



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2020 – 05:41 PM EST

PDB ID : 2KCU  
Title : NMR solution structure of an uncharacterized protein from *Chlorobium tepidum*. Northeast Structural Genomics target CtR107  
Authors : Mills, J.L.; Zhang, Q.; Sukumaran, D.K.; Wang, D.; Jiang, M.; Foote, E.L.; Xiao, R.; Nair, R.; Everett, J.K.; Swapna, G.V.T.; Acton, T.B.; Rost, B.; Montelione, G.T.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2008-12-29

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.

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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	:	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	:	2.4
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.4

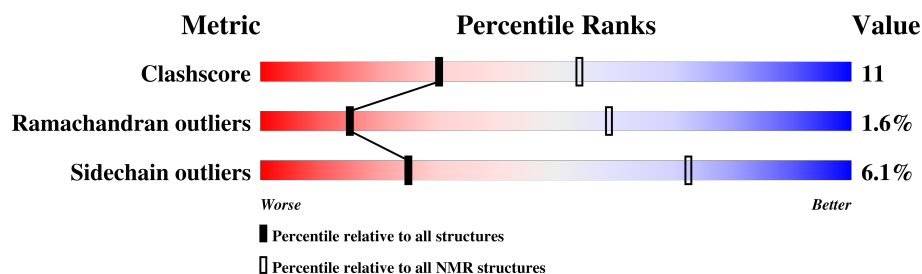
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 76%.

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	136327	12091
Ramachandran outliers	132723	10835
Sidechain outliers	132532	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	166	 74% 15% 11%

## 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:7-A:154 (148)	1.26	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 4 clusters and 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2495 atoms, of which 1218 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called protein Ctr107.

Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2495	813	1218	209	248	7	

There are 9 discrepancies between the modelled and reference sequences:

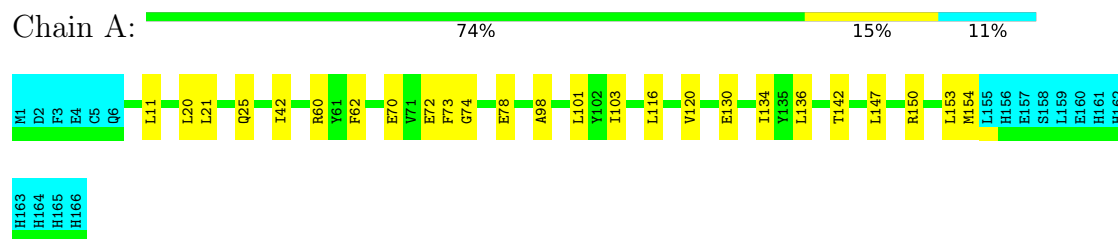
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	THR	SEE REMARK 999	UNP Q8KFZ1
A	159	LEU	-	expression tag	UNP Q8KFZ1
A	160	GLU	-	expression tag	UNP Q8KFZ1
A	161	HIS	-	expression tag	UNP Q8KFZ1
A	162	HIS	-	expression tag	UNP Q8KFZ1
A	163	HIS	-	expression tag	UNP Q8KFZ1
A	164	HIS	-	expression tag	UNP Q8KFZ1
A	165	HIS	-	expression tag	UNP Q8KFZ1
A	166	HIS	-	expression tag	UNP Q8KFZ1

## 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: protein Ctr107

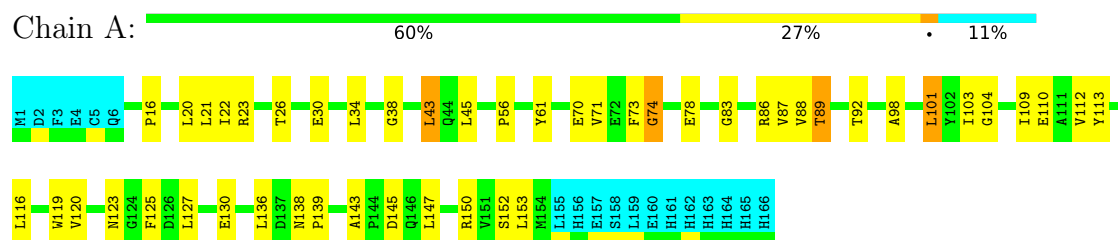


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

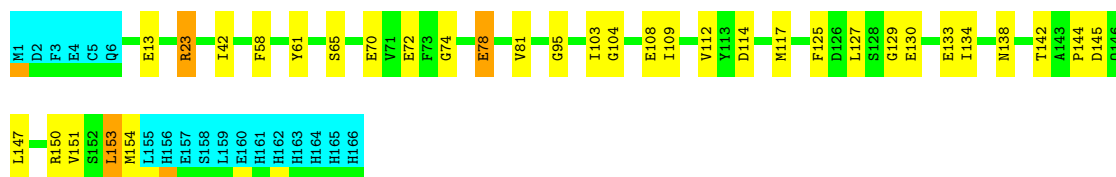
- Molecule 1: protein Ctr107



#### 4.2.2 Score per residue for model 2

- Molecule 1: protein Ctr107





### 4.2.3 Score per residue for model 3

- Molecule 1: protein CtR107

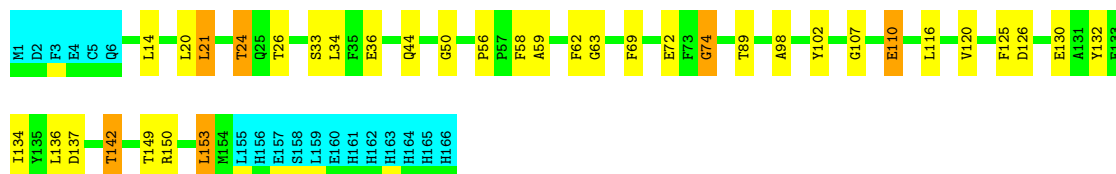
Chain A: 67% 22% 11%



### 4.2.4 Score per residue for model 4

- Molecule 1: protein CtR107

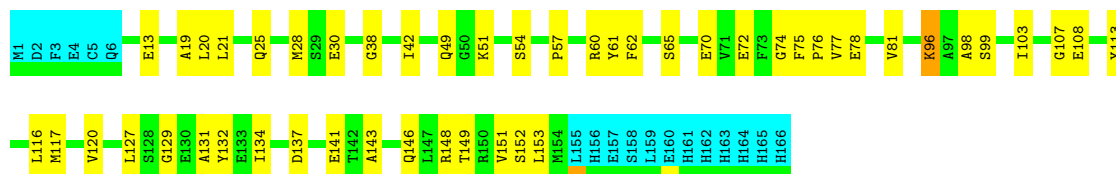
Chain A: 67% 18% 11%



### 4.2.5 Score per residue for model 5

- Molecule 1: protein CtR107

Chain A: 60% 29% 11%



### 4.2.6 Score per residue for model 6

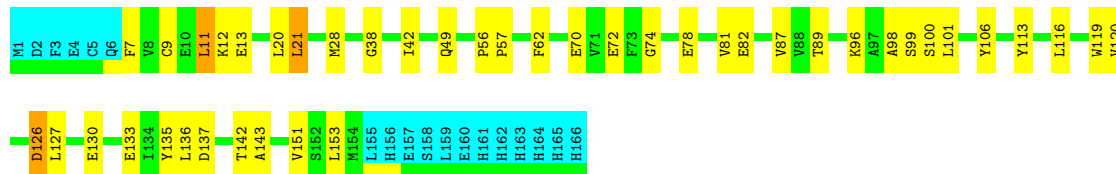
- Molecule 1: protein CtR107



### 4.2.10 Score per residue for model 10

- Molecule 1: protein CtR107

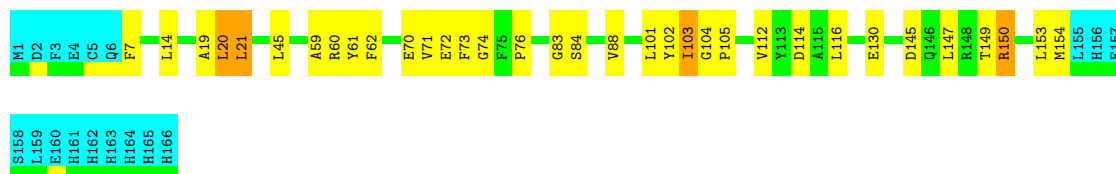
Chain A:  63% 24% 11%



### 4.2.11 Score per residue for model 11

- Molecule 1: protein CtR107

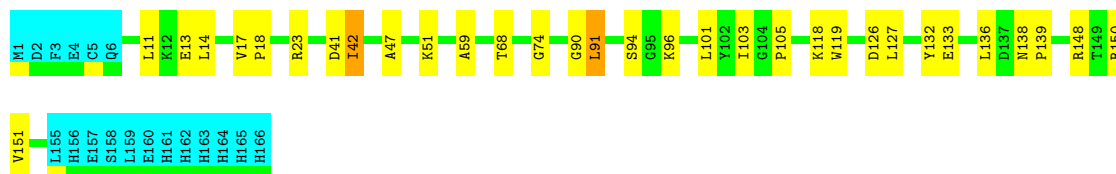
Chain A:  69% 18% 11%



### 4.2.12 Score per residue for model 12

- Molecule 1: protein CtR107

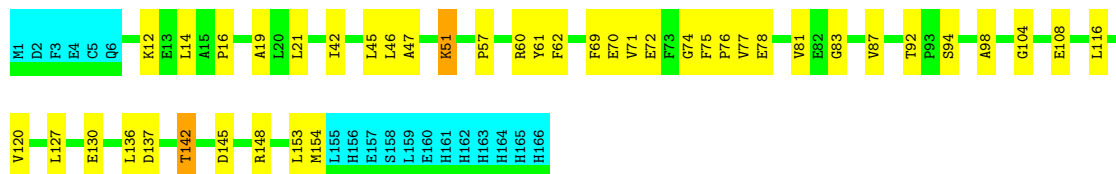
Chain A:  70% 18% 11%



### 4.2.13 Score per residue for model 13

- Molecule 1: protein CtR107

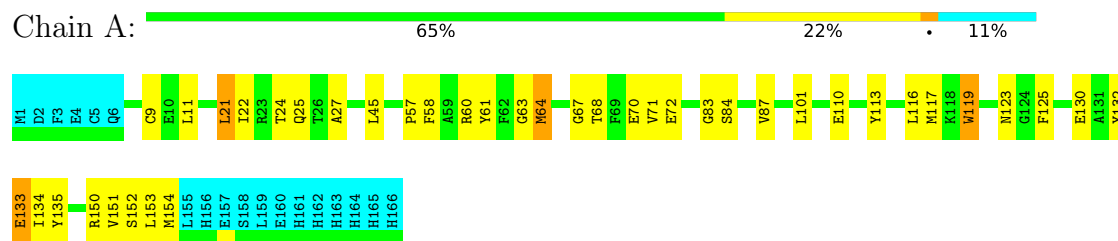
Chain A:  64% 24% 11%





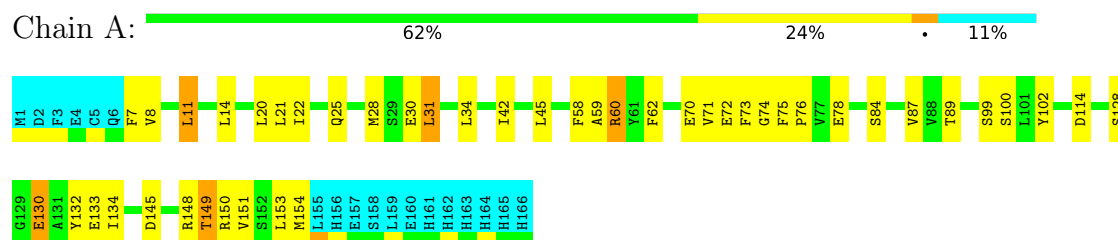
#### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: protein CtR107



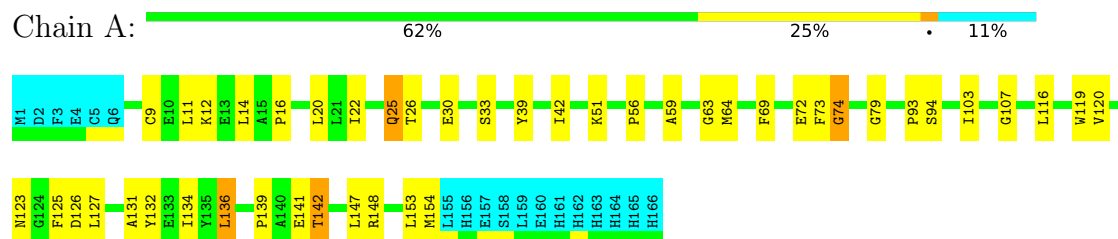
#### 4.2.15 Score per residue for model 15

- Molecule 1: protein CtR107



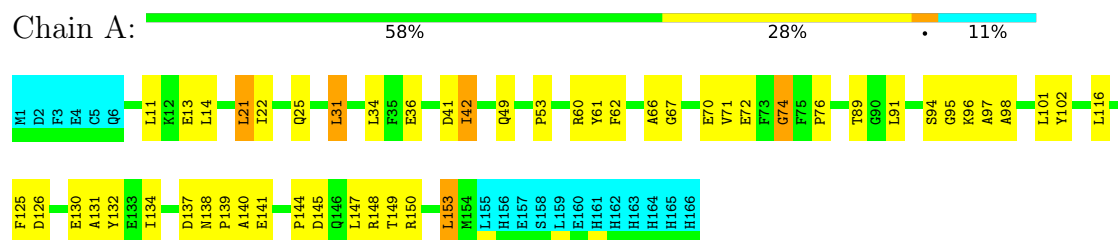
#### 4.2.16 Score per residue for model 16

- Molecule 1: protein CtR107



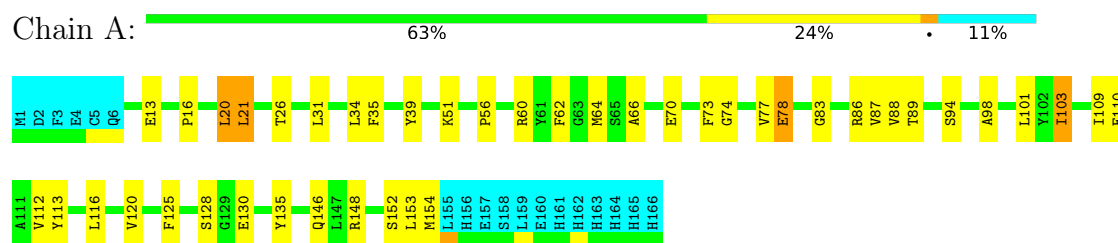
#### 4.2.17 Score per residue for model 17

- Molecule 1: protein CtR107



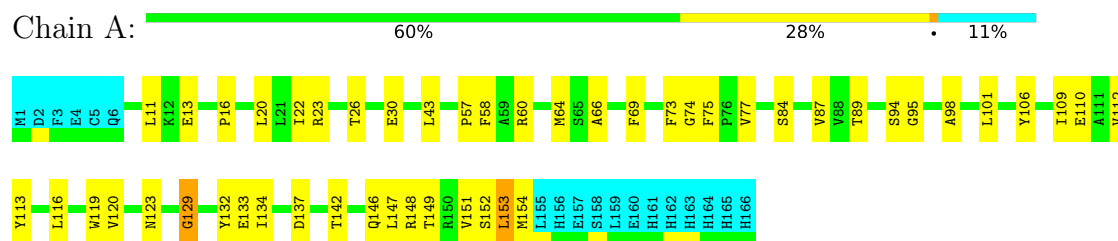
### 4.2.18 Score per residue for model 18

- Molecule 1: protein CtR107



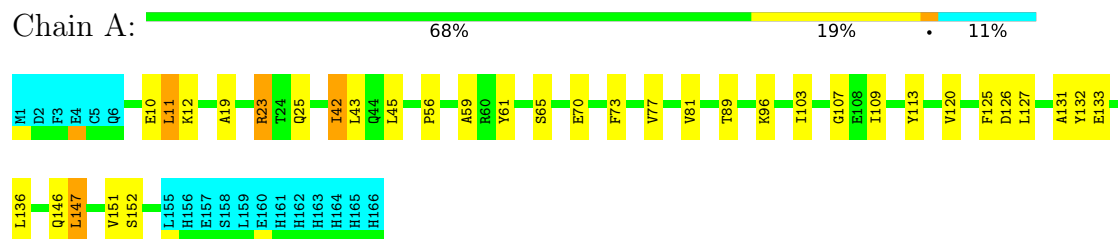
### 4.2.19 Score per residue for model 19

- Molecule 1: protein CtR107



### 4.2.20 Score per residue for model 20

- Molecule 1: protein CtR107



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CSI	structure solution	
TALOS	structure solution	
CYANA	structure solution	
CNS	geometry optimization	
PSVS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2kcu_cs.cif
Number of chemical shift lists	1
Total number of shifts	1677
Number of shifts mapped to atoms	1677
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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	1115	1080	1079	24±6
All	All	22300	21600	21580	476

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 11.

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:HB3	1:A:74:GLY:HA3	0.90	1.42	5	3
1:A:19:ALA:HA	1:A:76:PRO:HA	0.89	1.42	11	4
1:A:120:VAL:HA	1:A:123:ASN:HD22	0.83	1.34	19	3
1:A:62:PHE:HB2	1:A:70:GLU:HB3	0.81	1.49	18	2
1:A:102:TYR:HB3	1:A:149:THR:HB	0.77	1.54	17	2
1:A:120:VAL:HA	1:A:123:ASN:ND2	0.77	1.93	8	3
1:A:62:PHE:HB3	1:A:70:GLU:HB3	0.77	1.55	13	3
1:A:61:TYR:HB2	1:A:131:ALA:HB3	0.76	1.54	5	4
1:A:22:ILE:HB	1:A:87:VAL:HG22	0.75	1.57	1	2
1:A:100:SER:HB2	1:A:112:VAL:HG23	0.74	1.60	3	1
1:A:54:SER:HB3	1:A:76:PRO:HB2	0.73	1.59	9	2
1:A:60:ARG:HB3	1:A:132:TYR:HD1	0.73	1.42	15	1
1:A:57:PRO:HA	1:A:75:PHE:HB3	0.72	1.60	5	2
1:A:62:PHE:HB3	1:A:70:GLU:HB2	0.72	1.60	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ASP:HB3	1:A:142:THR:HG21	0.71	1.62	19	4
1:A:116:LEU:HG	1:A:153:LEU:HD21	0.71	1.61	17	1
1:A:132:TYR:HB3	1:A:152:SER:HB2	0.71	1.61	20	1
1:A:139:PRO:HA	1:A:147:LEU:HD21	0.71	1.61	1	1
1:A:21:LEU:HG	1:A:72:GLU:HB3	0.71	1.61	11	2
1:A:110:GLU:HA	1:A:113:TYR:HD2	0.69	1.46	18	3
1:A:25:GLN:HA	1:A:70:GLU:HA	0.69	1.61	20	4
1:A:23:ARG:HA	1:A:72:GLU:HG2	0.67	1.66	2	2
1:A:46:LEU:HG	1:A:51:LYS:HG3	0.66	1.68	13	1
1:A:110:GLU:HA	1:A:113:TYR:HB3	0.66	1.67	14	1
1:A:131:ALA:HB2	1:A:154:MET:HG3	0.66	1.68	7	2
1:A:21:LEU:HB2	1:A:72:GLU:HG2	0.65	1.68	10	1
1:A:12:LYS:HA	1:A:12:LYS:HE3	0.65	1.67	3	2
1:A:59:ALA:HA	1:A:73:PHE:HA	0.65	1.67	3	6
1:A:101:LEU:HD13	1:A:148:ARG:HD3	0.65	1.67	17	1
1:A:20:LEU:HD13	1:A:77:VAL:HG21	0.65	1.68	19	1
1:A:23:ARG:HB3	1:A:72:GLU:HG2	0.65	1.69	7	1
1:A:120:VAL:HG23	1:A:125:PHE:HB2	0.64	1.69	7	2
1:A:101:LEU:HB3	1:A:150:ARG:HG2	0.64	1.69	11	1
1:A:102:TYR:O	1:A:148:ARG:HA	0.64	1.92	15	1
1:A:11:LEU:HD11	1:A:96:LYS:HD3	0.64	1.69	20	1
1:A:84:SER:HB3	1:A:87:VAL:HB	0.64	1.70	6	1
1:A:31:LEU:HD13	1:A:31:LEU:H	0.64	1.51	15	1
1:A:45:LEU:HD21	1:A:83:GLY:HA2	0.63	1.70	13	1
1:A:83:GLY:HA3	1:A:88:VAL:HA	0.63	1.71	11	3
1:A:133:GLU:HB3	1:A:151:VAL:HA	0.63	1.69	15	1
1:A:116:LEU:HG	1:A:153:LEU:HD23	0.63	1.70	14	1
1:A:23:ARG:HD3	1:A:23:ARG:H	0.63	1.53	20	1
1:A:112:VAL:HG21	1:A:151:VAL:HG13	0.63	1.71	3	1
1:A:153:LEU:H	1:A:153:LEU:HD13	0.63	1.52	19	1
1:A:113:TYR:CD2	1:A:153:LEU:HD13	0.63	2.29	5	1
1:A:103:ILE:HD12	1:A:148:ARG:HG2	0.63	1.69	16	1
1:A:134:ILE:HB	1:A:150:ARG:HB2	0.62	1.69	17	2
1:A:96:LYS:HD2	1:A:127:LEU:HD22	0.62	1.71	20	1
1:A:61:TYR:HB3	1:A:71:VAL:HG12	0.62	1.72	14	3
1:A:22:ILE:O	1:A:72:GLU:HA	0.62	1.95	16	2
1:A:84:SER:H	1:A:87:VAL:HG13	0.62	1.54	9	2
1:A:116:LEU:HD21	1:A:153:LEU:HD12	0.62	1.70	5	1
1:A:56:PRO:HG2	1:A:134:ILE:HD11	0.61	1.71	16	1
1:A:57:PRO:HG2	1:A:135:TYR:HB2	0.61	1.71	3	1
1:A:136:LEU:H	1:A:136:LEU:HD23	0.61	1.54	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:LEU:HB3	1:A:153:LEU:HD21	0.61	1.71	4	1
1:A:60:ARG:HB3	1:A:132:TYR:HB3	0.61	1.72	19	2
1:A:136:LEU:HD13	1:A:136:LEU:H	0.61	1.55	9	2
1:A:116:LEU:HD11	1:A:153:LEU:HD22	0.61	1.71	13	1
1:A:11:LEU:H	1:A:11:LEU:HD23	0.61	1.55	19	1
1:A:104:GLY:HA2	1:A:144:PRO:HB2	0.61	1.72	2	1
1:A:11:LEU:HD21	1:A:96:LYS:HB3	0.60	1.73	20	1
1:A:102:TYR:HE2	1:A:106:TYR:HA	0.60	1.56	7	1
1:A:11:LEU:HB2	1:A:119:TRP:HH2	0.60	1.57	10	2
1:A:129:GLY:HA2	1:A:154:MET:SD	0.59	2.38	2	1
1:A:116:LEU:HD13	1:A:153:LEU:HD21	0.59	1.73	11	1
1:A:11:LEU:HB2	1:A:119:TRP:CH2	0.59	2.31	10	4
1:A:127:LEU:HD12	1:A:127:LEU:H	0.59	1.57	16	3
1:A:10:GLU:HB2	1:A:12:LYS:HE2	0.59	1.75	20	1
1:A:133:GLU:HB2	1:A:135:TYR:CE2	0.58	2.34	7	1
1:A:109:ILE:O	1:A:112:VAL:HG12	0.58	1.96	18	6
1:A:104:GLY:HA2	1:A:145:ASP:HA	0.58	1.76	1	2
1:A:132:TYR:HB3	1:A:152:SER:HB3	0.58	1.73	14	2
1:A:16:PRO:HG3	1:A:94:SER:HB3	0.57	1.75	13	2
1:A:139:PRO:HB3	1:A:147:LEU:HD11	0.57	1.75	9	1
1:A:60:ARG:HG3	1:A:72:GLU:HB2	0.57	1.73	9	1
1:A:137:ASP:HB3	1:A:142:THR:HB	0.57	1.75	10	1
1:A:103:ILE:HA	1:A:147:LEU:O	0.57	2.00	20	3
1:A:138:ASN:OD1	1:A:139:PRO:HD2	0.57	1.98	3	4
1:A:25:GLN:HG2	1:A:70:GLU:HG2	0.57	1.77	15	1
1:A:22:ILE:HG13	1:A:87:VAL:HB	0.57	1.75	15	1
1:A:11:LEU:HG	1:A:96:LYS:HB3	0.57	1.77	8	1
1:A:16:PRO:HD3	1:A:94:SER:HB3	0.57	1.76	19	1
1:A:21:LEU:HD22	1:A:72:GLU:HB3	0.56	1.77	13	2
1:A:20:LEU:HD13	1:A:87:VAL:HG21	0.56	1.77	15	1
1:A:58:PHE:CZ	1:A:76:PRO:HG3	0.56	2.35	15	1
1:A:116:LEU:HA	1:A:119:TRP:CD1	0.56	2.35	1	1
1:A:99:SER:HB3	1:A:152:SER:HB2	0.56	1.76	8	1
1:A:120:VAL:CG2	1:A:125:PHE:HA	0.56	2.31	20	1
1:A:20:LEU:HA	1:A:89:THR:HA	0.56	1.76	15	2
1:A:23:ARG:H	1:A:23:ARG:HD2	0.56	1.61	2	1
1:A:24:THR:HG21	1:A:34:LEU:HD21	0.56	1.77	6	2
1:A:102:TYR:CG	1:A:149:THR:HG22	0.56	2.36	15	1
1:A:101:LEU:HA	1:A:150:ARG:HA	0.56	1.76	14	2
1:A:60:ARG:HB3	1:A:132:TYR:CD1	0.56	2.31	15	1
1:A:43:LEU:HD23	1:A:43:LEU:H	0.56	1.60	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:98:ALA:O	1:A:152:SER:HA	0.55	2.02	19	5
1:A:96:LYS:HD2	1:A:96:LYS:O	0.55	2.01	7	1
1:A:13:GLU:HB3	1:A:96:LYS:HD3	0.55	1.79	17	1
1:A:45:LEU:HD23	1:A:84:SER:HB3	0.54	1.79	14	1
1:A:24:THR:HB	1:A:34:LEU:HD21	0.54	1.79	4	1
1:A:8:VAL:O	1:A:100:SER:HA	0.54	2.02	15	1
1:A:20:LEU:HD13	1:A:77:VAL:HG11	0.54	1.78	8	1
1:A:103:ILE:HB	1:A:145:ASP:O	0.54	2.02	11	1
1:A:98:ALA:HB2	1:A:119:TRP:HZ2	0.54	1.62	19	1
1:A:62:PHE:HD1	1:A:130:GLU:HG2	0.54	1.63	15	1
1:A:39:TYR:HA	1:A:42:ILE:HG22	0.54	1.80	16	1
1:A:26:THR:HG21	1:A:31:LEU:HD22	0.54	1.78	18	1
1:A:77:VAL:HG21	1:A:81:VAL:HB	0.53	1.80	13	1
1:A:61:TYR:HB3	1:A:69:PHE:CE2	0.53	2.38	13	1
1:A:137:ASP:O	1:A:139:PRO:HD3	0.53	2.03	17	1
1:A:59:ALA:HB3	1:A:133:GLU:HB2	0.53	1.79	20	1
1:A:62:PHE:HB2	1:A:70:GLU:HB2	0.53	1.79	11	1
1:A:110:GLU:HA	1:A:113:TYR:CB	0.53	2.33	14	1
1:A:22:ILE:HD13	1:A:73:PHE:HB3	0.53	1.79	16	1
1:A:98:ALA:HB1	1:A:116:LEU:HD12	0.53	1.79	17	2
1:A:60:ARG:HG3	1:A:72:GLU:O	0.53	2.03	15	1
1:A:34:LEU:HG	1:A:73:PHE:HZ	0.53	1.63	1	1
1:A:42:ILE:HG22	1:A:43:LEU:H	0.53	1.64	20	1
1:A:62:PHE:HD1	1:A:130:GLU:HB3	0.52	1.63	9	2
1:A:136:LEU:H	1:A:136:LEU:HD13	0.52	1.63	16	2
1:A:102:TYR:CD1	1:A:149:THR:HG22	0.52	2.39	15	1
1:A:43:LEU:HD22	1:A:45:LEU:HD23	0.52	1.81	1	1
1:A:26:THR:HG21	1:A:34:LEU:HD22	0.52	1.82	1	1
1:A:21:LEU:HD23	1:A:74:GLY:HA3	0.52	1.82	15	1
1:A:110:GLU:HA	1:A:113:TYR:CD2	0.52	2.40	19	2
1:A:51:LYS:HE2	1:A:51:LYS:O	0.52	2.03	13	1
1:A:26:THR:O	1:A:69:PHE:HB3	0.52	2.05	19	1
1:A:133:GLU:HB3	1:A:151:VAL:HG23	0.51	1.81	2	1
1:A:98:ALA:HB3	1:A:153:LEU:HD21	0.51	1.82	13	1
1:A:31:LEU:O	1:A:35:PHE:HB2	0.51	2.05	7	1
1:A:139:PRO:HB3	1:A:147:LEU:HD13	0.51	1.83	16	1
1:A:38:GLY:HA3	1:A:73:PHE:CE2	0.51	2.40	1	1
1:A:101:LEU:HD13	1:A:103:ILE:HD11	0.51	1.83	7	1
1:A:61:TYR:O	1:A:130:GLU:HA	0.51	2.05	11	1
1:A:24:THR:O	1:A:71:VAL:HG22	0.51	2.06	7	4
1:A:41:ASP:O	1:A:44:GLN:HG2	0.51	2.06	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:LEU:HD23	1:A:153:LEU:H	0.51	1.66	13	1
1:A:41:ASP:O	1:A:42:ILE:HG12	0.51	2.06	12	2
1:A:36:GLU:HA	1:A:39:TYR:CE2	0.51	2.41	7	1
1:A:20:LEU:HD23	1:A:77:VAL:HG21	0.51	1.82	18	1
1:A:134:ILE:HG12	1:A:150:ARG:HB2	0.51	1.83	6	1
1:A:136:LEU:HB2	1:A:148:ARG:HG3	0.51	1.83	12	1
1:A:60:ARG:HD3	1:A:72:GLU:OE1	0.50	2.06	11	4
1:A:56:PRO:HB3	1:A:136:LEU:HA	0.50	1.82	20	2
1:A:116:LEU:O	1:A:120:VAL:HG12	0.50	2.07	3	2
1:A:31:LEU:CD1	1:A:31:LEU:H	0.50	2.20	15	1
1:A:11:LEU:O	1:A:11:LEU:HD12	0.50	2.06	17	2
1:A:132:TYR:CE2	1:A:152:SER:HB3	0.50	2.42	8	1
1:A:109:ILE:HD11	1:A:151:VAL:HG21	0.50	1.82	20	1
1:A:59:ALA:O	1:A:132:TYR:HA	0.50	2.07	4	3
1:A:61:TYR:HD1	1:A:71:VAL:HG12	0.50	1.65	11	1
1:A:64:MET:HG2	1:A:129:GLY:O	0.49	2.07	19	1
1:A:56:PRO:CB	1:A:136:LEU:HA	0.49	2.37	4	3
1:A:20:LEU:HD12	1:A:87:VAL:HG22	0.49	1.83	9	1
1:A:114:ASP:O	1:A:117:MET:HG2	0.49	2.08	2	1
1:A:20:LEU:HB3	1:A:89:THR:HG22	0.49	1.84	7	1
1:A:109:ILE:O	1:A:112:VAL:HG22	0.49	2.07	2	1
1:A:101:LEU:HG	1:A:150:ARG:HG2	0.49	1.84	12	1
1:A:120:VAL:HG22	1:A:125:PHE:HA	0.49	1.83	20	1
1:A:25:GLN:NE2	1:A:25:GLN:H	0.49	2.04	16	1
1:A:14:LEU:HB2	1:A:94:SER:HB3	0.49	1.84	16	1
1:A:20:LEU:HD11	1:A:45:LEU:HD23	0.49	1.84	11	1
1:A:24:THR:HG22	1:A:26:THR:HG23	0.49	1.84	7	1
1:A:24:THR:HG23	1:A:71:VAL:HG23	0.49	1.85	9	1
1:A:58:PHE:CD1	1:A:134:ILE:HD12	0.49	2.43	15	1
1:A:143:ALA:HB1	1:A:146:GLN:HB2	0.48	1.85	7	3
1:A:42:ILE:HG13	1:A:87:VAL:HG13	0.48	1.84	13	1
1:A:133:GLU:HA	1:A:151:VAL:HA	0.48	1.85	19	1
1:A:120:VAL:HG21	1:A:153:LEU:HD11	0.48	1.84	13	1
1:A:49:GLN:HB3	1:A:51:LYS:HE3	0.48	1.83	5	1
1:A:54:SER:CB	1:A:78:GLU:HG3	0.48	2.39	5	1
1:A:24:THR:HG21	1:A:34:LEU:HD22	0.48	1.85	7	1
1:A:46:LEU:O	1:A:51:LYS:HB3	0.48	2.08	13	1
1:A:103:ILE:CG2	1:A:145:ASP:HA	0.48	2.38	2	1
1:A:14:LEU:O	1:A:94:SER:HA	0.48	2.08	12	3
1:A:30:GLU:HG3	1:A:33:SER:HB2	0.48	1.84	16	1
1:A:56:PRO:HB2	1:A:135:TYR:O	0.48	2.08	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:GLU:OE2	1:A:81:VAL:HG23	0.48	2.08	2	1
1:A:64:MET:CE	1:A:64:MET:HA	0.48	2.39	7	1
1:A:99:SER:HB3	1:A:152:SER:CB	0.48	2.38	8	1
1:A:134:ILE:HD11	1:A:150:ARG:HB3	0.48	1.85	9	1
1:A:45:LEU:HD23	1:A:87:VAL:HB	0.48	1.85	13	1
1:A:64:MET:HG3	1:A:129:GLY:C	0.47	2.29	8	1
1:A:9:CYS:HA	1:A:100:SER:OG	0.47	2.10	10	1
1:A:60:ARG:HG3	1:A:132:TYR:CE2	0.47	2.43	17	1
1:A:120:VAL:HA	1:A:125:PHE:CE1	0.47	2.44	18	1
1:A:45:LEU:HD23	1:A:45:LEU:H	0.47	1.69	20	1
1:A:13:GLU:HA	1:A:95:GLY:O	0.47	2.09	19	3
1:A:43:LEU:HD21	1:A:87:VAL:HB	0.47	1.86	1	1
1:A:56:PRO:HG2	1:A:136:LEU:HG	0.47	1.85	1	1
1:A:20:LEU:HD12	1:A:87:VAL:HG12	0.47	1.84	18	2
1:A:102:TYR:CD1	1:A:112:VAL:HG11	0.47	2.45	9	1
1:A:11:LEU:HD13	1:A:123:ASN:HD21	0.47	1.70	14	1
1:A:64:MET:N	1:A:64:MET:SD	0.47	2.87	14	1
1:A:51:LYS:HE2	1:A:79:GLY:O	0.47	2.09	16	1
1:A:60:ARG:HD2	1:A:72:GLU:OE1	0.47	2.10	8	2
1:A:101:LEU:HA	1:A:149:THR:O	0.47	2.10	9	1
1:A:46:LEU:HG	1:A:51:LYS:CG	0.47	2.37	13	1
1:A:31:LEU:HB3	1:A:71:VAL:HG11	0.47	1.85	15	1
1:A:61:TYR:HB3	1:A:69:PHE:CZ	0.47	2.44	6	1
1:A:27:ALA:HB2	1:A:68:THR:HA	0.47	1.85	14	1
1:A:83:GLY:HA3	1:A:87:VAL:O	0.47	2.10	14	1
1:A:116:LEU:HA	1:A:119:TRP:HD1	0.47	1.68	1	2
1:A:130:GLU:HG3	1:A:154:MET:HG3	0.47	1.87	9	1
1:A:77:VAL:HB	1:A:81:VAL:HG21	0.47	1.87	20	3
1:A:113:TYR:HA	1:A:153:LEU:HD11	0.47	1.88	10	1
1:A:21:LEU:HB3	1:A:74:GLY:CA	0.47	2.37	11	1
1:A:20:LEU:HD11	1:A:89:THR:HG22	0.46	1.86	19	1
1:A:58:PHE:HB3	1:A:134:ILE:HG12	0.46	1.85	19	1
1:A:58:PHE:CE1	1:A:76:PRO:HG3	0.46	2.46	3	1
1:A:18:PRO:HA	1:A:90:GLY:O	0.46	2.11	12	1
1:A:21:LEU:HB3	1:A:74:GLY:H	0.46	1.70	1	1
1:A:63:GLY:HA3	1:A:69:PHE:CE2	0.46	2.44	16	1
1:A:116:LEU:HB3	1:A:153:LEU:HB2	0.46	1.88	14	1
1:A:142:THR:HG23	1:A:147:LEU:HD23	0.46	1.86	2	1
1:A:63:GLY:HA3	1:A:69:PHE:CD2	0.46	2.45	4	1
1:A:43:LEU:HG	1:A:46:LEU:HB3	0.46	1.87	6	1
1:A:61:TYR:CE2	1:A:131:ALA:HB3	0.46	2.46	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:ILE:HG13	1:A:148:ARG:HG2	0.46	1.85	5	1
1:A:150:ARG:HG3	1:A:150:ARG:O	0.46	2.11	14	1
1:A:120:VAL:HG22	1:A:125:PHE:CZ	0.46	2.46	18	1
1:A:23:ARG:HB3	1:A:72:GLU:CG	0.46	2.40	7	1
1:A:22:ILE:HB	1:A:73:PHE:HD2	0.46	1.70	19	1
1:A:110:GLU:HA	1:A:113:TYR:CD1	0.46	2.46	3	1
1:A:98:ALA:HB1	1:A:116:LEU:HD22	0.46	1.88	3	1
1:A:38:GLY:O	1:A:42:ILE:HG12	0.46	2.11	10	2
1:A:101:LEU:O	1:A:101:LEU:HD12	0.46	2.11	10	1
1:A:21:LEU:HB3	1:A:74:GLY:HA2	0.46	1.88	4	2
1:A:45:LEU:O	1:A:49:GLN:HB2	0.46	2.11	6	1
1:A:104:GLY:HA2	1:A:145:ASP:H	0.46	1.71	11	1
1:A:31:LEU:HD21	1:A:71:VAL:HG11	0.46	1.87	17	1
1:A:42:ILE:HB	1:A:87:VAL:HG21	0.45	1.86	6	1
1:A:14:LEU:HD22	1:A:150:ARG:HH22	0.45	1.72	15	1
1:A:20:LEU:HD11	1:A:75:PHE:CZ	0.45	2.46	15	1
1:A:116:LEU:CB	1:A:153:LEU:HD21	0.45	2.41	4	1
1:A:142:THR:HG23	1:A:143:ALA:H	0.45	1.72	8	1
1:A:120:VAL:HG13	1:A:125:PHE:O	0.45	2.12	18	1
1:A:99:SER:HA	1:A:151:VAL:O	0.45	2.12	15	2
1:A:42:ILE:HG22	1:A:43:LEU:N	0.45	2.27	20	1
1:A:22:ILE:HD13	1:A:87:VAL:HB	0.45	1.88	9	1
1:A:51:LYS:HD3	1:A:51:LYS:H	0.45	1.71	13	1
1:A:102:TYR:CE1	1:A:149:THR:HB	0.45	2.47	11	1
1:A:23:ARG:HD3	1:A:70:GLU:OE1	0.45	2.12	1	1
1:A:153:LEU:HG	1:A:154:MET:H	0.45	1.71	7	1
1:A:22:ILE:HG13	1:A:86:ARG:HD2	0.45	1.88	7	1
1:A:103:ILE:H	1:A:103:ILE:HD13	0.45	1.72	11	1
1:A:136:LEU:CD1	1:A:136:LEU:H	0.45	2.24	8	1
1:A:127:LEU:HD12	1:A:130:GLU:HB3	0.45	1.88	13	1
1:A:61:TYR:HA	1:A:70:GLU:O	0.44	2.11	11	2
1:A:113:TYR:HD2	1:A:153:LEU:HD13	0.44	1.69	5	1
1:A:142:THR:O	1:A:146:GLN:HB3	0.44	2.12	9	1
1:A:16:PRO:HB3	1:A:93:PRO:HA	0.44	1.88	16	1
1:A:58:PHE:HB3	1:A:134:ILE:HG13	0.44	1.88	4	1
1:A:39:TYR:HB3	1:A:73:PHE:CE2	0.44	2.47	18	1
1:A:153:LEU:HD13	1:A:154:MET:H	0.44	1.72	2	1
1:A:62:PHE:HB2	1:A:130:GLU:HG3	0.44	1.89	4	1
1:A:153:LEU:HG	1:A:154:MET:N	0.44	2.27	7	1
1:A:56:PRO:HG2	1:A:136:LEU:HA	0.44	1.89	9	1
1:A:133:GLU:HG2	1:A:151:VAL:HG23	0.44	1.89	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ARG:HG2	1:A:72:GLU:HB2	0.44	1.89	11	1
1:A:127:LEU:HG	1:A:129:GLY:H	0.44	1.71	5	1
1:A:101:LEU:HB3	1:A:150:ARG:HB3	0.44	1.87	14	1
1:A:134:ILE:HD11	1:A:150:ARG:HG2	0.44	1.88	14	1
1:A:139:PRO:C	1:A:141:GLU:H	0.44	2.15	17	1
1:A:20:LEU:HB3	1:A:89:THR:HB	0.44	1.89	15	1
1:A:123:ASN:HB3	1:A:125:PHE:HD2	0.44	1.72	1	1
1:A:46:LEU:HG	1:A:51:LYS:CB	0.44	2.43	13	1
1:A:139:PRO:HG3	1:A:147:LEU:HD21	0.44	1.88	17	1
1:A:57:PRO:HB3	1:A:75:PHE:CE2	0.44	2.47	3	2
1:A:136:LEU:HD13	1:A:136:LEU:N	0.44	2.27	16	2
1:A:57:PRO:HD2	1:A:135:TYR:O	0.44	2.13	14	2
1:A:62:PHE:CD1	1:A:130:GLU:HG3	0.44	2.48	17	1
1:A:154:MET:HA	1:A:154:MET:CE	0.43	2.43	15	1
1:A:61:TYR:HB3	1:A:69:PHE:HE2	0.43	1.71	13	1
1:A:34:LEU:HG	1:A:73:PHE:CZ	0.43	2.48	1	1
1:A:12:LYS:HA	1:A:12:LYS:CE	0.43	2.43	3	1
1:A:127:LEU:HD21	1:A:130:GLU:HB2	0.43	1.91	2	1
1:A:147:LEU:HD12	1:A:147:LEU:O	0.43	2.13	2	1
1:A:28:MET:HG2	1:A:28:MET:O	0.43	2.14	7	1
1:A:136:LEU:N	1:A:136:LEU:HD13	0.43	2.27	9	1
1:A:17:VAL:O	1:A:91:LEU:HA	0.43	2.13	12	1
1:A:49:GLN:HE22	1:A:81:VAL:HG13	0.43	1.74	10	1
1:A:128:SER:OG	1:A:153:LEU:HG	0.43	2.14	15	1
1:A:23:ARG:CD	1:A:23:ARG:H	0.43	2.25	20	1
1:A:60:ARG:O	1:A:71:VAL:HA	0.43	2.14	13	1
1:A:128:SER:CB	1:A:154:MET:HB3	0.43	2.44	18	1
1:A:60:ARG:HA	1:A:132:TYR:HA	0.43	1.90	19	1
1:A:20:LEU:HD12	1:A:89:THR:HB	0.42	1.91	4	1
1:A:64:MET:H	1:A:69:PHE:HE1	0.42	1.57	6	1
1:A:123:ASN:HB3	1:A:125:PHE:CD2	0.42	2.49	1	1
1:A:142:THR:HG23	1:A:143:ALA:N	0.42	2.27	8	1
1:A:9:CYS:HB2	1:A:119:TRP:CD1	0.42	2.49	14	1
1:A:21:LEU:N	1:A:21:LEU:HD13	0.42	2.30	14	2
1:A:19:ALA:HA	1:A:77:VAL:HG22	0.42	1.92	20	1
1:A:26:THR:HB	1:A:34:LEU:HD22	0.42	1.90	4	1
1:A:47:ALA:HA	1:A:51:LYS:O	0.42	2.14	12	1
1:A:30:GLU:O	1:A:34:LEU:HG	0.42	2.14	15	1
1:A:101:LEU:HD11	1:A:148:ARG:CG	0.42	2.44	19	1
1:A:103:ILE:N	1:A:103:ILE:HD13	0.42	2.29	18	1
1:A:64:MET:SD	1:A:130:GLU:HB2	0.42	2.54	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ARG:HG2	1:A:72:GLU:HG2	0.42	1.91	14	1
1:A:58:PHE:HD1	1:A:134:ILE:HG12	0.42	1.74	2	2
1:A:51:LYS:HG3	1:A:81:VAL:HG22	0.42	1.91	7	1
1:A:112:VAL:O	1:A:116:LEU:HG	0.42	2.15	11	1
1:A:47:ALA:HA	1:A:51:LYS:CD	0.42	2.44	13	1
1:A:12:LYS:CB	1:A:99:SER:HB3	0.42	2.44	10	1
1:A:63:GLY:HA3	1:A:69:PHE:HD2	0.42	1.74	4	1
1:A:20:LEU:HD23	1:A:77:VAL:HG12	0.42	1.91	7	1
1:A:25:GLN:CD	1:A:25:GLN:H	0.42	2.19	7	1
1:A:20:LEU:O	1:A:74:GLY:HA2	0.42	2.15	16	1
1:A:11:LEU:O	1:A:11:LEU:HG	0.42	2.14	19	1
1:A:134:ILE:O	1:A:149:THR:HG23	0.42	2.15	5	1
1:A:64:MET:HG3	1:A:154:MET:SD	0.42	2.55	6	1
1:A:98:ALA:HB2	1:A:119:TRP:CZ2	0.41	2.48	19	1
1:A:143:ALA:O	1:A:147:LEU:HG	0.41	2.15	7	1
1:A:154:MET:SD	1:A:154:MET:N	0.41	2.93	14	1
1:A:110:GLU:HA	1:A:113:TYR:HD1	0.41	1.76	3	1
1:A:9:CYS:SG	1:A:116:LEU:HG	0.41	2.55	16	1
1:A:77:VAL:HG12	1:A:78:GLU:H	0.41	1.75	18	1
1:A:137:ASP:CB	1:A:142:THR:HG21	0.41	2.44	3	1
1:A:54:SER:HB2	1:A:78:GLU:HG3	0.41	1.91	5	1
1:A:13:GLU:HA	1:A:96:LYS:HA	0.41	1.91	5	1
1:A:45:LEU:HD21	1:A:84:SER:HB3	0.41	1.93	15	1
1:A:113:TYR:HA	1:A:116:LEU:HD12	0.41	1.92	18	1
1:A:106:TYR:OH	1:A:149:THR:HG21	0.41	2.14	19	1
1:A:23:ARG:O	1:A:86:ARG:HD3	0.41	2.16	1	1
1:A:119:TRP:O	1:A:119:TRP:HE3	0.41	1.98	14	1
1:A:60:ARG:HG2	1:A:72:GLU:CG	0.41	2.45	14	1
1:A:26:THR:HG22	1:A:69:PHE:HB3	0.41	1.92	16	1
1:A:21:LEU:HG	1:A:60:ARG:NH2	0.41	2.29	18	1
1:A:20:LEU:HB3	1:A:89:THR:HG23	0.41	1.93	1	1
1:A:136:LEU:O	1:A:137:ASP:HB2	0.41	2.16	3	1
1:A:62:PHE:CZ	1:A:65:SER:HB2	0.41	2.50	5	1
1:A:101:LEU:HD12	1:A:101:LEU:O	0.41	2.14	11	1
1:A:116:LEU:HD22	1:A:153:LEU:HB3	0.41	1.91	16	1
1:A:53:PRO:HA	1:A:76:PRO:O	0.41	2.16	17	1
1:A:58:PHE:CB	1:A:134:ILE:HG12	0.41	2.46	19	1
1:A:129:GLY:HA2	1:A:154:MET:HG3	0.41	1.93	2	1
1:A:73:PHE:HB3	1:A:75:PHE:HE1	0.41	1.76	8	1
1:A:123:ASN:OD1	1:A:125:PHE:HB2	0.41	2.16	14	1
1:A:104:GLY:HA2	1:A:145:ASP:O	0.41	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LYS:HD2	1:A:78:GLU:HB3	0.41	1.91	7	1
1:A:62:PHE:CD1	1:A:130:GLU:HG2	0.41	2.50	15	1
1:A:101:LEU:HD11	1:A:148:ARG:HG2	0.41	1.93	19	1
1:A:11:LEU:HD11	1:A:96:LYS:HB3	0.40	1.92	6	1
1:A:20:LEU:HD21	1:A:46:LEU:HD21	0.40	1.93	7	1
1:A:61:TYR:CD1	1:A:71:VAL:HG12	0.40	2.50	11	1
1:A:35:PHE:HB2	1:A:73:PHE:CD1	0.40	2.50	18	1
1:A:77:VAL:HB	1:A:81:VAL:CG2	0.40	2.46	5	1
1:A:49:GLN:OE1	1:A:81:VAL:HA	0.40	2.17	7	1
1:A:103:ILE:HD13	1:A:103:ILE:N	0.40	2.31	11	1
1:A:136:LEU:HB2	1:A:148:ARG:HB3	0.40	1.92	13	1
1:A:7:PHE:HA	1:A:101:LEU:O	0.40	2.17	11	1
1:A:16:PRO:HA	1:A:92:THR:O	0.40	2.16	1	1
1:A:129:GLY:HA2	1:A:154:MET:CG	0.40	2.46	2	1
1:A:110:GLU:CD	1:A:110:GLU:H	0.40	2.20	4	1
1:A:21:LEU:HD13	1:A:21:LEU:N	0.40	2.31	7	1
1:A:144:PRO:O	1:A:145:ASP:HB3	0.40	2.17	17	1
1:A:150:ARG:O	1:A:150:ARG:HG3	0.40	2.16	1	1
1:A:138:ASN:O	1:A:142:THR:HG22	0.40	2.16	2	1
1:A:20:LEU:HD11	1:A:83:GLY:HA2	0.40	1.93	18	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	148/166 (89%)	133±3 (90±2%)	13±3 (9±2%)	2±1 (2±1%)	15	59
All	All	2960/3320 (89%)	2650 (90%)	264 (9%)	46 (2%)	15	59

All 20 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	74	GLY	11
1	A	42	ILE	5

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Mol	Chain	Res	Type	Models (Total)
1	A	107	GLY	5
1	A	66	ALA	4
1	A	28	MET	3
1	A	143	ALA	2
1	A	43	LEU	2
1	A	67	GLY	2
1	A	129	GLY	1
1	A	49	GLN	1
1	A	142	THR	1
1	A	108	GLU	1
1	A	105	PRO	1
1	A	140	ALA	1
1	A	50	GLY	1
1	A	137	ASP	1
1	A	30	GLU	1
1	A	7	PHE	1
1	A	65	SER	1
1	A	63	GLY	1

### 6.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/134 (87%)	109±2 (94±2%)	7±2 (6±2%)	25	72
All	All	2320/2680 (87%)	2179 (94%)	141 (6%)	25	72

All 57 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	21	LEU	9
1	A	78	GLU	6
1	A	136	LEU	5
1	A	89	THR	5
1	A	153	LEU	5
1	A	96	LYS	4
1	A	141	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	23	ARG	4
1	A	25	GLN	4
1	A	117	MET	4
1	A	12	LYS	4
1	A	101	LEU	4
1	A	11	LEU	3
1	A	103	ILE	3
1	A	20	LEU	3
1	A	142	THR	3
1	A	13	GLU	3
1	A	154	MET	3
1	A	148	ARG	3
1	A	14	LEU	3
1	A	130	GLU	3
1	A	126	ASP	3
1	A	118	LYS	3
1	A	51	LYS	2
1	A	31	LEU	2
1	A	91	LEU	2
1	A	34	LEU	2
1	A	133	GLU	2
1	A	110	GLU	2
1	A	147	LEU	2
1	A	114	ASP	2
1	A	64	MET	2
1	A	146	GLN	2
1	A	86	ARG	2
1	A	60	ARG	2
1	A	30	GLU	2
1	A	10	GLU	2
1	A	36	GLU	2
1	A	150	ARG	2
1	A	119	TRP	1
1	A	33	SER	1
1	A	108	GLU	1
1	A	68	THR	1
1	A	44	GLN	1
1	A	24	THR	1
1	A	113	TYR	1
1	A	123	ASN	1
1	A	138	ASN	1
1	A	122	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	106	TYR	1
1	A	22	ILE	1
1	A	58	PHE	1
1	A	84	SER	1
1	A	149	THR	1
1	A	82	GLU	1
1	A	116	LEU	1
1	A	92	THR	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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 76% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2kcu\_cs.cif

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

#### 7.1.1 Bookkeeping [i](#)

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	1677
Number of shifts mapped to atoms	1677
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	156	$0.12 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	138	$-0.05 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	149	$-0.10 \pm 0.33$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 1298 atoms were assigned a chemical shift out of a possible 1697. 23 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	545/720 (76%)	273/286 (95%)	139/296 (47%)	133/138 (96%)
Sidechain	650/829 (78%)	400/486 (82%)	246/318 (77%)	4/25 (16%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	103/148 (70%)	67/78 (86%)	35/67 (52%)	1/3 (33%)
Overall	1298/1697 (76%)	740/850 (87%)	420/681 (62%)	138/166 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 1476 atoms were assigned a chemical shift out of a possible 1943. 25 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	611/810 (75%)	306/322 (95%)	156/332 (47%)	149/156 (96%)
Sidechain	727/920 (79%)	449/541 (83%)	273/353 (77%)	5/26 (19%)
Aromatic	138/213 (65%)	86/111 (77%)	51/85 (60%)	1/17 (6%)
Overall	1476/1943 (76%)	841/974 (86%)	480/770 (62%)	155/199 (78%)

#### 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	22	ILE	HB	0.24	3.24 – 0.34	-5.4

#### 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:

