



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 19, 2018 – 11:44 am GMT

PDB ID : 2M7F  
Title : The C-terminal Region of Disintegrin Modulate its 3D Conformation and Co-operate with RGD Loop in Regulating Integrins Recognitions  
Authors : Chuang, W.; Chang, Y.  
Deposited on : 2013-04-22

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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 : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk30686  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

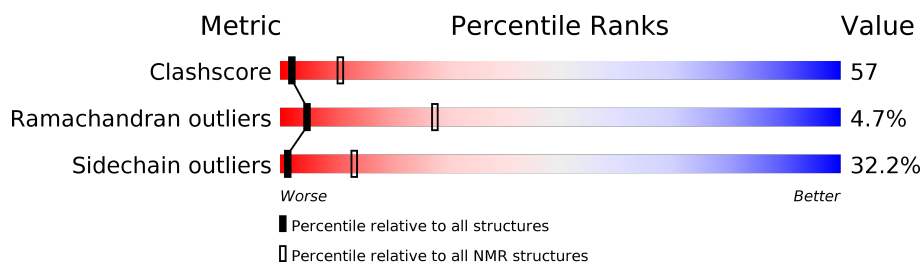
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 54%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	79	

## 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:68 (66)	0.54	1

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 5 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 989 atoms, of which 470 are hydrogens and 0 are deuteriums.

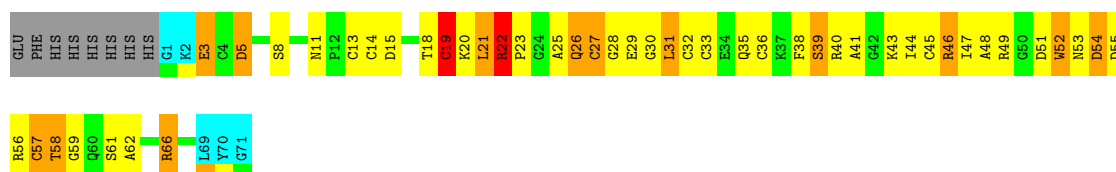
- Molecule 1 is a protein called Zinc metalloproteinase/disintegrin.

Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			989	302	470	100	105	12	

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLU	-	EXPRESSION TAG	UNP P30403
A	-6	PHE	-	EXPRESSION TAG	UNP P30403
A	-5	HIS	-	EXPRESSION TAG	UNP P30403
A	-4	HIS	-	EXPRESSION TAG	UNP P30403
A	-3	HIS	-	EXPRESSION TAG	UNP P30403
A	-2	HIS	-	EXPRESSION TAG	UNP P30403
A	-1	HIS	-	EXPRESSION TAG	UNP P30403
A	0	HIS	-	EXPRESSION TAG	UNP P30403
A	48	ALA	PRO	ENGINEERED MUTATION	UNP P30403
A	52	TRP	MET	ENGINEERED MUTATION	UNP P30403
A	53	ASN	PRO	ENGINEERED MUTATION	UNP P30403
A	67	ASN	TYR	ENGINEERED MUTATION	UNP P30403
A	68	GLY	HIS	ENGINEERED MUTATION	UNP P30403
A	69	LEU	SER	ENGINEERED MUTATION	UNP P30403
A	70	TYR	HIS	ENGINEERED MUTATION	UNP P30403
A	71	GLY	ALA	ENGINEERED MUTATION	UNP P30403

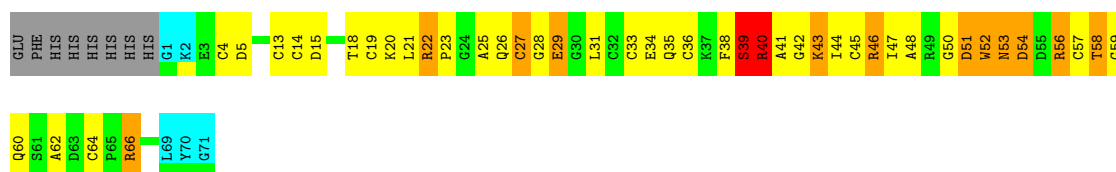




### 4.2.3 Score per residue for model 3

- Molecule 1: Zinc metalloproteinase/disintegrin

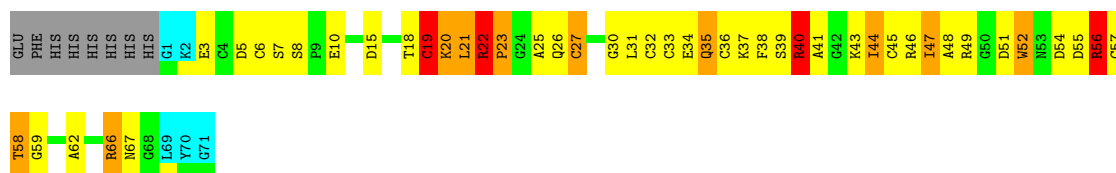
Chain A: 27% 39% 15% 6% 10%



### 4.2.4 Score per residue for model 4

- Molecule 1: Zinc metalloproteinase/disintegrin

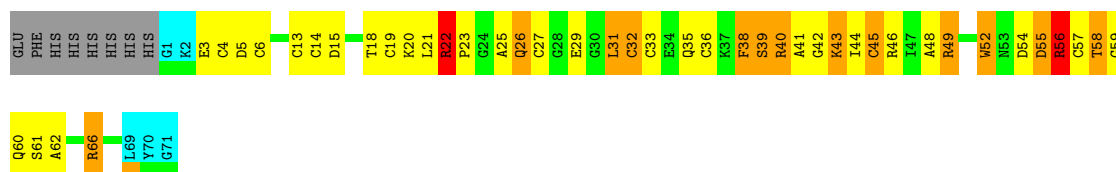
Chain A: 25% 41% 13% 5% 6% 10%



### 4.2.5 Score per residue for model 5

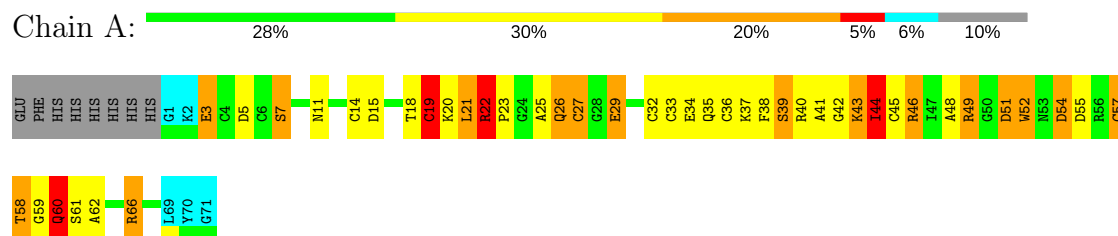
- Molecule 1: Zinc metalloproteinase/disintegrin

Chain A: 28% 37% 16% 6% 10%



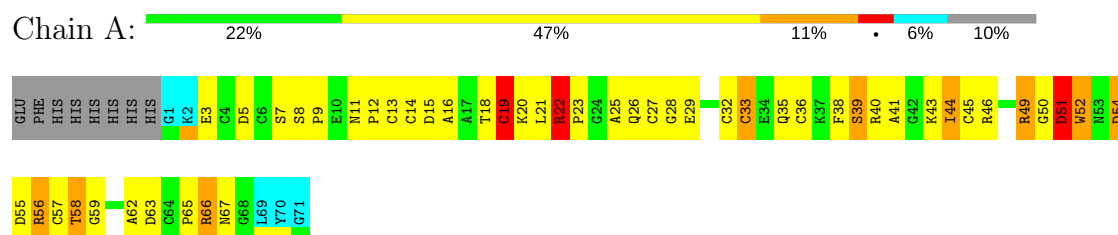
### 4.2.6 Score per residue for model 6

- Molecule 1: Zinc metalloproteinase/disintegrin



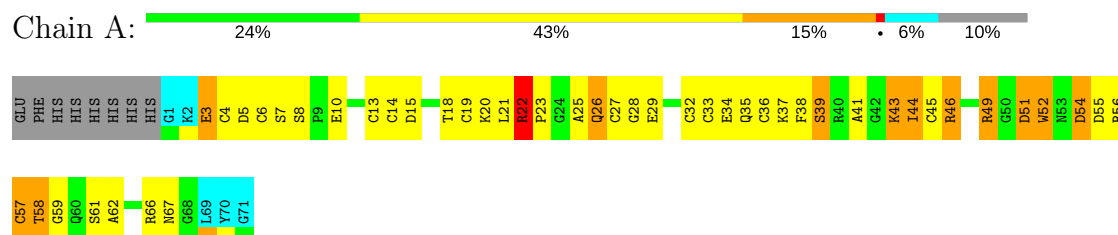
#### 4.2.7 Score per residue for model 7

- Molecule 1: Zinc metalloproteinase/disintegrin



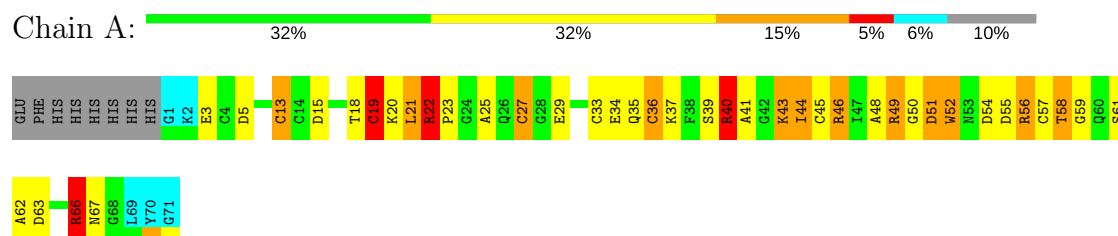
#### 4.2.8 Score per residue for model 8

- Molecule 1: Zinc metalloproteinase/disintegrin



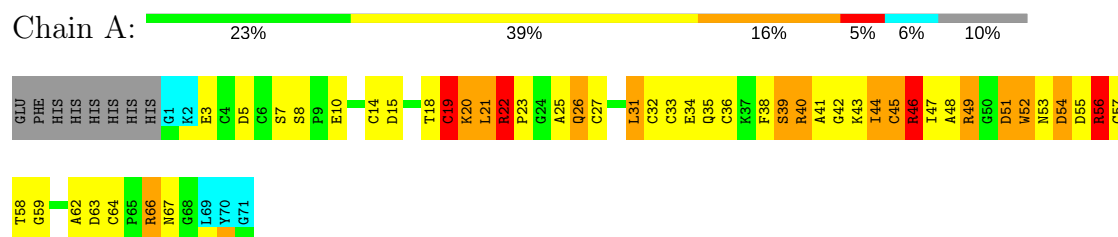
#### 4.2.9 Score per residue for model 9

- Molecule 1: Zinc metalloproteinase/disintegrin



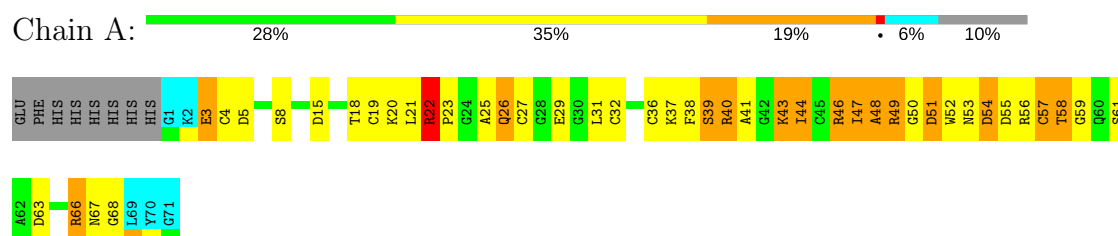
### 4.2.10 Score per residue for model 10

- Molecule 1: Zinc metalloproteinase/disintegrin



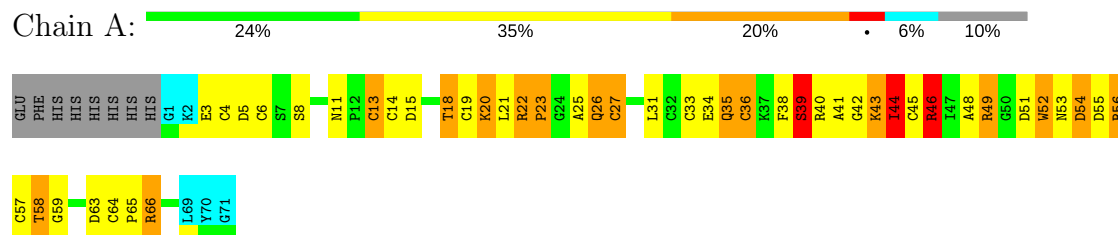
### 4.2.11 Score per residue for model 11

- Molecule 1: Zinc metalloproteinase/disintegrin



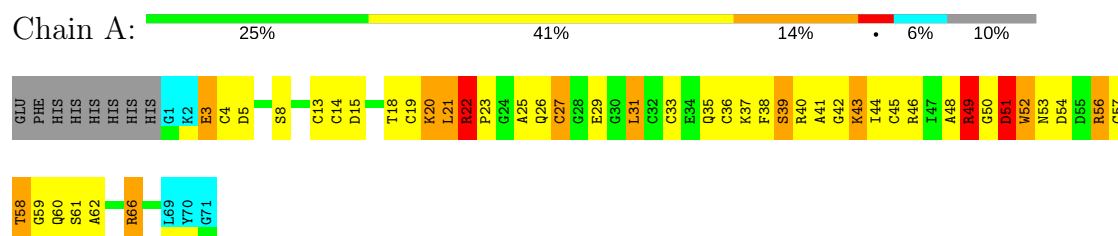
### 4.2.12 Score per residue for model 12

- Molecule 1: Zinc metalloproteinase/disintegrin



### 4.2.13 Score per residue for model 13

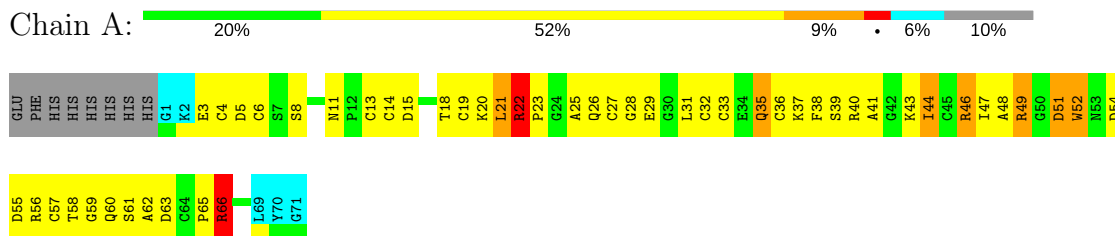
- Molecule 1: Zinc metalloproteinase/disintegrin





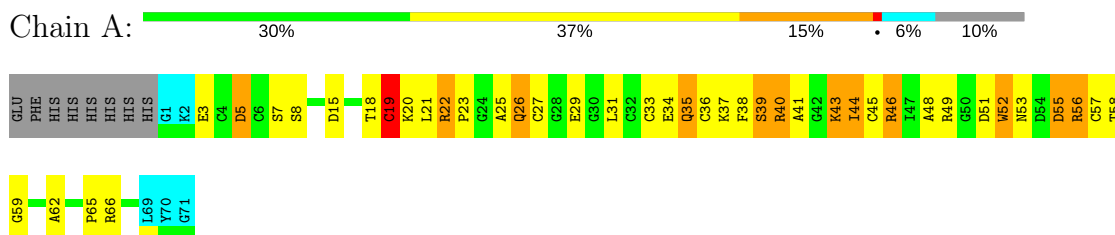
#### 4.2.14 Score per residue for model 14

- Molecule 1: Zinc metalloproteinase/disintegrin



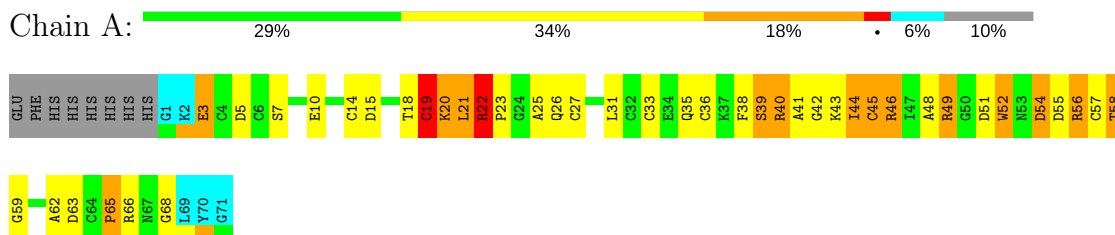
#### 4.2.15 Score per residue for model 15

- Molecule 1: Zinc metalloproteinase/disintegrin



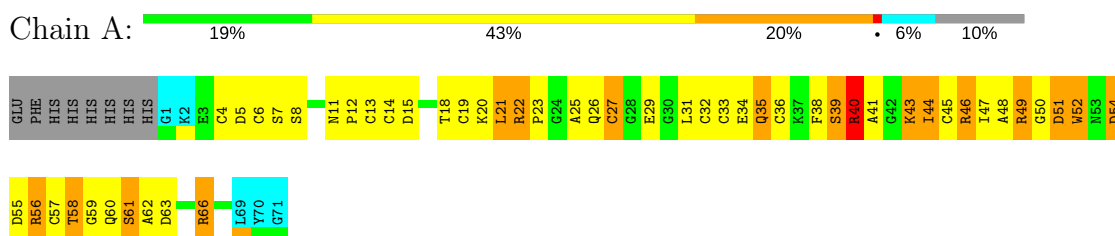
#### 4.2.16 Score per residue for model 16

- Molecule 1: Zinc metalloproteinase/disintegrin



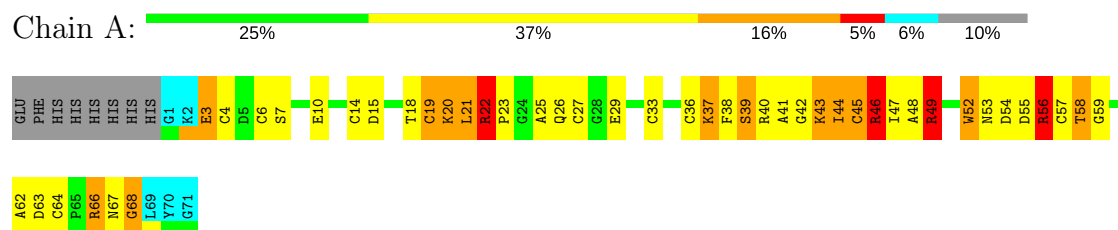
#### 4.2.17 Score per residue for model 17

- Molecule 1: Zinc metalloproteinase/disintegrin



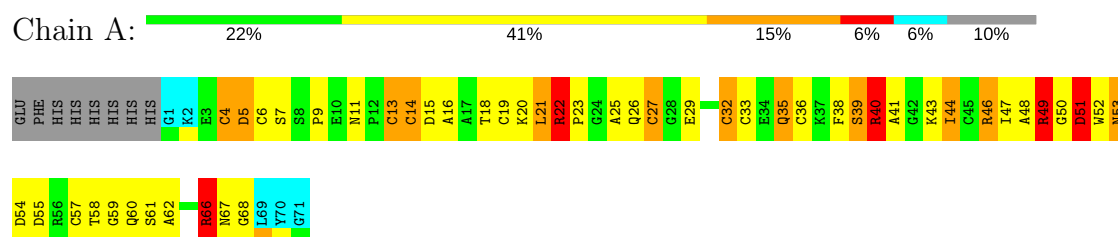
### 4.2.18 Score per residue for model 18

- Molecule 1: Zinc metalloproteinase/disintegrin



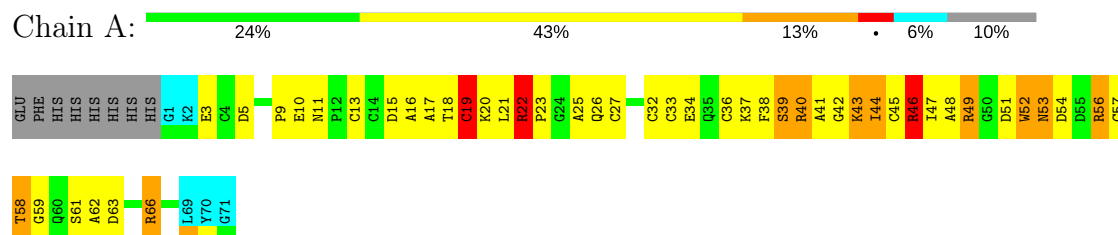
### 4.2.19 Score per residue for model 19

- Molecule 1: Zinc metalloproteinase/disintegrin



### 4.2.20 Score per residue for model 20

- Molecule 1: Zinc metalloproteinase/disintegrin



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing*.

Of the 200 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
X-PLOR	refinement	3.185

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)	2m7f_cs.str
Number of chemical shift lists	1
Total number of shifts	471
Number of shifts mapped to atoms	471
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

There are no covalent bond-length or bond-angle outliers.

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.7±0.5
All	All	0	113

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	66	ARG	Sidechain	20
1	A	40	ARG	Sidechain	19
1	A	22	ARG	Sidechain	19
1	A	46	ARG	Sidechain	19
1	A	49	ARG	Sidechain	19
1	A	56	ARG	Sidechain	17

### 6.2 Too-close contacts [i](#)

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	481	431	431	52±5
All	All	9620	8620	8620	1034

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD22	1:A:25:ALA:O	0.95	1.60	17	13
1:A:33:CYS:SG	1:A:62:ALA:HB1	0.91	2.05	3	11
1:A:25:ALA:HB1	1:A:36:CYS:O	0.91	1.64	6	8
1:A:21:LEU:HD23	1:A:25:ALA:HB3	0.91	1.42	11	11
1:A:21:LEU:CD2	1:A:25:ALA:HB3	0.88	1.98	13	12
1:A:41:ALA:HB2	1:A:58:THR:O	0.88	1.67	18	19
1:A:48:ALA:HB2	1:A:53:ASN:O	0.86	1.71	10	6
1:A:38:PHE:CE1	1:A:62:ALA:HB2	0.83	2.07	3	7
1:A:25:ALA:HB1	1:A:36:CYS:HB3	0.82	1.51	16	12
1:A:44:ILE:O	1:A:44:ILE:HG23	0.80	1.76	12	5
1:A:44:ILE:HD11	1:A:54:ASP:HB2	0.80	1.52	7	6
1:A:21:LEU:HD21	1:A:27:CYS:C	0.79	1.96	1	2
1:A:21:LEU:HD21	1:A:27:CYS:N	0.78	1.93	10	3
1:A:48:ALA:HB1	1:A:52:TRP:CD1	0.75	2.16	18	12
1:A:44:ILE:HD11	1:A:46:ARG:O	0.74	1.81	2	7
1:A:21:LEU:HD22	1:A:25:ALA:C	0.74	2.03	4	8
1:A:21:LEU:HD23	1:A:36:CYS:SG	0.74	2.22	8	1
1:A:9:PRO:O	1:A:16:ALA:HB2	0.73	1.84	7	3
1:A:44:ILE:HD11	1:A:54:ASP:CB	0.71	2.15	4	9
1:A:44:ILE:HD13	1:A:55:ASP:O	0.71	1.85	7	5
1:A:25:ALA:CB	1:A:36:CYS:SG	0.69	2.80	8	3
1:A:48:ALA:HB1	1:A:52:TRP:NE1	0.68	2.03	18	2
1:A:33:CYS:HB2	1:A:62:ALA:HB1	0.64	1.69	20	2
1:A:44:ILE:O	1:A:44:ILE:HG22	0.64	1.92	4	1
1:A:25:ALA:HB1	1:A:36:CYS:C	0.64	2.11	8	1
1:A:21:LEU:HD23	1:A:25:ALA:CB	0.64	2.21	15	4
1:A:44:ILE:HD12	1:A:55:ASP:O	0.64	1.92	18	1
1:A:33:CYS:SG	1:A:62:ALA:HB2	0.63	2.32	7	3
1:A:44:ILE:HD11	1:A:46:ARG:C	0.62	2.13	6	1
1:A:25:ALA:HB3	1:A:36:CYS:SG	0.62	2.34	8	1
1:A:48:ALA:HB2	1:A:54:ASP:HA	0.62	1.70	4	9
1:A:27:CYS:HB2	1:A:62:ALA:HB2	0.62	1.70	5	2
1:A:21:LEU:HD22	1:A:25:ALA:HB3	0.62	1.72	13	5
1:A:49:ARG:O	1:A:52:TRP:CZ2	0.61	2.53	13	13
1:A:43:LYS:O	1:A:45:CYS:N	0.61	2.33	12	4
1:A:50:GLY:O	1:A:52:TRP:CE3	0.61	2.54	11	1
1:A:44:ILE:HG22	1:A:44:ILE:O	0.61	1.95	7	3
1:A:22:ARG:N	1:A:23:PRO:CD	0.61	2.63	20	18
1:A:15:ASP:HB3	1:A:18:THR:HG22	0.60	1.72	19	4
1:A:38:PHE:HE1	1:A:62:ALA:HB2	0.60	1.55	8	5
1:A:50:GLY:O	1:A:52:TRP:CZ3	0.59	2.55	11	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:42:GLY:HA2	1:A:56:ARG:CG	0.59	2.27	1	4
1:A:52:TRP:CD1	1:A:68:GLY:O	0.59	2.55	11	1
1:A:38:PHE:CE2	1:A:60:GLN:O	0.58	2.56	17	6
1:A:41:ALA:HB2	1:A:59:GLY:HA3	0.58	1.74	10	5
1:A:49:ARG:O	1:A:52:TRP:CE2	0.58	2.56	13	2
1:A:58:THR:HG22	1:A:65:PRO:HG3	0.58	1.75	16	3
1:A:5:ASP:N	1:A:19:CYS:O	0.58	2.37	20	16
1:A:38:PHE:CD2	1:A:60:GLN:O	0.58	2.57	6	2
1:A:13:CYS:SG	1:A:28:GLY:CA	0.58	2.91	8	1
1:A:26:GLN:O	1:A:38:PHE:CZ	0.58	2.57	10	2
1:A:15:ASP:N	1:A:20:LYS:O	0.57	2.37	18	20
1:A:43:LYS:O	1:A:57:CYS:N	0.57	2.38	6	13
1:A:27:CYS:SG	1:A:62:ALA:HB1	0.57	2.40	19	4
1:A:15:ASP:O	1:A:19:CYS:N	0.57	2.38	14	20
1:A:44:ILE:CD1	1:A:54:ASP:CB	0.57	2.83	2	4
1:A:44:ILE:HD11	1:A:54:ASP:HB3	0.57	1.77	4	5
1:A:44:ILE:HG23	1:A:44:ILE:O	0.57	2.00	5	4
1:A:38:PHE:CD1	1:A:59:GLY:O	0.56	2.57	5	1
1:A:21:LEU:CD2	1:A:25:ALA:CB	0.56	2.81	13	4
1:A:48:ALA:HB1	1:A:52:TRP:HD1	0.56	1.60	2	4
1:A:43:LYS:HB3	1:A:57:CYS:HB2	0.56	1.78	12	3
1:A:48:ALA:CB	1:A:52:TRP:CD1	0.56	2.88	18	1
1:A:25:ALA:CB	1:A:36:CYS:HB3	0.56	2.31	5	13
1:A:22:ARG:CB	1:A:23:PRO:HD3	0.56	2.31	18	12
1:A:22:ARG:N	1:A:23:PRO:HD2	0.55	2.17	9	18
1:A:47:ILE:N	1:A:47:ILE:HD13	0.55	2.16	11	1
1:A:3:GLU:O	1:A:18:THR:O	0.55	2.25	16	15
1:A:5:ASP:OD2	1:A:21:LEU:HD12	0.54	2.02	9	2
1:A:43:LYS:O	1:A:56:ARG:HA	0.54	2.02	12	10
1:A:27:CYS:SG	1:A:38:PHE:N	0.54	2.80	5	1
1:A:5:ASP:CG	1:A:21:LEU:HD12	0.54	2.23	13	2
1:A:27:CYS:CB	1:A:62:ALA:HB2	0.54	2.33	5	1
1:A:44:ILE:O	1:A:44:ILE:CG2	0.54	2.49	12	3
1:A:26:GLN:HG2	1:A:38:PHE:CZ	0.54	2.38	5	1
1:A:45:CYS:SG	1:A:55:ASP:CB	0.54	2.96	18	6
1:A:26:GLN:HB3	1:A:38:PHE:CD2	0.54	2.37	5	5
1:A:3:GLU:O	1:A:20:LYS:CG	0.54	2.56	18	7
1:A:18:THR:O	1:A:20:LYS:N	0.54	2.41	16	7
1:A:41:ALA:HB2	1:A:58:THR:C	0.54	2.23	13	4
1:A:22:ARG:CB	1:A:23:PRO:CD	0.54	2.86	18	7
1:A:50:GLY:O	1:A:51:ASP:CB	0.54	2.55	11	4

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:THR:O	1:A:19:CYS:CB	0.54	2.56	18	6
1:A:21:LEU:HD11	1:A:28:GLY:N	0.53	2.17	7	1
1:A:26:GLN:O	1:A:38:PHE:CE1	0.53	2.60	1	1
1:A:26:GLN:HG2	1:A:38:PHE:CD2	0.53	2.39	8	4
1:A:21:LEU:HD11	1:A:26:GLN:O	0.53	2.04	6	1
1:A:33:CYS:SG	1:A:62:ALA:CB	0.53	2.97	16	11
1:A:27:CYS:SG	1:A:37:LYS:N	0.53	2.81	1	2
1:A:44:ILE:CD1	1:A:46:ARG:O	0.53	2.57	2	6
1:A:26:GLN:HB3	1:A:38:PHE:CD1	0.53	2.38	4	3
1:A:41:ALA:CB	1:A:58:THR:O	0.53	2.57	8	12
1:A:35:GLN:O	1:A:36:CYS:CB	0.52	2.56	8	6
1:A:25:ALA:CB	1:A:36:CYS:CB	0.52	2.88	8	1
1:A:31:LEU:N	1:A:31:LEU:HD23	0.52	2.18	10	1
1:A:41:ALA:N	1:A:59:GLY:HA3	0.52	2.19	6	13
1:A:31:LEU:CD1	1:A:45:CYS:O	0.52	2.57	13	2
1:A:18:THR:O	1:A:20:LYS:CG	0.52	2.57	4	4
1:A:47:ILE:O	1:A:47:ILE:HG23	0.52	2.04	14	2
1:A:32:CYS:SG	1:A:39:SER:CB	0.52	2.98	20	1
1:A:41:ALA:HB2	1:A:59:GLY:CA	0.52	2.34	13	4
1:A:44:ILE:C	1:A:44:ILE:HD12	0.52	2.25	6	1
1:A:26:GLN:CG	1:A:38:PHE:CD2	0.52	2.93	16	1
1:A:49:ARG:O	1:A:52:TRP:NE1	0.52	2.43	20	1
1:A:43:LYS:CD	1:A:43:LYS:C	0.52	2.78	12	2
1:A:41:ALA:N	1:A:59:GLY:CA	0.52	2.73	6	10
1:A:35:GLN:O	1:A:36:CYS:HB2	0.52	2.05	5	11
1:A:31:LEU:O	1:A:43:LYS:NZ	0.51	2.43	12	1
1:A:25:ALA:HB1	1:A:36:CYS:CB	0.51	2.35	9	2
1:A:14:CYS:CA	1:A:20:LYS:O	0.51	2.57	5	3
1:A:44:ILE:CD1	1:A:54:ASP:HB2	0.51	2.35	3	3
1:A:23:PRO:O	1:A:25:ALA:N	0.51	2.43	10	1
1:A:31:LEU:HD12	1:A:45:CYS:O	0.51	2.05	13	1
1:A:42:GLY:N	1:A:57:CYS:O	0.51	2.42	13	5
1:A:45:CYS:SG	1:A:57:CYS:CA	0.51	2.98	10	1
1:A:43:LYS:CB	1:A:57:CYS:HB2	0.51	2.34	11	4
1:A:27:CYS:SG	1:A:38:PHE:CD1	0.51	3.04	12	1
1:A:15:ASP:O	1:A:19:CYS:CA	0.50	2.59	9	11
1:A:53:ASN:OD1	1:A:53:ASN:N	0.50	2.44	15	1
1:A:48:ALA:HB2	1:A:53:ASN:C	0.50	2.26	11	1
1:A:27:CYS:SG	1:A:62:ALA:CB	0.50	3.00	14	2
1:A:48:ALA:HB1	1:A:52:TRP:HE1	0.50	1.64	18	1
1:A:18:THR:O	1:A:19:CYS:C	0.49	2.50	4	10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:CYS:SG	1:A:57:CYS:N	0.49	2.85	10	1
1:A:44:ILE:CD1	1:A:46:ARG:C	0.49	2.81	12	1
1:A:38:PHE:O	1:A:39:SER:O	0.49	2.31	2	9
1:A:26:GLN:HG2	1:A:38:PHE:CE2	0.49	2.42	6	3
1:A:22:ARG:HB3	1:A:23:PRO:HD3	0.49	1.82	18	10
1:A:48:ALA:CB	1:A:53:ASN:O	0.49	2.60	3	3
1:A:26:GLN:CG	1:A:38:PHE:CE2	0.49	2.95	5	1
1:A:52:TRP:CG	1:A:68:GLY:O	0.49	2.66	16	1
1:A:3:GLU:O	1:A:20:LYS:HG2	0.49	2.07	18	5
1:A:27:CYS:SG	1:A:29:GLU:O	0.49	2.71	19	6
1:A:44:ILE:O	1:A:44:ILE:HD12	0.49	2.07	12	1
1:A:14:CYS:SG	1:A:15:ASP:N	0.49	2.86	6	1
1:A:38:PHE:CZ	1:A:60:GLN:HA	0.49	2.43	5	1
1:A:18:THR:HB	1:A:20:LYS:CD	0.49	2.38	18	1
1:A:29:GLU:OE2	1:A:30:GLY:N	0.49	2.45	2	2
1:A:45:CYS:N	1:A:55:ASP:O	0.49	2.41	5	1
1:A:21:LEU:CD1	1:A:26:GLN:O	0.49	2.61	6	1
1:A:25:ALA:CB	1:A:36:CYS:O	0.49	2.57	8	2
1:A:15:ASP:O	1:A:19:CYS:HA	0.48	2.08	20	10
1:A:27:CYS:HB3	1:A:38:PHE:CE1	0.48	2.43	10	1
1:A:34:GLU:N	1:A:37:LYS:O	0.48	2.46	6	1
1:A:11:ASN:OD1	1:A:13:CYS:N	0.48	2.46	19	3
1:A:50:GLY:O	1:A:51:ASP:HB2	0.48	2.08	11	3
1:A:21:LEU:CD2	1:A:25:ALA:C	0.48	2.81	15	1
1:A:43:LYS:CG	1:A:57:CYS:HB2	0.48	2.39	9	9
1:A:44:ILE:CD1	1:A:44:ILE:C	0.48	2.81	12	1
1:A:25:ALA:HB1	1:A:36:CYS:SG	0.48	2.48	9	2
1:A:44:ILE:CG2	1:A:44:ILE:O	0.48	2.62	7	2
1:A:15:ASP:HB3	1:A:18:THR:CG2	0.48	2.39	13	2
1:A:19:CYS:O	1:A:19:CYS:SG	0.48	2.72	19	3
1:A:21:LEU:HD22	1:A:25:ALA:CB	0.48	2.39	20	2
1:A:47:ILE:O	1:A:48:ALA:O	0.47	2.33	11	1
1:A:43:LYS:C	1:A:43:LYS:CD	0.47	2.80	18	1
1:A:54:ASP:OD1	1:A:54:ASP:N	0.47	2.47	2	1
1:A:43:LYS:HB3	1:A:57:CYS:CB	0.47	2.39	13	5
1:A:32:CYS:O	1:A:39:SER:OG	0.47	2.33	7	1
1:A:26:GLN:NE2	1:A:38:PHE:CD2	0.47	2.82	2	1
1:A:4:CYS:SG	1:A:6:CYS:O	0.47	2.73	12	6
1:A:31:LEU:HD12	1:A:46:ARG:HG3	0.47	1.87	10	1
1:A:3:GLU:O	1:A:19:CYS:SG	0.47	2.73	9	8
1:A:4:CYS:HA	1:A:19:CYS:O	0.47	2.09	8	10

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:GLU:O	1:A:35:GLN:CB	0.47	2.62	17	3
1:A:45:CYS:SG	1:A:55:ASP:O	0.47	2.73	12	2
1:A:50:GLY:O	1:A:51:ASP:OD1	0.47	2.33	9	2
1:A:54:ASP:N	1:A:54:ASP:OD1	0.47	2.47	10	2
1:A:42:GLY:C	1:A:56:ARG:HG3	0.47	2.31	1	1
1:A:13:CYS:SG	1:A:28:GLY:HA2	0.46	2.49	8	2
1:A:51:ASP:O	1:A:52:TRP:O	0.46	2.32	3	2
1:A:32:CYS:O	1:A:39:SER:N	0.46	2.45	4	1
1:A:27:CYS:O	1:A:36:CYS:HA	0.46	2.10	8	3
1:A:52:TRP:O	1:A:53:ASN:O	0.46	2.34	19	2
1:A:31:LEU:HD22	1:A:46:ARG:HD2	0.46	1.87	11	1
1:A:55:ASP:OD1	1:A:55:ASP:N	0.46	2.47	16	1
1:A:14:CYS:SG	1:A:14:CYS:O	0.46	2.73	3	2
1:A:53:ASN:OD1	1:A:54:ASP:N	0.46	2.47	3	1
1:A:22:ARG:CG	1:A:23:PRO:HD3	0.46	2.40	18	2
1:A:38:PHE:CE1	1:A:59:GLY:O	0.46	2.69	5	1
1:A:58:THR:CG2	1:A:61:SER:HB3	0.46	2.40	19	1
1:A:54:ASP:OD1	1:A:56:ARG:NH1	0.46	2.43	10	1
1:A:41:ALA:CB	1:A:58:THR:C	0.46	2.83	13	3
1:A:52:TRP:CD1	1:A:53:ASN:N	0.46	2.84	13	1
1:A:14:CYS:O	1:A:14:CYS:SG	0.46	2.73	12	5
1:A:27:CYS:O	1:A:36:CYS:SG	0.46	2.74	9	2
1:A:58:THR:HG23	1:A:65:PRO:CG	0.46	2.41	14	1
1:A:27:CYS:SG	1:A:36:CYS:O	0.46	2.74	5	1
1:A:25:ALA:HB2	1:A:36:CYS:HB3	0.46	1.87	8	2
1:A:56:ARG:NH1	1:A:56:ARG:CG	0.46	2.78	10	1
1:A:42:GLY:CA	1:A:56:ARG:HG3	0.46	2.40	5	1
1:A:13:CYS:HB3	1:A:28:GLY:HA2	0.46	1.88	2	2
1:A:41:ALA:HA	1:A:57:CYS:O	0.46	2.10	11	19
1:A:13:CYS:CB	1:A:28:GLY:HA2	0.46	2.41	3	2
1:A:45:CYS:SG	1:A:55:ASP:HB3	0.46	2.51	16	4
1:A:44:ILE:CD1	1:A:54:ASP:HB3	0.45	2.41	4	3
1:A:18:THR:O	1:A:20:LYS:HG3	0.45	2.11	20	3
1:A:21:LEU:HD11	1:A:27:CYS:HA	0.45	1.89	1	2
1:A:18:THR:C	1:A:19:CYS:SG	0.45	2.95	7	10
1:A:27:CYS:O	1:A:33:CYS:SG	0.45	2.74	5	1
1:A:38:PHE:CE1	1:A:60:GLN:HA	0.45	2.46	5	1
1:A:22:ARG:HG2	1:A:23:PRO:N	0.45	2.26	11	2
1:A:21:LEU:HD11	1:A:27:CYS:C	0.45	2.32	7	1
1:A:39:SER:O	1:A:59:GLY:O	0.45	2.35	14	2
1:A:43:LYS:HE2	1:A:44:ILE:N	0.45	2.27	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:7:SER:OG	1:A:29:GLU:OE2	0.45	2.35	6	1
1:A:46:ARG:CB	1:A:55:ASP:OD2	0.45	2.65	11	1
1:A:42:GLY:HA2	1:A:56:ARG:HB3	0.45	1.88	20	3
1:A:43:LYS:HB3	1:A:57:CYS:HB3	0.45	1.88	20	2
1:A:4:CYS:SG	1:A:19:CYS:O	0.45	2.75	5	2
1:A:9:PRO:O	1:A:16:ALA:CB	0.45	2.62	7	1
1:A:34:GLU:CG	1:A:39:SER:OG	0.45	2.65	8	2
1:A:43:LYS:O	1:A:45:CYS:SG	0.45	2.75	10	1
1:A:67:ASN:O	1:A:67:ASN:OD1	0.45	2.34	10	1
1:A:32:CYS:SG	1:A:43:LYS:HG2	0.45	2.52	7	2
1:A:32:CYS:SG	1:A:32:CYS:O	0.45	2.75	10	1
1:A:43:LYS:HD3	1:A:44:ILE:N	0.44	2.26	12	2
1:A:58:THR:HG23	1:A:65:PRO:HG3	0.44	1.88	14	1
1:A:11:ASN:ND2	1:A:14:CYS:SG	0.44	2.90	2	2
1:A:45:CYS:SG	1:A:55:ASP:CG	0.44	2.95	17	1
1:A:58:THR:OG1	1:A:61:SER:CB	0.44	2.66	14	1
1:A:50:GLY:O	1:A:51:ASP:OD2	0.44	2.36	7	1
1:A:13:CYS:O	1:A:23:PRO:CD	0.44	2.65	9	1
1:A:45:CYS:SG	1:A:55:ASP:HB2	0.44	2.53	6	4
1:A:32:CYS:SG	1:A:39:SER:HB2	0.44	2.51	20	1
1:A:58:THR:CG2	1:A:65:PRO:HG3	0.44	2.42	15	1
1:A:48:ALA:O	1:A:50:GLY:N	0.44	2.50	3	1
1:A:57:CYS:HA	1:A:64:CYS:SG	0.44	2.53	3	1
1:A:43:LYS:O	1:A:43:LYS:HG3	0.44	2.12	9	1
1:A:48:ALA:N	1:A:54:ASP:OD2	0.44	2.44	9	1
1:A:18:THR:O	1:A:19:CYS:HB3	0.44	2.13	19	3
1:A:32:CYS:C	1:A:39:SER:OG	0.44	2.57	14	3
1:A:32:CYS:HB3	1:A:39:SER:OG	0.44	2.13	19	1
1:A:15:ASP:CB	1:A:22:ARG:HG3	0.44	2.43	17	1
1:A:30:GLY:HA3	1:A:33:CYS:SG	0.44	2.53	4	1
1:A:27:CYS:HB2	1:A:38:PHE:CE1	0.44	2.48	4	2
1:A:13:CYS:O	1:A:23:PRO:HD2	0.44	2.13	5	2
1:A:21:LEU:CD2	1:A:25:ALA:O	0.43	2.61	15	2
1:A:18:THR:CB	1:A:20:LYS:HD3	0.43	2.43	18	1
1:A:45:CYS:SG	1:A:55:ASP:C	0.43	2.96	18	1
1:A:44:ILE:HG13	1:A:44:ILE:O	0.43	2.13	6	3
1:A:57:CYS:HA	1:A:65:PRO:CD	0.43	2.43	7	1
1:A:13:CYS:O	1:A:21:LEU:HD23	0.43	2.13	12	1
1:A:6:CYS:SG	1:A:8:SER:OG	0.43	2.74	4	1
1:A:13:CYS:HB3	1:A:28:GLY:CA	0.43	2.43	3	2
1:A:40:ARG:C	1:A:59:GLY:CA	0.43	2.87	19	4

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:CYS:SG	1:A:38:PHE:CE1	0.43	3.12	12	1
1:A:33:CYS:HA	1:A:37:LYS:O	0.43	2.14	15	3
1:A:51:ASP:O	1:A:52:TRP:C	0.43	2.55	3	3
1:A:48:ALA:N	1:A:54:ASP:HA	0.43	2.28	11	1
1:A:27:CYS:SG	1:A:38:PHE:CA	0.43	3.07	5	1
1:A:32:CYS:HB3	1:A:62:ALA:O	0.43	2.13	10	1
1:A:33:CYS:SG	1:A:36:CYS:C	0.43	2.96	12	1
1:A:43:LYS:C	1:A:43:LYS:HD3	0.43	2.33	12	1
1:A:44:ILE:HA	1:A:55:ASP:O	0.43	2.14	12	3
1:A:32:CYS:SG	1:A:62:ALA:O	0.43	2.77	19	2
1:A:21:LEU:HD21	1:A:27:CYS:CA	0.43	2.44	10	2
1:A:46:ARG:HB3	1:A:55:ASP:OD2	0.43	2.13	11	1
1:A:27:CYS:SG	1:A:36:CYS:C	0.43	2.97	20	1
1:A:14:CYS:SG	1:A:19:CYS:C	0.43	2.97	6	1
1:A:42:GLY:HA2	1:A:56:ARG:HG2	0.43	1.90	1	2
1:A:58:THR:CG2	1:A:61:SER:CB	0.43	2.97	19	1
1:A:14:CYS:HA	1:A:20:LYS:O	0.43	2.14	8	4
1:A:46:ARG:C	1:A:47:ILE:HD13	0.43	2.34	11	1
1:A:40:ARG:O	1:A:57:CYS:HB3	0.42	2.14	10	4
1:A:67:ASN:O	1:A:68:GLY:O	0.42	2.36	18	1
1:A:31:LEU:HD23	1:A:45:CYS:HB2	0.42	1.91	4	1
1:A:35:GLN:O	1:A:36:CYS:HB3	0.42	2.15	8	1
1:A:10:GLU:N	1:A:10:GLU:OE1	0.42	2.52	18	1
1:A:40:ARG:C	1:A:59:GLY:HA2	0.42	2.35	9	6
1:A:27:CYS:N	1:A:36:CYS:O	0.42	2.52	8	1
1:A:66:ARG:CD	1:A:66:ARG:O	0.42	2.68	14	1
1:A:11:ASN:O	1:A:14:CYS:O	0.42	2.38	6	1
1:A:44:ILE:O	1:A:44:ILE:CG1	0.42	2.68	6	1
1:A:31:LEU:C	1:A:32:CYS:SG	0.42	2.98	5	1
1:A:21:LEU:CD2	1:A:36:CYS:SG	0.42	3.04	8	1
1:A:31:LEU:HD23	1:A:45:CYS:HB3	0.42	1.91	3	1
1:A:47:ILE:CG2	1:A:47:ILE:O	0.42	2.67	14	1
1:A:34:GLU:O	1:A:35:GLN:HB2	0.42	2.15	3	2
1:A:14:CYS:CB	1:A:20:LYS:O	0.42	2.68	5	1
1:A:26:GLN:O	1:A:38:PHE:CD2	0.42	2.73	5	1
1:A:63:ASP:N	1:A:63:ASP:OD1	0.42	2.52	18	1
1:A:34:GLU:HG3	1:A:39:SER:OG	0.42	2.15	8	1
1:A:45:CYS:HB3	1:A:57:CYS:SG	0.42	2.55	1	2
1:A:27:CYS:O	1:A:36:CYS:C	0.41	2.58	8	1
1:A:27:CYS:SG	1:A:37:LYS:O	0.41	2.78	11	1
1:A:42:GLY:C	1:A:56:ARG:CD	0.41	2.89	12	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:GLY:CA	1:A:33:CYS:SG	0.41	3.08	4	1
1:A:13:CYS:SG	1:A:14:CYS:SG	0.41	3.18	8	1
1:A:32:CYS:SG	1:A:43:LYS:CG	0.41	3.08	7	1
1:A:35:GLN:C	1:A:36:CYS:SG	0.41	2.98	15	1
1:A:32:CYS:HB2	1:A:61:SER:O	0.41	2.15	17	1
1:A:43:LYS:HD2	1:A:44:ILE:N	0.41	2.30	4	1
1:A:58:THR:OG1	1:A:61:SER:HB2	0.41	2.15	14	1
1:A:26:GLN:HB3	1:A:38:PHE:CE2	0.41	2.51	15	1
1:A:34:GLU:HG2	1:A:39:SER:OG	0.41	2.15	3	1
1:A:32:CYS:N	1:A:62:ALA:O	0.41	2.43	20	1
1:A:44:ILE:O	1:A:44:ILE:CD1	0.41	2.68	12	1
1:A:6:CYS:O	1:A:19:CYS:SG	0.41	2.79	8	1
1:A:11:ASN:OD1	1:A:12:PRO:HD2	0.41	2.16	17	2
1:A:39:SER:O	1:A:59:GLY:HA2	0.41	2.16	4	3
1:A:22:ARG:HB3	1:A:23:PRO:CD	0.41	2.45	18	1
1:A:15:ASP:OD2	1:A:17:ALA:HB3	0.41	2.16	20	1
1:A:47:ILE:HG13	1:A:48:ALA:N	0.41	2.31	19	1
1:A:43:LYS:HG3	1:A:43:LYS:O	0.41	2.16	17	2
1:A:42:GLY:HA2	1:A:56:ARG:CD	0.41	2.45	18	1
1:A:46:ARG:NH1	1:A:46:ARG:HG3	0.41	2.30	20	1
1:A:42:GLY:CA	1:A:56:ARG:HB3	0.41	2.46	20	1
1:A:47:ILE:O	1:A:47:ILE:CG2	0.40	2.69	4	1
1:A:43:LYS:HD2	1:A:44:ILE:O	0.40	2.17	20	1
1:A:66:ARG:O	1:A:66:ARG:CG	0.40	2.68	19	1
1:A:46:ARG:CB	1:A:55:ASP:HB2	0.40	2.45	10	1
1:A:27:CYS:SG	1:A:38:PHE:HB3	0.40	2.57	5	1
1:A:3:GLU:O	1:A:20:LYS:HG3	0.40	2.15	7	1
1:A:14:CYS:HB2	1:A:20:LYS:O	0.40	2.16	18	1
1:A:48:ALA:CB	1:A:52:TRP:O	0.40	2.69	11	1
1:A:26:GLN:CG	1:A:38:PHE:CZ	0.40	3.04	5	1
1:A:41:ALA:N	1:A:59:GLY:HA2	0.40	2.30	8	1
1:A:63:ASP:C	1:A:63:ASP:OD1	0.40	2.60	11	1
1:A:46:ARG:HB2	1:A:55:ASP:HB2	0.40	1.93	10	1
1:A:11:ASN:CG	1:A:14:CYS:SG	0.40	2.99	19	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	66/79 (84%)	54±2 (82±3%)	9±2 (13±4%)	3±1 (5±2%)	5	27
All	All	1320/1580 (84%)	1088 (82%)	170 (13%)	62 (5%)	5	27

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	39	SER	14
1	A	51	ASP	11
1	A	19	CYS	10
1	A	44	ILE	7
1	A	54	ASP	5
1	A	3	GLU	3
1	A	52	TRP	2
1	A	53	ASN	2
1	A	23	PRO	2
1	A	48	ALA	2
1	A	68	GLY	1
1	A	65	PRO	1
1	A	22	ARG	1
1	A	60	GLN	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	53/64 (83%)	36±3 (68±5%)	17±3 (32±5%)	1	13
All	All	1060/1280 (83%)	719 (68%)	341 (32%)	1	13

All 47 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	58	THR	17
1	A	66	ARG	16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	52	TRP	16
1	A	51	ASP	15
1	A	43	LYS	15
1	A	22	ARG	15
1	A	26	GLN	13
1	A	21	LEU	12
1	A	46	ARG	11
1	A	44	ILE	11
1	A	19	CYS	11
1	A	27	CYS	11
1	A	8	SER	11
1	A	29	GLU	10
1	A	7	SER	10
1	A	61	SER	9
1	A	47	ILE	9
1	A	39	SER	8
1	A	63	ASP	8
1	A	31	LEU	8
1	A	35	GLN	7
1	A	54	ASP	7
1	A	67	ASN	6
1	A	20	LYS	6
1	A	45	CYS	6
1	A	37	LYS	6
1	A	32	CYS	5
1	A	40	ARG	5
1	A	56	ARG	5
1	A	55	ASP	5
1	A	13	CYS	5
1	A	5	ASP	5
1	A	3	GLU	5
1	A	10	GLU	5
1	A	57	CYS	4
1	A	49	ARG	4
1	A	64	CYS	3
1	A	34	GLU	3
1	A	53	ASN	3
1	A	36	CYS	2
1	A	60	GLN	2
1	A	38	PHE	1
1	A	6	CYS	1
1	A	18	THR	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	4	CYS	1
1	A	33	CYS	1
1	A	14	CYS	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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 54% for the well-defined parts and 53% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2m7f\_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	471
Number of shifts mapped to atoms	471
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	67	$0.36 \pm 0.36$	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 54%, i.e. 396 atoms were assigned a chemical shift out of a possible 739. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	190/322 (59%)	128/128 (100%)	0/132 (0%)	62/62 (100%)
Sidechain	196/396 (49%)	192/238 (81%)	0/131 (0%)	4/27 (15%)

*Continued on next page...*



Continued from previous page...

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	10/21 (48%)	10/11 (91%)	0/9 (0%)	0/1 (0%)
Overall	396/739 (54%)	330/377 (88%)	0/272 (0%)	66/90 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 53%, i.e. 425 atoms were assigned a chemical shift out of a possible 797. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	204/347 (59%)	137/138 (99%)	0/142 (0%)	67/67 (100%)
Sidechain	207/421 (49%)	203/253 (80%)	0/140 (0%)	4/28 (14%)
Aromatic	14/29 (48%)	14/15 (93%)	0/13 (0%)	0/1 (0%)
Overall	425/797 (53%)	354/406 (87%)	0/295 (0%)	71/96 (74%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 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:

