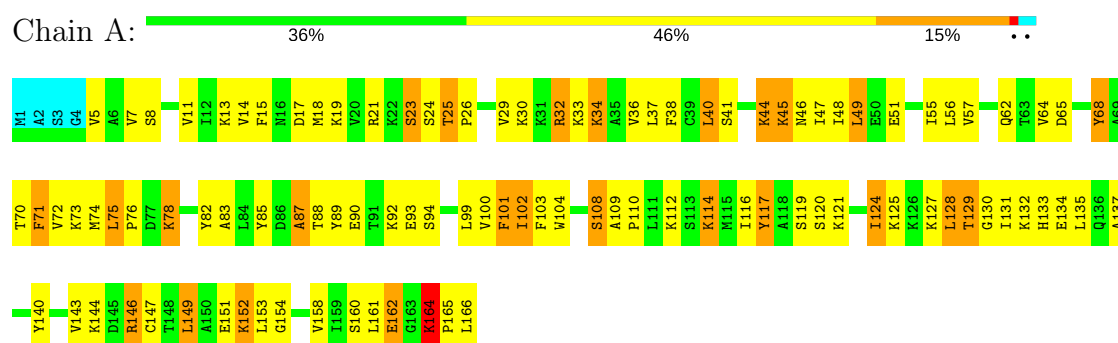
### 4.2.18 Score per residue for model 18

- Molecule 1: Cofilin, non-muscle isoform



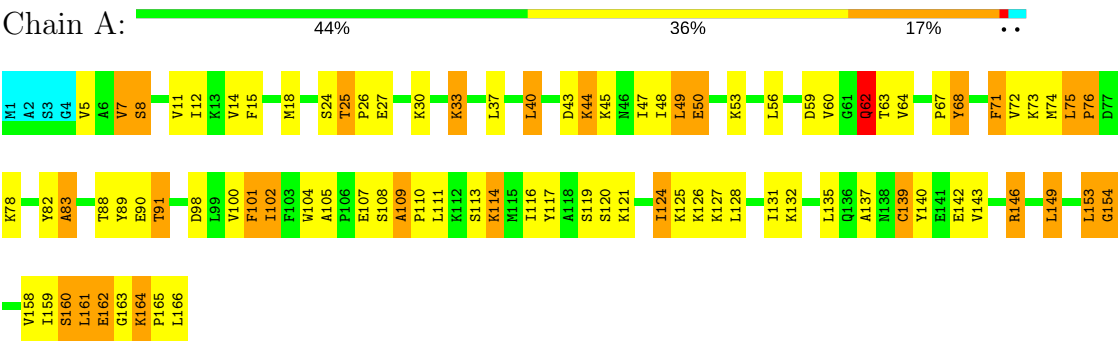
### 4.2.19 Score per residue for model 19

- Molecule 1: Cofilin, non-muscle isoform



4.2.20 Score per residue for model 20

● Molecule 1: Cofilin, non-muscle isoform



## 5 Refinement protocol and experimental data overview

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

Of the 140 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
CNS	structure solution	1.1
CNS	refinement	1.1

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)	BMRB entry 6004
Number of chemical shift lists	1
Total number of shifts	1864
Number of shifts mapped to atoms	1864
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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	1273	1322	1321	85±11
All	All	25460	26440	26420	1708

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:100:VAL:HG21	1:A:149:LEU:HD21	1.09	1.20	1	1
1:A:100:VAL:HG11	1:A:149:LEU:HD21	1.05	1.18	12	2
1:A:87:ALA:HB2	1:A:149:LEU:HD12	1.01	1.27	17	11
1:A:55:ILE:HD13	1:A:70:THR:HG23	1.01	1.30	16	3
1:A:47:ILE:HG21	1:A:124:ILE:HD12	0.87	1.45	4	12
1:A:89:TYR:CD1	1:A:153:LEU:HD22	0.86	2.05	19	6
1:A:135:LEU:HD22	1:A:149:LEU:HD22	0.85	1.47	6	3
1:A:89:TYR:CD1	1:A:153:LEU:HD13	0.84	2.08	3	7
1:A:12:ILE:HD11	1:A:127:LYS:CD	0.84	2.02	20	2
1:A:153:LEU:HD12	1:A:158:VAL:HG21	0.83	1.49	20	1
1:A:12:ILE:HD12	1:A:127:LYS:CG	0.83	2.04	13	1
1:A:15:PHE:CE1	1:A:128:LEU:HD22	0.82	2.10	17	2
1:A:153:LEU:CD1	1:A:158:VAL:HG21	0.82	2.05	20	10
1:A:87:ALA:HB2	1:A:149:LEU:CD1	0.81	2.06	17	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ALA:HB1	1:A:110:PRO:HD2	0.81	1.53	6	20
1:A:105:ALA:HB2	1:A:117:TYR:CE1	0.80	2.12	10	8
1:A:12:ILE:HD11	1:A:127:LYS:HD3	0.80	1.53	17	2
1:A:8:SER:OG	1:A:48:ILE:HG22	0.80	1.77	10	2
1:A:135:LEU:CD2	1:A:148:THR:HG22	0.80	2.07	16	2
1:A:15:PHE:CZ	1:A:131:ILE:HD12	0.79	2.11	14	9
1:A:109:ALA:HB3	1:A:114:LYS:HG3	0.79	1.52	7	19
1:A:120:SER:O	1:A:124:ILE:HG22	0.78	1.78	4	4
1:A:55:ILE:CD1	1:A:70:THR:HG23	0.78	2.08	16	2
1:A:44:LYS:O	1:A:116:ILE:HD13	0.77	1.77	19	5
1:A:146:ARG:CD	1:A:161:LEU:HD22	0.77	2.09	1	3
1:A:153:LEU:HD13	1:A:158:VAL:HG21	0.77	1.57	1	2
1:A:154:GLY:O	1:A:158:VAL:HG23	0.77	1.80	20	16
1:A:87:ALA:CB	1:A:149:LEU:HD12	0.76	2.10	17	10
1:A:137:ALA:HB3	1:A:143:VAL:HG22	0.76	1.58	17	17
1:A:161:LEU:O	1:A:161:LEU:HD13	0.76	1.81	6	6
1:A:84:LEU:HD22	1:A:99:LEU:HD11	0.76	1.56	2	2
1:A:146:ARG:HG3	1:A:161:LEU:HD22	0.76	1.55	2	4
1:A:67:PRO:O	1:A:70:THR:HG22	0.76	1.80	16	2
1:A:89:TYR:CE1	1:A:153:LEU:HD22	0.76	2.16	9	3
1:A:153:LEU:HD12	1:A:154:GLY:N	0.76	1.96	19	8
1:A:47:ILE:HD11	1:A:120:SER:OG	0.75	1.80	20	5
1:A:71:PHE:CE2	1:A:102:ILE:HG21	0.74	2.17	2	8
1:A:100:VAL:HG21	1:A:149:LEU:CD2	0.74	2.09	1	1
1:A:12:ILE:HD12	1:A:127:LYS:HG3	0.74	1.59	13	1
1:A:35:ALA:HB2	1:A:85:TYR:CD2	0.74	2.18	13	7
1:A:88:THR:HG23	1:A:162:GLU:HG2	0.73	1.58	11	6
1:A:109:ALA:HB3	1:A:114:LYS:CG	0.73	2.13	7	5
1:A:60:VAL:HG21	1:A:162:GLU:OE2	0.73	1.84	10	1
1:A:101:PHE:CE2	1:A:128:LEU:HD11	0.73	2.19	11	15
1:A:161:LEU:HD13	1:A:161:LEU:O	0.72	1.84	13	5
1:A:139:CYS:O	1:A:143:VAL:HG12	0.72	1.83	4	1
1:A:68:TYR:OH	1:A:149:LEU:HD23	0.72	1.84	19	5
1:A:60:VAL:HG22	1:A:67:PRO:HD3	0.72	1.60	1	1
1:A:149:LEU:O	1:A:149:LEU:HD13	0.71	1.85	3	6
1:A:84:LEU:HD21	1:A:131:ILE:HD11	0.71	1.60	18	6
1:A:72:VAL:HG11	1:A:144:LYS:HB2	0.71	1.62	18	4
1:A:5:VAL:HG11	1:A:120:SER:HB2	0.71	1.61	12	5
1:A:85:TYR:O	1:A:100:VAL:HG12	0.71	1.85	19	1
1:A:72:VAL:HG11	1:A:144:LYS:CD	0.71	2.15	8	1
1:A:40:LEU:CD2	1:A:47:ILE:HD13	0.71	2.16	20	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ALA:HB3	1:A:114:LYS:HG2	0.71	1.61	3	1
1:A:47:ILE:CG2	1:A:124:ILE:HD12	0.70	2.15	19	3
1:A:18:MET:SD	1:A:99:LEU:HD11	0.70	2.26	12	2
1:A:162:GLU:HB2	1:A:165:PRO:HG3	0.70	1.62	2	20
1:A:8:SER:HB3	1:A:48:ILE:HG22	0.70	1.63	11	6
1:A:8:SER:HB2	1:A:48:ILE:HG22	0.70	1.63	3	8
1:A:59:ASP:HB3	1:A:64:VAL:HG21	0.70	1.63	10	3
1:A:72:VAL:HG22	1:A:143:VAL:HG12	0.70	1.63	1	4
1:A:104:TRP:CZ3	1:A:143:VAL:HG21	0.70	2.22	1	13
1:A:87:ALA:HB1	1:A:161:LEU:HD11	0.70	1.63	8	3
1:A:57:VAL:O	1:A:60:VAL:HG23	0.69	1.86	13	6
1:A:8:SER:CB	1:A:48:ILE:HG22	0.69	2.17	12	12
1:A:89:TYR:CE1	1:A:153:LEU:HD13	0.69	2.22	10	3
1:A:100:VAL:HG11	1:A:152:LYS:HG2	0.69	1.64	14	3
1:A:75:LEU:HD22	1:A:143:VAL:HG11	0.69	1.63	5	6
1:A:137:ALA:HB1	1:A:142:GLU:HB2	0.69	1.64	17	13
1:A:135:LEU:HD12	1:A:149:LEU:HD22	0.69	1.62	3	4
1:A:60:VAL:HG22	1:A:67:PRO:HG2	0.69	1.64	4	1
1:A:87:ALA:HB3	1:A:153:LEU:HD21	0.68	1.63	16	3
1:A:40:LEU:HD13	1:A:44:LYS:HG3	0.68	1.66	12	1
1:A:23:SER:CB	1:A:29:VAL:HG12	0.68	2.19	1	6
1:A:100:VAL:HG12	1:A:133:HIS:HB2	0.68	1.64	5	5
1:A:111:LEU:HD23	1:A:111:LEU:O	0.67	1.89	8	1
1:A:75:LEU:HD22	1:A:104:TRP:CD1	0.67	2.25	7	1
1:A:59:ASP:CB	1:A:64:VAL:HG21	0.67	2.20	10	1
1:A:5:VAL:CG1	1:A:47:ILE:HD11	0.66	2.21	4	1
1:A:106:PRO:HG2	1:A:109:ALA:HB2	0.66	1.67	1	9
1:A:100:VAL:HG12	1:A:133:HIS:CB	0.66	2.20	5	4
1:A:16:ASN:O	1:A:20:VAL:HG22	0.66	1.89	3	3
1:A:47:ILE:HG21	1:A:124:ILE:CD1	0.66	2.21	15	4
1:A:87:ALA:HB1	1:A:153:LEU:HD11	0.65	1.68	6	4
1:A:72:VAL:HG21	1:A:144:LYS:HD3	0.65	1.66	15	2
1:A:62:GLN:OE1	1:A:63:THR:HG22	0.65	1.91	20	1
1:A:18:MET:O	1:A:99:LEU:HD21	0.65	1.91	13	2
1:A:87:ALA:HB2	1:A:149:LEU:HD11	0.65	1.68	3	2
1:A:139:CYS:O	1:A:143:VAL:HG23	0.65	1.91	12	9
1:A:149:LEU:HD22	1:A:152:LYS:HE2	0.65	1.67	1	1
1:A:102:ILE:HD11	1:A:149:LEU:HD21	0.64	1.68	7	2
1:A:87:ALA:HB3	1:A:149:LEU:CD1	0.64	2.21	2	1
1:A:5:VAL:HG13	1:A:47:ILE:HG12	0.64	1.69	10	1
1:A:134:GLU:O	1:A:135:LEU:HD12	0.64	1.92	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:LEU:HD13	1:A:104:TRP:CE2	0.64	2.28	12	5
1:A:146:ARG:CG	1:A:161:LEU:HD22	0.64	2.23	19	2
1:A:20:VAL:HG23	1:A:22:LYS:HG2	0.64	1.68	2	1
1:A:104:TRP:CH2	1:A:143:VAL:HG11	0.64	2.27	4	1
1:A:72:VAL:HG22	1:A:140:TYR:CE2	0.64	2.26	9	4
1:A:150:ALA:HB2	1:A:161:LEU:HD23	0.64	1.69	5	3
1:A:100:VAL:HG11	1:A:152:LYS:CG	0.64	2.23	14	3
1:A:128:LEU:HD12	1:A:131:ILE:HG21	0.64	1.70	3	1
1:A:84:LEU:HD22	1:A:99:LEU:CD1	0.63	2.24	9	2
1:A:5:VAL:CG1	1:A:40:LEU:HD11	0.63	2.23	6	2
1:A:5:VAL:HG13	1:A:123:ALA:CB	0.63	2.24	3	5
1:A:49:LEU:HD13	1:A:49:LEU:N	0.63	2.09	9	1
1:A:49:LEU:N	1:A:49:LEU:HD13	0.63	2.09	6	1
1:A:84:LEU:HD22	1:A:99:LEU:HD22	0.63	1.71	11	1
1:A:75:LEU:HD13	1:A:104:TRP:CD1	0.63	2.28	18	3
1:A:5:VAL:HG11	1:A:40:LEU:HD21	0.63	1.71	6	1
1:A:36:VAL:HG23	1:A:38:PHE:CE1	0.63	2.29	18	3
1:A:57:VAL:O	1:A:60:VAL:HG12	0.63	1.94	15	4
1:A:161:LEU:N	1:A:166:LEU:HB2	0.62	2.09	14	13
1:A:7:VAL:HG13	1:A:11:VAL:HG21	0.62	1.69	16	14
1:A:100:VAL:HG21	1:A:149:LEU:HD11	0.62	1.72	16	1
1:A:100:VAL:HG11	1:A:149:LEU:CD2	0.62	2.10	12	1
1:A:75:LEU:HD12	1:A:143:VAL:HG11	0.62	1.71	9	4
1:A:7:VAL:HG21	1:A:127:LYS:HG3	0.62	1.70	8	6
1:A:60:VAL:HG22	1:A:67:PRO:HG3	0.62	1.71	13	1
1:A:12:ILE:HD12	1:A:127:LYS:HG2	0.62	1.72	13	1
1:A:15:PHE:CE1	1:A:131:ILE:HD12	0.62	2.29	11	3
1:A:75:LEU:CD2	1:A:143:VAL:HG11	0.61	2.24	19	6
1:A:10:GLY:HA2	1:A:13:LYS:HB2	0.61	1.70	18	6
1:A:84:LEU:HD21	1:A:131:ILE:CD1	0.61	2.25	2	9
1:A:84:LEU:HD11	1:A:131:ILE:CD1	0.61	2.25	4	1
1:A:100:VAL:CG2	1:A:149:LEU:HD21	0.61	2.13	1	1
1:A:153:LEU:HD11	1:A:158:VAL:HG21	0.61	1.72	15	2
1:A:7:VAL:HG13	1:A:11:VAL:CG2	0.61	2.26	16	5
1:A:84:LEU:HB3	1:A:99:LEU:HD11	0.61	1.72	15	1
1:A:72:VAL:HG12	1:A:140:TYR:CE2	0.61	2.30	16	11
1:A:40:LEU:CD1	1:A:47:ILE:HD13	0.61	2.26	10	1
1:A:37:LEU:HD21	1:A:75:LEU:CD1	0.61	2.25	15	1
1:A:32:ARG:NH1	1:A:57:VAL:HG11	0.61	2.10	19	2
1:A:5:VAL:HG21	1:A:47:ILE:CD1	0.61	2.26	17	2
1:A:71:PHE:CZ	1:A:75:LEU:HD11	0.61	2.31	10	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:LEU:CD1	1:A:149:LEU:HD22	0.61	2.26	3	3
1:A:5:VAL:HG11	1:A:120:SER:CB	0.61	2.25	3	4
1:A:25:THR:HG22	1:A:26:PRO:HD3	0.60	1.73	4	18
1:A:60:VAL:HG23	1:A:67:PRO:HG3	0.60	1.73	10	3
1:A:153:LEU:HD21	1:A:161:LEU:CD2	0.60	2.26	13	2
1:A:75:LEU:HD13	1:A:104:TRP:NE1	0.60	2.12	8	5
1:A:15:PHE:CD1	1:A:84:LEU:HD13	0.60	2.32	1	2
1:A:18:MET:CE	1:A:99:LEU:HD11	0.60	2.26	16	1
1:A:150:ALA:HB2	1:A:161:LEU:CD2	0.60	2.25	16	2
1:A:88:THR:HG23	1:A:162:GLU:CG	0.59	2.26	11	3
1:A:89:TYR:HE1	1:A:153:LEU:HD22	0.59	1.58	3	2
1:A:37:LEU:HD23	1:A:74:MET:HE3	0.59	1.73	10	1
1:A:86:ASP:OD2	1:A:99:LEU:HD13	0.59	1.97	14	1
1:A:40:LEU:HD22	1:A:47:ILE:HD13	0.59	1.74	20	2
1:A:33:LYS:HA	1:A:56:LEU:HD23	0.59	1.74	17	9
1:A:146:ARG:HD2	1:A:161:LEU:HD22	0.59	1.72	3	3
1:A:57:VAL:O	1:A:57:VAL:HG22	0.59	1.97	3	1
1:A:135:LEU:HD13	1:A:149:LEU:HD22	0.59	1.75	7	2
1:A:87:ALA:HB1	1:A:153:LEU:HD22	0.59	1.74	17	1
1:A:7:VAL:HG13	1:A:47:ILE:HB	0.59	1.73	10	1
1:A:5:VAL:HG22	1:A:47:ILE:HG12	0.58	1.74	16	8
1:A:11:VAL:HG21	1:A:47:ILE:HG22	0.58	1.75	8	6
1:A:72:VAL:HG11	1:A:144:LYS:HD3	0.58	1.75	8	1
1:A:34:LYS:HE3	1:A:88:THR:HG22	0.58	1.73	13	1
1:A:15:PHE:CD1	1:A:128:LEU:HD22	0.58	2.33	17	2
1:A:109:ALA:HB1	1:A:110:PRO:CD	0.58	2.29	14	13
1:A:104:TRP:CZ3	1:A:143:VAL:HG11	0.58	2.34	4	1
1:A:72:VAL:HG22	1:A:140:TYR:CD2	0.57	2.34	7	3
1:A:5:VAL:HG21	1:A:47:ILE:HD11	0.57	1.75	1	4
1:A:5:VAL:HG13	1:A:123:ALA:HB3	0.57	1.75	3	2
1:A:72:VAL:HG21	1:A:144:LYS:HB2	0.57	1.76	12	4
1:A:37:LEU:HD11	1:A:75:LEU:CD1	0.57	2.28	14	4
1:A:87:ALA:HB1	1:A:153:LEU:CD2	0.57	2.28	17	3
1:A:5:VAL:O	1:A:5:VAL:HG12	0.57	1.98	4	2
1:A:60:VAL:HG13	1:A:67:PRO:HG3	0.57	1.76	8	2
1:A:60:VAL:HG22	1:A:67:PRO:CG	0.57	2.29	13	1
1:A:7:VAL:HG22	1:A:47:ILE:HB	0.57	1.74	18	5
1:A:89:TYR:HB2	1:A:158:VAL:HG13	0.57	1.76	20	2
1:A:14:VAL:HB	1:A:49:LEU:HD13	0.57	1.77	19	6
1:A:135:LEU:HD22	1:A:149:LEU:CD2	0.56	2.24	6	2
1:A:14:VAL:CB	1:A:49:LEU:HD13	0.56	2.30	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:LEU:HD21	1:A:131:ILE:HD13	0.56	1.76	2	2
1:A:116:ILE:O	1:A:120:SER:N	0.56	2.37	7	17
1:A:88:THR:HG23	1:A:88:THR:O	0.56	2.00	10	5
1:A:37:LEU:HD22	1:A:74:MET:HE3	0.56	1.75	5	1
1:A:60:VAL:HG21	1:A:162:GLU:OE1	0.56	2.01	5	1
1:A:18:MET:SD	1:A:99:LEU:HD21	0.56	2.40	3	1
1:A:25:THR:HG22	1:A:26:PRO:CD	0.56	2.30	12	5
1:A:149:LEU:HD13	1:A:149:LEU:O	0.56	2.00	15	1
1:A:103:PHE:HB2	1:A:135:LEU:O	0.56	1.99	19	1
1:A:49:LEU:HD12	1:A:49:LEU:O	0.56	2.01	12	1
1:A:40:LEU:HD23	1:A:117:TYR:CE1	0.56	2.35	15	2
1:A:12:ILE:HD12	1:A:12:ILE:N	0.56	2.15	4	2
1:A:60:VAL:HG22	1:A:67:PRO:CD	0.56	2.30	1	1
1:A:128:LEU:N	1:A:128:LEU:HD23	0.56	2.15	19	1
1:A:75:LEU:N	1:A:76:PRO:HD3	0.56	2.15	18	18
1:A:161:LEU:H	1:A:166:LEU:HB2	0.56	1.61	14	15
1:A:18:MET:SD	1:A:99:LEU:HD13	0.56	2.41	9	1
1:A:131:ILE:HG23	1:A:131:ILE:O	0.56	2.01	15	3
1:A:72:VAL:HG12	1:A:140:TYR:CD2	0.56	2.36	3	8
1:A:12:ILE:HD13	1:A:127:LYS:HB3	0.56	1.77	6	1
1:A:15:PHE:CD2	1:A:128:LEU:HD22	0.56	2.36	16	2
1:A:160:SER:HA	1:A:166:LEU:CB	0.55	2.32	10	20
1:A:37:LEU:HD12	1:A:83:ALA:HB2	0.55	1.77	16	4
1:A:100:VAL:HG21	1:A:135:LEU:HD12	0.55	1.77	10	3
1:A:5:VAL:HG11	1:A:40:LEU:HD11	0.55	1.78	6	1
1:A:59:ASP:HB2	1:A:64:VAL:HG21	0.55	1.77	20	1
1:A:84:LEU:HD22	1:A:99:LEU:CG	0.54	2.32	9	1
1:A:36:VAL:O	1:A:83:ALA:HB1	0.54	2.03	13	2
1:A:11:VAL:HA	1:A:49:LEU:HD12	0.54	1.78	9	2
1:A:32:ARG:O	1:A:56:LEU:HD22	0.54	2.02	19	1
1:A:62:GLN:HG3	1:A:63:THR:HG22	0.54	1.78	11	1
1:A:37:LEU:HD21	1:A:71:PHE:CE2	0.54	2.37	12	1
1:A:87:ALA:HB1	1:A:153:LEU:HD23	0.54	1.80	19	1
1:A:111:LEU:HD13	1:A:111:LEU:O	0.54	2.03	16	3
1:A:87:ALA:CB	1:A:153:LEU:HD11	0.54	2.33	9	2
1:A:57:VAL:HG22	1:A:57:VAL:O	0.54	2.02	18	1
1:A:84:LEU:HD22	1:A:99:LEU:HD21	0.54	1.78	15	1
1:A:49:LEU:HD22	1:A:49:LEU:O	0.54	2.03	9	2
1:A:164:LYS:N	1:A:165:PRO:HD2	0.54	2.18	2	20
1:A:18:MET:O	1:A:99:LEU:HD22	0.54	2.02	16	1
1:A:160:SER:HA	1:A:166:LEU:HB2	0.53	1.79	13	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:TYR:CE1	1:A:117:TYR:CE2	0.53	2.96	11	9
1:A:164:LYS:HG3	1:A:165:PRO:N	0.53	2.19	14	20
1:A:87:ALA:HB3	1:A:149:LEU:HD11	0.53	1.79	2	1
1:A:72:VAL:HG11	1:A:144:LYS:HD2	0.53	1.78	8	1
1:A:101:PHE:HB2	1:A:131:ILE:HD13	0.53	1.79	17	1
1:A:12:ILE:HD12	1:A:127:LYS:HD3	0.53	1.79	12	1
1:A:23:SER:HB3	1:A:29:VAL:HG12	0.53	1.80	2	4
1:A:82:TYR:O	1:A:83:ALA:HB2	0.53	2.04	20	5
1:A:40:LEU:HD23	1:A:117:TYR:CD1	0.53	2.38	15	2
1:A:137:ALA:CB	1:A:143:VAL:HG22	0.53	2.33	19	7
1:A:40:LEU:HD22	1:A:44:LYS:HA	0.53	1.80	12	1
1:A:7:VAL:CG1	1:A:11:VAL:HG21	0.53	2.32	10	1
1:A:82:TYR:CD2	1:A:124:ILE:HD13	0.53	2.39	19	1
1:A:99:LEU:C	1:A:99:LEU:HD13	0.53	2.24	2	1
1:A:75:LEU:N	1:A:76:PRO:CD	0.53	2.72	18	16
1:A:5:VAL:HG13	1:A:47:ILE:HD11	0.53	1.79	4	1
1:A:12:ILE:HD11	1:A:127:LYS:HD2	0.53	1.75	20	1
1:A:100:VAL:HG13	1:A:100:VAL:O	0.53	2.04	12	4
1:A:60:VAL:O	1:A:60:VAL:HG12	0.53	2.04	8	1
1:A:36:VAL:O	1:A:36:VAL:HG23	0.52	2.05	5	2
1:A:100:VAL:O	1:A:100:VAL:HG13	0.52	2.04	10	3
1:A:37:LEU:HD21	1:A:75:LEU:HD11	0.52	1.81	15	1
1:A:135:LEU:HD11	1:A:152:LYS:NZ	0.52	2.19	1	1
1:A:31:LYS:O	1:A:56:LEU:HD22	0.52	2.04	13	2
1:A:114:LYS:NZ	1:A:118:ALA:HB2	0.52	2.19	10	1
1:A:149:LEU:HD13	1:A:152:LYS:HD2	0.52	1.80	19	2
1:A:40:LEU:HD12	1:A:44:LYS:HA	0.52	1.81	6	3
1:A:89:TYR:CG	1:A:153:LEU:HD22	0.52	2.40	2	1
1:A:116:ILE:HG22	1:A:116:ILE:O	0.52	2.05	15	1
1:A:153:LEU:C	1:A:153:LEU:HD12	0.52	2.26	15	2
1:A:131:ILE:HG23	1:A:132:LYS:H	0.52	1.64	11	1
1:A:88:THR:O	1:A:88:THR:HG23	0.52	2.05	6	6
1:A:71:PHE:CZ	1:A:102:ILE:HG21	0.52	2.39	1	5
1:A:146:ARG:HG2	1:A:161:LEU:CB	0.52	2.35	20	4
1:A:153:LEU:HD12	1:A:154:GLY:H	0.52	1.64	1	1
1:A:87:ALA:CB	1:A:149:LEU:HD11	0.52	2.35	3	1
1:A:5:VAL:HG12	1:A:45:LYS:C	0.51	2.24	6	1
1:A:89:TYR:CD2	1:A:153:LEU:HD13	0.51	2.40	17	1
1:A:66:ASP:HB3	1:A:69:ALA:HB3	0.51	1.82	13	1
1:A:76:PRO:O	1:A:104:TRP:NE1	0.51	2.43	3	16
1:A:153:LEU:HD21	1:A:161:LEU:HD21	0.51	1.80	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:VAL:HG22	1:A:143:VAL:CG1	0.51	2.34	16	4
1:A:40:LEU:HD22	1:A:44:LYS:CA	0.51	2.34	12	1
1:A:82:TYR:CZ	1:A:117:TYR:CD2	0.51	2.97	14	6
1:A:105:ALA:HB2	1:A:117:TYR:HE1	0.51	1.58	3	3
1:A:100:VAL:O	1:A:100:VAL:HG23	0.51	2.06	1	1
1:A:149:LEU:HA	1:A:152:LYS:HE2	0.51	1.80	1	1
1:A:20:VAL:HG23	1:A:22:LYS:CG	0.51	2.36	2	1
1:A:85:TYR:O	1:A:100:VAL:HG22	0.51	2.05	6	1
1:A:60:VAL:HG13	1:A:67:PRO:HD3	0.51	1.83	9	1
1:A:37:LEU:HD11	1:A:75:LEU:HD12	0.51	1.82	15	2
1:A:101:PHE:CE1	1:A:103:PHE:CE1	0.51	2.99	19	1
1:A:82:TYR:CE1	1:A:103:PHE:CE2	0.51	2.99	5	1
1:A:5:VAL:HG13	1:A:5:VAL:O	0.50	2.06	19	4
1:A:114:LYS:HZ1	1:A:118:ALA:HB2	0.50	1.66	10	1
1:A:84:LEU:HD23	1:A:101:PHE:N	0.50	2.22	12	2
1:A:86:ASP:OD1	1:A:99:LEU:HD12	0.50	2.05	10	1
1:A:149:LEU:HD22	1:A:152:LYS:CE	0.50	2.36	1	1
1:A:37:LEU:HD22	1:A:74:MET:CE	0.50	2.37	5	1
1:A:82:TYR:CD1	1:A:117:TYR:CE2	0.50	2.99	3	4
1:A:68:TYR:CD2	1:A:85:TYR:CZ	0.50	3.00	11	1
1:A:25:THR:O	1:A:29:VAL:HG22	0.50	2.05	18	2
1:A:8:SER:O	1:A:9:ASP:CB	0.50	2.59	16	4
1:A:37:LEU:HD13	1:A:74:MET:HE3	0.50	1.83	5	1
1:A:116:ILE:O	1:A:116:ILE:HG22	0.50	2.07	19	1
1:A:146:ARG:HG3	1:A:161:LEU:HD13	0.50	1.83	1	1
1:A:135:LEU:HD21	1:A:148:THR:HG22	0.50	1.79	16	1
1:A:75:LEU:CD2	1:A:104:TRP:CD1	0.49	2.95	7	4
1:A:75:LEU:HD13	1:A:104:TRP:CG	0.49	2.43	7	3
1:A:100:VAL:HG11	1:A:152:LYS:CB	0.49	2.36	8	2
1:A:82:TYR:CE2	1:A:117:TYR:CZ	0.49	3.01	19	1
1:A:82:TYR:CE1	1:A:117:TYR:CD2	0.49	3.00	20	4
1:A:146:ARG:HG3	1:A:161:LEU:HG	0.49	1.83	8	8
1:A:14:VAL:CG2	1:A:36:VAL:HG11	0.49	2.37	18	2
1:A:23:SER:HB2	1:A:29:VAL:HG12	0.49	1.84	1	5
1:A:82:TYR:CE2	1:A:117:TYR:CE2	0.49	3.00	1	2
1:A:5:VAL:HG13	1:A:47:ILE:CD1	0.49	2.37	4	1
1:A:75:LEU:HD23	1:A:104:TRP:CD2	0.49	2.43	5	1
1:A:75:LEU:CD1	1:A:104:TRP:CG	0.49	2.96	7	3
1:A:104:TRP:CH2	1:A:143:VAL:HG21	0.49	2.43	12	1
1:A:37:LEU:HD11	1:A:75:LEU:HD11	0.49	1.84	2	1
1:A:84:LEU:CD2	1:A:99:LEU:HD11	0.49	2.33	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:ARG:O	1:A:161:LEU:HD13	0.49	2.08	1	1
1:A:82:TYR:CZ	1:A:117:TYR:CE2	0.49	3.00	1	3
1:A:82:TYR:CD2	1:A:117:TYR:CE2	0.49	3.01	19	1
1:A:131:ILE:O	1:A:131:ILE:HG23	0.49	2.06	3	1
1:A:25:THR:CB	1:A:26:PRO:CD	0.49	2.91	20	20
1:A:7:VAL:HG11	1:A:127:LYS:HG3	0.49	1.84	10	1
1:A:146:ARG:HG2	1:A:165:PRO:HB2	0.49	1.84	13	7
1:A:5:VAL:HG13	1:A:40:LEU:HD11	0.49	1.85	9	1
1:A:159:ILE:HG23	1:A:160:SER:N	0.49	2.22	20	1
1:A:15:PHE:HE2	1:A:131:ILE:HD12	0.49	1.67	13	1
1:A:84:LEU:HD23	1:A:101:PHE:HA	0.48	1.83	16	2
1:A:111:LEU:O	1:A:111:LEU:HD23	0.48	2.07	3	2
1:A:11:VAL:CG2	1:A:47:ILE:HG22	0.48	2.36	8	3
1:A:135:LEU:HD23	1:A:148:THR:HG22	0.48	1.83	16	1
1:A:72:VAL:HG21	1:A:144:LYS:CB	0.48	2.38	12	2
1:A:110:PRO:O	1:A:114:LYS:HB2	0.48	2.08	3	3
1:A:15:PHE:CE1	1:A:84:LEU:HD13	0.48	2.43	1	1
1:A:55:ILE:HD13	1:A:70:THR:HB	0.48	1.85	14	2
1:A:27:GLU:CG	1:A:27:GLU:O	0.48	2.61	20	6
1:A:104:TRP:CE3	1:A:104:TRP:HA	0.48	2.43	12	2
1:A:75:LEU:CD1	1:A:104:TRP:CE2	0.48	2.96	12	3
1:A:131:ILE:HG23	1:A:132:LYS:N	0.48	2.24	6	1
1:A:140:TYR:HA	1:A:143:VAL:HG13	0.48	1.85	4	1
1:A:152:LYS:CE	1:A:153:LEU:HD23	0.48	2.38	16	1
1:A:25:THR:HB	1:A:26:PRO:CD	0.48	2.38	17	12
1:A:161:LEU:N	1:A:166:LEU:HD12	0.48	2.24	20	4
1:A:161:LEU:CD1	1:A:161:LEU:O	0.48	2.61	20	3
1:A:37:LEU:HD21	1:A:75:LEU:HD23	0.48	1.84	18	1
1:A:160:SER:C	1:A:166:LEU:HD12	0.47	2.29	11	3
1:A:72:VAL:CG1	1:A:140:TYR:CD2	0.47	2.97	5	9
1:A:47:ILE:HD12	1:A:82:TYR:CE2	0.47	2.44	10	1
1:A:37:LEU:HD11	1:A:75:LEU:CD2	0.47	2.39	8	1
1:A:99:LEU:HD22	1:A:100:VAL:N	0.47	2.24	2	1
1:A:71:PHE:CE2	1:A:75:LEU:CD2	0.47	2.97	6	11
1:A:104:TRP:CZ3	1:A:143:VAL:CG2	0.47	2.97	7	12
1:A:35:ALA:CB	1:A:85:TYR:CD2	0.47	2.98	15	4
1:A:103:PHE:CE2	1:A:121:LYS:CB	0.47	2.97	3	2
1:A:47:ILE:O	1:A:48:ILE:HG23	0.47	2.10	6	2
1:A:37:LEU:HD23	1:A:74:MET:CE	0.47	2.39	10	2
1:A:68:TYR:CD1	1:A:146:ARG:NH2	0.47	2.83	11	2
1:A:71:PHE:CE1	1:A:75:LEU:CD1	0.47	2.97	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:THR:HG23	1:A:162:GLU:CD	0.47	2.29	13	1
1:A:72:VAL:CG2	1:A:140:TYR:CD2	0.47	2.97	8	5
1:A:101:PHE:CE2	1:A:128:LEU:CD1	0.47	2.97	15	13
1:A:60:VAL:HG21	1:A:162:GLU:CD	0.47	2.29	10	1
1:A:72:VAL:HG21	1:A:144:LYS:CA	0.47	2.40	1	1
1:A:82:TYR:HB3	1:A:101:PHE:CE1	0.47	2.44	20	1
1:A:82:TYR:CE1	1:A:103:PHE:CE1	0.47	3.03	18	1
1:A:46:ASN:O	1:A:48:ILE:HG23	0.47	2.10	10	1
1:A:5:VAL:HG13	1:A:47:ILE:CG1	0.47	2.40	4	2
1:A:27:GLU:O	1:A:27:GLU:CG	0.47	2.63	15	5
1:A:35:ALA:HB3	1:A:55:ILE:HB	0.47	1.85	10	2
1:A:149:LEU:HD11	1:A:152:LYS:NZ	0.46	2.25	18	1
1:A:48:ILE:C	1:A:48:ILE:HD12	0.46	2.30	9	2
1:A:160:SER:CA	1:A:166:LEU:HB2	0.46	2.40	17	7
1:A:7:VAL:HG22	1:A:47:ILE:CG1	0.46	2.40	17	1
1:A:92:LYS:HD2	1:A:157:ALA:HB1	0.46	1.85	17	1
1:A:62:GLN:OE1	1:A:63:THR:HG23	0.46	2.10	18	1
1:A:104:TRP:HA	1:A:104:TRP:CE3	0.46	2.46	8	1
1:A:110:PRO:O	1:A:113:SER:N	0.46	2.47	3	1
1:A:162:GLU:HB2	1:A:165:PRO:CG	0.46	2.39	9	14
1:A:32:ARG:O	1:A:57:VAL:HG13	0.46	2.10	16	1
1:A:71:PHE:CZ	1:A:75:LEU:CD1	0.46	2.99	10	5
1:A:34:LYS:HB2	1:A:57:VAL:HG12	0.46	1.87	16	1
1:A:15:PHE:CE1	1:A:131:ILE:CD1	0.46	2.99	12	3
1:A:100:VAL:HG13	1:A:152:LYS:NZ	0.46	2.26	16	1
1:A:59:ASP:CG	1:A:64:VAL:HG21	0.46	2.31	10	1
1:A:104:TRP:CZ3	1:A:143:VAL:CG1	0.46	2.99	4	1
1:A:90:GLU:CB	1:A:159:ILE:HD11	0.46	2.40	8	1
1:A:40:LEU:HD23	1:A:46:ASN:O	0.46	2.11	12	1
1:A:35:ALA:HB2	1:A:85:TYR:CG	0.46	2.45	14	1
1:A:90:GLU:HB3	1:A:159:ILE:HD11	0.46	1.87	17	1
1:A:15:PHE:CZ	1:A:131:ILE:CD1	0.45	2.99	20	4
1:A:89:TYR:CE1	1:A:153:LEU:CB	0.45	2.99	1	1
1:A:83:ALA:HB3	1:A:102:ILE:HB	0.45	1.86	20	1
1:A:71:PHE:HE2	1:A:102:ILE:HG21	0.45	1.71	5	1
1:A:11:VAL:HG21	1:A:47:ILE:CG2	0.45	2.40	8	2
1:A:37:LEU:HD23	1:A:83:ALA:HB2	0.45	1.88	20	2
1:A:55:ILE:HD12	1:A:70:THR:CG2	0.45	2.41	19	1
1:A:44:LYS:NZ	1:A:116:ILE:HD13	0.45	2.25	11	1
1:A:37:LEU:HG	1:A:83:ALA:HB2	0.45	1.88	5	1
1:A:34:LYS:NZ	1:A:60:VAL:HG22	0.45	2.26	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:160:SER:OG	1:A:166:LEU:HB2	0.45	2.10	8	2
1:A:37:LEU:CD2	1:A:71:PHE:CE2	0.45	3.00	12	1
1:A:71:PHE:CZ	1:A:75:LEU:CD2	0.45	3.00	6	1
1:A:84:LEU:CD2	1:A:131:ILE:HD11	0.45	2.36	3	2
1:A:12:ILE:HD11	1:A:127:LYS:HB2	0.45	1.89	1	1
1:A:117:TYR:O	1:A:121:LYS:N	0.45	2.49	4	9
1:A:68:TYR:CD1	1:A:85:TYR:CE2	0.45	3.05	6	1
1:A:12:ILE:N	1:A:12:ILE:CD1	0.45	2.80	4	2
1:A:71:PHE:CE1	1:A:75:LEU:HD11	0.45	2.47	19	3
1:A:137:ALA:HB1	1:A:142:GLU:CB	0.45	2.41	1	2
1:A:85:TYR:CD1	1:A:86:ASP:N	0.45	2.84	1	5
1:A:12:ILE:CD1	1:A:128:LEU:HD23	0.45	2.42	6	1
1:A:36:VAL:HG23	1:A:38:PHE:CZ	0.45	2.47	16	2
1:A:36:VAL:CG2	1:A:38:PHE:CE2	0.45	2.99	10	1
1:A:103:PHE:N	1:A:135:LEU:O	0.45	2.50	15	2
1:A:84:LEU:HD21	1:A:101:PHE:CD2	0.45	2.46	17	1
1:A:40:LEU:HD21	1:A:47:ILE:CD1	0.44	2.41	11	2
1:A:49:LEU:CD1	1:A:49:LEU:N	0.44	2.80	9	1
1:A:15:PHE:CE1	1:A:19:LYS:CG	0.44	3.00	6	1
1:A:15:PHE:CZ	1:A:19:LYS:CG	0.44	3.00	8	2
1:A:72:VAL:HA	1:A:75:LEU:CB	0.44	2.43	2	10
1:A:71:PHE:CD2	1:A:75:LEU:HD13	0.44	2.48	1	1
1:A:154:GLY:C	1:A:158:VAL:HG23	0.44	2.32	16	1
1:A:11:VAL:N	1:A:49:LEU:HD22	0.44	2.28	15	1
1:A:55:ILE:CD1	1:A:70:THR:HG22	0.44	2.42	11	2
1:A:5:VAL:HG21	1:A:120:SER:HB2	0.44	1.90	4	2
1:A:113:SER:HA	1:A:116:ILE:HD12	0.44	1.90	17	2
1:A:44:LYS:O	1:A:116:ILE:HD12	0.44	2.12	12	1
1:A:80:CYS:HG	1:A:117:TYR:CB	0.44	2.26	4	2
1:A:111:LEU:O	1:A:111:LEU:HD13	0.44	2.12	7	1
1:A:5:VAL:O	1:A:5:VAL:HG13	0.44	2.12	7	3
1:A:37:LEU:HD21	1:A:75:LEU:HD12	0.44	1.88	10	1
1:A:55:ILE:HD11	1:A:74:MET:CE	0.44	2.42	6	1
1:A:161:LEU:O	1:A:161:LEU:CD1	0.44	2.66	8	3
1:A:75:LEU:CD2	1:A:143:VAL:HG21	0.44	2.43	4	1
1:A:99:LEU:HD23	1:A:100:VAL:H	0.44	1.73	8	1
1:A:47:ILE:HG21	1:A:124:ILE:HD13	0.44	1.90	15	1
1:A:60:VAL:HG22	1:A:67:PRO:HB3	0.44	1.88	17	1
1:A:101:PHE:HD2	1:A:131:ILE:HD13	0.44	1.72	5	1
1:A:83:ALA:O	1:A:102:ILE:N	0.43	2.51	9	3
1:A:78:LYS:N	1:A:78:LYS:CD	0.43	2.81	3	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ILE:O	1:A:132:LYS:CB	0.43	2.66	6	1
1:A:68:TYR:CD2	1:A:146:ARG:CD	0.43	3.01	13	2
1:A:100:VAL:HG21	1:A:135:LEU:CD1	0.43	2.43	19	1
1:A:55:ILE:HD13	1:A:70:THR:CG2	0.43	2.21	16	1
1:A:84:LEU:HD11	1:A:101:PHE:CD2	0.43	2.48	10	1
1:A:135:LEU:HD22	1:A:148:THR:CG2	0.43	2.43	11	1
1:A:34:LYS:N	1:A:55:ILE:O	0.43	2.51	16	2
1:A:15:PHE:CD1	1:A:128:LEU:CD2	0.43	3.01	17	1
1:A:72:VAL:CG1	1:A:140:TYR:CG	0.43	3.01	13	1
1:A:37:LEU:CD2	1:A:71:PHE:CE1	0.43	3.01	1	1
1:A:36:VAL:O	1:A:38:PHE:CE1	0.43	2.72	17	4
1:A:124:ILE:O	1:A:127:LYS:CG	0.43	2.67	1	1
1:A:82:TYR:CD2	1:A:117:TYR:CZ	0.43	3.06	19	2
1:A:78:LYS:CD	1:A:78:LYS:N	0.43	2.82	8	6
1:A:75:LEU:HD13	1:A:104:TRP:CD2	0.43	2.49	7	2
1:A:37:LEU:HD12	1:A:83:ALA:CB	0.43	2.43	2	1
1:A:160:SER:OG	1:A:161:LEU:N	0.43	2.52	20	4
1:A:149:LEU:C	1:A:149:LEU:HD13	0.43	2.33	3	1
1:A:135:LEU:HD11	1:A:152:LYS:HZ3	0.43	1.72	1	1
1:A:64:VAL:HG12	1:A:65:ASP:N	0.43	2.29	3	3
1:A:152:LYS:HZ2	1:A:153:LEU:HD21	0.43	1.74	3	1
1:A:60:VAL:HG23	1:A:67:PRO:CD	0.43	2.44	16	1
1:A:40:LEU:HD22	1:A:44:LYS:C	0.43	2.34	12	1
1:A:48:ILE:HD12	1:A:49:LEU:O	0.43	2.13	12	1
1:A:12:ILE:O	1:A:16:ASN:N	0.43	2.51	6	1
1:A:25:THR:HB	1:A:26:PRO:HD2	0.43	1.91	6	1
1:A:20:VAL:HG12	1:A:21:ARG:N	0.43	2.29	5	2
1:A:15:PHE:CD1	1:A:84:LEU:CD1	0.43	3.01	1	2
1:A:100:VAL:HG13	1:A:102:ILE:HG13	0.43	1.91	19	1
1:A:72:VAL:CG2	1:A:140:TYR:CE2	0.43	3.01	11	1
1:A:149:LEU:O	1:A:152:LYS:CD	0.43	2.67	1	3
1:A:131:ILE:O	1:A:133:HIS:N	0.43	2.52	4	1
1:A:89:TYR:CG	1:A:153:LEU:HD13	0.43	2.48	8	1
1:A:15:PHE:HZ	1:A:131:ILE:HD12	0.42	1.70	15	2
1:A:149:LEU:O	1:A:153:LEU:HD23	0.42	2.13	17	1
1:A:91:THR:O	1:A:93:GLU:N	0.42	2.51	13	1
1:A:161:LEU:O	1:A:162:GLU:CB	0.42	2.67	8	1
1:A:40:LEU:N	1:A:117:TYR:CE1	0.42	2.87	19	1
1:A:82:TYR:CG	1:A:117:TYR:CE2	0.42	3.07	19	1
1:A:87:ALA:HB3	1:A:152:LYS:NZ	0.42	2.29	3	2
1:A:75:LEU:HG	1:A:104:TRP:CD1	0.42	2.50	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:TYR:CE1	1:A:103:PHE:CD1	0.42	3.08	18	2
1:A:40:LEU:HD12	1:A:45:LYS:N	0.42	2.29	10	1
1:A:89:TYR:CB	1:A:158:VAL:HG13	0.42	2.44	20	1
1:A:37:LEU:HD13	1:A:74:MET:CE	0.42	2.44	17	1
1:A:100:VAL:HG12	1:A:133:HIS:HB3	0.42	1.90	7	1
1:A:55:ILE:HD11	1:A:74:MET:HE2	0.42	1.91	6	1
1:A:77:ASP:OD2	1:A:108:SER:CB	0.42	2.68	10	1
1:A:99:LEU:HD23	1:A:100:VAL:N	0.42	2.29	8	1
1:A:8:SER:CB	1:A:48:ILE:CG2	0.42	2.96	9	3
1:A:84:LEU:HD23	1:A:100:VAL:C	0.42	2.35	7	2
1:A:160:SER:OG	1:A:163:GLY:N	0.42	2.53	2	3
1:A:68:TYR:CG	1:A:146:ARG:CZ	0.42	3.02	20	1
1:A:75:LEU:O	1:A:104:TRP:CZ2	0.42	2.73	3	1
1:A:87:ALA:CB	1:A:152:LYS:CE	0.42	2.98	3	1
1:A:14:VAL:CG1	1:A:49:LEU:HD22	0.42	2.45	20	1
1:A:38:PHE:CZ	1:A:84:LEU:HD12	0.42	2.50	17	1
1:A:75:LEU:HD23	1:A:104:TRP:CE2	0.42	2.50	5	1
1:A:18:MET:O	1:A:99:LEU:HD11	0.42	2.14	5	1
1:A:44:LYS:O	1:A:116:ILE:HG21	0.42	2.14	3	1
1:A:57:VAL:O	1:A:57:VAL:CG2	0.42	2.68	3	1
1:A:164:LYS:CB	1:A:165:PRO:CD	0.42	2.97	1	8
1:A:7:VAL:CG1	1:A:11:VAL:CG2	0.42	2.98	15	5
1:A:72:VAL:CG2	1:A:140:TYR:CG	0.42	3.02	2	1
1:A:100:VAL:CG1	1:A:152:LYS:CD	0.42	2.98	2	1
1:A:25:THR:HG22	1:A:26:PRO:HD2	0.42	1.91	2	2
1:A:152:LYS:CD	1:A:152:LYS:C	0.42	2.88	6	1
1:A:24:SER:O	1:A:29:VAL:HG13	0.42	2.15	18	2
1:A:127:LYS:O	1:A:129:THR:HG23	0.42	2.14	14	1
1:A:5:VAL:CG1	1:A:5:VAL:O	0.42	2.67	4	1
1:A:84:LEU:HD21	1:A:101:PHE:HD2	0.42	1.73	17	1
1:A:19:LYS:HG3	1:A:20:VAL:HG13	0.42	1.91	15	1
1:A:89:TYR:CD2	1:A:158:VAL:HG22	0.41	2.49	9	1
1:A:40:LEU:HD21	1:A:47:ILE:HD13	0.41	1.91	3	1
1:A:5:VAL:CG1	1:A:46:ASN:N	0.41	2.83	9	1
1:A:45:LYS:O	1:A:46:ASN:ND2	0.41	2.54	19	2
1:A:7:VAL:HG12	1:A:11:VAL:CG2	0.41	2.45	10	1
1:A:57:VAL:HG23	1:A:58:GLY:N	0.41	2.30	1	1
1:A:49:LEU:HD23	1:A:49:LEU:N	0.41	2.31	5	1
1:A:15:PHE:CE2	1:A:131:ILE:HD12	0.41	2.50	13	1
1:A:80:CYS:O	1:A:117:TYR:CE1	0.41	2.73	13	1
1:A:124:ILE:HG23	1:A:125:LYS:N	0.41	2.30	9	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:ARG:NE	1:A:165:PRO:CB	0.41	2.84	9	1
1:A:72:VAL:HA	1:A:75:LEU:HB2	0.41	1.92	2	3
1:A:77:ASP:CG	1:A:77:ASP:O	0.41	2.59	10	1
1:A:113:SER:O	1:A:117:TYR:CE1	0.41	2.73	9	1
1:A:49:LEU:H	1:A:49:LEU:HD13	0.41	1.73	9	1
1:A:89:TYR:CZ	1:A:96:LYS:CB	0.41	3.03	7	1
1:A:10:GLY:CA	1:A:13:LYS:HB2	0.41	2.44	18	1
1:A:87:ALA:HB3	1:A:149:LEU:HD12	0.41	1.93	8	1
1:A:10:GLY:C	1:A:49:LEU:HD22	0.41	2.36	15	1
1:A:104:TRP:O	1:A:117:TYR:CE2	0.41	2.74	11	1
1:A:152:LYS:HD3	1:A:152:LYS:C	0.41	2.35	11	1
1:A:14:VAL:HG11	1:A:38:PHE:CE2	0.41	2.51	18	1
1:A:164:LYS:CG	1:A:165:PRO:HD3	0.41	2.46	18	3
1:A:71:PHE:CZ	1:A:102:ILE:CG2	0.41	3.04	1	1
1:A:159:ILE:CG2	1:A:160:SER:N	0.41	2.83	20	1
1:A:104:TRP:CZ3	1:A:137:ALA:O	0.41	2.74	19	1
1:A:7:VAL:HG12	1:A:8:SER:N	0.41	2.30	9	3
1:A:89:TYR:CE2	1:A:96:LYS:CD	0.41	3.03	7	1
1:A:130:GLY:O	1:A:132:LYS:N	0.41	2.54	4	1
1:A:135:LEU:HD12	1:A:149:LEU:CD2	0.41	2.46	1	1
1:A:44:LYS:HZ1	1:A:116:ILE:HD13	0.41	1.75	11	1
1:A:100:VAL:CG1	1:A:152:LYS:CE	0.41	2.98	17	1
1:A:135:LEU:CD1	1:A:152:LYS:CG	0.41	2.98	5	1
1:A:7:VAL:HG11	1:A:11:VAL:HB	0.41	1.92	12	1
1:A:16:ASN:OD1	1:A:17:ASP:N	0.41	2.54	5	4
1:A:25:THR:CG2	1:A:26:PRO:CD	0.41	2.99	14	2
1:A:8:SER:HB2	1:A:48:ILE:HG23	0.41	1.92	6	1
1:A:101:PHE:HE2	1:A:128:LEU:HD12	0.41	1.75	19	1
1:A:30:LYS:O	1:A:58:GLY:N	0.41	2.54	11	1
1:A:150:ALA:HA	1:A:153:LEU:HD12	0.41	1.92	3	1
1:A:80:CYS:O	1:A:117:TYR:CZ	0.41	2.74	18	4
1:A:150:ALA:HA	1:A:153:LEU:HD21	0.41	1.93	2	1
1:A:34:LYS:HE2	1:A:88:THR:HG22	0.41	1.92	18	1
1:A:91:THR:HG23	1:A:92:LYS:H	0.41	1.76	18	1
1:A:84:LEU:HD11	1:A:131:ILE:HD13	0.41	1.93	4	1
1:A:98:ASP:OD2	1:A:133:HIS:CD2	0.41	2.74	1	1
1:A:60:VAL:O	1:A:60:VAL:HG22	0.41	2.16	11	1
1:A:25:THR:O	1:A:29:VAL:HG13	0.41	2.16	3	1
1:A:5:VAL:CG1	1:A:123:ALA:HB3	0.41	2.46	3	1
1:A:14:VAL:HG21	1:A:36:VAL:HG11	0.41	1.92	16	1
1:A:6:ALA:O	1:A:7:VAL:O	0.41	2.39	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:ALA:CB	1:A:117:TYR:CE1	0.41	3.00	7	1
1:A:10:GLY:O	1:A:13:LYS:N	0.41	2.54	18	1
1:A:5:VAL:CG2	1:A:47:ILE:CD1	0.41	2.99	8	1
1:A:89:TYR:CE1	1:A:153:LEU:HB2	0.41	2.51	1	1
1:A:132:LYS:O	1:A:133:HIS:CG	0.41	2.73	19	2
1:A:89:TYR:CE2	1:A:96:LYS:HB2	0.40	2.51	7	1
1:A:33:LYS:CD	1:A:36:VAL:CG1	0.40	3.00	1	1
1:A:99:LEU:HD12	1:A:99:LEU:N	0.40	2.31	19	1
1:A:40:LEU:HD13	1:A:44:LYS:HA	0.40	1.94	12	1
1:A:88:THR:CG2	1:A:162:GLU:CG	0.40	2.98	2	1
1:A:75:LEU:CD1	1:A:104:TRP:CD1	0.40	3.05	6	1
1:A:146:ARG:HG3	1:A:161:LEU:CG	0.40	2.46	18	1
1:A:101:PHE:CE1	1:A:103:PHE:CZ	0.40	3.10	19	1
1:A:152:LYS:CD	1:A:153:LEU:N	0.40	2.84	12	3
1:A:25:THR:CB	1:A:26:PRO:HD2	0.40	2.47	14	1
1:A:149:LEU:CA	1:A:152:LYS:HE2	0.40	2.46	1	1
1:A:131:ILE:CG1	1:A:132:LYS:N	0.40	2.83	11	1
1:A:68:TYR:CE2	1:A:143:VAL:O	0.40	2.74	13	1
1:A:5:VAL:CG1	1:A:123:ALA:CB	0.40	3.00	7	1
1:A:15:PHE:CZ	1:A:19:LYS:HG3	0.40	2.52	6	1
1:A:80:CYS:SG	1:A:117:TYR:CG	0.40	3.14	1	1
1:A:152:LYS:CD	1:A:153:LEU:CD2	0.40	2.99	16	1
1:A:25:THR:CG2	1:A:26:PRO:HD2	0.40	2.47	14	1
1:A:146:ARG:CD	1:A:165:PRO:HB2	0.40	2.46	1	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	161/166 (97%)	116±5 (72±3%)	34±5 (21±3%)	11±3 (7±2%)	3	18
All	All	3220/3320 (97%)	2324 (72%)	681 (21%)	215 (7%)	3	18

All 38 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	164	LYS	20
1	A	24	SER	20
1	A	102	ILE	18
1	A	162	GLU	16
1	A	76	PRO	14
1	A	71	PHE	12
1	A	132	LYS	12
1	A	91	THR	11
1	A	5	VAL	9
1	A	21	ARG	6
1	A	22	LYS	6
1	A	7	VAL	6
1	A	101	PHE	5
1	A	93	GLU	5
1	A	9	ASP	5
1	A	154	GLY	5
1	A	35	ALA	4
1	A	108	SER	4
1	A	45	LYS	3
1	A	62	GLN	3
1	A	131	ILE	3
1	A	129	THR	3
1	A	116	ILE	3
1	A	50	GLU	2
1	A	92	LYS	2
1	A	87	ALA	2
1	A	33	LYS	2
1	A	109	ALA	2
1	A	83	ALA	2
1	A	67	PRO	2
1	A	130	GLY	1
1	A	32	ARG	1
1	A	53	LYS	1
1	A	25	THR	1
1	A	41	SER	1
1	A	156	SER	1
1	A	155	GLY	1
1	A	135	LEU	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	142/144 (99%)	102±3 (72±2%)	40±3 (28±2%)	2	20
All	All	2840/2880 (99%)	2041 (72%)	799 (28%)	2	20

All 101 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	124	ILE	20
1	A	78	LYS	20
1	A	75	LEU	19
1	A	152	LYS	19
1	A	30	LYS	19
1	A	164	LYS	18
1	A	18	MET	18
1	A	149	LEU	18
1	A	25	THR	18
1	A	114	LYS	18
1	A	53	LYS	16
1	A	40	LEU	16
1	A	108	SER	16
1	A	107	GLU	16
1	A	33	LYS	16
1	A	125	LYS	16
1	A	113	SER	15
1	A	49	LEU	15
1	A	161	LEU	15
1	A	146	ARG	14
1	A	50	GLU	13
1	A	98	ASP	12
1	A	44	LYS	12
1	A	90	GLU	12
1	A	112	LYS	12
1	A	32	ARG	12
1	A	19	LYS	12
1	A	68	TYR	11
1	A	77	ASP	11
1	A	74	MET	11
1	A	73	LYS	11
1	A	119	SER	10
1	A	162	GLU	10

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Mol	Chain	Res	Type	Models (Total)
1	A	43	ASP	9
1	A	103	PHE	9
1	A	54	GLU	9
1	A	126	LYS	9
1	A	91	THR	9
1	A	45	LYS	9
1	A	139	CYS	9
1	A	13	LYS	8
1	A	37	LEU	8
1	A	131	ILE	8
1	A	22	LYS	8
1	A	134	GLU	8
1	A	120	SER	8
1	A	95	LYS	8
1	A	62	GLN	7
1	A	127	LYS	7
1	A	23	SER	7
1	A	94	SER	7
1	A	132	LYS	7
1	A	92	LYS	6
1	A	129	THR	6
1	A	17	ASP	6
1	A	34	LYS	6
1	A	147	CYS	6
1	A	111	LEU	5
1	A	151	GLU	5
1	A	99	LEU	5
1	A	122	ASP	5
1	A	59	ASP	5
1	A	93	GLU	5
1	A	51	GLU	5
1	A	27	GLU	5
1	A	145	ASP	5
1	A	21	ARG	4
1	A	135	LEU	4
1	A	42	GLU	4
1	A	115	MET	4
1	A	160	SER	4
1	A	96	LYS	3
1	A	46	ASN	3
1	A	9	ASP	3
1	A	39	CYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	156	SER	3
1	A	117	TYR	3
1	A	65	ASP	3
1	A	66	ASP	3
1	A	104	TRP	3
1	A	136	GLN	3
1	A	153	LEU	3
1	A	79	ASP	2
1	A	100	VAL	2
1	A	12	ILE	2
1	A	86	ASP	2
1	A	56	LEU	2
1	A	8	SER	2
1	A	121	LYS	2
1	A	81	ARG	1
1	A	138	ASN	1
1	A	72	VAL	1
1	A	80	CYS	1
1	A	84	LEU	1
1	A	7	VAL	1
1	A	101	PHE	1
1	A	140	TYR	1
1	A	128	LEU	1
1	A	143	VAL	1
1	A	144	LYS	1
1	A	5	VAL	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 6004

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	1864
Number of shifts mapped to atoms	1864
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
$^{13}\text{C}_\alpha$	164	$-0.10 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	155	$0.00 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	157	$0.90 \pm 0.35$	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 82%, i.e. 1636 atoms were assigned a chemical shift out of a possible 2007. 28 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	634/798 (79%)	316/318 (99%)	162/324 (50%)	156/156 (100%)
Sidechain	904/1096 (82%)	581/642 (90%)	317/412 (77%)	6/42 (14%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	98/113 (87%)	55/59 (93%)	42/51 (82%)	1/3 (33%)
Overall	1636/2007 (82%)	952/1019 (93%)	521/787 (66%)	163/201 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1642 atoms were assigned a chemical shift out of a possible 2040. 28 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	639/818 (78%)	318/326 (98%)	164/332 (49%)	157/160 (98%)
Sidechain	905/1109 (82%)	581/650 (89%)	318/417 (76%)	6/42 (14%)
Aromatic	98/113 (87%)	55/59 (93%)	42/51 (82%)	1/3 (33%)
Overall	1642/2040 (80%)	954/1035 (92%)	524/800 (66%)	164/205 (80%)

#### 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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	106	PRO	HD2	0.63	5.45 – 1.85	-8.4
1	A	75	LEU	HB3	-0.88	3.34 – -0.26	-6.7
1	A	96	LYS	HB3	0.10	3.10 – 0.40	-6.1
1	A	75	LEU	HG	-0.47	3.16 – -0.14	-6.0
1	A	152	LYS	HG3	-0.05	2.76 – -0.04	-5.0

#### 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.

Random coil index (RCI) for chain A:

