



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:09 AM BST

PDB ID : 2U1A  
Title : RNA BINDING DOMAIN 2 OF HUMAN U1A PROTEIN, NMR, 20 STRUCTURES  
Authors : Lu, J.; Hall, K.B.  
Deposited on : 1997-03-26

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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.

---

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  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

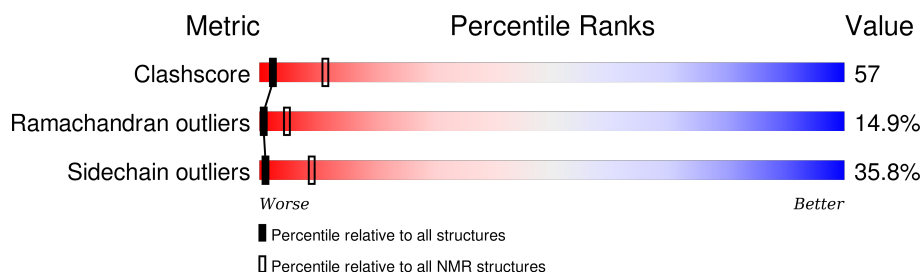
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	88	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:13-A:86 (74)	0.47	3

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 6 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1389 atoms, of which 693 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A.

Mol	Chain	Residues	Atoms						Trace
1	A	88	Total	C	H	N	O	S	0
			1389	445	693	119	128	4	

There is a discrepancy between the modelled and reference sequences:

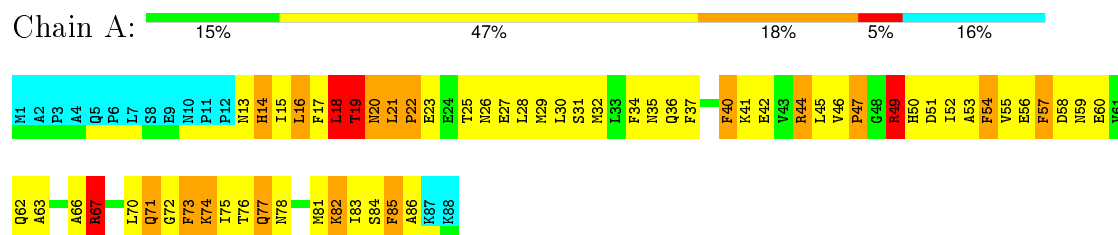
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	ENGINEERED	UNP P09012

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

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

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

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

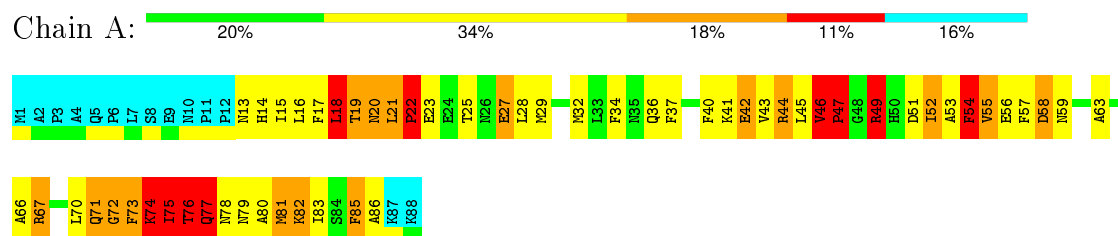


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

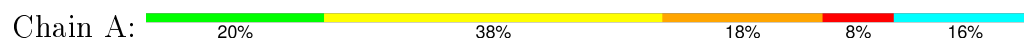
#### 4.2.1 Score per residue for model 1

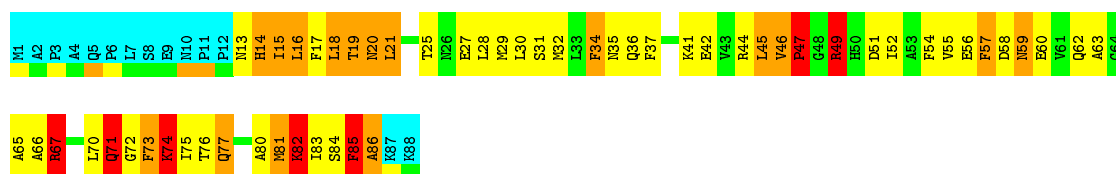
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



#### 4.2.2 Score per residue for model 2

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

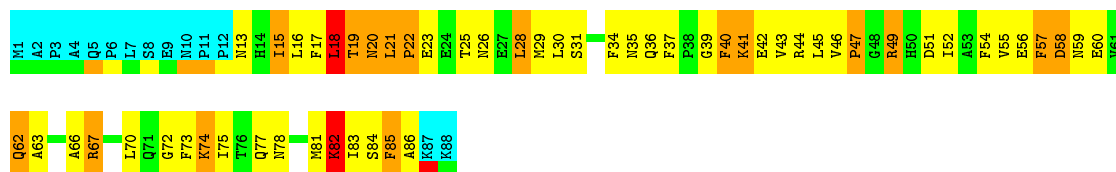




#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

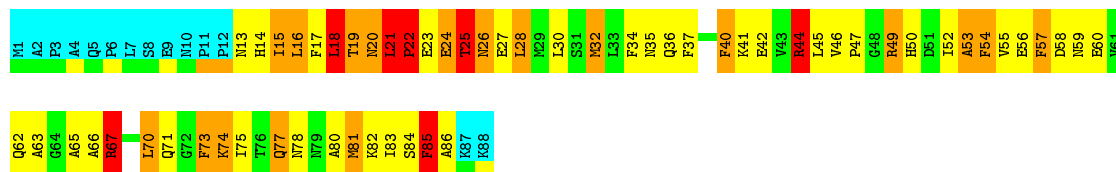
Chain A: 20% 43% 18% • 16%



#### 4.2.4 Score per residue for model 4

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

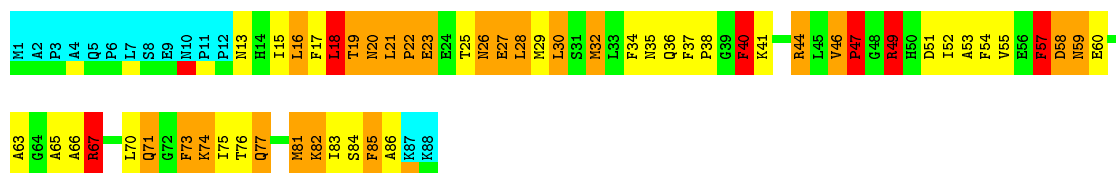
Chain A: 17% 39% 20% 8% 16%



#### 4.2.5 Score per residue for model 5

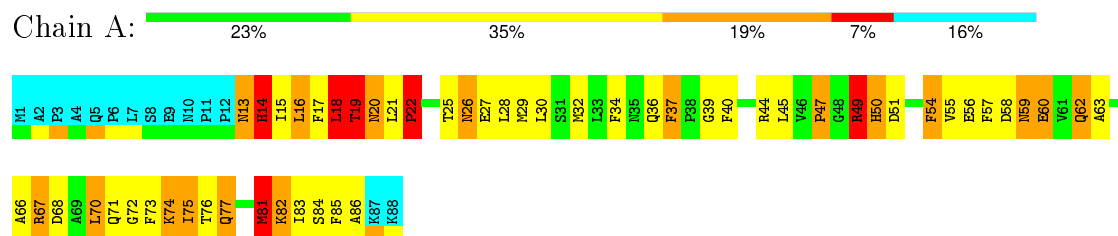
- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

Chain A: 23% 30% 25% 7% 16%



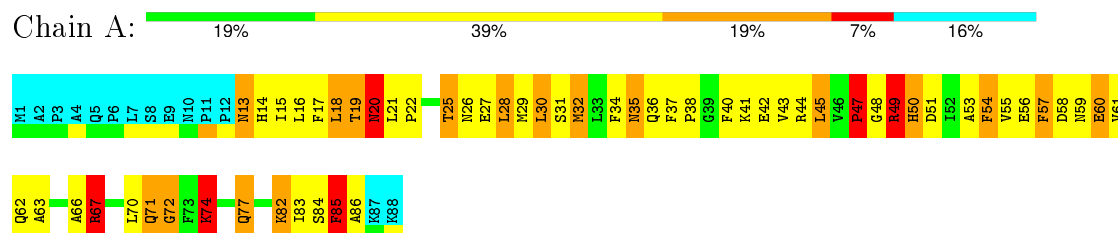
#### 4.2.6 Score per residue for model 6

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



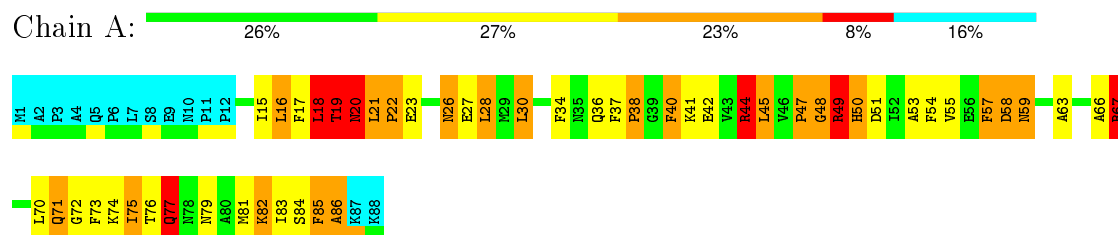
#### 4.2.7 Score per residue for model 7

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



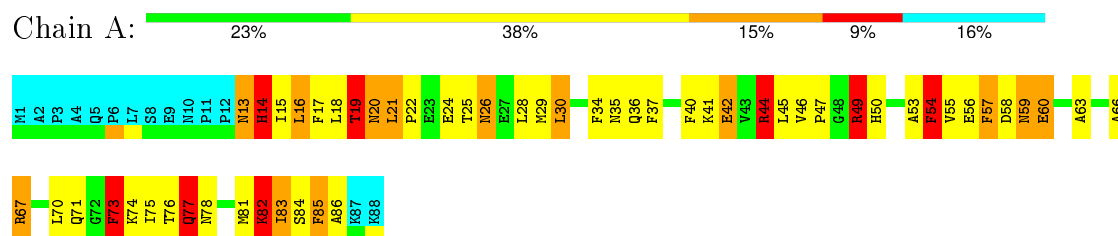
#### 4.2.8 Score per residue for model 8

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



#### 4.2.9 Score per residue for model 9

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A

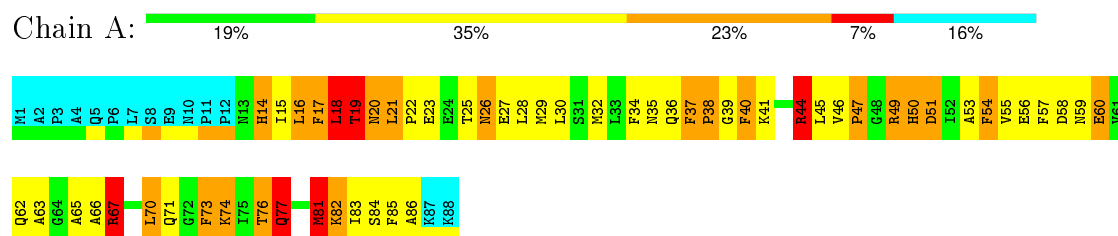






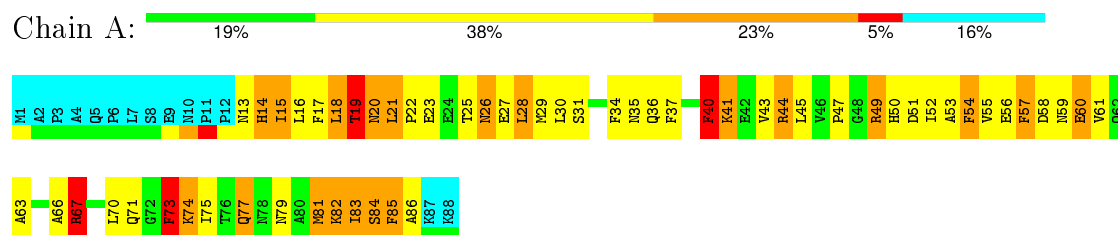
#### 4.2.14 Score per residue for model 14

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



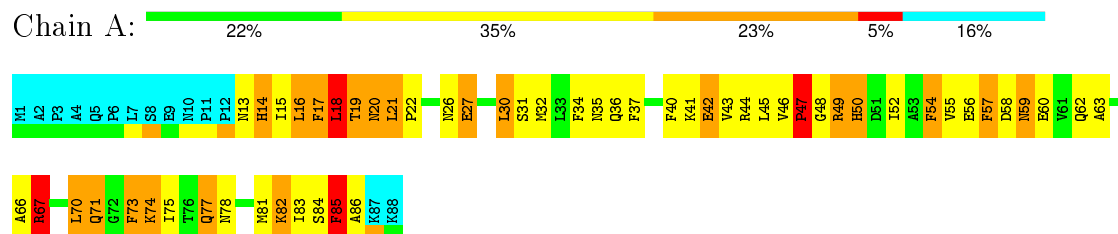
#### 4.2.15 Score per residue for model 15

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



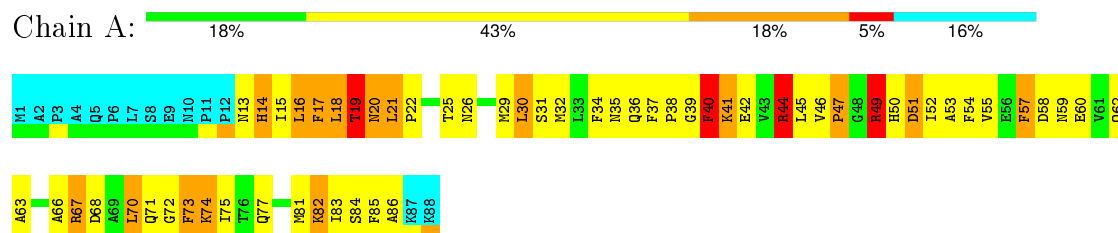
#### 4.2.16 Score per residue for model 16

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



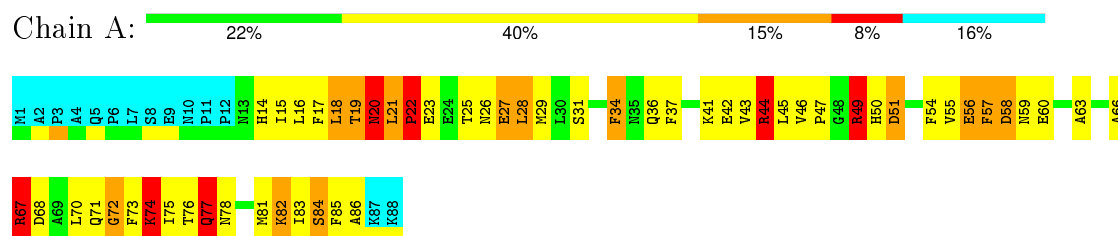
#### 4.2.17 Score per residue for model 17

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



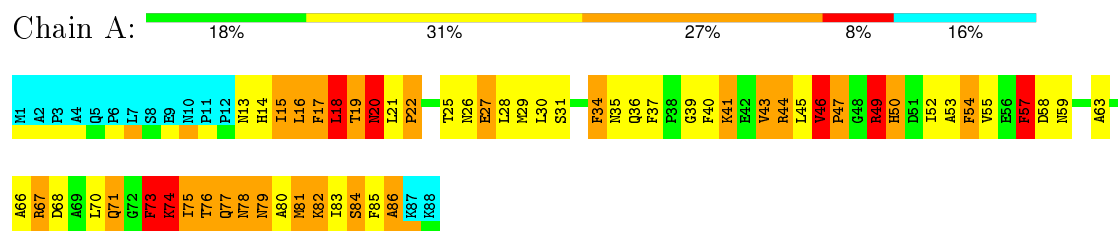
### 4.2.18 Score per residue for model 18

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



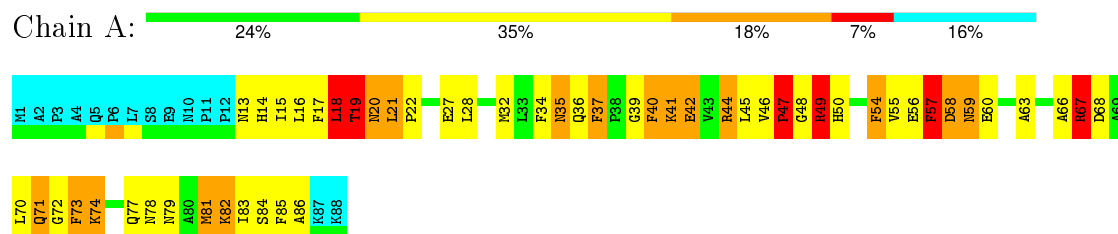
### 4.2.19 Score per residue for model 19

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



### 4.2.20 Score per residue for model 20

- Molecule 1: U1 SMALL NUCLEAR RIBONUCLEOPROTEIN A



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY*.

Of the 40 calculated structures, 20 were deposited, based on the following criterion: *LEAST ERROR FUNCTION*.

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

Software name	Classification	Version
TINKER	refinement	
TINKER	structure solution	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.28±0.02	1±0/604 (0.1±0.0%)	1.66±0.05	6±1/816 (0.7±0.1%)
All	All	1.28	18/12080 (0.1%)	1.66	111/16320 (0.7%)

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	3.0±0.0
All	All	0	60

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	19	THR	C-N	-5.38	1.21	1.34	5	18

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	57	PHE	CB-CG-CD1	-9.37	114.24	120.80	16	11
1	A	76	THR	CA-CB-CG2	-8.74	100.17	112.40	19	3
1	A	22	PRO	N-CA-CB	-8.49	93.11	103.30	18	2
1	A	79	ASN	O-C-N	-7.95	109.98	122.70	10	1
1	A	47	PRO	N-CA-CB	7.74	112.58	103.30	14	5
1	A	22	PRO	CA-N-CD	-7.67	100.76	111.50	4	4
1	A	40	PHE	CB-CG-CD1	-7.38	115.64	120.80	15	2
1	A	37	PHE	CB-CG-CD1	-7.25	115.72	120.80	14	2
1	A	57	PHE	CB-CG-CD2	-7.15	115.80	120.80	20	6
1	A	37	PHE	CB-CG-CD2	-6.88	115.98	120.80	11	2

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	48	GLY	N-CA-C	-6.72	96.29	113.10	7	2
1	A	47	PRO	N-CD-CG	-6.61	93.29	103.20	5	2
1	A	47	PRO	CA-N-CD	-6.60	102.26	111.50	12	2
1	A	40	PHE	CB-CG-CD2	-6.50	116.25	120.80	8	2
1	A	67	ARG	NE-CZ-NH1	-6.46	117.07	120.30	16	1
1	A	53	ALA	N-CA-CB	-6.43	101.10	110.10	4	1
1	A	54	PHE	CB-CG-CD2	-6.35	116.35	120.80	9	2
1	A	82	LYS	O-C-N	6.33	132.83	122.70	9	17
1	A	75	ILE	N-CA-C	-6.31	93.97	111.00	10	3
1	A	38	PRO	CA-N-CD	-6.28	102.71	111.50	12	2
1	A	85	PHE	CB-CG-CD1	6.25	125.17	120.80	3	2
1	A	67	ARG	NE-CZ-NH2	-6.10	117.25	120.30	14	2
1	A	76	THR	CB-CA-C	-6.09	95.15	111.60	19	2
1	A	18	LEU	N-CA-CB	6.00	122.41	110.40	1	18
1	A	34	PHE	CB-CG-CD2	-5.75	116.78	120.80	13	2
1	A	54	PHE	CB-CG-CD1	-5.72	116.80	120.80	11	2
1	A	85	PHE	CB-CG-CD2	-5.71	116.81	120.80	7	1
1	A	73	PHE	CB-CG-CD1	-5.69	116.82	120.80	6	1
1	A	17	PHE	CB-CG-CD2	-5.69	116.82	120.80	13	1
1	A	49	ARG	NE-CZ-NH1	-5.66	117.47	120.30	6	1
1	A	17	PHE	CB-CG-CD1	-5.46	116.98	120.80	17	1
1	A	34	PHE	CB-CG-CD1	-5.20	117.16	120.80	18	2
1	A	73	PHE	CB-CG-CD2	-5.11	117.22	120.80	9	1
1	A	77	GLN	N-CA-C	-5.04	97.39	111.00	10	1
1	A	68	ASP	CB-CG-OD2	-5.03	113.77	118.30	19	1
1	A	57	PHE	CB-CA-C	-5.02	100.37	110.40	15	1

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	44	ARG	Sidechain	20
1	A	49	ARG	Sidechain	20
1	A	67	ARG	Sidechain	20

## 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	591	582	579	67±14
All	All	11820	11640	11582	1333

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:76:THR:HA	1:A:79:ASN:CA	1.00	1.85	1	3
1:A:76:THR:CA	1:A:79:ASN:C	0.97	2.33	19	3
1:A:76:THR:N	1:A:79:ASN:C	0.95	2.19	19	3
1:A:76:THR:CA	1:A:79:ASN:O	0.95	2.14	10	1
1:A:16:LEU:HD11	1:A:63:ALA:HB1	0.91	1.37	7	8
1:A:76:THR:HA	1:A:79:ASN:C	0.91	1.84	19	3
1:A:16:LEU:HD21	1:A:85:PHE:CE1	0.90	2.02	20	3
1:A:76:THR:C	1:A:78:ASN:N	0.89	2.19	10	3
1:A:30:LEU:HD22	1:A:34:PHE:CE2	0.89	2.02	10	1
1:A:16:LEU:HD21	1:A:85:PHE:CZ	0.88	2.03	18	3
1:A:34:PHE:CZ	1:A:55:VAL:HG21	0.87	2.04	2	15
1:A:30:LEU:HD13	1:A:45:LEU:CD2	0.87	1.99	11	1
1:A:76:THR:OG1	1:A:79:ASN:O	0.87	1.92	10	1
1:A:76:THR:N	1:A:79:ASN:O	0.86	2.07	19	3
1:A:34:PHE:CE2	1:A:55:VAL:HG21	0.85	2.04	10	13
1:A:30:LEU:HD13	1:A:45:LEU:HD22	0.85	1.46	16	2
1:A:16:LEU:HD13	1:A:57:PHE:CE1	0.83	2.08	10	3
1:A:20:ASN:ND2	1:A:75:ILE:HD11	0.82	1.90	4	1
1:A:21:LEU:HD21	1:A:53:ALA:HB2	0.82	1.51	17	1
1:A:21:LEU:HD13	1:A:45:LEU:HD22	0.82	1.51	7	1
1:A:76:THR:CA	1:A:79:ASN:H	0.81	1.88	19	1
1:A:18:LEU:HD23	1:A:82:LYS:HB3	0.81	1.53	13	3
1:A:40:PHE:CZ	1:A:43:VAL:HG23	0.81	2.10	15	1
1:A:76:THR:OG1	1:A:80:ALA:CA	0.80	2.29	1	2
1:A:16:LEU:HD13	1:A:57:PHE:CD1	0.79	2.13	10	2
1:A:18:LEU:HB3	1:A:82:LYS:O	0.78	1.77	7	20
1:A:21:LEU:HD13	1:A:21:LEU:N	0.78	1.94	2	1
1:A:76:THR:C	1:A:78:ASN:H	0.77	1.82	10	3
1:A:76:THR:CA	1:A:79:ASN:N	0.77	2.47	19	3
1:A:67:ARG:NH2	1:A:83:ILE:HG21	0.77	1.94	5	1
1:A:18:LEU:HD13	1:A:84:SER:HB2	0.76	1.55	20	5
1:A:21:LEU:HD11	1:A:53:ALA:HB2	0.76	1.55	1	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HB3	1:A:25:THR:HG21	0.76	1.56	6	6
1:A:16:LEU:HB3	1:A:83:ILE:HG22	0.75	1.56	5	6
1:A:75:ILE:O	1:A:78:ASN:N	0.75	2.19	19	3
1:A:21:LEU:HD11	1:A:53:ALA:CB	0.75	2.11	1	2
1:A:76:THR:CB	1:A:79:ASN:O	0.74	2.35	10	1
1:A:21:LEU:HD12	1:A:21:LEU:N	0.74	1.97	12	2
1:A:27:GLU:HG2	1:A:46:VAL:HG23	0.73	1.58	1	2
1:A:70:LEU:HD12	1:A:81:MET:HE1	0.73	1.61	11	1
1:A:22:PRO:HG2	1:A:75:ILE:HG21	0.73	1.60	6	3
1:A:76:THR:HA	1:A:79:ASN:N	0.72	1.99	19	3
1:A:76:THR:CA	1:A:79:ASN:CA	0.72	2.67	1	3
1:A:34:PHE:CE2	1:A:55:VAL:HG11	0.72	2.19	19	1
1:A:19:THR:HG22	1:A:52:ILE:HA	0.72	1.59	2	2
1:A:70:LEU:HD12	1:A:81:MET:HE3	0.72	1.61	10	1
1:A:34:PHE:CD2	1:A:55:VAL:HG11	0.72	2.20	19	2
1:A:18:LEU:HD23	1:A:82:LYS:CB	0.71	2.14	8	7
1:A:57:PHE:HB2	1:A:63:ALA:HB2	0.71	1.63	18	10
1:A:55:VAL:HG12	1:A:57:PHE:CE1	0.71	2.20	10	2
1:A:30:LEU:HD23	1:A:34:PHE:CE2	0.71	2.20	11	2
1:A:76:THR:OG1	1:A:80:ALA:HB2	0.70	1.84	19	2
1:A:19:THR:CG2	1:A:52:ILE:HG22	0.70	2.17	5	3
1:A:18:LEU:HD13	1:A:84:SER:HB3	0.70	1.63	18	2
1:A:30:LEU:HD13	1:A:45:LEU:HD21	0.70	1.63	11	1
1:A:21:LEU:CD1	1:A:53:ALA:HB2	0.70	2.17	1	2
1:A:15:ILE:HG22	1:A:86:ALA:HB2	0.70	1.64	16	5
1:A:30:LEU:HD12	1:A:45:LEU:HD22	0.69	1.63	12	2
1:A:21:LEU:HD23	1:A:30:LEU:HD11	0.69	1.60	12	1
1:A:21:LEU:CD1	1:A:45:LEU:HD22	0.69	2.18	7	1
1:A:16:LEU:HB3	1:A:83:ILE:HG23	0.69	1.64	1	9
1:A:30:LEU:HD22	1:A:45:LEU:HD22	0.69	1.64	11	2
1:A:44:ARG:NH2	1:A:52:ILE:HD11	0.69	2.01	19	1
1:A:34:PHE:CD2	1:A:57:PHE:CE2	0.69	2.81	19	1
1:A:70:LEU:HD12	1:A:81:MET:CE	0.68	2.17	11	2
1:A:13:ASN:CG	1:A:86:ALA:HB3	0.68	2.07	6	1
1:A:15:ILE:CG2	1:A:86:ALA:HB2	0.68	2.18	3	7
1:A:22:PRO:HD3	1:A:75:ILE:HD12	0.68	1.65	10	1
1:A:18:LEU:HD12	1:A:19:THR:HG22	0.68	1.66	12	1
1:A:55:VAL:HG11	1:A:57:PHE:CE2	0.68	2.25	17	4
1:A:21:LEU:CB	1:A:25:THR:HG21	0.67	2.18	5	3
1:A:76:THR:OG1	1:A:80:ALA:CB	0.67	2.42	19	2
1:A:18:LEU:HD12	1:A:84:SER:CB	0.67	2.19	7	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:VAL:O	1:A:49:ARG:N	0.67	2.26	20	6
1:A:20:ASN:O	1:A:75:ILE:HD11	0.67	1.89	17	1
1:A:16:LEU:HD12	1:A:57:PHE:CE1	0.67	2.25	14	1
1:A:27:GLU:HA	1:A:45:LEU:HD23	0.67	1.66	2	1
1:A:49:ARG:HD2	1:A:52:ILE:HD12	0.66	1.67	1	1
1:A:34:PHE:CD2	1:A:55:VAL:CG1	0.66	2.78	19	3
1:A:76:THR:O	1:A:76:THR:HG22	0.66	1.89	1	1
1:A:30:LEU:HD22	1:A:34:PHE:CZ	0.66	2.26	10	1
1:A:75:ILE:C	1:A:79:ASN:H	0.66	1.94	10	2
1:A:57:PHE:CB	1:A:63:ALA:HB2	0.65	2.22	5	10
1:A:76:THR:HG22	1:A:76:THR:O	0.65	1.90	19	2
1:A:34:PHE:CD2	1:A:55:VAL:HG21	0.65	2.26	3	1
1:A:20:ASN:C	1:A:21:LEU:HD13	0.65	2.12	2	1
1:A:34:PHE:CE1	1:A:70:LEU:HD11	0.65	2.26	11	3
1:A:76:THR:O	1:A:78:ASN:N	0.65	2.30	10	3
1:A:21:LEU:N	1:A:21:LEU:HD23	0.65	2.07	20	1
1:A:34:PHE:CE2	1:A:55:VAL:CG2	0.64	2.81	9	15
1:A:18:LEU:CB	1:A:82:LYS:O	0.64	2.46	5	13
1:A:16:LEU:HB3	1:A:83:ILE:CG2	0.64	2.22	16	10
1:A:18:LEU:CD1	1:A:84:SER:CB	0.64	2.75	7	4
1:A:81:MET:SD	1:A:83:ILE:HD11	0.63	2.33	5	3
1:A:16:LEU:N	1:A:16:LEU:HD12	0.63	2.07	10	4
1:A:16:LEU:HD23	1:A:83:ILE:CG2	0.63	2.23	15	1
1:A:21:LEU:HD13	1:A:45:LEU:CD2	0.63	2.24	7	1
1:A:16:LEU:HD22	1:A:83:ILE:CG2	0.63	2.24	3	2
1:A:40:PHE:HZ	1:A:43:VAL:HG23	0.63	1.50	15	1
1:A:55:VAL:CG1	1:A:57:PHE:CZ	0.63	2.82	7	4
1:A:55:VAL:CG1	1:A:57:PHE:CE2	0.63	2.81	17	6
1:A:17:PHE:CG	1:A:54:PHE:CE2	0.62	2.87	13	2
1:A:21:LEU:HD12	1:A:51:ASP:C	0.62	2.14	11	1
1:A:16:LEU:CD1	1:A:57:PHE:CE1	0.62	2.82	14	2
1:A:46:VAL:H	1:A:47:PRO:CD	0.62	2.07	19	3
1:A:16:LEU:HD23	1:A:85:PHE:HA	0.62	1.70	2	1
1:A:57:PHE:CG	1:A:63:ALA:HA	0.62	2.30	4	14
1:A:18:LEU:HD12	1:A:84:SER:HB2	0.62	1.70	2	4
1:A:30:LEU:CD1	1:A:45:LEU:HD22	0.62	2.24	12	2
1:A:20:ASN:C	1:A:21:LEU:HD12	0.62	2.14	12	2
1:A:57:PHE:CZ	1:A:66:ALA:CB	0.61	2.83	13	14
1:A:15:ILE:C	1:A:16:LEU:HD12	0.61	2.16	10	1
1:A:76:THR:C	1:A:79:ASN:H	0.61	1.98	19	1
1:A:57:PHE:O	1:A:59:ASN:N	0.61	2.33	1	18

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD13	1:A:53:ALA:HB2	0.61	1.71	19	2
1:A:22:PRO:HG3	1:A:75:ILE:HG21	0.61	1.70	16	1
1:A:57:PHE:CE2	1:A:66:ALA:CB	0.61	2.83	7	11
1:A:18:LEU:CD1	1:A:84:SER:HB2	0.61	2.26	10	5
1:A:21:LEU:HD23	1:A:45:LEU:CD2	0.61	2.25	17	1
1:A:34:PHE:CE2	1:A:55:VAL:CG1	0.61	2.84	19	1
1:A:20:ASN:N	1:A:21:LEU:HD12	0.61	2.11	12	1
1:A:76:THR:CA	1:A:80:ALA:N	0.61	2.63	19	2
1:A:46:VAL:HG22	1:A:46:VAL:O	0.61	1.96	5	1
1:A:34:PHE:CD2	1:A:55:VAL:CG2	0.60	2.85	3	2
1:A:15:ILE:HB	1:A:86:ALA:HB2	0.60	1.71	15	2
1:A:16:LEU:HD12	1:A:55:VAL:O	0.60	1.95	17	2
1:A:37:PHE:CZ	1:A:66:ALA:HA	0.60	2.31	18	13
1:A:75:ILE:C	1:A:77:GLN:N	0.60	2.53	10	3
1:A:81:MET:CE	1:A:83:ILE:HD12	0.60	2.26	1	1
1:A:15:ILE:O	1:A:86:ALA:N	0.60	2.34	12	17
1:A:76:THR:OG1	1:A:80:ALA:HA	0.60	1.95	1	2
1:A:21:LEU:N	1:A:21:LEU:CD1	0.60	2.64	12	4
1:A:18:LEU:HD23	1:A:82:LYS:HB2	0.60	1.73	8	4
1:A:73:PHE:O	1:A:75:ILE:N	0.60	2.35	10	11
1:A:17:PHE:CD1	1:A:54:PHE:CD2	0.60	2.90	20	4
1:A:57:PHE:CD2	1:A:63:ALA:HA	0.60	2.32	17	14
1:A:19:THR:HG22	1:A:52:ILE:HG22	0.60	1.74	5	3
1:A:16:LEU:HD22	1:A:83:ILE:HG22	0.59	1.72	1	1
1:A:18:LEU:CD2	1:A:82:LYS:HB3	0.59	2.27	19	5
1:A:45:LEU:HD12	1:A:45:LEU:C	0.59	2.17	7	1
1:A:28:LEU:HD12	1:A:28:LEU:O	0.59	1.97	12	2
1:A:20:ASN:C	1:A:21:LEU:HD23	0.59	2.17	5	3
1:A:16:LEU:CB	1:A:83:ILE:CG2	0.59	2.80	4	6
1:A:26:ASN:C	1:A:45:LEU:HD23	0.59	2.18	16	4
1:A:16:LEU:CB	1:A:83:ILE:HG22	0.59	2.25	5	2
1:A:75:ILE:HB	1:A:80:ALA:N	0.59	2.13	10	1
1:A:18:LEU:CD2	1:A:82:LYS:CB	0.59	2.80	11	4
1:A:25:THR:HG23	1:A:46:VAL:HG22	0.59	1.72	11	1
1:A:55:VAL:CG1	1:A:57:PHE:CE1	0.59	2.86	14	2
1:A:45:LEU:O	1:A:46:VAL:HG23	0.58	1.98	11	1
1:A:30:LEU:HD22	1:A:45:LEU:CD1	0.58	2.29	9	1
1:A:70:LEU:HD11	1:A:83:ILE:HD12	0.58	1.74	2	1
1:A:30:LEU:HG	1:A:45:LEU:HD23	0.58	1.75	7	1
1:A:21:LEU:O	1:A:25:THR:HG21	0.58	1.99	18	1
1:A:13:ASN:OD1	1:A:86:ALA:HB3	0.58	1.98	6	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:VAL:HG22	1:A:50:HIS:HB3	0.58	1.75	11	1
1:A:75:ILE:HB	1:A:79:ASN:O	0.57	1.99	1	2
1:A:37:PHE:CE1	1:A:65:ALA:HB1	0.57	2.33	5	2
1:A:28:LEU:HD23	1:A:28:LEU:N	0.57	2.13	7	1
1:A:19:THR:O	1:A:20:ASN:HB2	0.57	1.99	1	12
1:A:13:ASN:HB3	1:A:85:PHE:CD1	0.57	2.34	9	1
1:A:70:LEU:CD1	1:A:73:PHE:CD2	0.57	2.88	4	1
1:A:18:LEU:HD23	1:A:82:LYS:O	0.57	1.99	11	4
1:A:22:PRO:CG	1:A:75:ILE:HG21	0.57	2.30	16	3
1:A:25:THR:HG23	1:A:46:VAL:CG2	0.57	2.30	11	1
1:A:31:SER:OG	1:A:43:VAL:HG21	0.57	2.00	16	1
1:A:75:ILE:HD12	1:A:80:ALA:N	0.57	2.15	4	1
1:A:18:LEU:HB3	1:A:82:LYS:C	0.56	2.20	16	17
1:A:76:THR:HA	1:A:80:ALA:N	0.56	2.15	19	2
1:A:19:THR:O	1:A:82:LYS:O	0.56	2.24	19	8
1:A:37:PHE:CD2	1:A:66:ALA:HB2	0.56	2.36	20	4
1:A:13:ASN:CB	1:A:85:PHE:CD1	0.56	2.88	9	1
1:A:34:PHE:CZ	1:A:70:LEU:HD11	0.56	2.36	11	2
1:A:75:ILE:HG22	1:A:79:ASN:HB2	0.56	1.76	19	1
1:A:18:LEU:HB2	1:A:83:ILE:CA	0.56	2.31	5	7
1:A:18:LEU:HD13	1:A:84:SER:CB	0.56	2.31	16	3
1:A:25:THR:HB	1:A:45:LEU:HD21	0.56	1.76	10	1
1:A:16:LEU:HD23	1:A:85:PHE:CA	0.56	2.30	2	1
1:A:42:GLU:CB	1:A:56:GLU:HB3	0.55	2.31	1	6
1:A:19:THR:O	1:A:20:ASN:CB	0.55	2.55	16	18
1:A:43:VAL:HG12	1:A:55:VAL:HG13	0.55	1.78	19	1
1:A:16:LEU:CD1	1:A:57:PHE:CD1	0.55	2.89	7	1
1:A:55:VAL:HG12	1:A:57:PHE:CD1	0.55	2.36	13	2
1:A:75:ILE:C	1:A:79:ASN:O	0.55	2.45	19	1
1:A:21:LEU:HD12	1:A:81:MET:HB2	0.55	1.77	2	2
1:A:75:ILE:O	1:A:77:GLN:N	0.55	2.40	10	1
1:A:34:PHE:CG	1:A:55:VAL:HG11	0.55	2.37	19	2
1:A:85:PHE:O	1:A:86:ALA:HB2	0.55	2.02	2	1
1:A:84:SER:O	1:A:86:ALA:N	0.55	2.40	8	2
1:A:17:PHE:CD1	1:A:18:LEU:N	0.55	2.75	13	12
1:A:57:PHE:CZ	1:A:66:ALA:HB2	0.55	2.37	6	5
1:A:50:HIS:ND1	1:A:50:HIS:N	0.55	2.54	8	1
1:A:16:LEU:CD2	1:A:85:PHE:CE1	0.55	2.90	8	2
1:A:17:PHE:O	1:A:18:LEU:CG	0.55	2.55	6	3
1:A:70:LEU:HD12	1:A:73:PHE:HB2	0.54	1.78	4	1
1:A:26:ASN:O	1:A:45:LEU:HD23	0.54	2.03	12	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:GLU:CG	1:A:46:VAL:HG23	0.54	2.30	1	1
1:A:15:ILE:CG1	1:A:56:GLU:HG3	0.54	2.33	10	4
1:A:34:PHE:CD2	1:A:55:VAL:HG23	0.54	2.37	1	1
1:A:37:PHE:CE2	1:A:66:ALA:HA	0.54	2.38	12	13
1:A:76:THR:O	1:A:77:GLN:C	0.54	2.45	1	3
1:A:21:LEU:HD23	1:A:81:MET:SD	0.53	2.43	15	1
1:A:34:PHE:CD1	1:A:55:VAL:HG11	0.53	2.38	7	3
1:A:30:LEU:HD22	1:A:45:LEU:HD13	0.53	1.79	3	2
1:A:22:PRO:CD	1:A:75:ILE:HG12	0.53	2.33	18	3
1:A:21:LEU:CD1	1:A:21:LEU:N	0.53	2.70	3	4
1:A:45:LEU:HD11	1:A:50:HIS:HA	0.53	1.80	10	1
1:A:25:THR:HG23	1:A:50:HIS:HB3	0.53	1.80	4	1
1:A:15:ILE:HD11	1:A:56:GLU:HG2	0.53	1.80	15	3
1:A:49:ARG:O	1:A:50:HIS:CG	0.53	2.61	10	3
1:A:16:LEU:CD1	1:A:63:ALA:HB1	0.53	2.34	20	3
1:A:57:PHE:HB3	1:A:63:ALA:HB2	0.53	1.80	19	3
1:A:75:ILE:HD12	1:A:80:ALA:CA	0.53	2.34	4	1
1:A:30:LEU:HB2	1:A:45:LEU:CD1	0.53	2.32	4	1
1:A:15:ILE:HD11	1:A:56:GLU:HG3	0.53	1.81	18	4
1:A:18:LEU:HB2	1:A:83:ILE:HA	0.53	1.80	5	7
1:A:60:GLU:HA	1:A:63:ALA:HB3	0.53	1.80	14	10
1:A:74:LYS:C	1:A:76:THR:N	0.53	2.57	10	3
1:A:21:LEU:HD22	1:A:30:LEU:HD21	0.53	1.81	15	1
1:A:45:LEU:C	1:A:46:VAL:HG23	0.53	2.24	11	1
1:A:45:LEU:HD11	1:A:50:HIS:C	0.53	2.24	12	1
1:A:15:ILE:CB	1:A:86:ALA:HB2	0.52	2.34	15	1
1:A:19:THR:OG1	1:A:20:ASN:N	0.52	2.42	20	8
1:A:21:LEU:N	1:A:21:LEU:HD13	0.52	2.20	3	1
1:A:44:ARG:HB3	1:A:54:PHE:CB	0.52	2.34	4	3
1:A:49:ARG:NE	1:A:49:ARG:HA	0.52	2.16	7	2
1:A:18:LEU:HG	1:A:84:SER:CB	0.52	2.34	5	3
1:A:70:LEU:HD12	1:A:81:MET:SD	0.52	2.45	16	2
1:A:26:ASN:OD1	1:A:28:LEU:N	0.52	2.42	7	12
1:A:46:VAL:HG12	1:A:46:VAL:O	0.52	2.05	11	1
1:A:17:PHE:HB2	1:A:54:PHE:CZ	0.52	2.40	13	1
1:A:25:THR:CG2	1:A:50:HIS:HB2	0.52	2.34	7	1
1:A:45:LEU:CD1	1:A:50:HIS:HA	0.52	2.35	8	2
1:A:17:PHE:O	1:A:18:LEU:HB2	0.52	2.03	3	11
1:A:49:ARG:HD3	1:A:52:ILE:HG23	0.51	1.82	15	2
1:A:15:ILE:CD1	1:A:56:GLU:HG2	0.51	2.35	11	1
1:A:26:ASN:C	1:A:45:LEU:HD12	0.51	2.24	17	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:ILE:O	1:A:78:ASN:C	0.51	2.49	19	1
1:A:21:LEU:HD13	1:A:45:LEU:CD1	0.51	2.36	11	1
1:A:46:VAL:O	1:A:46:VAL:HG12	0.51	2.05	16	1
1:A:37:PHE:CE1	1:A:66:ALA:HA	0.51	2.40	13	1
1:A:15:ILE:CG1	1:A:56:GLU:CG	0.51	2.89	10	1
1:A:30:LEU:HB2	1:A:45:LEU:HD22	0.51	1.83	2	1
1:A:70:LEU:HD13	1:A:81:MET:CE	0.51	2.34	2	1
1:A:57:PHE:CB	1:A:63:ALA:HA	0.51	2.36	4	1
1:A:59:ASN:ND2	1:A:62:GLN:NE2	0.51	2.59	12	1
1:A:67:ARG:NH1	1:A:85:PHE:CZ	0.51	2.78	16	2
1:A:34:PHE:CD2	1:A:55:VAL:HG13	0.51	2.41	14	1
1:A:22:PRO:HD2	1:A:25:THR:HG21	0.51	1.81	3	1
1:A:55:VAL:HG11	1:A:57:PHE:CZ	0.51	2.41	20	5
1:A:18:LEU:HG	1:A:19:THR:H	0.51	1.66	4	7
1:A:76:THR:H	1:A:79:ASN:C	0.51	2.04	10	1
1:A:39:GLY:HA3	1:A:62:GLN:NE2	0.51	2.21	6	1
1:A:40:PHE:CD1	1:A:41:LYS:N	0.51	2.78	15	1
1:A:21:LEU:HB2	1:A:22:PRO:HD3	0.51	1.83	4	1
1:A:22:PRO:HD2	1:A:75:ILE:HD13	0.51	1.83	11	1
1:A:28:LEU:O	1:A:28:LEU:HD12	0.51	2.05	3	1
1:A:76:THR:HA	1:A:79:ASN:O	0.51	1.93	10	1
1:A:76:THR:OG1	1:A:80:ALA:N	0.50	2.44	1	1
1:A:37:PHE:CE2	1:A:66:ALA:HB2	0.50	2.41	14	1
1:A:28:LEU:HA	1:A:31:SER:HB3	0.50	1.82	11	7
1:A:34:PHE:CZ	1:A:55:VAL:HG11	0.50	2.40	19	1
1:A:37:PHE:CE1	1:A:65:ALA:CB	0.50	2.95	5	5
1:A:45:LEU:HD11	1:A:50:HIS:O	0.50	2.05	12	1
1:A:14:HIS:CD2	1:A:14:HIS:C	0.50	2.84	6	1
1:A:15:ILE:HG12	1:A:56:GLU:CG	0.50	2.36	10	3
1:A:16:LEU:CD2	1:A:67:ARG:HG2	0.50	2.36	18	1
1:A:22:PRO:CD	1:A:75:ILE:HG21	0.50	2.36	16	2
1:A:17:PHE:O	1:A:18:LEU:HG	0.50	2.06	6	8
1:A:37:PHE:N	1:A:37:PHE:CD2	0.50	2.79	18	3
1:A:21:LEU:CD2	1:A:53:ALA:HB2	0.50	2.35	12	4
1:A:18:LEU:CD1	1:A:84:SER:HB3	0.50	2.37	7	1
1:A:46:VAL:HG13	1:A:46:VAL:O	0.50	2.07	19	1
1:A:16:LEU:CD2	1:A:83:ILE:CG2	0.50	2.89	3	1
1:A:45:LEU:HG	1:A:46:VAL:HG23	0.50	1.82	11	1
1:A:49:ARG:HD3	1:A:52:ILE:CG1	0.50	2.36	11	1
1:A:21:LEU:CB	1:A:22:PRO:HD3	0.50	2.36	4	1
1:A:34:PHE:CD1	1:A:57:PHE:CZ	0.50	3.00	14	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:N	1:A:21:LEU:CD2	0.50	2.72	20	2
1:A:67:ARG:CZ	1:A:83:ILE:HD13	0.49	2.37	5	1
1:A:21:LEU:HD23	1:A:45:LEU:HD21	0.49	1.84	17	1
1:A:34:PHE:CG	1:A:55:VAL:HG21	0.49	2.42	3	1
1:A:67:ARG:NH2	1:A:83:ILE:HD13	0.49	2.22	5	1
1:A:16:LEU:HD12	1:A:16:LEU:H	0.49	1.66	17	1
1:A:30:LEU:HD22	1:A:45:LEU:HG	0.49	1.84	17	1
1:A:16:LEU:HD22	1:A:67:ARG:HG3	0.49	1.82	13	1
1:A:13:ASN:HD21	1:A:86:ALA:HB3	0.49	1.67	3	1
1:A:20:ASN:HD21	1:A:75:ILE:HD11	0.49	1.65	4	1
1:A:37:PHE:CE2	1:A:66:ALA:CB	0.49	2.96	20	1
1:A:13:ASN:O	1:A:14:HIS:ND1	0.49	2.46	17	1
1:A:67:ARG:O	1:A:71:GLN:N	0.49	2.45	4	9
1:A:57:PHE:CD1	1:A:62:GLN:HG3	0.49	2.43	17	1
1:A:67:ARG:HH21	1:A:83:ILE:HG21	0.49	1.63	5	1
1:A:16:LEU:CD1	1:A:16:LEU:N	0.49	2.76	10	1
1:A:21:LEU:CD1	1:A:45:LEU:HD13	0.49	2.38	10	1
1:A:18:LEU:HG	1:A:19:THR:HG23	0.49	1.85	4	1
1:A:46:VAL:HG12	1:A:47:PRO:HD3	0.49	1.85	2	1
1:A:46:VAL:O	1:A:48:GLY:N	0.48	2.46	16	3
1:A:73:PHE:CE2	1:A:75:ILE:HG13	0.48	2.42	9	1
1:A:16:LEU:HD12	1:A:16:LEU:N	0.48	2.23	17	1
1:A:21:LEU:CB	1:A:22:PRO:CD	0.48	2.91	7	1
1:A:13:ASN:O	1:A:14:HIS:CG	0.48	2.67	9	6
1:A:44:ARG:CB	1:A:54:PHE:HB3	0.48	2.38	4	4
1:A:44:ARG:HE	1:A:45:LEU:N	0.48	2.06	9	1
1:A:17:PHE:HB2	1:A:54:PHE:CE2	0.48	2.43	15	4
1:A:17:PHE:HB2	1:A:54:PHE:CE1	0.48	2.44	13	4
1:A:30:LEU:HG	1:A:45:LEU:HD22	0.48	1.85	14	1
1:A:41:LYS:CD	1:A:41:LYS:C	0.48	2.80	17	1
1:A:22:PRO:HD3	1:A:75:ILE:HD11	0.48	1.86	8	1
1:A:37:PHE:CD1	1:A:66:ALA:HB2	0.48	2.43	13	1
1:A:76:THR:O	1:A:77:GLN:CB	0.48	2.60	2	9
1:A:18:LEU:HG	1:A:84:SER:HB2	0.48	1.83	5	2
1:A:16:LEU:CB	1:A:83:ILE:HG23	0.48	2.38	11	1
1:A:81:MET:HE3	1:A:83:ILE:HD12	0.48	1.85	1	1
1:A:16:LEU:CD2	1:A:83:ILE:HG22	0.48	2.38	1	1
1:A:37:PHE:CD1	1:A:37:PHE:N	0.48	2.76	20	1
1:A:18:LEU:HB3	1:A:83:ILE:CA	0.48	2.38	12	6
1:A:40:PHE:HE1	1:A:43:VAL:HG13	0.48	1.68	3	1
1:A:57:PHE:CB	1:A:63:ALA:CB	0.48	2.92	4	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:PRO:HD2	1:A:75:ILE:HG13	0.48	1.85	1	1
1:A:81:MET:SD	1:A:83:ILE:HD12	0.48	2.49	4	3
1:A:49:ARG:C	1:A:51:ASP:N	0.48	2.66	14	5
1:A:30:LEU:HD23	1:A:34:PHE:HE2	0.48	1.67	17	1
1:A:45:LEU:C	1:A:45:LEU:HD13	0.48	2.29	17	3
1:A:67:ARG:CZ	1:A:85:PHE:CE2	0.48	2.97	13	1
1:A:16:LEU:H	1:A:16:LEU:HD12	0.48	1.67	6	1
1:A:39:GLY:CA	1:A:62:GLN:NE2	0.48	2.77	10	3
1:A:67:ARG:NE	1:A:67:ARG:HA	0.48	2.23	5	1
1:A:17:PHE:HB2	1:A:54:PHE:CD2	0.47	2.44	18	4
1:A:42:GLU:HB3	1:A:56:GLU:CB	0.47	2.40	1	1
1:A:70:LEU:CD1	1:A:83:ILE:CD1	0.47	2.92	14	1
1:A:75:ILE:HB	1:A:80:ALA:H	0.47	1.69	10	1
1:A:49:ARG:C	1:A:50:HIS:CD2	0.47	2.87	11	1
1:A:18:LEU:HB2	1:A:84:SER:N	0.47	2.23	16	7
1:A:21:LEU:HD12	1:A:45:LEU:HD21	0.47	1.85	13	2
1:A:80:ALA:O	1:A:81:MET:C	0.47	2.53	4	1
1:A:75:ILE:C	1:A:79:ASN:N	0.47	2.68	10	1
1:A:30:LEU:HD12	1:A:45:LEU:HD13	0.47	1.85	2	1
1:A:15:ILE:HG22	1:A:86:ALA:CB	0.47	2.38	16	1
1:A:66:ALA:O	1:A:70:LEU:HD23	0.47	2.10	6	1
1:A:49:ARG:HD3	1:A:52:ILE:CG2	0.47	2.40	15	1
1:A:67:ARG:NH2	1:A:71:GLN:NE2	0.47	2.63	18	1
1:A:47:PRO:HA	1:A:50:HIS:CD2	0.47	2.45	18	3
1:A:49:ARG:C	1:A:50:HIS:CG	0.47	2.87	11	2
1:A:55:VAL:HG12	1:A:57:PHE:CD2	0.47	2.44	4	1
1:A:25:THR:CG2	1:A:50:HIS:HB3	0.47	2.40	4	1
1:A:42:GLU:CB	1:A:56:GLU:CB	0.47	2.93	1	1
1:A:21:LEU:HD21	1:A:53:ALA:CB	0.47	2.40	15	1
1:A:57:PHE:CE2	1:A:66:ALA:HB3	0.47	2.44	19	3
1:A:19:THR:CB	1:A:51:ASP:O	0.46	2.63	15	2
1:A:41:LYS:HG3	1:A:42:GLU:N	0.46	2.24	10	2
1:A:55:VAL:HG12	1:A:57:PHE:CE2	0.46	2.44	18	2
1:A:18:LEU:CG	1:A:19:THR:H	0.46	2.23	19	4
1:A:75:ILE:O	1:A:79:ASN:N	0.46	2.48	19	1
1:A:22:PRO:CD	1:A:75:ILE:HD12	0.46	2.39	10	1
1:A:75:ILE:CB	1:A:79:ASN:O	0.46	2.63	19	2
1:A:76:THR:N	1:A:79:ASN:N	0.46	2.64	10	1
1:A:34:PHE:CD1	1:A:57:PHE:CE2	0.46	3.03	11	4
1:A:21:LEU:HB3	1:A:22:PRO:HD2	0.46	1.88	7	1
1:A:30:LEU:HD22	1:A:45:LEU:HB2	0.46	1.86	16	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:CD1	1:A:53:ALA:CB	0.46	2.88	1	1
1:A:13:ASN:ND2	1:A:86:ALA:C	0.46	2.69	6	2
1:A:54:PHE:CD1	1:A:54:PHE:C	0.46	2.87	6	1
1:A:37:PHE:CD2	1:A:37:PHE:N	0.46	2.83	6	2
1:A:46:VAL:HB	1:A:47:PRO:CD	0.46	2.41	12	1
1:A:13:ASN:C	1:A:14:HIS:CG	0.46	2.87	9	2
1:A:13:ASN:C	1:A:14:HIS:CD2	0.46	2.89	13	1
1:A:16:LEU:HB2	1:A:83:ILE:CG2	0.46	2.40	4	1
1:A:17:PHE:CB	1:A:54:PHE:CZ	0.46	2.99	13	1
1:A:37:PHE:HB2	1:A:57:PHE:CE1	0.46	2.46	4	2
1:A:17:PHE:O	1:A:18:LEU:HD23	0.46	2.11	1	1
1:A:30:LEU:O	1:A:34:PHE:CD2	0.46	2.69	5	7
1:A:55:VAL:HG12	1:A:57:PHE:CZ	0.46	2.46	10	3
1:A:30:LEU:HD23	1:A:30:LEU:N	0.46	2.24	8	1
1:A:32:MET:HA	1:A:35:ASN:HB3	0.45	1.87	20	5
1:A:67:ARG:HG3	1:A:85:PHE:CZ	0.45	2.47	20	1
1:A:27:GLU:HG2	1:A:46:VAL:CG2	0.45	2.41	5	1
1:A:13:ASN:CB	1:A:85:PHE:HB3	0.45	2.41	3	1
1:A:21:LEU:H	1:A:21:LEU:HD12	0.45	1.71	16	1
1:A:28:LEU:HA	1:A:31:SER:CB	0.45	2.41	2	1
1:A:40:PHE:CD1	1:A:40:PHE:C	0.45	2.87	20	1
1:A:70:LEU:CD1	1:A:73:PHE:HB2	0.45	2.42	4	1
1:A:26:ASN:ND2	1:A:29:MET:HB2	0.45	2.26	15	2
1:A:17:PHE:CB	1:A:54:PHE:CE2	0.45	3.00	13	1
1:A:43:VAL:HG23	1:A:43:VAL:O	0.45	2.10	7	2
1:A:37:PHE:HB2	1:A:57:PHE:CZ	0.45	2.46	19	1
1:A:49:ARG:HD2	1:A:52:ILE:HG12	0.45	1.89	5	1
1:A:20:ASN:O	1:A:75:ILE:CG1	0.45	2.65	10	1
1:A:21:LEU:HB3	1:A:22:PRO:CD	0.45	2.41	7	1
1:A:85:PHE:O	1:A:86:ALA:HB3	0.45	2.12	4	1
1:A:67:ARG:NE	1:A:71:GLN:CG	0.45	2.80	14	1
1:A:81:MET:HG3	1:A:82:LYS:N	0.45	2.27	10	2
1:A:42:GLU:HB3	1:A:56:GLU:HB3	0.45	1.88	16	1
1:A:17:PHE:HB2	1:A:54:PHE:CD1	0.45	2.47	14	4
1:A:18:LEU:HB3	1:A:83:ILE:HA	0.45	1.89	4	2
1:A:18:LEU:HG	1:A:82:LYS:O	0.45	2.12	12	1
1:A:43:VAL:O	1:A:43:VAL:HG23	0.45	2.12	1	1
1:A:35:ASN:C	1:A:37:PHE:N	0.45	2.69	10	1
1:A:18:LEU:HG	1:A:84:SER:HB3	0.45	1.88	7	2
1:A:25:THR:HG23	1:A:50:HIS:HB2	0.45	1.89	7	1
1:A:37:PHE:CE1	1:A:65:ALA:HB3	0.45	2.47	2	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:GLU:O	1:A:31:SER:CB	0.45	2.65	7	3
1:A:34:PHE:CE1	1:A:55:VAL:HG21	0.45	2.47	3	1
1:A:67:ARG:CZ	1:A:71:GLN:NE2	0.45	2.80	18	1
1:A:22:PRO:CD	1:A:75:ILE:HD13	0.45	2.42	4	1
1:A:59:ASN:OD1	1:A:61:VAL:N	0.45	2.50	11	1
1:A:74:LYS:N	1:A:74:LYS:CD	0.45	2.80	2	1
1:A:37:PHE:CE1	1:A:66:ALA:CA	0.44	3.00	13	1
1:A:45:LEU:HD13	1:A:45:LEU:C	0.44	2.32	20	1
1:A:73:PHE:HB2	1:A:81:MET:HE3	0.44	1.88	2	1
1:A:16:LEU:HB2	1:A:55:VAL:HG12	0.44	1.89	1	1
1:A:49:ARG:CD	1:A:52:ILE:HG12	0.44	2.42	5	1
1:A:20:ASN:O	1:A:21:LEU:HB2	0.44	2.13	4	1
1:A:14:HIS:ND1	1:A:57:PHE:O	0.44	2.50	6	1
1:A:16:LEU:HA	1:A:85:PHE:HA	0.44	1.87	13	2
1:A:74:LYS:O	1:A:75:ILE:C	0.44	2.53	10	1
1:A:72:GLY:O	1:A:74:LYS:N	0.44	2.51	6	9
1:A:25:THR:HG22	1:A:30:LEU:HD13	0.44	1.90	17	1
1:A:74:LYS:HA	1:A:80:ALA:HA	0.44	1.87	2	1
1:A:28:LEU:HD12	1:A:28:LEU:C	0.44	2.33	12	1
1:A:42:GLU:HB2	1:A:56:GLU:HB3	0.44	1.90	1	3
1:A:13:ASN:HB3	1:A:85:PHE:HB3	0.44	1.90	3	1
1:A:48:GLY:O	1:A:49:ARG:HG2	0.44	2.13	8	1
1:A:18:LEU:CG	1:A:84:SER:HB3	0.44	2.43	7	1
1:A:15:ILE:O	1:A:85:PHE:HA	0.44	2.13	1	1
1:A:37:PHE:CE2	1:A:66:ALA:CA	0.44	3.01	2	2
1:A:62:GLN:HG2	1:A:63:ALA:N	0.44	2.26	14	1
1:A:22:PRO:CG	1:A:75:ILE:HG12	0.44	2.43	3	2
1:A:45:LEU:HD23	1:A:53:ALA:HA	0.44	1.90	4	1
1:A:67:ARG:NH1	1:A:85:PHE:CE2	0.44	2.86	13	2
1:A:79:ASN:O	1:A:80:ALA:HB2	0.44	2.13	10	1
1:A:45:LEU:O	1:A:46:VAL:CG2	0.44	2.66	11	1
1:A:67:ARG:CD	1:A:67:ARG:C	0.44	2.87	7	1
1:A:22:PRO:HD3	1:A:75:ILE:HG21	0.44	1.90	19	1
1:A:15:ILE:HG22	1:A:15:ILE:O	0.44	2.13	2	1
1:A:49:ARG:HD3	1:A:52:ILE:HG13	0.43	1.90	11	1
1:A:34:PHE:HB2	1:A:43:VAL:HG21	0.43	1.90	15	1
1:A:47:PRO:HA	1:A:50:HIS:CE1	0.43	2.49	15	2
1:A:27:GLU:HG2	1:A:46:VAL:HG21	0.43	1.88	19	1
1:A:67:ARG:CD	1:A:71:GLN:HG3	0.43	2.44	2	1
1:A:49:ARG:HD3	1:A:52:ILE:HG12	0.43	1.90	17	1
1:A:78:ASN:O	1:A:79:ASN:CB	0.43	2.66	19	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LYS:CB	1:A:56:GLU:O	0.43	2.66	3	4
1:A:39:GLY:O	1:A:58:ASP:N	0.43	2.52	20	1
1:A:16:LEU:HD22	1:A:67:ARG:HG2	0.43	1.91	18	1
1:A:73:PHE:CB	1:A:81:MET:CE	0.43	2.97	2	1
1:A:84:SER:O	1:A:85:PHE:C	0.43	2.57	2	1
1:A:37:PHE:CZ	1:A:66:ALA:CA	0.43	3.02	15	3
1:A:39:GLY:O	1:A:40:PHE:C	0.43	2.56	17	4
1:A:75:ILE:C	1:A:77:GLN:H	0.43	2.14	10	1
1:A:57:PHE:CB	1:A:63:ALA:CA	0.43	2.97	4	1
1:A:37:PHE:CD1	1:A:65:ALA:CB	0.43	3.01	4	1
1:A:35:ASN:O	1:A:37:PHE:N	0.43	2.52	9	8
1:A:15:ILE:O	1:A:15:ILE:HG22	0.43	2.13	4	2
1:A:57:PHE:CE2	1:A:66:ALA:HB2	0.43	2.48	13	2
1:A:47:PRO:C	1:A:49:ARG:N	0.43	2.71	2	1
1:A:20:ASN:N	1:A:21:LEU:CD1	0.43	2.81	12	1
1:A:49:ARG:O	1:A:50:HIS:CD2	0.43	2.71	6	1
1:A:79:ASN:N	1:A:79:ASN:ND2	0.43	2.67	20	1
1:A:70:LEU:CD1	1:A:83:ILE:HD12	0.43	2.42	2	1
1:A:18:LEU:HD23	1:A:82:LYS:C	0.43	2.34	20	1
1:A:16:LEU:HD12	1:A:57:PHE:CD1	0.43	2.48	14	1
1:A:49:ARG:O	1:A:50:HIS:ND1	0.43	2.51	14	1
1:A:19:THR:HB	1:A:51:ASP:O	0.43	2.13	14	3
1:A:21:LEU:HB2	1:A:25:THR:HG21	0.43	1.89	13	1
1:A:41:LYS:C	1:A:41:LYS:CD	0.43	2.87	20	1
1:A:30:LEU:HB2	1:A:45:LEU:HD23	0.43	1.91	11	1
1:A:39:GLY:O	1:A:41:LYS:N	0.43	2.52	19	1
1:A:21:LEU:CD2	1:A:81:MET:SD	0.42	3.07	20	1
1:A:24:GLU:O	1:A:26:ASN:N	0.42	2.52	4	1
1:A:21:LEU:HA	1:A:75:ILE:CD1	0.42	2.44	12	1
1:A:18:LEU:HD23	1:A:18:LEU:HA	0.42	1.74	2	2
1:A:18:LEU:HD22	1:A:84:SER:HB3	0.42	1.90	15	1
1:A:32:MET:HA	1:A:35:ASN:HB2	0.42	1.92	13	1
1:A:46:VAL:O	1:A:46:VAL:HG13	0.42	2.15	14	1
1:A:34:PHE:CD1	1:A:55:VAL:HG21	0.42	2.49	3	1
1:A:67:ARG:NE	1:A:67:ARG:CA	0.42	2.82	5	1
1:A:57:PHE:HB2	1:A:63:ALA:CB	0.42	2.44	4	1
1:A:13:ASN:O	1:A:14:HIS:CB	0.42	2.67	6	1
1:A:13:ASN:HB3	1:A:85:PHE:CB	0.42	2.45	5	1
1:A:21:LEU:HD23	1:A:45:LEU:HD23	0.42	1.90	17	1
1:A:15:ILE:HD13	1:A:55:VAL:O	0.42	2.15	3	1
1:A:51:ASP:OD1	1:A:52:ILE:HG23	0.42	2.13	3	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:ILE:CD1	1:A:56:GLU:HG3	0.42	2.44	10	1
1:A:30:LEU:CD2	1:A:45:LEU:HD22	0.42	2.40	11	1
1:A:44:ARG:HB2	1:A:54:PHE:HB3	0.42	1.91	4	1
1:A:37:PHE:HA	1:A:38:PRO:HD2	0.42	1.75	8	4
1:A:27:GLU:N	1:A:45:LEU:HD12	0.42	2.29	18	1
1:A:13:ASN:ND2	1:A:86:ALA:O	0.42	2.53	19	1
1:A:15:ILE:CG2	1:A:86:ALA:CB	0.42	2.98	16	1
1:A:34:PHE:CE1	1:A:55:VAL:HG11	0.42	2.49	15	1
1:A:47:PRO:O	1:A:50:HIS:ND1	0.42	2.53	16	1
1:A:44:ARG:CB	1:A:54:PHE:CB	0.42	2.97	4	1
1:A:34:PHE:CG	1:A:55:VAL:CG1	0.42	3.03	14	2
1:A:74:LYS:N	1:A:74:LYS:HD2	0.42	2.30	14	1
1:A:81:MET:HG2	1:A:82:LYS:N	0.42	2.28	6	1
1:A:13:ASN:OD1	1:A:14:HIS:N	0.42	2.52	1	1
1:A:46:VAL:N	1:A:47:PRO:CD	0.41	2.82	2	2
1:A:21:LEU:HD22	1:A:53:ALA:HB2	0.41	1.91	12	1
1:A:40:PHE:CE1	1:A:43:VAL:HG23	0.41	2.49	15	1
1:A:60:GLU:OE2	1:A:61:VAL:HG23	0.41	2.13	7	2
1:A:37:PHE:CD2	1:A:66:ALA:CB	0.41	3.03	20	1
1:A:20:ASN:O	1:A:20:ASN:ND2	0.41	2.54	3	2
1:A:46:VAL:N	1:A:47:PRO:HD3	0.41	2.29	5	1
1:A:76:THR:HA	1:A:79:ASN:HA	0.41	1.83	10	1
1:A:67:ARG:HG3	1:A:85:PHE:CE2	0.41	2.51	18	1
1:A:73:PHE:HB3	1:A:81:MET:HB2	0.41	1.91	4	1
1:A:75:ILE:N	1:A:79:ASN:O	0.41	2.52	15	1
1:A:73:PHE:HB3	1:A:81:MET:HB3	0.41	1.92	3	1
1:A:21:LEU:HD22	1:A:81:MET:SD	0.41	2.55	5	1
1:A:46:VAL:O	1:A:46:VAL:CG2	0.41	2.65	5	1
1:A:39:GLY:N	1:A:62:GLN:NE2	0.41	2.67	10	1
1:A:22:PRO:HD2	1:A:75:ILE:CG1	0.41	2.45	18	1
1:A:67:ARG:C	1:A:67:ARG:HD2	0.41	2.36	11	1
1:A:30:LEU:HD22	1:A:45:LEU:CG	0.41	2.45	17	1
1:A:45:LEU:CD1	1:A:45:LEU:C	0.41	2.89	1	2
1:A:17:PHE:CG	1:A:54:PHE:CD2	0.41	3.08	4	1
1:A:21:LEU:HD23	1:A:21:LEU:N	0.41	2.30	5	1
1:A:16:LEU:HD22	1:A:67:ARG:HB2	0.41	1.92	11	1
1:A:27:GLU:N	1:A:27:GLU:OE1	0.41	2.54	16	1
1:A:22:PRO:CD	1:A:75:ILE:HG13	0.41	2.46	1	1
1:A:18:LEU:HA	1:A:18:LEU:HD22	0.41	1.80	1	1
1:A:44:ARG:HB3	1:A:54:PHE:HB3	0.41	1.91	5	1
1:A:22:PRO:HG3	1:A:75:ILE:CG2	0.41	2.41	16	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:LEU:HD12	1:A:18:LEU:HA	0.41	1.85	15	1
1:A:35:ASN:O	1:A:35:ASN:ND2	0.41	2.54	14	1
1:A:40:PHE:CG	1:A:40:PHE:O	0.41	2.74	5	1
1:A:70:LEU:O	1:A:72:GLY:N	0.41	2.54	2	1
1:A:45:LEU:HD13	1:A:50:HIS:HA	0.41	1.92	8	1
1:A:76:THR:O	1:A:76:THR:CG2	0.41	2.60	1	1
1:A:55:VAL:O	1:A:55:VAL:CG1	0.41	2.69	1	1
1:A:14:HIS:HB2	1:A:57:PHE:O	0.41	2.16	14	1
1:A:13:ASN:ND2	1:A:13:ASN:H	0.41	2.13	11	1
1:A:74:LYS:HD2	1:A:74:LYS:N	0.41	2.30	2	1
1:A:45:LEU:CD2	1:A:53:ALA:HA	0.41	2.46	4	1
1:A:19:THR:N	1:A:82:LYS:O	0.41	2.54	9	5
1:A:15:ILE:HG12	1:A:56:GLU:HG3	0.41	1.93	15	1
1:A:21:LEU:CD1	1:A:45:LEU:HD21	0.41	2.45	13	1
1:A:27:GLU:HG2	1:A:46:VAL:CB	0.41	2.46	5	1
1:A:70:LEU:N	1:A:70:LEU:HD23	0.41	2.31	10	1
1:A:27:GLU:OE2	1:A:43:VAL:HG12	0.41	2.15	11	1
1:A:46:VAL:O	1:A:50:HIS:N	0.41	2.53	9	1
1:A:42:GLU:HB2	1:A:56:GLU:CB	0.41	2.46	9	1
1:A:16:LEU:N	1:A:16:LEU:CD1	0.41	2.84	4	1
1:A:19:THR:OG1	1:A:21:LEU:HD21	0.41	2.16	4	1
1:A:34:PHE:CZ	1:A:55:VAL:CG2	0.41	3.00	8	1
1:A:30:LEU:CD2	1:A:30:LEU:N	0.41	2.84	8	1
1:A:32:MET:SD	1:A:32:MET:N	0.41	2.93	12	1
1:A:14:HIS:CG	1:A:14:HIS:O	0.41	2.73	14	1
1:A:34:PHE:HB2	1:A:43:VAL:HG11	0.40	1.92	3	1
1:A:47:PRO:HA	1:A:50:HIS:CG	0.40	2.50	7	1
1:A:32:MET:HA	1:A:35:ASN:CB	0.40	2.46	17	1
1:A:13:ASN:O	1:A:14:HIS:CD2	0.40	2.75	2	1
1:A:47:PRO:O	1:A:50:HIS:NE2	0.40	2.53	4	1
1:A:57:PHE:O	1:A:58:ASP:C	0.40	2.59	1	2
1:A:55:VAL:O	1:A:55:VAL:HG12	0.40	2.16	3	1
1:A:73:PHE:HB3	1:A:81:MET:CB	0.40	2.46	10	1
1:A:30:LEU:HD23	1:A:34:PHE:CZ	0.40	2.51	11	1
1:A:42:GLU:HB2	1:A:56:GLU:HB2	0.40	1.93	11	1
1:A:76:THR:N	1:A:79:ASN:CA	0.40	2.80	10	1
1:A:28:LEU:CA	1:A:31:SER:HB3	0.40	2.47	18	1
1:A:25:THR:HG23	1:A:50:HIS:CB	0.40	2.45	7	1
1:A:20:ASN:HB3	1:A:81:MET:HA	0.40	1.91	14	1
1:A:22:PRO:HD2	1:A:75:ILE:HG12	0.40	1.93	18	1
1:A:45:LEU:O	1:A:46:VAL:CB	0.40	2.70	11	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:LEU:CG	1:A:45:LEU:HD23	0.40	2.44	7	1
1:A:73:PHE:HB2	1:A:81:MET:CE	0.40	2.46	2	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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	74/88 (84%)	53±3 (71±4%)	10±3 (14±3%)	11±2 (15±3%)	<b>1</b>	<b>5</b>
All	All	1480/1760 (84%)	1057 (71%)	202 (14%)	221 (15%)	<b>1</b>	<b>5</b>

All 27 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	58	ASP	20
1	A	20	ASN	19
1	A	77	GLN	18
1	A	36	GLN	18
1	A	22	PRO	17
1	A	40	PHE	15
1	A	74	LYS	15
1	A	47	PRO	14
1	A	85	PHE	12
1	A	73	PHE	12
1	A	14	HIS	8
1	A	49	ARG	7
1	A	72	GLY	7
1	A	46	VAL	6
1	A	23	GLU	6
1	A	13	ASN	4
1	A	86	ALA	4
1	A	81	MET	3
1	A	18	LEU	3
1	A	38	PRO	3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	71	GLN	3
1	A	76	THR	2
1	A	21	LEU	1
1	A	80	ALA	1
1	A	25	THR	1
1	A	79	ASN	1
1	A	78	ASN	1

### 6.3.2 Protein sidechains [i](#)

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	63/75 (84%)	40±4 (64±6%)	23±4 (36±6%)	1	9
All	All	1260/1500 (84%)	809 (64%)	451 (36%)	1	9

All 58 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	70	LEU	19
1	A	67	ARG	19
1	A	74	LYS	18
1	A	21	LEU	17
1	A	41	LYS	15
1	A	71	GLN	15
1	A	54	PHE	14
1	A	29	MET	14
1	A	44	ARG	12
1	A	19	THR	12
1	A	28	LEU	12
1	A	16	LEU	12
1	A	81	MET	11
1	A	27	GLU	11
1	A	60	GLU	11
1	A	14	HIS	11
1	A	18	LEU	10
1	A	77	GLN	10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	85	PHE	9
1	A	26	ASN	9
1	A	30	LEU	9
1	A	59	ASN	9
1	A	73	PHE	9
1	A	62	GLN	8
1	A	32	MET	8
1	A	49	ARG	8
1	A	82	LYS	8
1	A	50	HIS	8
1	A	42	GLU	8
1	A	22	PRO	7
1	A	51	ASP	7
1	A	25	THR	7
1	A	78	ASN	7
1	A	47	PRO	7
1	A	15	ILE	7
1	A	20	ASN	5
1	A	45	LEU	5
1	A	40	PHE	5
1	A	46	VAL	5
1	A	84	SER	5
1	A	23	GLU	5
1	A	68	ASP	5
1	A	58	ASP	4
1	A	13	ASN	4
1	A	35	ASN	3
1	A	75	ILE	3
1	A	17	PHE	3
1	A	57	PHE	3
1	A	36	GLN	3
1	A	83	ILE	2
1	A	56	GLU	2
1	A	43	VAL	2
1	A	52	ILE	2
1	A	24	GLU	2
1	A	79	ASN	2
1	A	55	VAL	1
1	A	76	THR	1
1	A	31	SER	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

No chemical shift data were provided