



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:35 PM BST

PDB ID : 1L3X  
Title : Solution Structure of Novel Disintegrin Salmosin  
Authors : Shin, J.; Lee, W.  
Deposited on : 2002-03-01

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

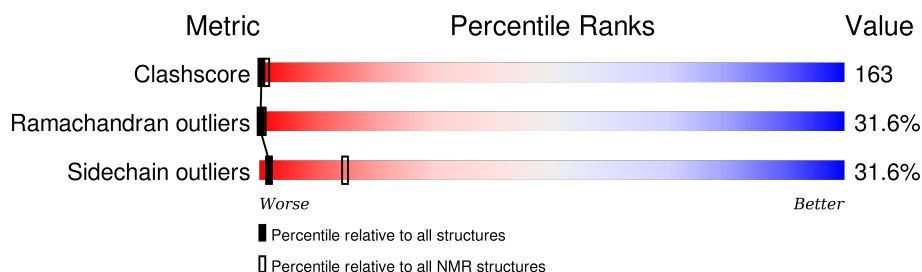
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 43%.

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	73	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 18 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:4-A:49, A:56-A:73 (64)	0.49	18

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 5 single-model clusters were found.

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

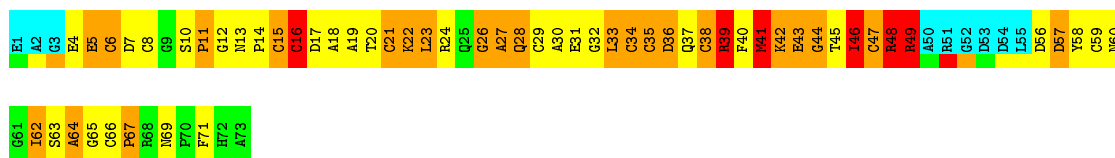
### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1003 atoms, of which 472 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called platelet aggregation inhibitor disintegrin.

Mol	Chain	Residues	Atoms						Trace
1	A	73	Total	C	H	N	O	S	0
			1003	308	472	101	109	13	

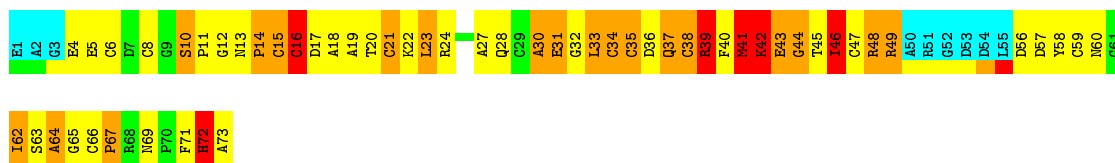




#### 4.2.3 Score per residue for model 3

- Molecule 1: platelet aggregation inhibitor disintegrin

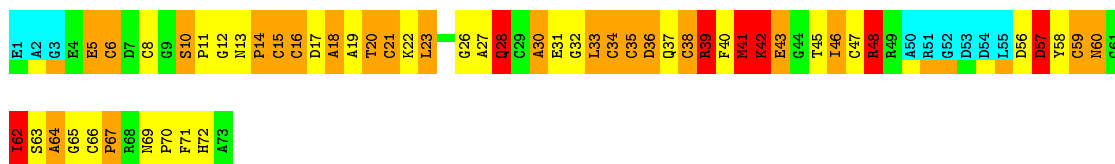
Chain A: 11% 42% 26% 8% 12%



#### 4.2.4 Score per residue for model 4

- Molecule 1: platelet aggregation inhibitor disintegrin

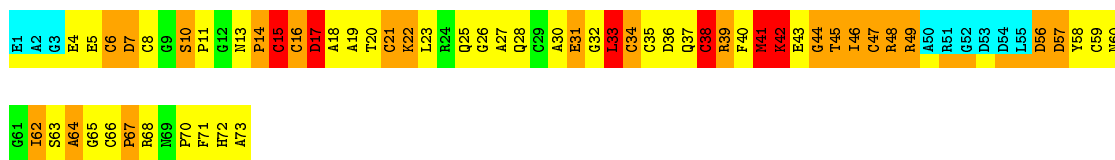
Chain A: 15% 33% 30% 10% 12%



#### 4.2.5 Score per residue for model 5

- Molecule 1: platelet aggregation inhibitor disintegrin

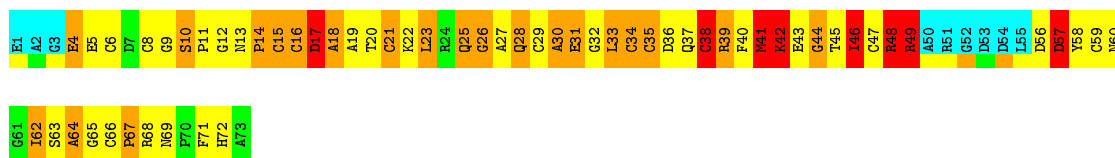
Chain A: 8% 42% 29% 8% 12%



#### 4.2.6 Score per residue for model 6

- Molecule 1: platelet aggregation inhibitor disintegrin

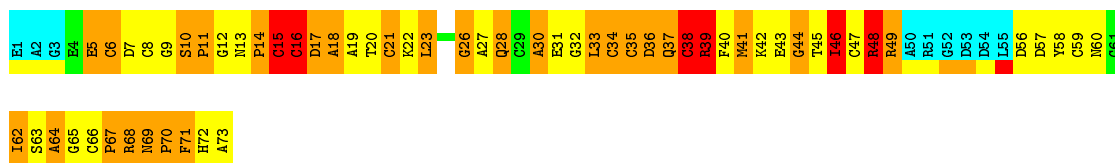
Chain A: 7% 41% 29% 11% 12%



#### 4.2.7 Score per residue for model 7

- Molecule 1: platelet aggregation inhibitor disintegrin

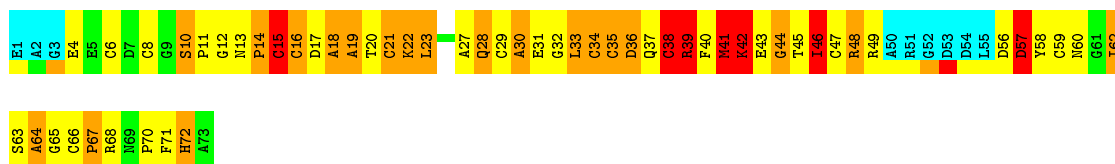
Chain A: 7% 36% 37% 8% 12%



#### 4.2.8 Score per residue for model 8

- Molecule 1: platelet aggregation inhibitor disintegrin

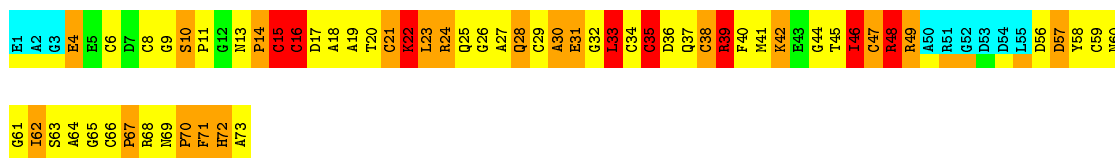
Chain A: 12% 38% 27% 10% 12%



#### 4.2.9 Score per residue for model 9

- Molecule 1: platelet aggregation inhibitor disintegrin

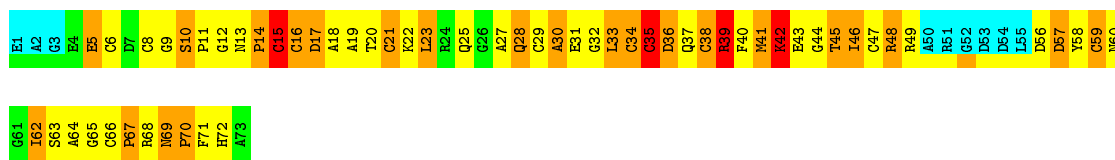
Chain A: 5% 45% 26% 11% 12%



#### 4.2.10 Score per residue for model 10

- Molecule 1: platelet aggregation inhibitor disintegrin

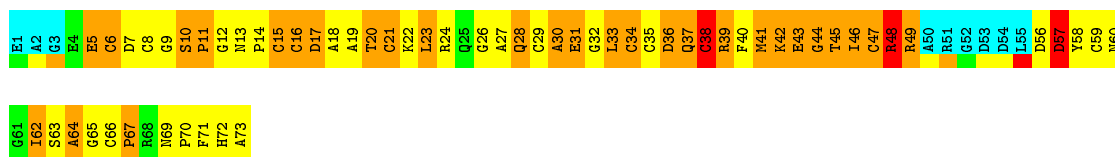
Chain A: 8% 42% 32% 5% 12%



#### 4.2.11 Score per residue for model 11

- Molecule 1: platelet aggregation inhibitor disintegrin

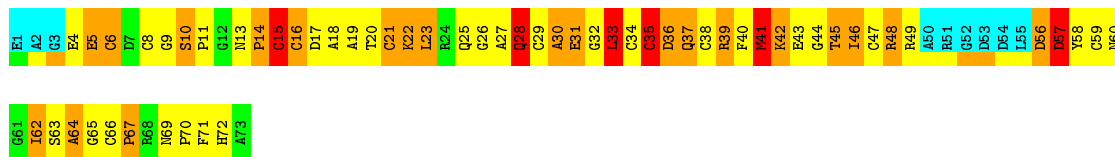
Chain A: 5% 38% 40% • 12%



#### 4.2.12 Score per residue for model 12

- Molecule 1: platelet aggregation inhibitor disintegrin

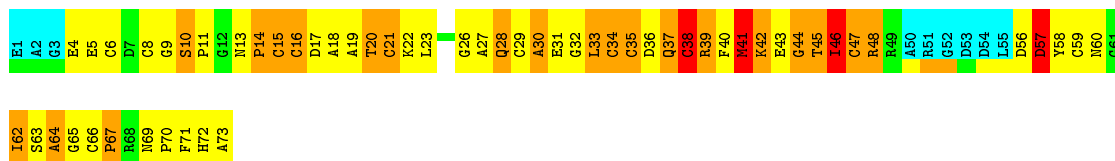
Chain A: 8% 42% 29% 8% 12%



#### 4.2.13 Score per residue for model 13

- Molecule 1: platelet aggregation inhibitor disintegrin

Chain A: 10% 44% 29% 5% 12%

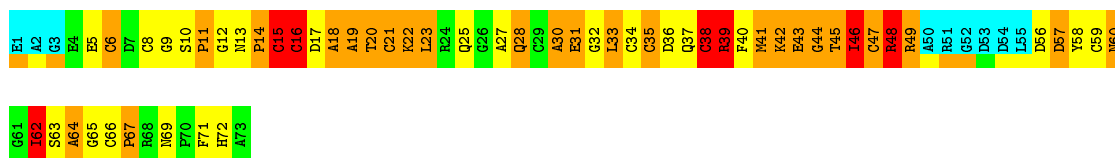


#### 4.2.14 Score per residue for model 14

- Molecule 1: platelet aggregation inhibitor disintegrin

Chain A: 12% 32% 34% 10% 12%

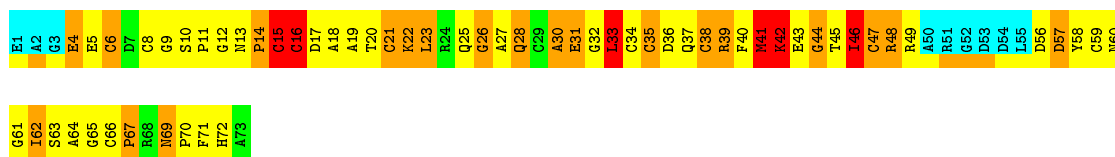




#### 4.2.15 Score per residue for model 15

- Molecule 1: platelet aggregation inhibitor disintegrin

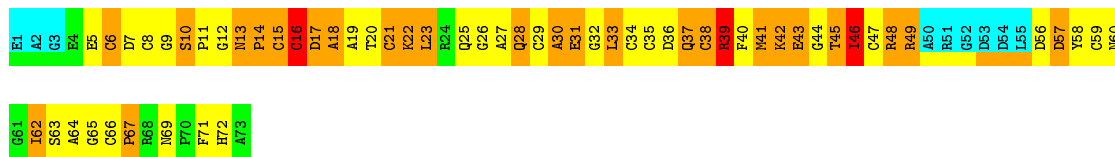
Chain A: 7% 45% 27% 8% 12%



#### 4.2.16 Score per residue for model 16

- Molecule 1: platelet aggregation inhibitor disintegrin

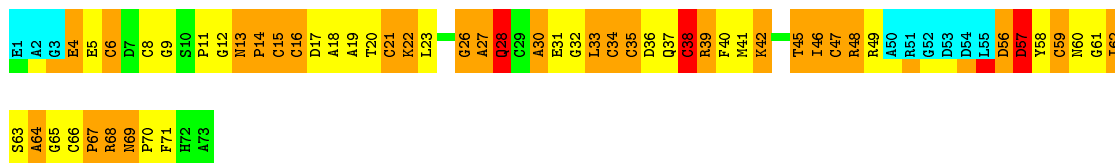
Chain A: 8% 41% 34% 12%



#### 4.2.17 Score per residue for model 17

- Molecule 1: platelet aggregation inhibitor disintegrin

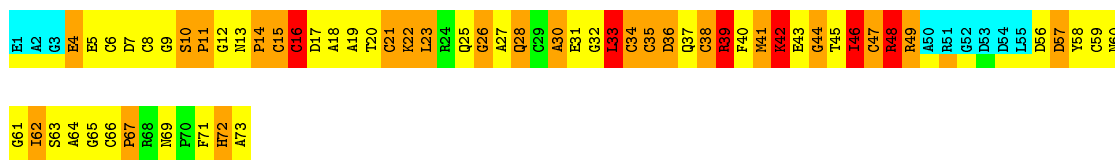
Chain A: 12% 34% 37% 12%



#### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: platelet aggregation inhibitor disintegrin

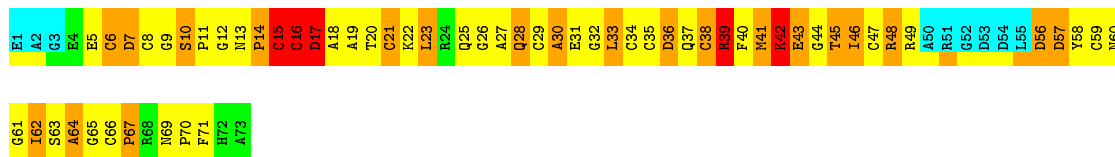
Chain A: 5% 42% 32% 8% 12%



#### 4.2.19 Score per residue for model 19

- Molecule 1: platelet aggregation inhibitor disintegrin

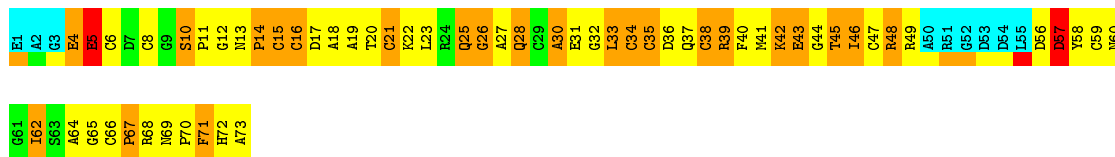
Chain A: 7% 45% 29% 7% 12%



#### 4.2.20 Score per residue for model 20

- Molecule 1: platelet aggregation inhibitor disintegrin

Chain A: 8% 45% 32% 12%



## 5 Refinement protocol and experimental data overview

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

Of the 90 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.0

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

Chemical shift file(s)	BMRB entry 5346
Number of chemical shift lists	1
Total number of shifts	391
Number of shifts mapped to atoms	391
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	43%

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.

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 [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	469	416	415	144±11
All	All	9380	8320	8300	2884

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 163.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:PHE:HB3	1:A:62:ILE:HD13	0.92	1.41	15	3
1:A:23:LEU:HD11	1:A:27:ALA:N	0.92	1.79	4	15
1:A:45:THR:O	1:A:46:ILE:HD12	0.90	1.66	7	13
1:A:33:LEU:HD11	1:A:64:ALA:C	0.90	1.86	19	8
1:A:15:CYS:O	1:A:23:LEU:HD13	0.89	1.67	3	10
1:A:4:GLU:HG3	1:A:46:ILE:HD13	0.88	1.43	2	2
1:A:62:ILE:HG22	1:A:65:GLY:O	0.87	1.69	18	6
1:A:40:PHE:HB2	1:A:62:ILE:HD13	0.87	1.47	20	7
1:A:16:CYS:O	1:A:23:LEU:HD22	0.87	1.69	18	6
1:A:33:LEU:HD23	1:A:47:CYS:HA	0.86	1.47	15	8
1:A:40:PHE:CB	1:A:62:ILE:HD13	0.85	2.01	18	9
1:A:45:THR:HG23	1:A:59:CYS:CB	0.84	2.01	19	1
1:A:40:PHE:CZ	1:A:64:ALA:HB2	0.84	2.07	15	11
1:A:62:ILE:HD13	1:A:62:ILE:O	0.80	1.76	7	8

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:ILE:O	1:A:62:ILE:HD13	0.80	1.76	14	9
1:A:62:ILE:HG22	1:A:66:CYS:HA	0.80	1.51	9	5
1:A:19:ALA:O	1:A:20:THR:HG23	0.79	1.77	8	2
1:A:27:ALA:HB3	1:A:34:CYS:SG	0.79	2.18	14	6
1:A:33:LEU:HD12	1:A:64:ALA:C	0.79	1.97	8	2
1:A:15:CYS:N	1:A:27:ALA:HB1	0.78	1.93	14	17
1:A:15:CYS:HB2	1:A:27:ALA:HB1	0.77	1.57	19	8
1:A:41:MET:CB	1:A:45:THR:HG21	0.77	2.09	19	1
1:A:62:ILE:HD12	1:A:62:ILE:N	0.77	1.95	20	8
1:A:42:LYS:N	1:A:62:ILE:HD11	0.77	1.95	20	3
1:A:33:LEU:HD13	1:A:34:CYS:N	0.77	1.95	6	9
1:A:15:CYS:O	1:A:23:LEU:HD12	0.77	1.80	7	7
1:A:14:PRO:O	1:A:23:LEU:HD13	0.74	1.82	1	2
1:A:33:LEU:HD11	1:A:65:GLY:N	0.73	1.98	18	5
1:A:60:ASN:O	1:A:62:ILE:HD12	0.73	1.82	14	2
1:A:23:LEU:HD22	1:A:23:LEU:H	0.72	1.44	2	1
1:A:46:ILE:HG23	1:A:48:ARG:CG	0.72	2.14	12	18
1:A:15:CYS:O	1:A:16:CYS:HB2	0.71	1.85	16	20
1:A:34:CYS:HB3	1:A:40:PHE:CE2	0.70	2.20	9	8
1:A:8:CYS:CB	1:A:16:CYS:N	0.70	2.54	12	19
1:A:10:SER:CB	1:A:11:PRO:CD	0.70	2.69	5	17
1:A:62:ILE:HG23	1:A:67:PRO:HD3	0.70	1.63	18	13
1:A:23:LEU:HD11	1:A:27:ALA:H	0.70	1.47	4	7
1:A:62:ILE:H	1:A:62:ILE:HD12	0.70	1.47	11	12
1:A:23:LEU:HD22	1:A:23:LEU:N	0.69	2.02	2	2
1:A:45:THR:HG22	1:A:46:ILE:N	0.69	2.03	11	3
1:A:33:LEU:HD13	1:A:34:CYS:H	0.68	1.46	7	14
1:A:46:ILE:HG23	1:A:48:ARG:HG3	0.68	1.66	1	18
1:A:62:ILE:N	1:A:62:ILE:HD12	0.68	2.03	6	9
1:A:40:PHE:CE1	1:A:64:ALA:HB2	0.68	2.24	1	5
1:A:58:TYR:CG	1:A:71:PHE:CD2	0.68	2.82	4	2
1:A:8:CYS:HB3	1:A:16:CYS:N	0.67	2.04	15	20
1:A:46:ILE:HG22	1:A:46:ILE:O	0.67	1.88	14	12
1:A:40:PHE:CZ	1:A:64:ALA:CB	0.67	2.78	5	9
1:A:46:ILE:O	1:A:46:ILE:HG22	0.67	1.90	15	8
1:A:35:CYS:HA	1:A:64:ALA:HB1	0.67	1.67	11	11
1:A:15:CYS:SG	1:A:30:ALA:HB1	0.67	2.30	19	3
1:A:15:CYS:CB	1:A:27:ALA:HB1	0.67	2.18	5	13
1:A:33:LEU:HD13	1:A:34:CYS:O	0.66	1.90	6	9
1:A:40:PHE:CZ	1:A:64:ALA:CA	0.66	2.79	6	17
1:A:23:LEU:H	1:A:23:LEU:HD23	0.65	1.52	16	5

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:CYS:HB3	1:A:27:ALA:CB	0.65	2.22	17	12
1:A:23:LEU:HD11	1:A:27:ALA:CB	0.65	2.21	12	8
1:A:34:CYS:SG	1:A:40:PHE:CZ	0.65	2.90	20	11
1:A:45:THR:OG1	1:A:46:ILE:N	0.65	2.29	19	1
1:A:4:GLU:CG	1:A:46:ILE:HD13	0.65	2.20	2	1
1:A:15:CYS:CB	1:A:27:ALA:CB	0.64	2.76	2	15
1:A:33:LEU:CD1	1:A:40:PHE:CE2	0.64	2.81	12	2
1:A:23:LEU:CD2	1:A:23:LEU:N	0.64	2.61	7	4
1:A:72:HIS:O	1:A:73:ALA:HB2	0.64	1.93	13	3
1:A:14:PRO:O	1:A:16:CYS:N	0.63	2.30	2	18
1:A:72:HIS:O	1:A:73:ALA:HB3	0.63	1.94	7	1
1:A:41:MET:O	1:A:42:LYS:CB	0.63	2.46	13	15
1:A:46:ILE:CG2	1:A:46:ILE:O	0.63	2.47	13	13
1:A:41:MET:HB2	1:A:45:THR:HG21	0.62	1.71	19	1
1:A:45:THR:HG23	1:A:59:CYS:HB2	0.62	1.68	19	1
1:A:23:LEU:HD23	1:A:23:LEU:H	0.62	1.54	17	3
1:A:16:CYS:O	1:A:23:LEU:HD12	0.62	1.94	14	1
1:A:23:LEU:N	1:A:23:LEU:CD2	0.62	2.63	8	5
1:A:15:CYS:N	1:A:27:ALA:CB	0.62	2.61	11	16
1:A:33:LEU:HD23	1:A:59:CYS:SG	0.62	2.35	17	4
1:A:47:CYS:SG	1:A:62:ILE:HG22	0.62	2.35	8	5
1:A:39:ARG:O	1:A:40:PHE:CG	0.62	2.53	12	18
1:A:45:THR:HB	1:A:59:CYS:HB2	0.62	1.71	5	15
1:A:62:ILE:HD12	1:A:62:ILE:H	0.62	1.54	17	5
1:A:17:ASP:O	1:A:18:ALA:HB3	0.62	1.94	19	14
1:A:23:LEU:HD23	1:A:23:LEU:N	0.61	2.10	3	6
1:A:69:ASN:N	1:A:70:PRO:CD	0.61	2.63	11	1
1:A:62:ILE:O	1:A:62:ILE:CD1	0.61	2.47	14	8
1:A:63:SER:O	1:A:64:ALA:HB2	0.61	1.95	12	4
1:A:34:CYS:SG	1:A:40:PHE:CE2	0.61	2.93	8	8
1:A:30:ALA:O	1:A:46:ILE:HG21	0.61	1.94	2	3
1:A:41:MET:HB3	1:A:45:THR:HG21	0.61	1.72	19	1
1:A:23:LEU:HD11	1:A:27:ALA:HB2	0.61	1.72	5	10
1:A:28:GLN:CG	1:A:38:CYS:O	0.60	2.48	19	18
1:A:39:ARG:C	1:A:40:PHE:CD1	0.60	2.75	18	18
1:A:40:PHE:CZ	1:A:64:ALA:HA	0.60	2.31	6	16
1:A:45:THR:CG2	1:A:46:ILE:N	0.60	2.64	16	3
1:A:38:CYS:O	1:A:39:ARG:CB	0.60	2.49	1	20
1:A:33:LEU:HD12	1:A:64:ALA:O	0.60	1.96	7	2
1:A:10:SER:HB3	1:A:11:PRO:CD	0.60	2.27	11	6
1:A:69:ASN:O	1:A:71:PHE:CG	0.60	2.54	10	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:CYS:HB3	1:A:40:PHE:CE1	0.60	2.31	4	2
1:A:40:PHE:CG	1:A:62:ILE:O	0.60	2.54	20	12
1:A:15:CYS:O	1:A:16:CYS:CB	0.60	2.50	13	13
1:A:14:PRO:C	1:A:27:ALA:CB	0.60	2.70	1	14
1:A:39:ARG:C	1:A:40:PHE:CG	0.59	2.75	11	18
1:A:62:ILE:N	1:A:62:ILE:CD1	0.59	2.65	4	4
1:A:16:CYS:O	1:A:23:LEU:HD13	0.59	1.98	2	1
1:A:45:THR:HG23	1:A:59:CYS:HB3	0.59	1.70	19	1
1:A:63:SER:O	1:A:64:ALA:CB	0.59	2.51	8	16
1:A:8:CYS:HB2	1:A:16:CYS:N	0.59	2.12	12	19
1:A:63:SER:O	1:A:64:ALA:HB3	0.59	1.97	13	14
1:A:39:ARG:O	1:A:40:PHE:CD2	0.59	2.55	7	11
1:A:23:LEU:HD12	1:A:25:GLN:HG3	0.59	1.73	18	1
1:A:23:LEU:N	1:A:23:LEU:HD23	0.58	2.13	18	6
1:A:62:ILE:CB	1:A:65:GLY:O	0.58	2.50	10	4
1:A:69:ASN:O	1:A:71:PHE:CZ	0.58	2.56	15	3
1:A:23:LEU:CD1	1:A:27:ALA:HB2	0.58	2.28	7	10
1:A:46:ILE:O	1:A:46:ILE:CG2	0.58	2.52	18	7
1:A:10:SER:HB2	1:A:11:PRO:CD	0.58	2.28	3	11
1:A:46:ILE:HD13	1:A:57:ASP:O	0.58	1.97	4	1
1:A:20:THR:O	1:A:22:LYS:N	0.58	2.37	4	18
1:A:70:PRO:O	1:A:71:PHE:CG	0.58	2.56	7	5
1:A:59:CYS:HB3	1:A:62:ILE:CG1	0.58	2.29	12	12
1:A:62:ILE:CD1	1:A:62:ILE:O	0.58	2.52	5	7
1:A:34:CYS:SG	1:A:35:CYS:N	0.58	2.77	20	11
1:A:57:ASP:OD1	1:A:71:PHE:CD2	0.58	2.57	13	3
1:A:69:ASN:CB	1:A:70:PRO:CD	0.58	2.82	17	3
1:A:15:CYS:O	1:A:23:LEU:CD1	0.58	2.52	7	10
1:A:46:ILE:HG23	1:A:48:ARG:HG2	0.58	1.76	5	11
1:A:8:CYS:HB2	1:A:15:CYS:C	0.58	2.20	1	8
1:A:33:LEU:HD13	1:A:40:PHE:CE2	0.58	2.34	12	2
1:A:16:CYS:O	1:A:23:LEU:CD1	0.58	2.51	2	2
1:A:62:ILE:CG2	1:A:67:PRO:HD3	0.57	2.29	14	15
1:A:23:LEU:HD23	1:A:36:ASP:OD2	0.57	2.00	16	2
1:A:70:PRO:O	1:A:71:PHE:CD2	0.57	2.57	9	1
1:A:69:ASN:O	1:A:71:PHE:CE2	0.57	2.58	16	7
1:A:69:ASN:O	1:A:71:PHE:CD2	0.57	2.57	10	2
1:A:57:ASP:OD2	1:A:71:PHE:CG	0.57	2.57	18	1
1:A:41:MET:CB	1:A:45:THR:OG1	0.57	2.53	17	13
1:A:23:LEU:HG	1:A:27:ALA:HB2	0.57	1.76	14	1
1:A:56:ASP:OD1	1:A:72:HIS:CD2	0.57	2.57	16	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:ASP:O	1:A:19:ALA:N	0.57	2.38	4	6
1:A:15:CYS:HB2	1:A:30:ALA:HB3	0.57	1.74	11	7
1:A:57:ASP:OD1	1:A:71:PHE:CD1	0.57	2.58	17	1
1:A:69:ASN:O	1:A:71:PHE:CE1	0.57	2.58	12	4
1:A:43:GLU:O	1:A:45:THR:N	0.57	2.38	1	7
1:A:14:PRO:O	1:A:15:CYS:C	0.57	2.42	16	17
1:A:30:ALA:O	1:A:32:GLY:N	0.56	2.38	15	18
1:A:62:ILE:O	1:A:62:ILE:CG1	0.56	2.52	4	2
1:A:11:PRO:CG	1:A:48:ARG:O	0.56	2.54	14	5
1:A:40:PHE:CZ	1:A:64:ALA:N	0.56	2.74	20	2
1:A:40:PHE:CD1	1:A:62:ILE:O	0.56	2.58	20	1
1:A:15:CYS:HB3	1:A:27:ALA:HB2	0.56	1.78	1	6
1:A:40:PHE:CE2	1:A:64:ALA:HA	0.56	2.35	8	15
1:A:56:ASP:OD1	1:A:72:HIS:CG	0.56	2.59	16	1
1:A:8:CYS:HB3	1:A:16:CYS:CA	0.56	2.30	7	18
1:A:10:SER:HB2	1:A:11:PRO:HD2	0.56	1.78	5	1
1:A:40:PHE:CE1	1:A:63:SER:O	0.56	2.57	12	2
1:A:10:SER:OG	1:A:32:GLY:N	0.56	2.38	8	8
1:A:39:ARG:C	1:A:40:PHE:CD2	0.56	2.78	2	1
1:A:37:GLN:O	1:A:38:CYS:C	0.56	2.44	11	20
1:A:10:SER:CB	1:A:11:PRO:HD3	0.56	2.31	8	11
1:A:16:CYS:O	1:A:23:LEU:CB	0.56	2.54	15	2
1:A:33:LEU:HD22	1:A:47:CYS:HA	0.56	1.77	9	1
1:A:40:PHE:CB	1:A:62:ILE:O	0.56	2.54	12	15
1:A:14:PRO:CB	1:A:36:ASP:OD2	0.56	2.54	12	1
1:A:14:PRO:CG	1:A:36:ASP:OD1	0.55	2.54	19	1
1:A:28:GLN:HG2	1:A:38:CYS:O	0.55	2.02	6	18
1:A:47:CYS:SG	1:A:62:ILE:CG2	0.55	2.94	8	5
1:A:33:LEU:HD12	1:A:34:CYS:N	0.55	2.16	9	1
1:A:72:HIS:O	1:A:72:HIS:CG	0.55	2.59	7	1
1:A:33:LEU:CD1	1:A:65:GLY:N	0.55	2.69	11	4
1:A:62:ILE:CD1	1:A:62:ILE:N	0.55	2.65	20	6
1:A:23:LEU:HD22	1:A:36:ASP:OD2	0.55	2.02	8	3
1:A:33:LEU:CD2	1:A:47:CYS:HA	0.55	2.31	9	1
1:A:14:PRO:CD	1:A:35:CYS:SG	0.55	2.94	11	1
1:A:23:LEU:CD2	1:A:36:ASP:OD2	0.55	2.55	8	2
1:A:46:ILE:HD12	1:A:48:ARG:CG	0.55	2.32	4	1
1:A:46:ILE:HD12	1:A:48:ARG:HG2	0.55	1.78	4	1
1:A:45:THR:HG22	1:A:46:ILE:H	0.55	1.61	16	2
1:A:62:ILE:CG2	1:A:65:GLY:O	0.55	2.55	16	3
1:A:33:LEU:HD12	1:A:34:CYS:H	0.55	1.61	9	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:GLY:N	1:A:60:ASN:ND2	0.55	2.54	16	2
1:A:69:ASN:N	1:A:70:PRO:HD3	0.55	2.16	11	1
1:A:56:ASP:O	1:A:57:ASP:CB	0.55	2.55	10	15
1:A:47:CYS:O	1:A:48:ARG:C	0.55	2.45	8	20
1:A:23:LEU:CD2	1:A:36:ASP:OD1	0.55	2.55	9	4
1:A:70:PRO:O	1:A:71:PHE:CD1	0.55	2.60	19	5
1:A:27:ALA:N	1:A:38:CYS:HB2	0.55	2.16	18	4
1:A:44:GLY:N	1:A:59:CYS:O	0.54	2.41	16	8
1:A:34:CYS:CB	1:A:40:PHE:CE1	0.54	2.90	2	2
1:A:49:ARG:CG	1:A:66:CYS:SG	0.54	2.95	6	1
1:A:47:CYS:CB	1:A:58:TYR:O	0.54	2.55	19	4
1:A:37:GLN:O	1:A:39:ARG:N	0.54	2.40	16	9
1:A:19:ALA:O	1:A:20:THR:CG2	0.54	2.56	16	2
1:A:16:CYS:O	1:A:23:LEU:CD2	0.54	2.55	4	2
1:A:32:GLY:CA	1:A:48:ARG:HB2	0.54	2.32	4	9
1:A:14:PRO:O	1:A:23:LEU:CD1	0.54	2.56	2	1
1:A:36:ASP:OD1	1:A:36:ASP:N	0.54	2.41	19	1
1:A:38:CYS:SG	1:A:39:ARG:N	0.54	2.80	17	5
1:A:33:LEU:CD2	1:A:59:CYS:SG	0.54	2.95	7	6
1:A:15:CYS:CB	1:A:30:ALA:HB3	0.54	2.31	18	1
1:A:33:LEU:CD1	1:A:34:CYS:O	0.54	2.55	6	2
1:A:8:CYS:HB3	1:A:16:CYS:HA	0.54	1.80	16	14
1:A:5:GLU:O	1:A:6:CYS:CB	0.54	2.55	19	3
1:A:69:ASN:HB2	1:A:70:PRO:CD	0.54	2.32	17	2
1:A:13:ASN:N	1:A:14:PRO:CD	0.54	2.70	6	10
1:A:49:ARG:CG	1:A:56:ASP:O	0.54	2.55	14	1
1:A:58:TYR:CD1	1:A:71:PHE:HB3	0.54	2.38	14	3
1:A:33:LEU:CD1	1:A:40:PHE:CD2	0.54	2.91	12	1
1:A:10:SER:CB	1:A:11:PRO:HD2	0.54	2.33	5	5
1:A:59:CYS:SG	1:A:62:ILE:HD11	0.54	2.43	10	2
1:A:40:PHE:CE1	1:A:63:SER:C	0.54	2.81	7	6
1:A:14:PRO:CB	1:A:38:CYS:SG	0.54	2.96	3	1
1:A:59:CYS:CB	1:A:62:ILE:HG13	0.54	2.33	4	7
1:A:45:THR:CG2	1:A:59:CYS:HB2	0.54	2.33	19	1
1:A:33:LEU:HD12	1:A:64:ALA:CA	0.54	2.32	8	2
1:A:27:ALA:O	1:A:34:CYS:CB	0.54	2.56	1	6
1:A:17:ASP:O	1:A:18:ALA:CB	0.54	2.56	16	14
1:A:59:CYS:HA	1:A:62:ILE:HG21	0.54	1.79	20	8
1:A:42:LYS:CD	1:A:60:ASN:O	0.54	2.56	11	3
1:A:47:CYS:O	1:A:47:CYS:SG	0.53	2.65	15	4
1:A:42:LYS:O	1:A:43:GLU:CB	0.53	2.55	20	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:CD2	1:A:40:PHE:CD1	0.53	2.91	4	1
1:A:36:ASP:O	1:A:38:CYS:N	0.53	2.41	3	3
1:A:28:GLN:HG2	1:A:39:ARG:HB2	0.53	1.81	15	1
1:A:39:ARG:O	1:A:40:PHE:CD1	0.53	2.61	4	1
1:A:23:LEU:CD1	1:A:27:ALA:CB	0.53	2.87	12	2
1:A:36:ASP:CG	1:A:37:GLN:N	0.53	2.62	10	6
1:A:34:CYS:CB	1:A:40:PHE:CE2	0.53	2.92	3	4
1:A:15:CYS:SG	1:A:30:ALA:CB	0.53	2.95	19	5
1:A:62:ILE:CG1	1:A:62:ILE:O	0.53	2.57	19	2
1:A:60:ASN:O	1:A:62:ILE:CD1	0.53	2.57	14	1
1:A:59:CYS:O	1:A:60:ASN:ND2	0.53	2.42	15	9
1:A:31:GLU:O	1:A:48:ARG:NE	0.53	2.41	8	4
1:A:8:CYS:O	1:A:13:ASN:O	0.53	2.27	17	3
1:A:57:ASP:OD2	1:A:71:PHE:CD2	0.53	2.61	3	3
1:A:41:MET:CG	1:A:45:THR:OG1	0.53	2.57	16	3
1:A:38:CYS:O	1:A:39:ARG:CG	0.53	2.57	13	5
1:A:29:CYS:CB	1:A:45:THR:CG2	0.53	2.87	16	1
1:A:45:THR:CB	1:A:59:CYS:HB2	0.53	2.33	17	9
1:A:69:ASN:O	1:A:71:PHE:N	0.53	2.41	7	3
1:A:10:SER:OG	1:A:32:GLY:CA	0.53	2.57	8	2
1:A:21:CYS:O	1:A:22:LYS:CD	0.53	2.56	19	1
1:A:57:ASP:OD1	1:A:71:PHE:CB	0.53	2.57	10	1
1:A:20:THR:O	1:A:21:CYS:C	0.53	2.46	5	17
1:A:14:PRO:CG	1:A:21:CYS:SG	0.53	2.97	18	9
1:A:58:TYR:CD2	1:A:71:PHE:CE2	0.53	2.97	4	1
1:A:27:ALA:N	1:A:38:CYS:HB3	0.52	2.19	20	3
1:A:27:ALA:CB	1:A:34:CYS:SG	0.52	2.98	4	2
1:A:41:MET:O	1:A:42:LYS:HB3	0.52	2.04	17	6
1:A:45:THR:O	1:A:46:ILE:CD1	0.52	2.57	13	8
1:A:22:LYS:CA	1:A:36:ASP:OD2	0.52	2.57	15	1
1:A:6:CYS:O	1:A:31:GLU:CB	0.52	2.57	15	2
1:A:14:PRO:CB	1:A:36:ASP:OD1	0.52	2.57	18	1
1:A:9:GLY:CA	1:A:31:GLU:OE1	0.52	2.57	1	1
1:A:9:GLY:O	1:A:15:CYS:CA	0.52	2.58	12	3
1:A:47:CYS:SG	1:A:65:GLY:O	0.52	2.67	12	9
1:A:11:PRO:CD	1:A:48:ARG:O	0.52	2.57	14	1
1:A:40:PHE:CE1	1:A:64:ALA:HA	0.52	2.40	2	1
1:A:13:ASN:O	1:A:15:CYS:N	0.52	2.43	5	3
1:A:14:PRO:CG	1:A:36:ASP:OD2	0.52	2.56	2	2
1:A:27:ALA:O	1:A:30:ALA:N	0.52	2.42	2	1
1:A:49:ARG:CG	1:A:57:ASP:OD1	0.52	2.57	11	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:PRO:HG3	1:A:36:ASP:OD1	0.52	2.05	19	1
1:A:72:HIS:O	1:A:73:ALA:CB	0.52	2.57	20	3
1:A:27:ALA:O	1:A:28:GLN:C	0.52	2.48	2	4
1:A:4:GLU:O	1:A:5:GLU:CG	0.52	2.57	17	1
1:A:57:ASP:OD1	1:A:58:TYR:N	0.52	2.42	3	2
1:A:29:CYS:SG	1:A:33:LEU:CD2	0.52	2.97	11	1
1:A:15:CYS:HB2	1:A:30:ALA:CB	0.52	2.35	6	9
1:A:67:PRO:HG2	1:A:71:PHE:CE2	0.52	2.40	7	3
1:A:40:PHE:CE2	1:A:64:ALA:HB2	0.52	2.39	2	1
1:A:21:CYS:HA	1:A:36:ASP:OD1	0.52	2.05	19	1
1:A:48:ARG:NH1	1:A:56:ASP:OD2	0.52	2.43	5	2
1:A:43:GLU:O	1:A:44:GLY:C	0.52	2.48	13	13
1:A:62:ILE:O	1:A:64:ALA:N	0.51	2.42	10	6
1:A:65:GLY:O	1:A:66:CYS:SG	0.51	2.68	5	14
1:A:59:CYS:HB3	1:A:62:ILE:HG12	0.51	1.83	2	9
1:A:41:MET:HE2	1:A:45:THR:HG21	0.51	1.83	14	1
1:A:49:ARG:CD	1:A:66:CYS:SG	0.51	2.97	5	1
1:A:40:PHE:HB3	1:A:62:ILE:CD1	0.51	2.35	10	1
1:A:72:HIS:O	1:A:72:HIS:ND1	0.51	2.43	14	2
1:A:9:GLY:O	1:A:15:CYS:N	0.51	2.44	19	1
1:A:33:LEU:CD1	1:A:64:ALA:C	0.51	2.79	10	8
1:A:28:GLN:HG2	1:A:38:CYS:CB	0.51	2.36	2	1
1:A:67:PRO:HG2	1:A:71:PHE:CE1	0.51	2.41	15	4
1:A:49:ARG:O	1:A:49:ARG:NE	0.51	2.43	6	1
1:A:16:CYS:O	1:A:23:LEU:HB3	0.51	2.06	9	11
1:A:8:CYS:CB	1:A:16:CYS:CA	0.51	2.88	2	10
1:A:69:ASN:O	1:A:71:PHE:CD1	0.51	2.63	4	2
1:A:67:PRO:HG2	1:A:71:PHE:CZ	0.51	2.41	19	7
1:A:59:CYS:C	1:A:60:ASN:ND2	0.51	2.64	2	10
1:A:66:CYS:O	1:A:67:PRO:O	0.51	2.29	4	11
1:A:38:CYS:O	1:A:39:ARG:HB2	0.51	2.04	9	18
1:A:10:SER:CB	1:A:32:GLY:HA3	0.51	2.35	8	3
1:A:40:PHE:CE1	1:A:64:ALA:N	0.51	2.79	20	3
1:A:47:CYS:SG	1:A:47:CYS:O	0.51	2.68	1	5
1:A:34:CYS:HB3	1:A:40:PHE:CZ	0.51	2.40	10	2
1:A:40:PHE:HB3	1:A:62:ILE:HD11	0.51	1.83	10	1
1:A:56:ASP:OD1	1:A:72:HIS:CE1	0.51	2.64	16	1
1:A:41:MET:HB3	1:A:45:THR:CG2	0.51	2.35	19	1
1:A:10:SER:HB3	1:A:33:LEU:N	0.51	2.21	12	9
1:A:60:ASN:C	1:A:62:ILE:HD12	0.51	2.27	14	2
1:A:6:CYS:CB	1:A:31:GLU:HB2	0.51	2.36	13	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:CYS:HB3	1:A:27:ALA:HB1	0.51	1.83	15	1
1:A:13:ASN:OD1	1:A:13:ASN:N	0.51	2.44	1	1
1:A:10:SER:HA	1:A:14:PRO:HA	0.51	1.83	19	1
1:A:42:LYS:HA	1:A:60:ASN:O	0.50	2.05	10	10
1:A:26:GLY:O	1:A:28:GLN:NE2	0.50	2.44	11	2
1:A:41:MET:O	1:A:42:LYS:HB2	0.50	2.07	7	14
1:A:14:PRO:CD	1:A:21:CYS:SG	0.50	2.99	5	2
1:A:6:CYS:HB3	1:A:31:GLU:CB	0.50	2.36	13	5
1:A:36:ASP:O	1:A:37:GLN:C	0.50	2.49	3	1
1:A:6:CYS:SG	1:A:7:ASP:N	0.50	2.83	18	3
1:A:57:ASP:CG	1:A:71:PHE:CD1	0.50	2.84	17	1
1:A:45:THR:CG2	1:A:59:CYS:CB	0.50	2.83	19	1
1:A:46:ILE:CG2	1:A:48:ARG:HG3	0.50	2.36	19	11
1:A:15:CYS:HB2	1:A:27:ALA:CB	0.50	2.34	10	3
1:A:47:CYS:HB2	1:A:58:TYR:O	0.50	2.07	12	10
1:A:14:PRO:HG2	1:A:21:CYS:CB	0.50	2.37	14	3
1:A:40:PHE:CD1	1:A:63:SER:HA	0.50	2.41	14	2
1:A:8:CYS:O	1:A:15:CYS:CA	0.50	2.59	2	1
1:A:69:ASN:HB2	1:A:70:PRO:HD3	0.50	1.83	17	3
1:A:15:CYS:CB	1:A:27:ALA:HA	0.50	2.37	2	1
1:A:28:GLN:N	1:A:38:CYS:HB2	0.50	2.22	4	2
1:A:33:LEU:HD13	1:A:64:ALA:HA	0.50	1.83	4	1
1:A:36:ASP:OD1	1:A:37:GLN:N	0.50	2.42	16	1
1:A:48:ARG:NH1	1:A:56:ASP:OD1	0.50	2.44	1	1
1:A:4:GLU:OE1	1:A:4:GLU:N	0.50	2.44	9	1
1:A:59:CYS:SG	1:A:59:CYS:O	0.50	2.70	4	2
1:A:36:ASP:O	1:A:38:CYS:SG	0.50	2.70	15	9
1:A:35:CYS:HA	1:A:64:ALA:CB	0.50	2.36	20	5
1:A:8:CYS:O	1:A:15:CYS:HA	0.50	2.06	2	2
1:A:21:CYS:C	1:A:36:ASP:CB	0.50	2.80	6	4
1:A:21:CYS:CA	1:A:36:ASP:OD2	0.50	2.60	12	1
1:A:33:LEU:HD11	1:A:64:ALA:O	0.50	2.06	19	2
1:A:59:CYS:CB	1:A:62:ILE:HG12	0.50	2.37	1	8
1:A:67:PRO:HD2	1:A:71:PHE:CZ	0.50	2.42	10	1
1:A:57:ASP:OD1	1:A:71:PHE:CE2	0.50	2.65	13	1
1:A:58:TYR:CD1	1:A:71:PHE:CB	0.50	2.95	5	2
1:A:28:GLN:HA	1:A:38:CYS:SG	0.50	2.47	1	4
1:A:42:LYS:CG	1:A:60:ASN:O	0.49	2.60	11	2
1:A:58:TYR:HB2	1:A:71:PHE:CE2	0.49	2.41	4	1
1:A:32:GLY:HA2	1:A:48:ARG:HB2	0.49	1.83	14	13
1:A:6:CYS:O	1:A:31:GLU:CG	0.49	2.60	2	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:LEU:CD1	1:A:64:ALA:CA	0.49	2.90	8	4
1:A:31:GLU:OE2	1:A:48:ARG:NH2	0.49	2.45	4	1
1:A:41:MET:O	1:A:42:LYS:CG	0.49	2.60	12	4
1:A:14:PRO:O	1:A:16:CYS:O	0.49	2.30	5	7
1:A:5:GLU:O	1:A:31:GLU:CB	0.49	2.60	4	1
1:A:48:ARG:NH2	1:A:56:ASP:OD2	0.49	2.45	18	1
1:A:70:PRO:HG2	1:A:71:PHE:CE2	0.49	2.41	11	1
1:A:23:LEU:CD2	1:A:36:ASP:CG	0.49	2.81	6	1
1:A:56:ASP:N	1:A:56:ASP:OD1	0.49	2.45	17	1
1:A:60:ASN:N	1:A:62:ILE:HG13	0.49	2.22	15	2
1:A:14:PRO:HB3	1:A:38:CYS:SG	0.49	2.47	3	1
1:A:58:TYR:HB2	1:A:71:PHE:CG	0.49	2.42	5	3
1:A:33:LEU:CD1	1:A:64:ALA:HA	0.49	2.37	11	6
1:A:14:PRO:HG3	1:A:35:CYS:SG	0.49	2.47	19	2
1:A:58:TYR:HB2	1:A:71:PHE:CE1	0.49	2.42	11	3
1:A:69:ASN:HB3	1:A:70:PRO:CD	0.49	2.37	15	1
1:A:62:ILE:C	1:A:62:ILE:CD1	0.49	2.80	16	2
1:A:28:GLN:HB3	1:A:40:PHE:HA	0.49	1.85	2	2
1:A:42:LYS:CD	1:A:61:GLY:HA2	0.49	2.37	18	3
1:A:49:ARG:O	1:A:49:ARG:CD	0.49	2.61	6	1
1:A:60:ASN:N	1:A:62:ILE:HG23	0.49	2.23	19	1
1:A:28:GLN:HA	1:A:39:ARG:O	0.49	2.08	7	6
1:A:23:LEU:O	1:A:25:GLN:N	0.49	2.45	9	1
1:A:44:GLY:HA2	1:A:60:ASN:ND2	0.49	2.23	20	4
1:A:15:CYS:CB	1:A:27:ALA:HB2	0.49	2.37	2	2
1:A:28:GLN:CG	1:A:38:CYS:HB2	0.49	2.38	2	1
1:A:10:SER:HB3	1:A:11:PRO:HD3	0.49	1.85	5	2
1:A:62:ILE:CD1	1:A:62:ILE:H	0.48	2.20	19	2
1:A:28:GLN:CG	1:A:38:CYS:C	0.48	2.81	10	5
1:A:57:ASP:HA	1:A:71:PHE:CG	0.48	2.43	13	1
1:A:14:PRO:C	1:A:27:ALA:HB1	0.48	2.28	3	1
1:A:36:ASP:OD1	1:A:38:CYS:SG	0.48	2.71	12	2
1:A:21:CYS:CB	1:A:36:ASP:HB2	0.48	2.38	11	1
1:A:17:ASP:N	1:A:17:ASP:OD1	0.48	2.46	10	5
1:A:17:ASP:O	1:A:18:ALA:C	0.48	2.51	8	5
1:A:11:PRO:HG2	1:A:48:ARG:O	0.48	2.08	18	3
1:A:28:GLN:HB3	1:A:40:PHE:CA	0.48	2.38	2	1
1:A:30:ALA:C	1:A:32:GLY:N	0.48	2.66	13	18
1:A:33:LEU:HG	1:A:47:CYS:SG	0.48	2.49	4	10
1:A:45:THR:HB	1:A:59:CYS:HB3	0.48	1.84	10	2
1:A:14:PRO:HG2	1:A:21:CYS:SG	0.48	2.49	14	9

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:CYS:HB3	1:A:45:THR:CG2	0.48	2.38	16	1
1:A:41:MET:O	1:A:42:LYS:HG2	0.48	2.09	1	2
1:A:11:PRO:HB3	1:A:49:ARG:CG	0.48	2.39	3	1
1:A:49:ARG:CG	1:A:57:ASP:CG	0.48	2.81	11	1
1:A:21:CYS:O	1:A:36:ASP:OD1	0.48	2.32	20	5
1:A:71:PHE:O	1:A:73:ALA:N	0.48	2.47	3	3
1:A:49:ARG:NH1	1:A:69:ASN:OD1	0.48	2.46	11	1
1:A:47:CYS:HB3	1:A:58:TYR:O	0.48	2.09	17	8
1:A:25:GLN:O	1:A:26:GLY:C	0.48	2.52	6	4
1:A:10:SER:HB3	1:A:11:PRO:HD2	0.48	1.86	14	3
1:A:21:CYS:C	1:A:36:ASP:HB3	0.48	2.29	9	4
1:A:59:CYS:CA	1:A:62:ILE:HG13	0.48	2.38	13	6
1:A:57:ASP:OD1	1:A:71:PHE:CG	0.48	2.67	15	2
1:A:8:CYS:N	1:A:31:GLU:OE1	0.48	2.47	18	1
1:A:23:LEU:HD11	1:A:26:GLY:C	0.48	2.29	9	2
1:A:47:CYS:N	1:A:57:ASP:O	0.48	2.46	19	1
1:A:28:GLN:HG2	1:A:38:CYS:C	0.48	2.29	2	4
1:A:59:CYS:HB3	1:A:62:ILE:HG13	0.48	1.85	12	4
1:A:59:CYS:HA	1:A:62:ILE:CG2	0.48	2.38	20	7
1:A:67:PRO:HD2	1:A:71:PHE:CE1	0.48	2.43	10	1
1:A:68:ARG:HB3	1:A:68:ARG:CZ	0.48	2.39	20	1
1:A:9:GLY:O	1:A:31:GLU:O	0.48	2.32	18	1
1:A:33:LEU:CD2	1:A:65:GLY:O	0.48	2.61	9	1
1:A:17:ASP:HB2	1:A:20:THR:O	0.47	2.08	11	5
1:A:41:MET:HB3	1:A:45:THR:OG1	0.47	2.07	10	6
1:A:34:CYS:SG	1:A:40:PHE:CE1	0.47	3.08	2	1
1:A:23:LEU:CD2	1:A:36:ASP:HB3	0.47	2.39	15	1
1:A:57:ASP:CG	1:A:71:PHE:CD2	0.47	2.87	15	1
1:A:21:CYS:HB3	1:A:36:ASP:CA	0.47	2.39	16	6
1:A:16:CYS:O	1:A:22:LYS:O	0.47	2.32	14	1
1:A:33:LEU:HD21	1:A:40:PHE:CD1	0.47	2.43	4	1
1:A:6:CYS:SG	1:A:9:GLY:O	0.47	2.71	16	2
1:A:38:CYS:SG	1:A:39:ARG:O	0.47	2.73	17	3
1:A:42:LYS:HG2	1:A:62:ILE:HD12	0.47	1.86	16	1
1:A:9:GLY:O	1:A:15:CYS:HA	0.47	2.08	16	5
1:A:26:GLY:O	1:A:28:GLN:OE1	0.47	2.33	17	5
1:A:56:ASP:CB	1:A:72:HIS:HA	0.47	2.39	8	2
1:A:40:PHE:CD2	1:A:63:SER:HA	0.47	2.44	4	1
1:A:43:GLU:N	1:A:59:CYS:O	0.47	2.45	16	1
1:A:60:ASN:N	1:A:60:ASN:ND2	0.47	2.59	4	1
1:A:47:CYS:O	1:A:66:CYS:SG	0.47	2.72	12	6

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:CYS:O	1:A:22:LYS:CG	0.47	2.63	19	1
1:A:47:CYS:SG	1:A:57:ASP:HB3	0.47	2.49	1	7
1:A:59:CYS:CB	1:A:62:ILE:CG1	0.47	2.92	11	8
1:A:5:GLU:O	1:A:6:CYS:O	0.47	2.33	11	5
1:A:58:TYR:HB2	1:A:71:PHE:CD1	0.47	2.45	2	2
1:A:72:HIS:CG	1:A:73:ALA:N	0.47	2.82	9	2
1:A:30:ALA:O	1:A:46:ILE:CG2	0.47	2.63	1	1
1:A:10:SER:C	1:A:33:LEU:O	0.47	2.53	13	7
1:A:39:ARG:HG3	1:A:40:PHE:N	0.47	2.25	14	1
1:A:17:ASP:OD2	1:A:20:THR:N	0.47	2.48	2	1
1:A:31:GLU:OE1	1:A:32:GLY:N	0.47	2.47	16	1
1:A:34:CYS:O	1:A:64:ALA:HA	0.47	2.10	7	12
1:A:32:GLY:O	1:A:33:LEU:O	0.47	2.33	18	4
1:A:10:SER:O	1:A:33:LEU:O	0.47	2.32	3	4
1:A:10:SER:HB2	1:A:11:PRO:HD3	0.47	1.85	10	9
1:A:10:SER:HB3	1:A:32:GLY:CA	0.47	2.40	13	3
1:A:40:PHE:O	1:A:41:MET:O	0.47	2.33	14	1
1:A:62:ILE:CG2	1:A:66:CYS:HA	0.47	2.39	14	3
1:A:27:ALA:O	1:A:34:CYS:HB2	0.47	2.10	18	8
1:A:34:CYS:SG	1:A:36:ASP:OD1	0.47	2.73	2	2
1:A:36:ASP:OD2	1:A:38:CYS:SG	0.47	2.73	8	3
1:A:5:GLU:O	1:A:31:GLU:CG	0.47	2.63	4	1
1:A:60:ASN:OD1	1:A:70:PRO:CG	0.47	2.63	17	1
1:A:33:LEU:HD13	1:A:40:PHE:CD2	0.47	2.45	12	1
1:A:49:ARG:CD	1:A:57:ASP:OD1	0.47	2.63	11	1
1:A:46:ILE:CG2	1:A:48:ARG:CG	0.47	2.93	5	2
1:A:28:GLN:HG2	1:A:39:ARG:CG	0.47	2.40	14	2
1:A:27:ALA:O	1:A:29:CYS:N	0.47	2.48	2	1
1:A:29:CYS:O	1:A:30:ALA:O	0.47	2.33	8	4
1:A:59:CYS:SG	1:A:62:ILE:HG21	0.47	2.50	11	3
1:A:56:ASP:O	1:A:57:ASP:HB2	0.47	2.10	8	13
1:A:15:CYS:O	1:A:15:CYS:SG	0.47	2.72	3	1
1:A:22:LYS:O	1:A:22:LYS:CG	0.47	2.63	3	1
1:A:30:ALA:O	1:A:31:GLU:C	0.47	2.54	10	18
1:A:56:ASP:O	1:A:57:ASP:OD1	0.47	2.32	8	2
1:A:49:ARG:HG2	1:A:66:CYS:SG	0.47	2.50	6	3
1:A:44:GLY:CA	1:A:60:ASN:ND2	0.47	2.78	16	3
1:A:47:CYS:SG	1:A:57:ASP:OD2	0.47	2.73	11	4
1:A:60:ASN:OD1	1:A:70:PRO:HG2	0.47	2.10	17	1
1:A:6:CYS:O	1:A:31:GLU:OE1	0.47	2.33	1	1
1:A:9:GLY:O	1:A:15:CYS:SG	0.46	2.73	9	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:CYS:SG	1:A:62:ILE:HG12	0.46	2.50	2	8
1:A:47:CYS:O	1:A:48:ARG:O	0.46	2.33	8	4
1:A:27:ALA:O	1:A:34:CYS:HB3	0.46	2.10	7	4
1:A:14:PRO:HB3	1:A:36:ASP:OD1	0.46	2.10	18	3
1:A:70:PRO:C	1:A:71:PHE:CD1	0.46	2.89	5	1
1:A:58:TYR:HB2	1:A:71:PHE:CD2	0.46	2.44	5	2
1:A:13:ASN:O	1:A:14:PRO:C	0.46	2.54	14	10
1:A:11:PRO:CG	1:A:49:ARG:HG3	0.46	2.39	2	1
1:A:12:GLY:C	1:A:14:PRO:HD2	0.46	2.31	6	10
1:A:28:GLN:O	1:A:34:CYS:HB2	0.46	2.09	14	1
1:A:56:ASP:O	1:A:57:ASP:OD2	0.46	2.33	1	3
1:A:10:SER:O	1:A:13:ASN:N	0.46	2.43	2	3
1:A:28:GLN:CG	1:A:28:GLN:O	0.46	2.64	4	1
1:A:4:GLU:OE1	1:A:48:ARG:NH1	0.46	2.48	18	1
1:A:42:LYS:CA	1:A:59:CYS:O	0.46	2.63	9	1
1:A:23:LEU:HD21	1:A:27:ALA:CB	0.46	2.39	11	1
1:A:42:LYS:HD2	1:A:61:GLY:CA	0.46	2.41	19	1
1:A:10:SER:O	1:A:12:GLY:N	0.46	2.49	2	1
1:A:56:ASP:HB2	1:A:72:HIS:CB	0.46	2.40	4	1
1:A:5:GLU:O	1:A:6:CYS:HB2	0.46	2.09	17	5
1:A:21:CYS:HB3	1:A:36:ASP:CB	0.46	2.40	10	4
1:A:6:CYS:O	1:A:15:CYS:SG	0.46	2.73	14	2
1:A:31:GLU:HG2	1:A:48:ARG:NH2	0.46	2.26	13	1
1:A:21:CYS:HA	1:A:36:ASP:OD2	0.46	2.10	12	2
1:A:22:LYS:HA	1:A:36:ASP:OD2	0.46	2.08	15	2
1:A:41:MET:HG3	1:A:45:THR:CG2	0.46	2.41	10	2
1:A:35:CYS:O	1:A:35:CYS:SG	0.46	2.74	13	1
1:A:60:ASN:O	1:A:61:GLY:C	0.46	2.53	18	4
1:A:14:PRO:HB2	1:A:36:ASP:OD2	0.46	2.11	18	3
1:A:42:LYS:HD3	1:A:62:ILE:HD12	0.46	1.87	12	1
1:A:70:PRO:HG2	1:A:71:PHE:CZ	0.46	2.46	11	1
1:A:57:ASP:OD2	1:A:66:CYS:SG	0.46	2.74	13	2
1:A:38:CYS:O	1:A:39:ARG:HG2	0.46	2.11	14	2
1:A:15:CYS:O	1:A:16:CYS:SG	0.46	2.74	6	4
1:A:69:ASN:CB	1:A:70:PRO:HD3	0.46	2.40	17	1
1:A:25:GLN:O	1:A:26:GLY:O	0.46	2.33	15	1
1:A:46:ILE:O	1:A:59:CYS:SG	0.46	2.74	15	6
1:A:40:PHE:HB2	1:A:62:ILE:O	0.46	2.11	17	7
1:A:71:PHE:O	1:A:72:HIS:C	0.46	2.54	10	6
1:A:17:ASP:OD2	1:A:20:THR:CA	0.46	2.64	2	1
1:A:56:ASP:OD1	1:A:72:HIS:O	0.46	2.34	13	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:PHE:CD1	1:A:64:ALA:N	0.46	2.84	1	1
1:A:41:MET:HB2	1:A:45:THR:OG1	0.46	2.11	9	2
1:A:62:ILE:CD1	1:A:62:ILE:C	0.46	2.84	9	1
1:A:23:LEU:HD23	1:A:23:LEU:O	0.46	2.11	1	3
1:A:4:GLU:OE2	1:A:29:CYS:O	0.46	2.34	8	3
1:A:9:GLY:O	1:A:15:CYS:CB	0.46	2.64	12	1
1:A:46:ILE:HA	1:A:57:ASP:O	0.45	2.11	10	7
1:A:38:CYS:O	1:A:39:ARG:HG3	0.45	2.11	13	3
1:A:27:ALA:O	1:A:34:CYS:SG	0.45	2.74	10	2
1:A:11:PRO:CB	1:A:49:ARG:HG2	0.45	2.41	9	2
1:A:21:CYS:HB2	1:A:36:ASP:HB2	0.45	1.86	11	2
1:A:22:LYS:N	1:A:36:ASP:OD2	0.45	2.49	12	1
1:A:56:ASP:OD1	1:A:56:ASP:N	0.45	2.49	12	1
1:A:56:ASP:O	1:A:57:ASP:CG	0.45	2.55	14	4
1:A:42:LYS:O	1:A:43:GLU:HB2	0.45	2.11	20	3
1:A:48:ARG:HA	1:A:57:ASP:HB2	0.45	1.88	13	2
1:A:47:CYS:SG	1:A:58:TYR:O	0.45	2.74	17	1
1:A:23:LEU:HD23	1:A:36:ASP:OD1	0.45	2.12	9	1
1:A:21:CYS:HB3	1:A:36:ASP:N	0.45	2.26	16	1
1:A:9:GLY:O	1:A:10:SER:OG	0.45	2.33	7	4
1:A:68:ARG:O	1:A:69:ASN:OD1	0.45	2.34	20	1
1:A:4:GLU:O	1:A:5:GLU:HG2	0.45	2.11	17	1
1:A:47:CYS:SG	1:A:57:ASP:CB	0.45	3.04	1	1
1:A:12:GLY:O	1:A:14:PRO:HD2	0.45	2.12	17	6
1:A:28:GLN:HG3	1:A:38:CYS:C	0.45	2.32	3	8
1:A:31:GLU:OE1	1:A:31:GLU:O	0.45	2.34	5	1
1:A:21:CYS:O	1:A:36:ASP:CG	0.45	2.55	14	2
1:A:49:ARG:HG2	1:A:56:ASP:O	0.45	2.10	14	1
1:A:23:LEU:O	1:A:25:GLN:O	0.45	2.34	9	1
1:A:33:LEU:HD11	1:A:64:ALA:CA	0.45	2.41	6	2
1:A:33:LEU:HD22	1:A:34:CYS:N	0.45	2.26	10	2
1:A:62:ILE:HG22	1:A:66:CYS:CA	0.45	2.41	14	1
1:A:10:SER:HB3	1:A:32:GLY:C	0.45	2.31	9	3
1:A:34:CYS:SG	1:A:36:ASP:O	0.45	2.74	11	1
1:A:21:CYS:CA	1:A:36:ASP:OD1	0.45	2.64	19	1
1:A:14:PRO:HG2	1:A:36:ASP:OD2	0.45	2.12	2	1
1:A:43:GLU:C	1:A:59:CYS:O	0.45	2.55	1	7
1:A:47:CYS:SG	1:A:57:ASP:OD1	0.45	2.74	15	1
1:A:21:CYS:HB2	1:A:36:ASP:CB	0.45	2.40	3	1
1:A:62:ILE:CA	1:A:65:GLY:O	0.45	2.64	10	1
1:A:27:ALA:C	1:A:34:CYS:SG	0.45	2.95	4	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:GLY:HA3	1:A:13:ASN:O	0.45	2.12	11	4
1:A:14:PRO:HG2	1:A:21:CYS:HA	0.45	1.89	14	2
1:A:36:ASP:CG	1:A:38:CYS:SG	0.45	2.96	8	2
1:A:15:CYS:O	1:A:27:ALA:HB2	0.45	2.12	9	1
1:A:40:PHE:O	1:A:41:MET:C	0.45	2.55	11	1
1:A:40:PHE:HZ	1:A:64:ALA:HB2	0.45	1.72	6	1
1:A:41:MET:HA	1:A:41:MET:CE	0.44	2.42	10	1
1:A:6:CYS:O	1:A:31:GLU:HB2	0.44	2.13	14	3
1:A:15:CYS:HB3	1:A:27:ALA:CA	0.44	2.42	2	1
1:A:36:ASP:C	1:A:38:CYS:N	0.44	2.70	16	6
1:A:34:CYS:O	1:A:64:ALA:CA	0.44	2.65	7	1
1:A:28:GLN:HB3	1:A:39:ARG:O	0.44	2.12	9	7
1:A:29:CYS:C	1:A:32:GLY:O	0.44	2.56	9	5
1:A:9:GLY:O	1:A:31:GLU:OE1	0.44	2.35	14	1
1:A:33:LEU:HG	1:A:65:GLY:O	0.44	2.11	17	5
1:A:21:CYS:HB3	1:A:36:ASP:HB3	0.44	1.89	4	3
1:A:33:LEU:CD1	1:A:34:CYS:N	0.44	2.80	9	1
1:A:41:MET:SD	1:A:45:THR:OG1	0.44	2.74	16	1
1:A:25:GLN:O	1:A:25:GLN:OE1	0.44	2.35	16	1
1:A:43:GLU:O	1:A:45:THR:OG1	0.44	2.35	1	1
1:A:10:SER:OG	1:A:32:GLY:HA3	0.44	2.13	3	1
1:A:21:CYS:C	1:A:36:ASP:OD2	0.44	2.55	12	1
1:A:58:TYR:HB2	1:A:71:PHE:CZ	0.44	2.48	11	1
1:A:59:CYS:SG	1:A:62:ILE:CG1	0.44	3.06	17	2
1:A:14:PRO:HG3	1:A:36:ASP:N	0.44	2.28	17	4
1:A:59:CYS:SG	1:A:62:ILE:HG13	0.44	2.52	17	2
1:A:43:GLU:O	1:A:43:GLU:CG	0.44	2.66	4	1
1:A:58:TYR:CG	1:A:71:PHE:CE2	0.44	3.05	4	1
1:A:62:ILE:HB	1:A:65:GLY:O	0.44	2.13	4	3
1:A:32:GLY:O	1:A:46:ILE:O	0.44	2.36	4	2
1:A:42:LYS:O	1:A:42:LYS:HG3	0.44	2.12	20	1
1:A:21:CYS:C	1:A:36:ASP:OD1	0.44	2.56	15	1
1:A:46:ILE:C	1:A:59:CYS:SG	0.44	2.96	11	10
1:A:42:LYS:NZ	1:A:42:LYS:HB2	0.44	2.27	10	1
1:A:11:PRO:HG3	1:A:48:ARG:O	0.44	2.13	2	2
1:A:41:MET:CE	1:A:45:THR:HG21	0.44	2.43	14	1
1:A:47:CYS:SG	1:A:57:ASP:CG	0.44	2.96	13	3
1:A:6:CYS:SG	1:A:9:GLY:N	0.44	2.91	17	2
1:A:14:PRO:HB3	1:A:34:CYS:HB2	0.44	1.89	11	1
1:A:23:LEU:HD21	1:A:36:ASP:OD1	0.44	2.13	10	1
1:A:57:ASP:HA	1:A:71:PHE:CB	0.44	2.43	20	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:HIS:CG	1:A:72:HIS:O	0.44	2.70	15	1
1:A:41:MET:CG	1:A:45:THR:HG21	0.43	2.43	17	1
1:A:42:LYS:O	1:A:42:LYS:HD2	0.43	2.12	9	1
1:A:21:CYS:O	1:A:22:LYS:HG2	0.43	2.13	19	1
1:A:62:ILE:HD13	1:A:62:ILE:C	0.43	2.33	17	3
1:A:58:TYR:N	1:A:58:TYR:CD1	0.43	2.84	14	1
1:A:62:ILE:CG2	1:A:67:PRO:CD	0.43	2.96	16	2
1:A:35:CYS:SG	1:A:35:CYS:O	0.43	2.77	15	1
1:A:62:ILE:HA	1:A:65:GLY:O	0.43	2.14	10	1
1:A:47:CYS:HB3	1:A:57:ASP:HB3	0.43	1.90	14	1
1:A:6:CYS:HB3	1:A:31:GLU:HB2	0.43	1.88	16	2
1:A:23:LEU:O	1:A:24:ARG:C	0.43	2.56	9	1
1:A:68:ARG:O	1:A:69:ASN:CG	0.43	2.57	7	3
1:A:21:CYS:O	1:A:36:ASP:HB2	0.43	2.13	4	2
1:A:20:THR:CG2	1:A:20:THR:O	0.43	2.65	3	1
1:A:49:ARG:HD3	1:A:57:ASP:OD1	0.43	2.13	16	1
1:A:14:PRO:HB3	1:A:34:CYS:CB	0.43	2.43	2	3
1:A:43:GLU:N	1:A:60:ASN:HA	0.43	2.29	14	1
1:A:5:GLU:O	1:A:6:CYS:HB3	0.43	2.14	4	4
1:A:31:GLU:O	1:A:48:ARG:CZ	0.43	2.66	9	1
1:A:14:PRO:CG	1:A:21:CYS:CB	0.43	2.97	16	1
1:A:28:GLN:O	1:A:29:CYS:C	0.43	2.57	19	2
1:A:14:PRO:HD2	1:A:21:CYS:SG	0.43	2.54	5	2
1:A:28:GLN:CB	1:A:39:ARG:O	0.43	2.66	10	5
1:A:17:ASP:CB	1:A:21:CYS:HA	0.43	2.44	2	1
1:A:32:GLY:HA3	1:A:48:ARG:HB2	0.43	1.89	4	1
1:A:23:LEU:C	1:A:25:GLN:N	0.43	2.72	9	1
1:A:21:CYS:O	1:A:22:LYS:HG3	0.43	2.14	5	1
1:A:45:THR:OG1	1:A:59:CYS:SG	0.43	2.77	10	1
1:A:40:PHE:CD1	1:A:40:PHE:N	0.43	2.87	18	1
1:A:14:PRO:CG	1:A:21:CYS:HB3	0.43	2.44	16	1
1:A:42:LYS:HG3	1:A:60:ASN:O	0.43	2.14	5	2
1:A:28:GLN:HG2	1:A:40:PHE:HA	0.43	1.91	4	1
1:A:14:PRO:CD	1:A:35:CYS:HB3	0.43	2.43	15	3
1:A:15:CYS:CB	1:A:27:ALA:CA	0.43	2.97	2	1
1:A:43:GLU:O	1:A:43:GLU:HG2	0.43	2.13	4	1
1:A:6:CYS:CB	1:A:31:GLU:CB	0.43	2.96	13	1
1:A:37:GLN:O	1:A:39:ARG:CZ	0.43	2.67	19	1
1:A:47:CYS:SG	1:A:66:CYS:N	0.43	2.92	10	1
1:A:28:GLN:O	1:A:29:CYS:HB2	0.43	2.14	2	1
1:A:5:GLU:O	1:A:31:GLU:HB2	0.43	2.14	2	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:LEU:HD11	1:A:27:ALA:HB3	0.43	1.91	15	2
1:A:29:CYS:CB	1:A:45:THR:HG21	0.43	2.44	16	1
1:A:6:CYS:O	1:A:31:GLU:CD	0.43	2.57	1	2
1:A:17:ASP:HB2	1:A:20:THR:C	0.43	2.34	7	1
1:A:17:ASP:HB2	1:A:21:CYS:CA	0.42	2.44	2	1
1:A:14:PRO:HG3	1:A:35:CYS:N	0.42	2.29	6	3
1:A:29:CYS:SG	1:A:62:ILE:HG12	0.42	2.55	19	2
1:A:10:SER:CA	1:A:33:LEU:O	0.42	2.67	19	1
1:A:6:CYS:C	1:A:7:ASP:OD1	0.42	2.57	5	1
1:A:57:ASP:OD1	1:A:71:PHE:HB3	0.42	2.13	10	1
1:A:57:ASP:N	1:A:71:PHE:HB3	0.42	2.29	13	1
1:A:6:CYS:O	1:A:7:ASP:CG	0.42	2.57	11	1
1:A:12:GLY:C	1:A:14:PRO:CD	0.42	2.87	19	2
1:A:45:THR:HB	1:A:59:CYS:SG	0.42	2.55	10	1
1:A:11:PRO:HB3	1:A:48:ARG:O	0.42	2.13	4	1
1:A:38:CYS:SG	1:A:40:PHE:CZ	0.42	3.13	18	1
1:A:39:ARG:HB2	1:A:39:ARG:NH1	0.42	2.30	18	1
1:A:14:PRO:HB3	1:A:34:CYS:SG	0.42	2.54	16	5
1:A:29:CYS:HA	1:A:32:GLY:O	0.42	2.15	9	3
1:A:31:GLU:CG	1:A:31:GLU:O	0.42	2.66	15	1
1:A:41:MET:HG3	1:A:45:THR:OG1	0.42	2.14	20	1
1:A:33:LEU:HD12	1:A:40:PHE:CE2	0.42	2.48	9	1
1:A:42:LYS:HD3	1:A:60:ASN:O	0.42	2.14	11	1
1:A:22:LYS:NZ	1:A:37:GLN:HG3	0.42	2.29	19	1
1:A:47:CYS:C	1:A:57:ASP:HB3	0.42	2.34	8	1
1:A:31:GLU:OE1	1:A:31:GLU:C	0.42	2.58	16	1
1:A:42:LYS:HD3	1:A:62:ILE:CD1	0.42	2.44	12	1
1:A:13:ASN:O	1:A:14:PRO:O	0.42	2.38	19	1
1:A:31:GLU:O	1:A:48:ARG:HG3	0.42	2.15	10	4
1:A:49:ARG:HG3	1:A:57:ASP:OD2	0.42	2.14	17	1
1:A:4:GLU:C	1:A:5:GLU:CG	0.42	2.88	17	1
1:A:4:GLU:OE1	1:A:48:ARG:HD2	0.42	2.14	15	1
1:A:44:GLY:CA	1:A:60:ASN:HD21	0.42	2.28	9	2
1:A:15:CYS:CB	1:A:30:ALA:CB	0.42	2.97	3	2
1:A:14:PRO:CG	1:A:35:CYS:HB3	0.42	2.45	14	2
1:A:45:THR:HB	1:A:59:CYS:CB	0.42	2.45	4	1
1:A:22:LYS:HA	1:A:36:ASP:CG	0.42	2.35	11	1
1:A:49:ARG:HG3	1:A:57:ASP:OD1	0.42	2.14	11	1
1:A:41:MET:HG2	1:A:45:THR:OG1	0.42	2.15	6	1
1:A:28:GLN:HG3	1:A:38:CYS:O	0.42	2.13	19	3
1:A:60:ASN:O	1:A:62:ILE:HG23	0.42	2.15	19	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASN:C	1:A:62:ILE:N	0.42	2.72	1	3
1:A:28:GLN:O	1:A:34:CYS:HB3	0.42	2.15	8	1
1:A:40:PHE:O	1:A:42:LYS:HG2	0.42	2.15	4	1
1:A:17:ASP:HB2	1:A:21:CYS:N	0.42	2.29	2	1
1:A:67:PRO:CG	1:A:71:PHE:CE1	0.42	3.03	4	1
1:A:34:CYS:O	1:A:40:PHE:CE2	0.41	2.73	15	1
1:A:6:CYS:O	1:A:31:GLU:HB3	0.41	2.14	15	1
1:A:7:ASP:CB	1:A:31:GLU:OE1	0.41	2.68	7	1
1:A:56:ASP:HA	1:A:72:HIS:CB	0.41	2.44	13	1
1:A:22:LYS:N	1:A:36:ASP:CG	0.41	2.73	15	1
1:A:57:ASP:OD1	1:A:70:PRO:HA	0.41	2.14	12	1
1:A:33:LEU:HD12	1:A:65:GLY:N	0.41	2.30	11	1
1:A:14:PRO:O	1:A:27:ALA:CB	0.41	2.68	5	1
1:A:38:CYS:O	1:A:39:ARG:HB3	0.41	2.15	14	1
1:A:28:GLN:HG2	1:A:38:CYS:HB2	0.41	1.89	2	1
1:A:32:GLY:O	1:A:33:LEU:C	0.41	2.58	18	2
1:A:21:CYS:CA	1:A:36:ASP:HB3	0.41	2.44	9	1
1:A:31:GLU:HG3	1:A:48:ARG:NH2	0.41	2.29	9	1
1:A:25:GLN:NE2	1:A:25:GLN:HA	0.41	2.30	6	1
1:A:39:ARG:NH1	1:A:39:ARG:HB2	0.41	2.31	19	1
1:A:36:ASP:HB3	1:A:38:CYS:SG	0.41	2.55	5	1
1:A:32:GLY:HA2	1:A:46:ILE:CG2	0.41	2.45	10	1
1:A:14:PRO:C	1:A:27:ALA:HB2	0.41	2.35	2	1
1:A:69:ASN:HB2	1:A:71:PHE:CZ	0.41	2.50	3	1
1:A:42:LYS:HD2	1:A:61:GLY:HA2	0.41	1.92	17	2
1:A:69:ASN:HB3	1:A:70:PRO:HD2	0.41	1.92	13	1
1:A:21:CYS:HB3	1:A:36:ASP:HB2	0.41	1.93	16	1
1:A:70:PRO:C	1:A:71:PHE:CG	0.41	2.94	19	1
1:A:62:ILE:HG21	1:A:67:PRO:HD3	0.41	1.92	10	1
1:A:10:SER:CB	1:A:32:GLY:N	0.41	2.84	20	1
1:A:41:MET:HG3	1:A:45:THR:HG21	0.41	1.93	2	1
1:A:36:ASP:OD1	1:A:38:CYS:N	0.41	2.48	8	1
1:A:45:THR:O	1:A:46:ILE:HB	0.41	2.15	13	1
1:A:42:LYS:HG2	1:A:62:ILE:CD1	0.41	2.45	16	1
1:A:23:LEU:CD2	1:A:23:LEU:H	0.41	2.28	1	1
1:A:21:CYS:HB3	1:A:36:ASP:OD1	0.41	2.15	19	1
1:A:15:CYS:HB3	1:A:27:ALA:HA	0.41	1.91	4	1
1:A:72:HIS:O	1:A:73:ALA:C	0.41	2.58	9	1
1:A:14:PRO:O	1:A:17:ASP:OD1	0.41	2.38	12	1
1:A:20:THR:C	1:A:22:LYS:N	0.41	2.73	11	1
1:A:14:PRO:HG3	1:A:21:CYS:SG	0.41	2.56	5	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ARG:NE	1:A:66:CYS:SG	0.41	2.94	5	1
1:A:10:SER:CB	1:A:32:GLY:CA	0.41	2.99	10	2
1:A:45:THR:CB	1:A:59:CYS:SG	0.41	3.09	10	1
1:A:14:PRO:HG3	1:A:35:CYS:HB3	0.41	1.91	14	1
1:A:44:GLY:HA2	1:A:58:TYR:HB3	0.41	1.90	14	1
1:A:68:ARG:HB3	1:A:68:ARG:NH1	0.41	2.30	20	1
1:A:21:CYS:O	1:A:36:ASP:HB3	0.41	2.16	2	1
1:A:6:CYS:N	1:A:31:GLU:HB2	0.41	2.31	13	1
1:A:10:SER:HB3	1:A:33:LEU:O	0.41	2.15	9	1
1:A:56:ASP:HB2	1:A:72:HIS:O	0.41	2.16	11	1
1:A:7:ASP:HB3	1:A:31:GLU:OE1	0.41	2.16	7	1
1:A:49:ARG:CZ	1:A:49:ARG:HB3	0.41	2.46	7	1
1:A:45:THR:O	1:A:58:TYR:HA	0.41	2.16	17	1
1:A:4:GLU:C	1:A:5:GLU:HG3	0.41	2.36	17	1
1:A:42:LYS:HG3	1:A:42:LYS:O	0.41	2.16	18	2
1:A:14:PRO:HD3	1:A:35:CYS:HB3	0.41	1.92	15	1
1:A:60:ASN:H	1:A:62:ILE:HG23	0.41	1.76	15	1
1:A:14:PRO:CB	1:A:36:ASP:CG	0.41	2.89	18	1
1:A:41:MET:CB	1:A:45:THR:CB	0.41	2.99	16	1
1:A:46:ILE:N	1:A:59:CYS:HB3	0.40	2.30	10	1
1:A:33:LEU:HD21	1:A:62:ILE:HG12	0.40	1.92	4	1
1:A:25:GLN:O	1:A:25:GLN:CG	0.40	2.68	16	1
1:A:45:THR:O	1:A:46:ILE:CB	0.40	2.68	13	1
1:A:47:CYS:CB	1:A:62:ILE:HG21	0.40	2.46	13	1
1:A:41:MET:HG3	1:A:45:THR:HG23	0.40	1.93	17	1
1:A:25:GLN:O	1:A:25:GLN:HG3	0.40	2.16	16	1
1:A:48:ARG:CZ	1:A:56:ASP:OD1	0.40	2.69	7	1
1:A:26:GLY:O	1:A:28:GLN:N	0.40	2.55	2	1
1:A:6:CYS:HB3	1:A:31:GLU:HB3	0.40	1.93	13	1
1:A:37:GLN:O	1:A:39:ARG:HG2	0.40	2.16	13	1
1:A:46:ILE:N	1:A:59:CYS:HB2	0.40	2.31	17	1
1:A:23:LEU:HD21	1:A:27:ALA:H	0.40	1.76	11	1
1:A:71:PHE:O	1:A:72:HIS:HB3	0.40	2.17	11	1
1:A:9:GLY:HA3	1:A:31:GLU:OE1	0.40	2.16	1	1
1:A:10:SER:O	1:A:14:PRO:HA	0.40	2.17	19	1
1:A:44:GLY:C	1:A:58:TYR:HB3	0.40	2.37	14	1
1:A:49:ARG:HD2	1:A:57:ASP:OD2	0.40	2.17	8	1
1:A:28:GLN:HG3	1:A:38:CYS:CB	0.40	2.46	13	1
1:A:23:LEU:N	1:A:36:ASP:OD2	0.40	2.54	15	1
1:A:41:MET:CG	1:A:45:THR:CG2	0.40	2.99	17	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	63/73 (86%)	25±2 (40±4%)	18±3 (28±4%)	20±2 (32±3%)	0	0
All	All	1260/1460 (86%)	504 (40%)	358 (28%)	398 (32%)	0	0

All 40 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	21	CYS	20
1	A	15	CYS	20
1	A	39	ARG	20
1	A	67	PRO	20
1	A	48	ARG	20
1	A	14	PRO	18
1	A	16	CYS	18
1	A	30	ALA	17
1	A	38	CYS	17
1	A	19	ALA	16
1	A	10	SER	15
1	A	57	ASP	15
1	A	6	CYS	15
1	A	42	LYS	14
1	A	64	ALA	13
1	A	41	MET	12
1	A	46	ILE	12
1	A	44	GLY	12
1	A	26	GLY	12
1	A	28	GLN	8
1	A	11	PRO	7
1	A	18	ALA	7
1	A	17	ASP	7
1	A	5	GLU	6
1	A	33	LEU	6
1	A	43	GLU	6
1	A	22	LYS	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	4	GLU	5
1	A	49	ARG	4
1	A	70	PRO	4
1	A	72	HIS	4
1	A	35	CYS	4
1	A	27	ALA	3
1	A	37	GLN	3
1	A	71	PHE	3
1	A	45	THR	3
1	A	69	ASN	3
1	A	62	ILE	2
1	A	60	ASN	1
1	A	24	ARG	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	51/56 (91%)	35±2 (68±3%)	16±2 (32±3%)	1	14
All	All	1020/1120 (91%)	698 (68%)	322 (32%)	1	14

All 37 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	62	ILE	20
1	A	46	ILE	20
1	A	33	LEU	20
1	A	35	CYS	18
1	A	23	LEU	16
1	A	41	MET	15
1	A	42	LYS	14
1	A	34	CYS	14
1	A	28	GLN	13
1	A	38	CYS	11
1	A	39	ARG	11
1	A	16	CYS	11

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	57	ASP	11
1	A	49	ARG	11
1	A	47	CYS	10
1	A	31	GLU	10
1	A	15	CYS	9
1	A	22	LYS	9
1	A	48	ARG	9
1	A	36	ASP	9
1	A	45	THR	7
1	A	25	GLN	7
1	A	68	ARG	6
1	A	20	THR	5
1	A	17	ASP	5
1	A	5	GLU	4
1	A	56	ASP	4
1	A	7	ASP	4
1	A	43	GLU	3
1	A	37	GLN	3
1	A	24	ARG	3
1	A	59	CYS	3
1	A	13	ASN	3
1	A	72	HIS	1
1	A	60	ASN	1
1	A	4	GLU	1
1	A	69	ASN	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 43% for the well-defined parts and 42% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5346

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	391
Number of shifts mapped to atoms	391
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

No chemical shift referencing corrections were calculated (not enough data).

#### 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 43%, i.e. 310 atoms were assigned a chemical shift out of a possible 715. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	124/312 (40%)	124/124 (100%)	0/128 (0%)	0/60 (0%)
Sidechain	174/369 (47%)	174/222 (78%)	0/124 (0%)	0/23 (0%)
Aromatic	12/34 (35%)	12/18 (67%)	0/14 (0%)	0/2 (0%)
Overall	310/715 (43%)	310/364 (85%)	0/266 (0%)	0/85 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 42%, i.e. 340 atoms were assigned a chemical shift out of a possible 806. 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	140/357 (39%)	140/142 (99%)	0/146 (0%)	0/69 (0%)
Sidechain	188/415 (45%)	188/248 (76%)	0/141 (0%)	0/26 (0%)
Aromatic	12/34 (35%)	12/18 (67%)	0/14 (0%)	0/2 (0%)
Overall	340/806 (42%)	340/408 (83%)	0/301 (0%)	0/97 (0%)

#### 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:

