



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:26 PM BST

PDB ID : 2GVA  
Title : REFINED SOLUTION STRUCTURE OF THE TYR 41-> HIS MUTANT OF THE M13 GENE V PROTEIN. A COMPARISON WITH THE CRYSTAL STRUCTURE  
Authors : Folkers, P.J.M.; Nilges, M.; Folmer, R.H.A.; Prompers, J.J.; Konings, R.N.H.; Hilbers, C.W.  
Deposited on : 1995-07-27

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

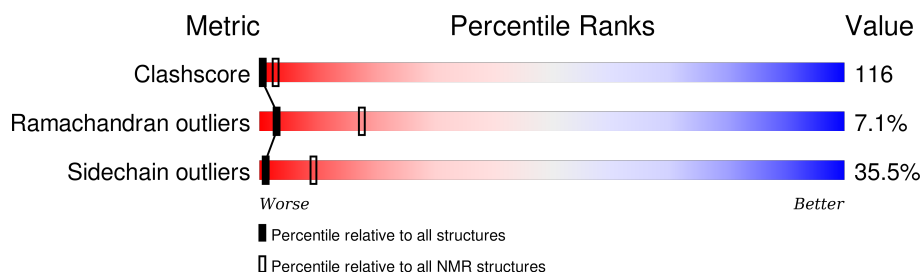
# 1 Overall quality at a glance

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	87	
1	B	87	

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 14 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:1-A:15, A:28-A:87, B:1-B:15, B:28-B:87 (150)	0.49	14

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5, 7, 10, 14, 15, 17, 19, 20, 24, 25, 26, 27, 28
2	1, 12, 16, 21, 29, 30
3	6, 22, 23
4	9, 13
Single-model clusters	8; 11; 18

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2760 atoms, of which 1400 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called GENE V PROTEIN.

Mol	Chain	Residues	Atoms						Trace
1	A	87	Total	C	H	N	O	S	0
			1380	435	700	117	125	3	
1	B	87	Total	C	H	N	O	S	0
			1380	435	700	117	125	3	

There are 2 discrepancies between the modelled and reference sequences:

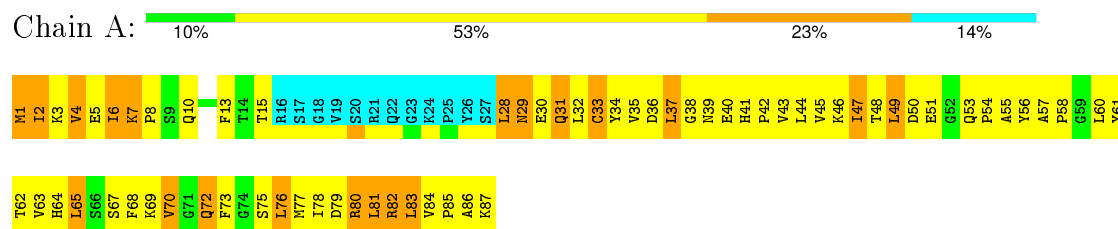
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	HIS	TYR	CONFLICT	UNP P69544
B	41	HIS	TYR	CONFLICT	UNP P69544

## 4 Residue-property plots

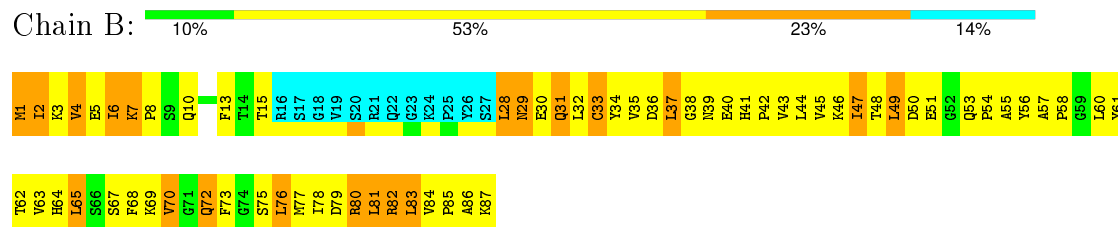
### 4.1 Average score per residue in the NMR ensemble

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

#### • Molecule 1: GENE V PROTEIN



#### • Molecule 1: GENE V PROTEIN

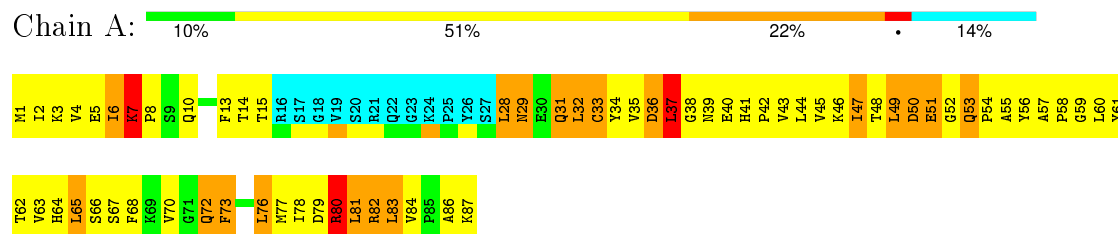


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

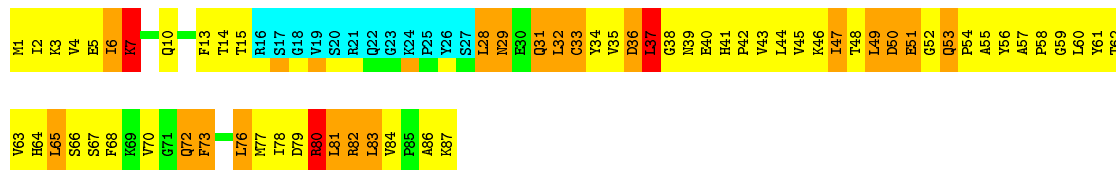
#### 4.2.1 Score per residue for model 1

#### • Molecule 1: GENE V PROTEIN



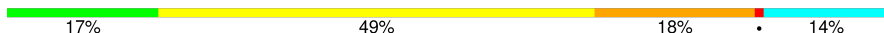
- Molecule 1: GENE V PROTEIN

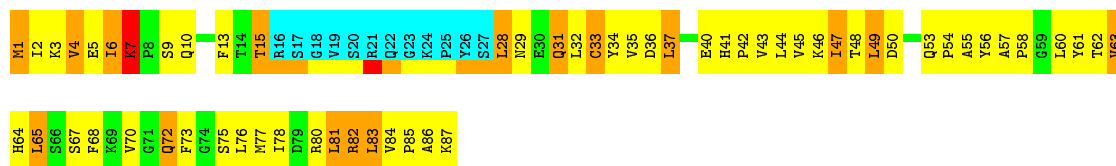
Chain B: 



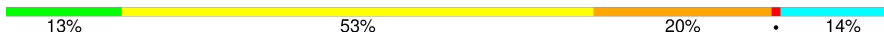
## 4.2.2 Score per residue for model 2

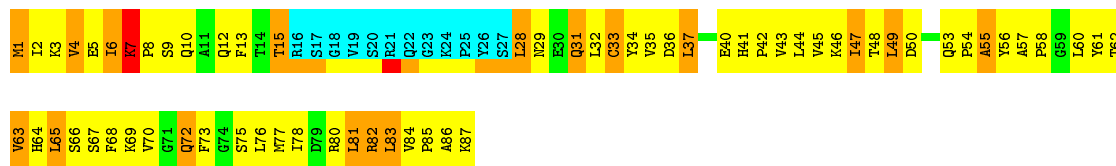
- Molecule 1: GENE V PROTEIN

Chain A: 



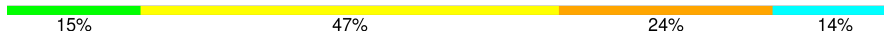
- Molecule 1: GENE V PROTEIN

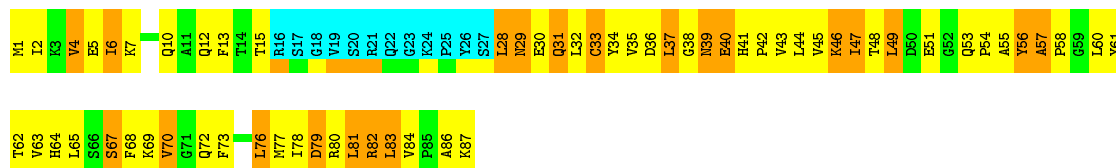
Chain B: 



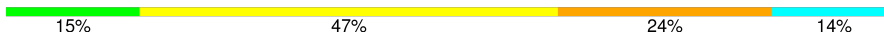
## 4.2.3 Score per residue for model 3

- Molecule 1: GENE V PROTEIN

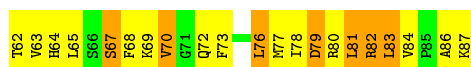
Chain A: 



- Molecule 1: GENE V PROTEIN

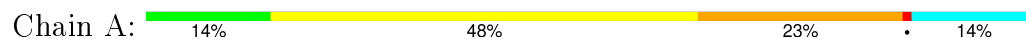
Chain B: 



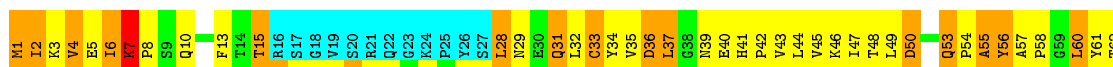
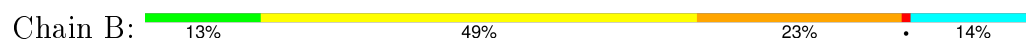


#### 4.2.4 Score per residue for model 4

- Molecule 1: GENE V PROTEIN

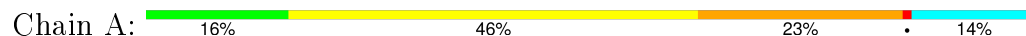


- Molecule 1: GENE V PROTEIN

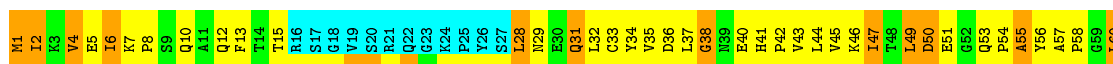
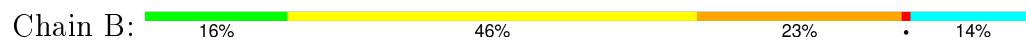


#### 4.2.5 Score per residue for model 5

- Molecule 1: GENE V PROTEIN

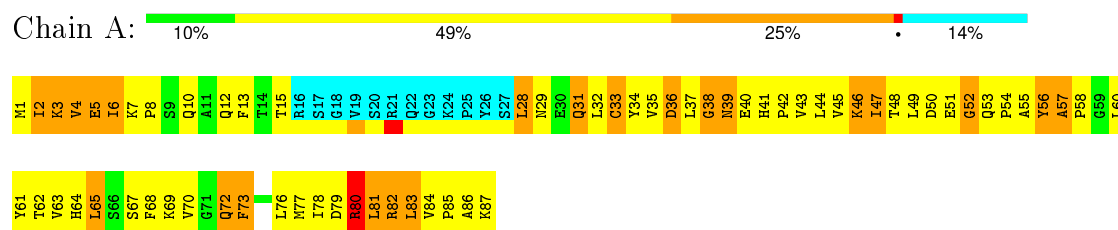


- Molecule 1: GENE V PROTEIN

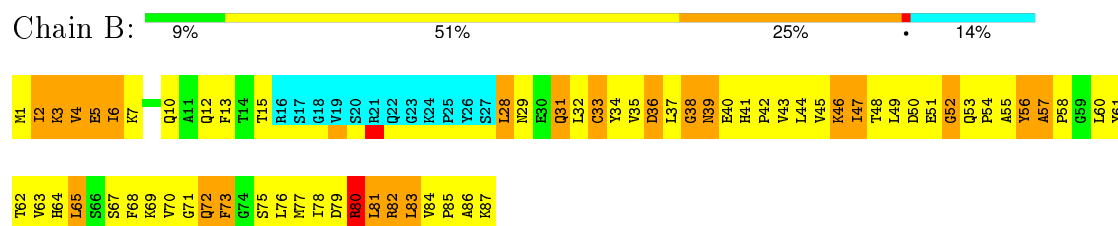


### 4.2.6 Score per residue for model 6

#### • Molecule 1: GENE V PROTEIN

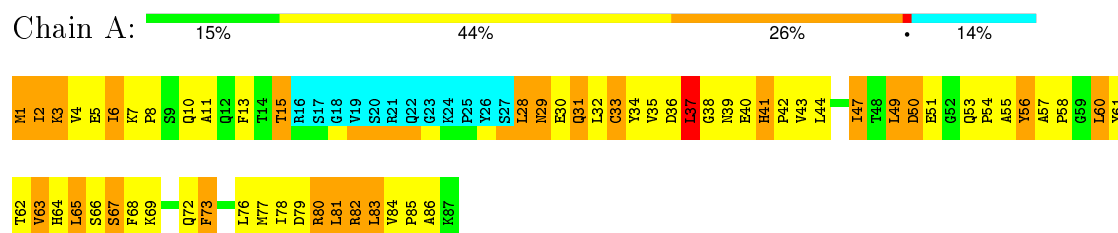


#### • Molecule 1: GENE V PROTEIN



### 4.2.7 Score per residue for model 7

#### • Molecule 1: GENE V PROTEIN

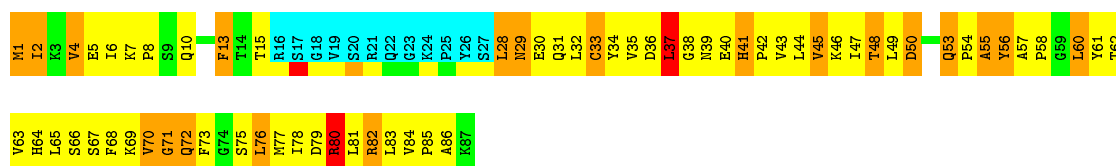






• Molecule 1: GENE V PROTEIN

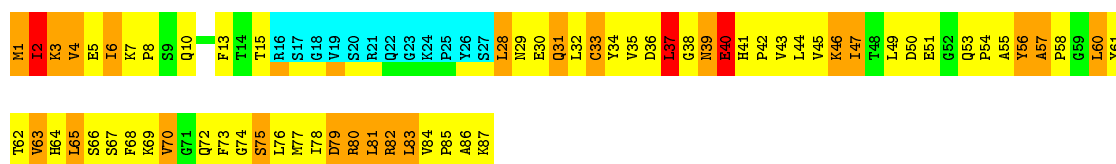
Chain B: 11% 49% 23% • 14%



#### 4.2.9 Score per residue for model 9

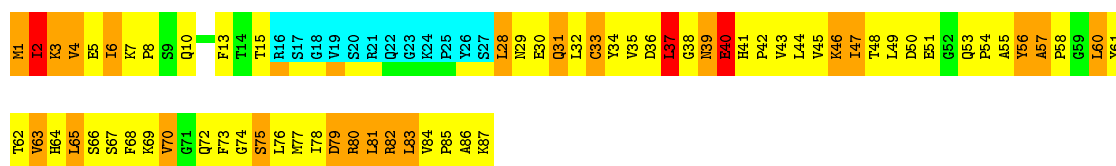
• Molecule 1: GENE V PROTEIN

Chain A: 9% 48% 25% • 14%



• Molecule 1: GENE V PROTEIN

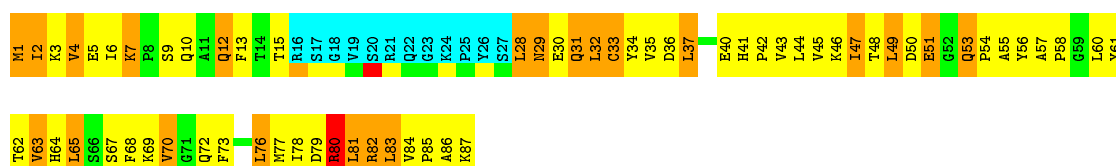
Chain B: 8% 49% 25% • 14%



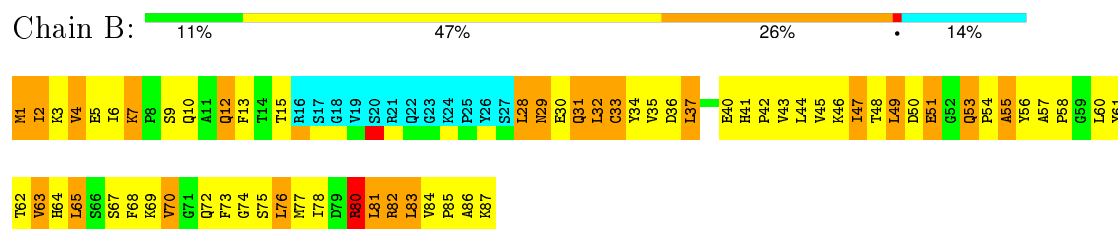
#### 4.2.10 Score per residue for model 10

• Molecule 1: GENE V PROTEIN

Chain A: 13% 47% 25% • 14%

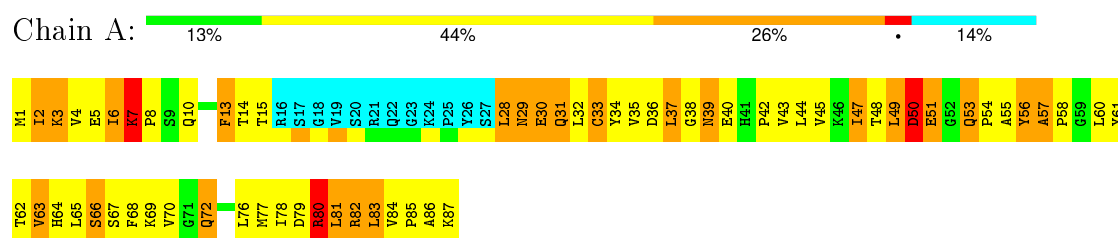


- Molecule 1: GENE V PROTEIN

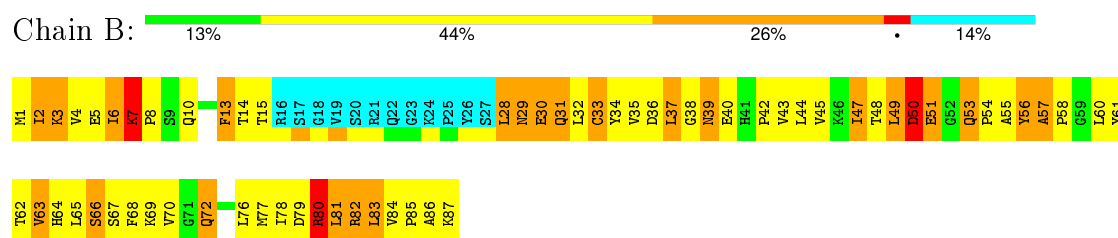


#### 4.2.11 Score per residue for model 11

- Molecule 1: GENE V PROTEIN

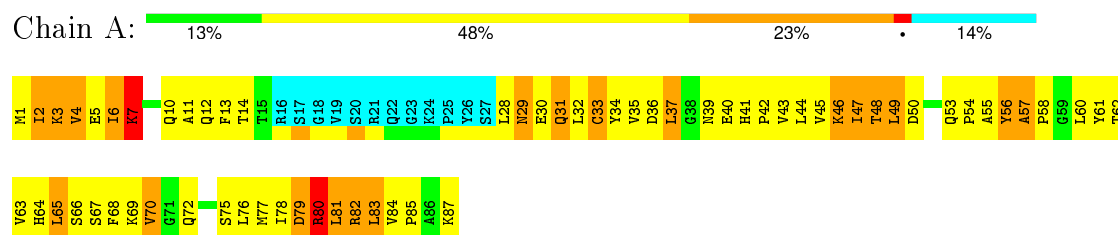


- Molecule 1: GENE V PROTEIN

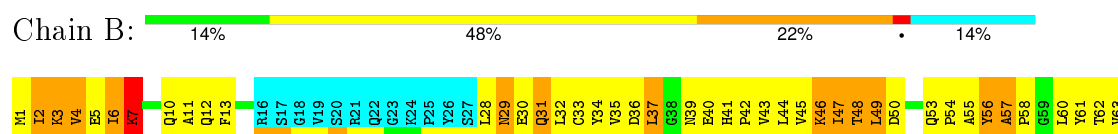


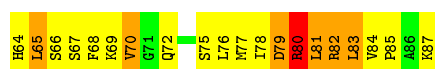
#### 4.2.12 Score per residue for model 12

- Molecule 1: GENE V PROTEIN



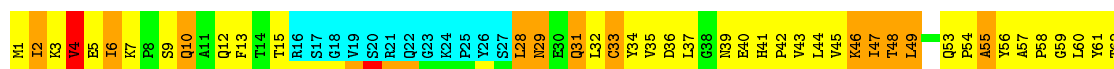
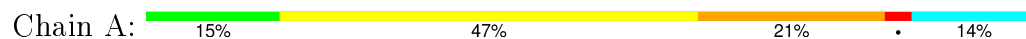
- Molecule 1: GENE V PROTEIN



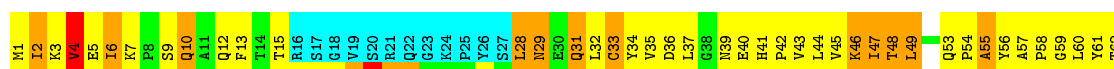
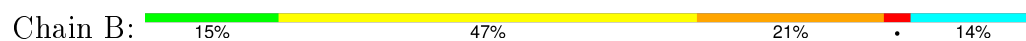


#### 4.2.13 Score per residue for model 13

- Molecule 1: GENE V PROTEIN



- Molecule 1: GENE V PROTEIN

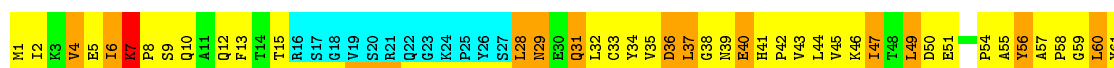
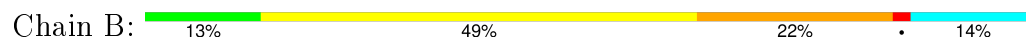


#### 4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: GENE V PROTEIN

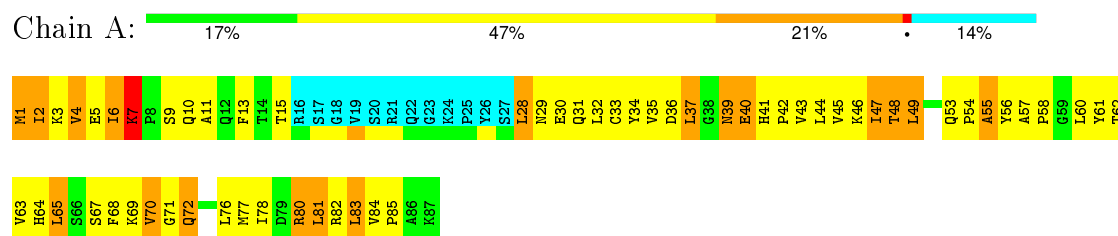


- Molecule 1: GENE V PROTEIN

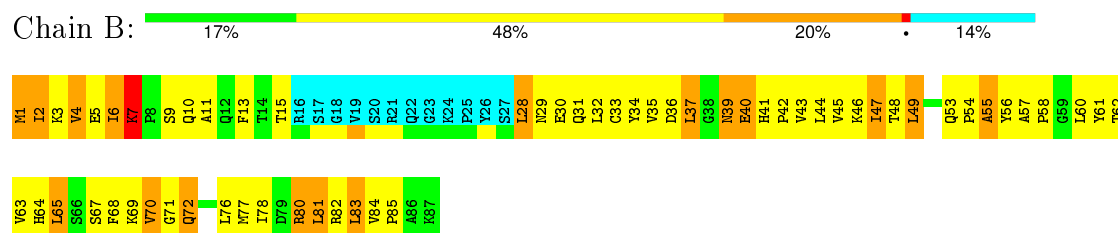


### 4.2.15 Score per residue for model 15

#### • Molecule 1: GENE V PROTEIN

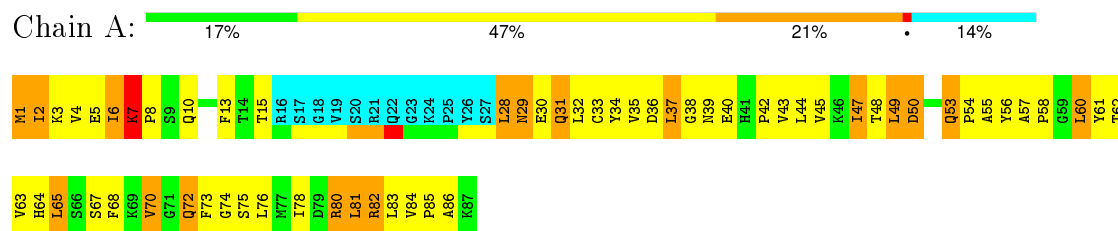


#### • Molecule 1: GENE V PROTEIN

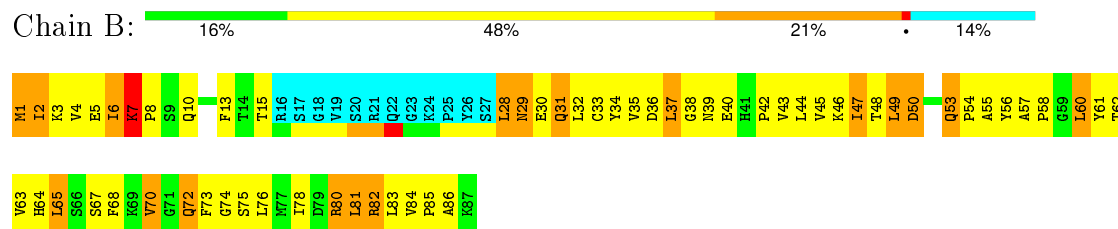


### 4.2.16 Score per residue for model 16

#### • Molecule 1: GENE V PROTEIN

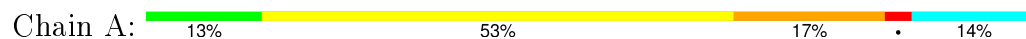


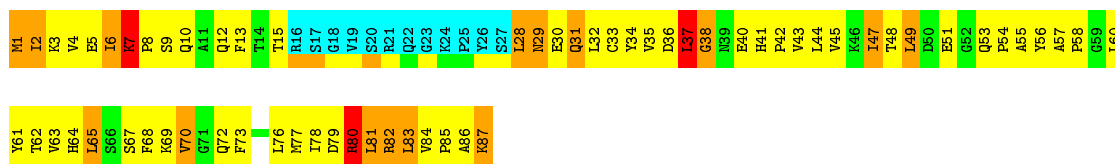
#### • Molecule 1: GENE V PROTEIN



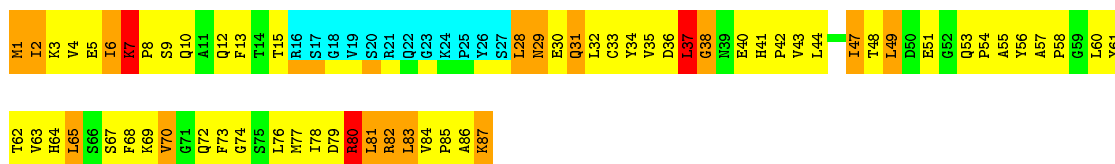
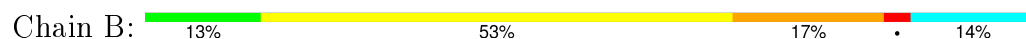
### 4.2.17 Score per residue for model 17

#### • Molecule 1: GENE V PROTEIN



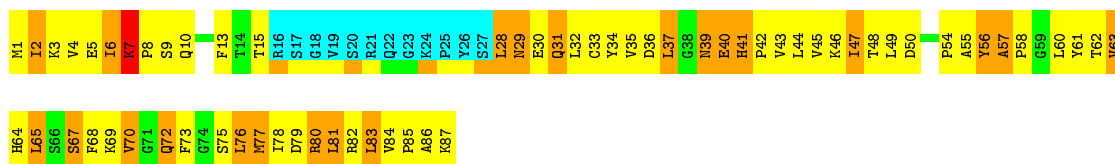


• Molecule 1: GENE V PROTEIN

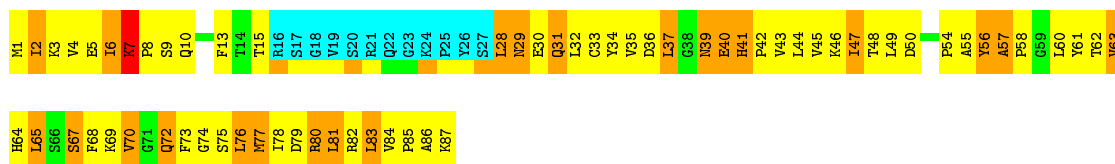


#### 4.2.18 Score per residue for model 18

• Molecule 1: GENE V PROTEIN

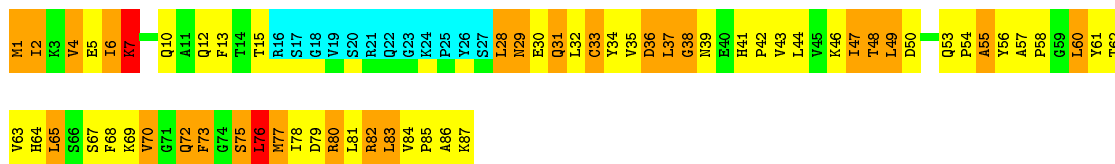


• Molecule 1: GENE V PROTEIN

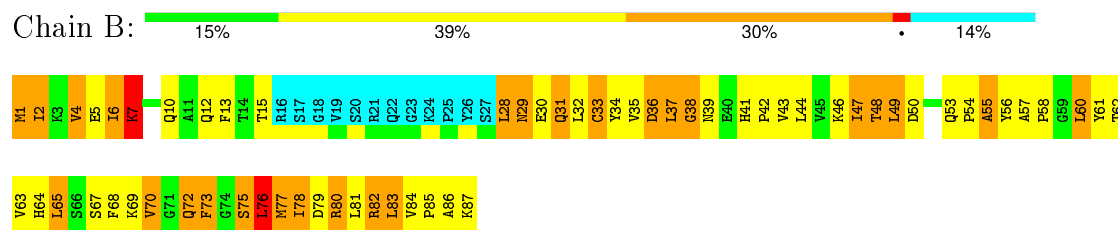


#### 4.2.19 Score per residue for model 19

• Molecule 1: GENE V PROTEIN

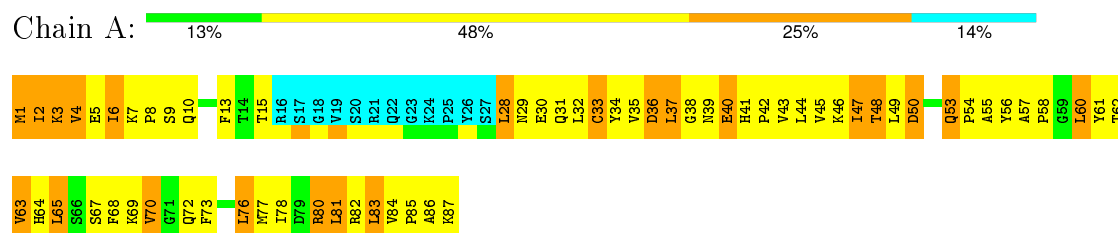


• Molecule 1: GENE V PROTEIN

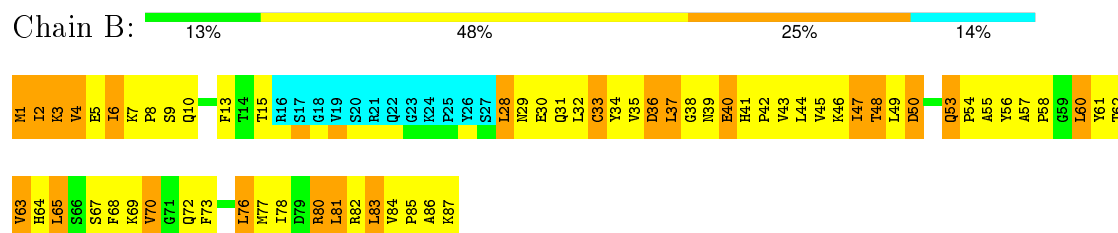


#### 4.2.20 Score per residue for model 20

- Molecule 1: GENE V PROTEIN

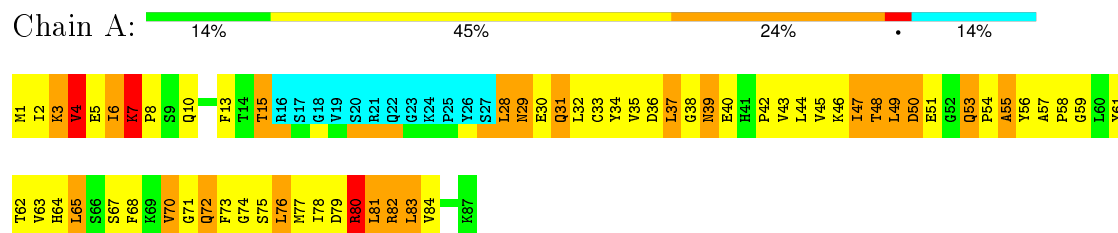


- Molecule 1: GENE V PROTEIN

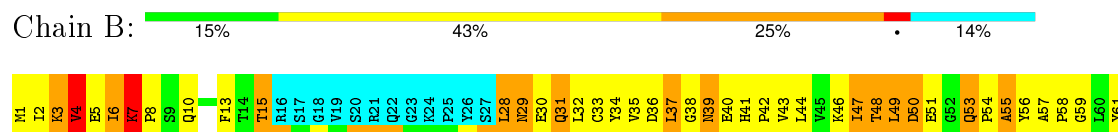


#### 4.2.21 Score per residue for model 21

- Molecule 1: GENE V PROTEIN



- Molecule 1: GENE V PROTEIN



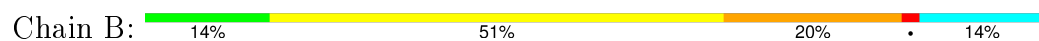


#### 4.2.22 Score per residue for model 22

- Molecule 1: GENE V PROTEIN

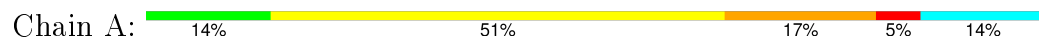


- Molecule 1: GENE V PROTEIN

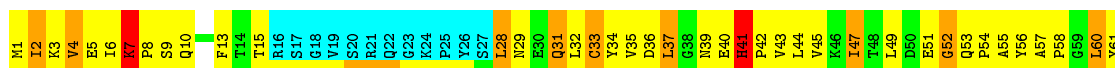
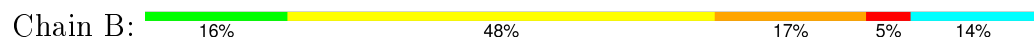


#### 4.2.23 Score per residue for model 23

- Molecule 1: GENE V PROTEIN

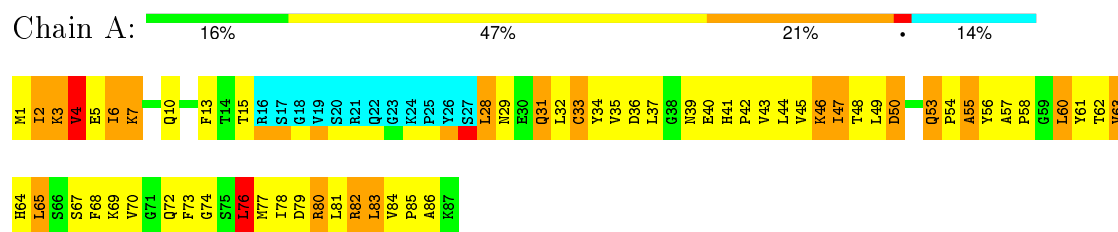


- Molecule 1: GENE V PROTEIN

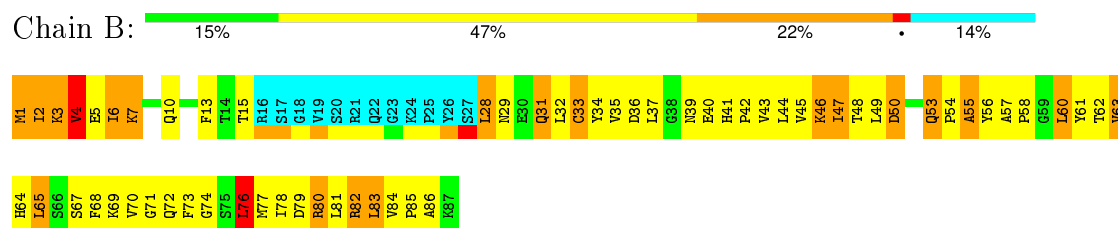


### 4.2.24 Score per residue for model 24

- Molecule 1: GENE V PROTEIN

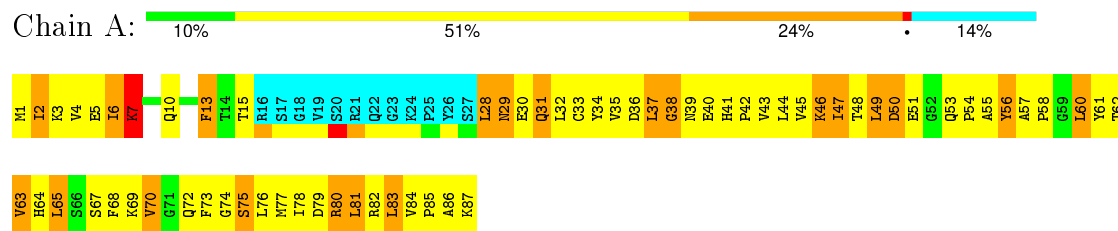


- Molecule 1: GENE V PROTEIN

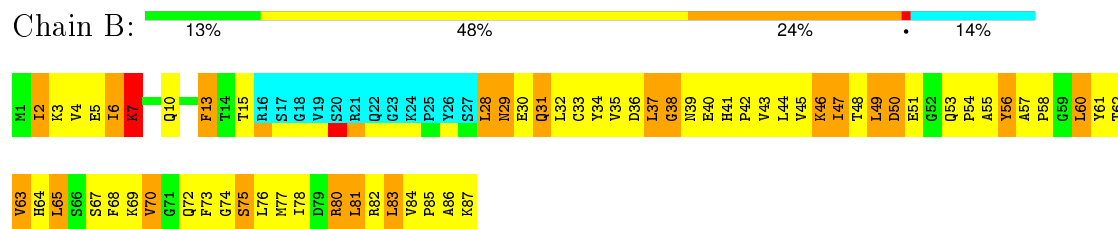


### 4.2.25 Score per residue for model 25

- Molecule 1: GENE V PROTEIN



- Molecule 1: GENE V PROTEIN

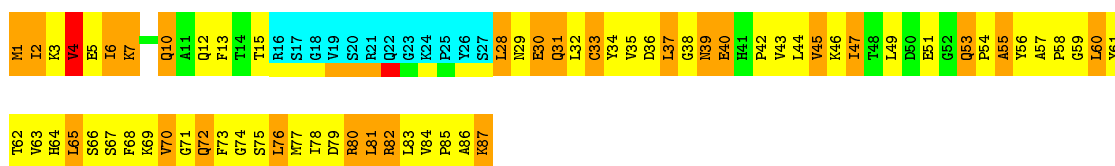


### 4.2.26 Score per residue for model 26

- Molecule 1: GENE V PROTEIN

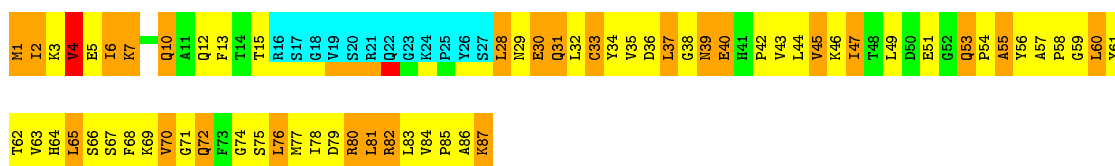






### • Molecule 1: GENE V PROTEIN

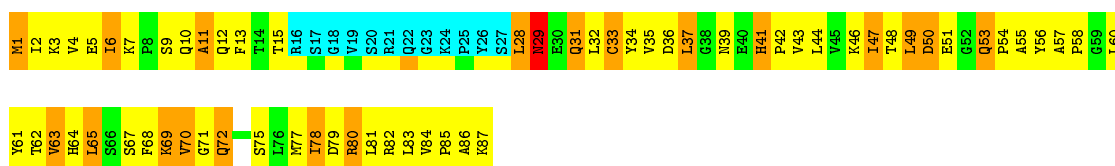
Chain B: 10% 46% 29% 14%



## 4.2.27 Score per residue for model 27

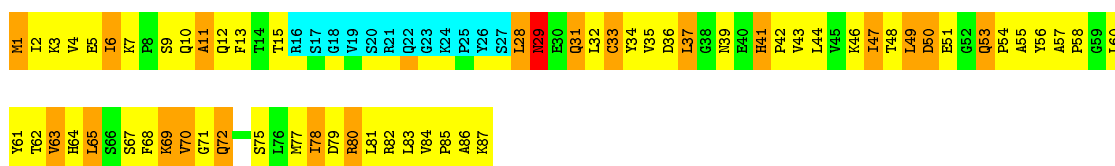
### • Molecule 1: GENE V PROTEIN

Chain A: 14% 49% 22% 14%



### • Molecule 1: GENE V PROTEIN

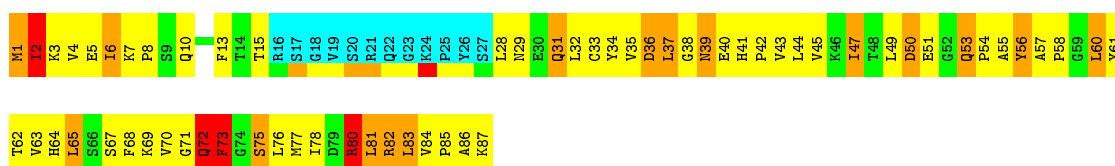
Chain B: 14% 49% 22% 14%



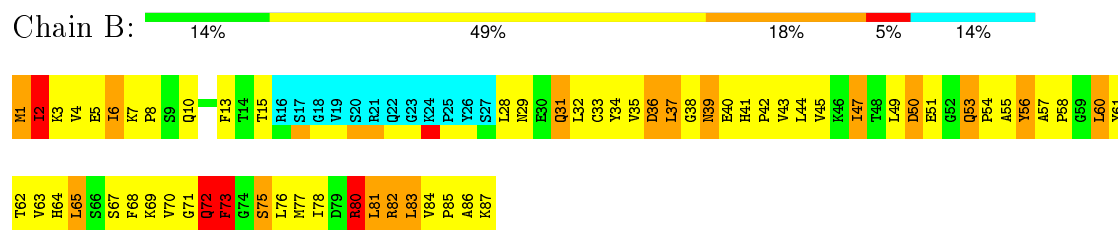
## 4.2.28 Score per residue for model 28

### • Molecule 1: GENE V PROTEIN

Chain A: 14% 49% 18% 5% 14%

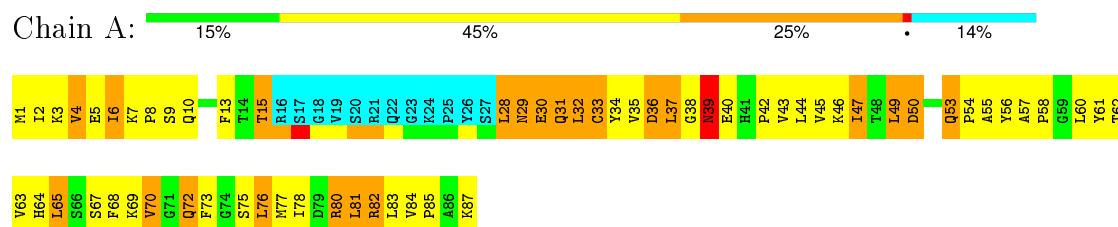


### • Molecule 1: GENE V PROTEIN

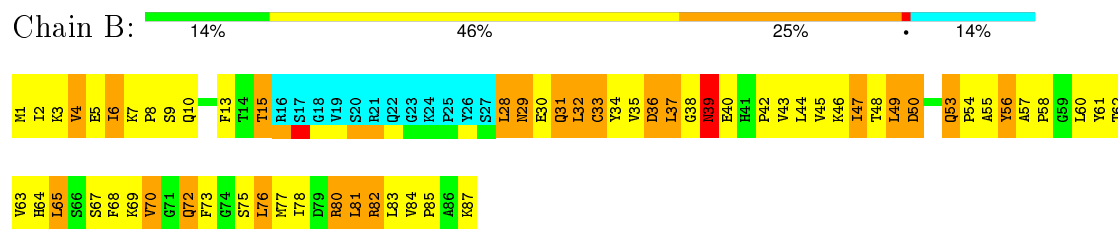


#### 4.2.29 Score per residue for model 29

- Molecule 1: GENE V PROTEIN

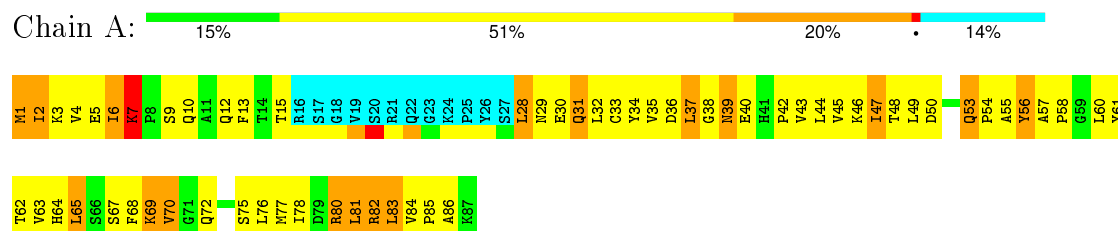


- Molecule 1: GENE V PROTEIN

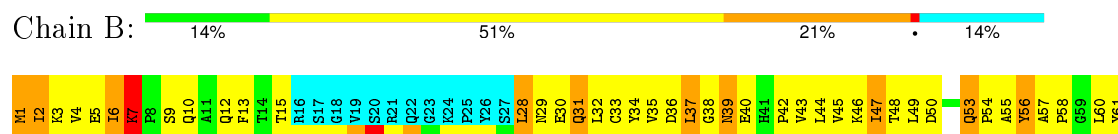


#### 4.2.30 Score per residue for model 30

- Molecule 1: GENE V PROTEIN



- Molecule 1: GENE V PROTEIN



T62	V63	H64	L65	S66	S67	F68	K69	V70	G71	Q72	F73	G74	S75	L76	M77	I78	D79	R80	L81	R82	L83	V84	P85	A86	R87
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 5 Refinement protocol and experimental data overview ⓘ

Of the ? calculated structures, 30 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DIANA	refinement	
X-PLOR	refinement	

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

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	588	607	607	153±10
1	B	588	607	607	152±10
All	All	35280	36420	36420	8286

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 116.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:VAL:HG22	1:B:35:VAL:HG22	1.14	1.20	1	11
1:A:43:VAL:HG21	1:B:70:VAL:HG21	1.12	1.18	29	19
1:A:4:VAL:HG22	1:A:35:VAL:HG22	1.06	1.20	1	11
1:A:70:VAL:HG21	1:B:43:VAL:HG21	1.05	1.15	29	17
1:A:63:VAL:HG13	1:A:81:LEU:HD13	1.03	1.29	8	1
1:B:63:VAL:HG13	1:B:81:LEU:HD13	1.01	1.29	8	1
1:A:37:LEU:HD12	1:A:38:GLY:N	0.98	1.72	28	2
1:B:37:LEU:HD12	1:B:38:GLY:N	0.98	1.73	28	2
1:A:4:VAL:CG2	1:A:35:VAL:HG22	0.98	1.89	7	11
1:A:65:LEU:CD1	1:B:37:LEU:HD13	0.97	1.89	28	1
1:B:4:VAL:CG2	1:B:35:VAL:HG22	0.97	1.89	7	11
1:A:37:LEU:HD13	1:B:65:LEU:CD1	0.97	1.89	28	1
1:A:4:VAL:HG13	1:A:61:TYR:CB	0.94	1.92	13	12

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLN:OE1	1:A:32:LEU:HD13	0.94	1.61	27	3
1:B:4:VAL:HG13	1:B:61:TYR:CB	0.94	1.92	13	12
1:A:47:ILE:HD11	1:A:83:LEU:HB2	0.93	1.40	8	16
1:B:10:GLN:OE1	1:B:32:LEU:HD13	0.93	1.61	27	3
1:A:47:ILE:HG21	1:A:56:TYR:CE1	0.92	1.99	15	11
1:A:3:LYS:N	1:A:37:LEU:HD12	0.91	1.79	1	1
1:B:47:ILE:HD11	1:B:83:LEU:HB2	0.91	1.40	8	16
1:B:3:LYS:N	1:B:37:LEU:HD12	0.91	1.79	1	1
1:B:47:ILE:HG21	1:B:56:TYR:CE1	0.91	1.99	15	11
1:B:47:ILE:HG21	1:B:56:TYR:CZ	0.90	2.01	15	1
1:A:65:LEU:CD2	1:B:2:ILE:HG23	0.90	1.96	9	2
1:B:35:VAL:O	1:B:43:VAL:HG22	0.90	1.66	10	28
1:A:47:ILE:HD13	1:A:83:LEU:HD12	0.90	1.43	28	13
1:B:65:LEU:HD23	1:B:68:PHE:CD2	0.90	2.02	9	2
1:A:65:LEU:HD23	1:A:68:PHE:CD2	0.89	2.02	9	2
1:A:2:ILE:HG23	1:B:65:LEU:CD2	0.89	1.97	9	2
1:A:47:ILE:HG21	1:A:56:TYR:CZ	0.89	2.02	15	1
1:A:35:VAL:O	1:A:43:VAL:HG22	0.89	1.67	18	28
1:B:47:ILE:HD13	1:B:83:LEU:HD12	0.89	1.43	28	13
1:B:4:VAL:HG13	1:B:61:TYR:HB2	0.89	1.44	24	7
1:A:2:ILE:N	1:B:65:LEU:HD22	0.89	1.83	18	23
1:B:57:ALA:HB1	1:B:58:PRO:HD2	0.88	1.44	1	30
1:A:49:LEU:HD11	1:A:53:GLN:O	0.88	1.67	20	8
1:A:57:ALA:HB1	1:A:58:PRO:HD2	0.88	1.44	1	30
1:A:65:LEU:HD22	1:B:2:ILE:N	0.88	1.84	18	24
1:A:4:VAL:HG13	1:A:61:TYR:HB2	0.88	1.44	24	7
1:B:47:ILE:CD1	1:B:83:LEU:HD12	0.88	1.99	17	15
1:A:63:VAL:CG1	1:A:81:LEU:HD12	0.88	1.99	18	7
1:B:49:LEU:HD11	1:B:53:GLN:O	0.88	1.67	20	8
1:A:6:ILE:HG21	1:A:56:TYR:O	0.88	1.68	7	24
1:A:47:ILE:CD1	1:A:83:LEU:HD12	0.88	1.99	24	15
1:B:63:VAL:CG1	1:B:81:LEU:HD12	0.88	1.99	18	7
1:B:6:ILE:HG21	1:B:56:TYR:O	0.87	1.68	7	24
1:A:31:GLN:OE1	1:A:55:ALA:HB1	0.87	1.69	22	2
1:A:33:CYS:SG	1:A:47:ILE:HD13	0.86	2.11	5	5
1:A:37:LEU:CG	1:B:65:LEU:HD11	0.86	2.00	30	4
1:A:2:ILE:HA	1:B:65:LEU:HD22	0.86	1.47	28	14
1:B:31:GLN:OE1	1:B:55:ALA:HB1	0.85	1.69	22	2
1:B:36:ASP:O	1:B:37:LEU:HD12	0.85	1.70	3	4
1:B:33:CYS:SG	1:B:47:ILE:HD13	0.85	2.10	5	5
1:A:15:THR:HG23	1:A:28:LEU:O	0.85	1.71	29	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:15:THR:HG23	1:B:28:LEU:O	0.84	1.72	29	1
1:A:36:ASP:O	1:A:37:LEU:HD12	0.84	1.70	3	4
1:A:65:LEU:HD11	1:B:37:LEU:CG	0.84	2.03	30	5
1:A:65:LEU:HD22	1:B:2:ILE:HA	0.84	1.47	28	14
1:B:76:LEU:HD23	1:B:77:MET:N	0.84	1.87	9	5
1:A:78:ILE:HD12	1:B:78:ILE:HD12	0.84	1.49	23	20
1:A:76:LEU:HD23	1:A:77:MET:N	0.83	1.88	9	5
1:A:2:ILE:HG23	1:B:65:LEU:HD13	0.83	1.49	21	8
1:A:65:LEU:CD1	1:B:2:ILE:HG23	0.82	2.04	2	5
1:B:62:THR:O	1:B:84:VAL:HG22	0.82	1.75	26	29
1:A:62:THR:O	1:A:84:VAL:HG22	0.81	1.75	26	29
1:A:65:LEU:HD13	1:B:37:LEU:HG	0.81	1.51	11	2
1:A:65:LEU:HD22	1:B:2:ILE:HG23	0.81	1.52	9	1
1:A:65:LEU:HD13	1:B:2:ILE:HG23	0.81	1.49	21	9
1:A:70:VAL:HG11	1:B:43:VAL:CG2	0.81	2.05	4	4
1:A:43:VAL:CG2	1:B:70:VAL:HG11	0.81	2.05	4	4
1:A:37:LEU:HG	1:B:65:LEU:HD13	0.81	1.51	11	1
1:A:32:LEU:HB3	1:A:44:LEU:HD11	0.80	1.54	3	29
1:A:43:VAL:HG21	1:B:70:VAL:HG11	0.80	1.54	4	4
1:A:31:GLN:HG3	1:A:55:ALA:HB1	0.80	1.53	5	17
1:A:70:VAL:HG11	1:B:43:VAL:HG21	0.80	1.53	4	4
1:A:70:VAL:HG21	1:B:43:VAL:CG2	0.80	2.04	29	4
1:A:2:ILE:CA	1:B:65:LEU:HD22	0.80	2.07	29	21
1:A:2:ILE:HG23	1:B:65:LEU:CD1	0.80	2.06	2	5
1:B:32:LEU:HB3	1:B:44:LEU:HD11	0.80	1.54	3	29
1:B:4:VAL:HG11	1:B:83:LEU:HD21	0.79	1.55	6	12
1:A:37:LEU:HB3	1:B:65:LEU:HD11	0.79	1.54	29	4
1:A:37:LEU:HG	1:B:65:LEU:HD11	0.79	1.54	30	4
1:A:4:VAL:HG11	1:A:83:LEU:HD21	0.78	1.55	6	12
1:B:31:GLN:HG3	1:B:55:ALA:HB1	0.78	1.54	5	17
1:A:37:LEU:HD13	1:B:65:LEU:HD11	0.78	1.55	28	1
1:A:2:ILE:HG23	1:B:65:LEU:HD22	0.78	1.54	9	1
1:A:65:LEU:HD22	1:B:2:ILE:CA	0.78	2.07	29	21
1:A:37:LEU:HD23	1:A:38:GLY:N	0.78	1.94	6	2
1:B:37:LEU:HD23	1:B:38:GLY:N	0.78	1.94	6	2
1:A:65:LEU:HD11	1:B:37:LEU:HD13	0.77	1.55	28	1
1:A:2:ILE:HG12	1:B:65:LEU:HD21	0.77	1.57	9	1
1:A:65:LEU:HD11	1:B:37:LEU:HB3	0.77	1.56	29	4
1:A:34:TYR:CE2	1:A:44:LEU:HD13	0.77	2.15	17	6
1:A:4:VAL:HG11	1:A:83:LEU:HD11	0.76	1.57	13	9
1:B:6:ILE:HD13	1:B:61:TYR:CE1	0.76	2.16	26	17

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:LYS:O	1:A:4:VAL:HG23	0.76	1.80	1	7
1:A:65:LEU:HD21	1:B:2:ILE:HG12	0.76	1.57	9	1
1:B:3:LYS:O	1:B:4:VAL:HG23	0.76	1.80	1	8
1:B:47:ILE:HD11	1:B:83:LEU:CB	0.76	2.11	22	6
1:A:65:LEU:HD11	1:B:37:LEU:HG	0.76	1.57	30	4
1:A:4:VAL:HB	1:A:35:VAL:HG22	0.76	1.58	3	18
1:B:4:VAL:HG11	1:B:83:LEU:HD11	0.76	1.58	29	9
1:A:43:VAL:CG2	1:B:70:VAL:HG21	0.76	2.06	29	5
1:B:34:TYR:CE2	1:B:44:LEU:HD13	0.75	2.16	17	6
1:A:47:ILE:HD11	1:A:83:LEU:CB	0.75	2.11	8	6
1:A:76:LEU:HD11	1:B:37:LEU:HD21	0.75	1.55	3	2
1:A:6:ILE:HD13	1:A:61:TYR:CE1	0.75	2.16	26	17
1:B:32:LEU:CD2	1:B:44:LEU:HD11	0.75	2.12	10	3
1:B:4:VAL:HB	1:B:35:VAL:HG22	0.75	1.58	9	18
1:A:32:LEU:CD2	1:A:44:LEU:HD11	0.75	2.11	10	3
1:A:63:VAL:HG13	1:A:81:LEU:HD12	0.75	1.59	18	4
1:B:2:ILE:HD12	1:B:63:VAL:HB	0.74	1.58	8	3
1:B:61:TYR:HB3	1:B:83:LEU:HD22	0.74	1.58	23	23
1:B:63:VAL:HG11	1:B:81:LEU:HB2	0.74	1.59	13	17
1:B:4:VAL:O	1:B:60:LEU:HD23	0.74	1.82	22	12
1:A:4:VAL:O	1:A:60:LEU:HD23	0.74	1.82	22	12
1:A:61:TYR:HB3	1:A:83:LEU:HD22	0.74	1.58	23	23
1:A:57:ALA:HB1	1:A:58:PRO:CD	0.74	2.13	1	28
1:A:70:VAL:CG2	1:B:43:VAL:HG21	0.73	2.08	29	11
1:A:2:ILE:H	1:B:65:LEU:HD22	0.73	1.43	5	5
1:A:65:LEU:HD22	1:B:2:ILE:H	0.73	1.43	15	5
1:A:2:ILE:HG21	1:A:63:VAL:HG21	0.73	1.61	5	11
1:B:63:VAL:HG13	1:B:81:LEU:HD12	0.73	1.59	18	4
1:A:37:LEU:CB	1:B:65:LEU:HD11	0.73	2.13	29	4
1:B:57:ALA:HB1	1:B:58:PRO:CD	0.72	2.13	1	28
1:A:63:VAL:HG11	1:A:81:LEU:HB2	0.72	1.60	13	16
1:A:48:THR:HG21	1:A:80:ARG:NH1	0.72	1.99	12	3
1:B:2:ILE:HG21	1:B:63:VAL:HG21	0.72	1.61	5	11
1:B:48:THR:HG21	1:B:80:ARG:NH1	0.72	1.99	12	3
1:A:2:ILE:HD12	1:A:63:VAL:HB	0.72	1.58	8	3
1:A:37:LEU:N	1:A:37:LEU:HD23	0.72	2.00	25	1
1:B:31:GLN:O	1:B:32:LEU:HD23	0.72	1.83	21	2
1:A:65:LEU:HD11	1:B:37:LEU:CB	0.72	2.12	29	4
1:B:49:LEU:HD12	1:B:53:GLN:O	0.72	1.85	22	7
1:A:43:VAL:HG21	1:B:70:VAL:CG2	0.72	2.10	29	12
1:A:37:LEU:HD11	1:B:69:LYS:CA	0.72	2.15	8	5

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:37:LEU:O	1:B:37:LEU:HD12	0.71	1.85	20	2
1:A:28:LEU:C	1:A:28:LEU:HD22	0.71	2.05	18	1
1:B:28:LEU:HD22	1:B:28:LEU:C	0.71	2.05	18	1
1:A:31:GLN:O	1:A:32:LEU:HD23	0.71	1.83	21	2
1:A:1:MET:SD	1:A:62:THR:HG21	0.71	2.25	6	9
1:B:33:CYS:SG	1:B:47:ILE:HD12	0.71	2.25	22	2
1:B:37:LEU:HD23	1:B:37:LEU:N	0.71	2.00	25	1
1:A:49:LEU:HD12	1:A:53:GLN:O	0.71	1.85	22	7
1:A:76:LEU:CD1	1:B:35:VAL:HG11	0.71	2.16	10	4
1:A:35:VAL:HG11	1:B:76:LEU:CD1	0.71	2.15	10	4
1:A:33:CYS:SG	1:A:47:ILE:HD12	0.71	2.24	22	2
1:B:39:ASN:ND2	1:B:43:VAL:HG11	0.71	2.01	29	2
1:A:4:VAL:HG22	1:A:35:VAL:CG2	0.71	2.15	7	9
1:A:39:ASN:ND2	1:A:43:VAL:HG11	0.70	2.01	29	2
1:A:37:LEU:HD11	1:B:68:PHE:C	0.70	2.06	6	9
1:A:65:LEU:HD11	1:B:37:LEU:O	0.70	1.86	19	6
1:A:37:LEU:O	1:A:37:LEU:HD12	0.70	1.86	20	1
1:B:1:MET:SD	1:B:62:THR:HG21	0.70	2.25	6	9
1:B:49:LEU:O	1:B:49:LEU:HD13	0.70	1.86	23	1
1:A:28:LEU:HD12	1:A:28:LEU:C	0.70	2.07	17	1
1:B:28:LEU:C	1:B:28:LEU:HD12	0.70	2.07	17	2
1:A:68:PHE:C	1:B:37:LEU:HD11	0.70	2.05	6	9
1:A:37:LEU:HD21	1:B:76:LEU:HD11	0.70	1.60	3	2
1:A:2:ILE:HA	1:B:65:LEU:HD21	0.70	1.62	11	1
1:A:37:LEU:O	1:B:65:LEU:HD11	0.70	1.86	19	6
1:A:49:LEU:HD13	1:A:49:LEU:O	0.70	1.86	23	1
1:A:35:VAL:HG12	1:A:37:LEU:H	0.69	1.47	25	3
1:A:49:LEU:HD13	1:A:50:ASP:O	0.69	1.87	24	3
1:B:49:LEU:HD13	1:B:50:ASP:O	0.69	1.87	24	3
1:A:35:VAL:HG21	1:B:76:LEU:HD13	0.69	1.64	26	1
1:A:6:ILE:HD11	1:A:33:CYS:SG	0.69	2.28	16	5
1:B:33:CYS:SG	1:B:47:ILE:HD11	0.69	2.27	15	1
1:A:47:ILE:HD11	1:A:83:LEU:HB3	0.69	1.65	22	1
1:B:36:ASP:C	1:B:37:LEU:HD12	0.69	2.07	3	2
1:B:4:VAL:HG22	1:B:35:VAL:CG2	0.69	2.15	7	9
1:A:69:LYS:CA	1:B:37:LEU:HD11	0.69	2.17	8	5
1:B:6:ILE:HD11	1:B:33:CYS:SG	0.69	2.27	21	5
1:A:37:LEU:CG	1:B:65:LEU:HD13	0.69	2.18	11	1
1:B:35:VAL:HG12	1:B:37:LEU:H	0.69	1.48	25	3
1:B:28:LEU:HD11	1:B:30:GLU:HG3	0.69	1.64	10	2
1:A:33:CYS:SG	1:A:47:ILE:HD11	0.69	2.28	15	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:HA	1:B:65:LEU:HD13	0.69	1.64	10	5
1:B:35:VAL:HG13	1:B:37:LEU:HD11	0.69	1.65	1	1
1:A:65:LEU:HD13	1:B:37:LEU:CG	0.69	2.18	11	1
1:A:65:LEU:HD21	1:B:2:ILE:HA	0.69	1.62	11	1
1:B:28:LEU:HD12	1:B:29:ASN:N	0.69	2.02	10	1
1:A:37:LEU:HG	1:B:65:LEU:HD21	0.68	1.65	16	3
1:A:81:LEU:HD12	1:A:81:LEU:C	0.68	2.08	8	1
1:B:81:LEU:C	1:B:81:LEU:HD12	0.68	2.09	8	1
1:A:36:ASP:C	1:A:37:LEU:HD12	0.68	2.07	3	2
1:A:76:LEU:HD13	1:B:35:VAL:HG21	0.68	1.64	26	1
1:A:48:THR:O	1:A:48:THR:HG22	0.68	1.89	25	1
1:B:6:ILE:HD13	1:B:61:TYR:CD1	0.68	2.23	26	7
1:A:65:LEU:HD13	1:B:2:ILE:HA	0.68	1.65	10	5
1:A:6:ILE:HD13	1:A:61:TYR:CD1	0.68	2.24	26	8
1:A:6:ILE:HD13	1:A:56:TYR:HB3	0.68	1.64	13	16
1:A:81:LEU:O	1:A:81:LEU:HD23	0.68	1.88	7	10
1:A:28:LEU:HD12	1:A:29:ASN:N	0.68	2.02	10	1
1:B:47:ILE:HD11	1:B:83:LEU:HB3	0.68	1.65	22	1
1:A:32:LEU:HD12	1:A:32:LEU:N	0.68	2.03	28	1
1:B:81:LEU:HD23	1:B:81:LEU:O	0.68	1.89	7	16
1:A:7:LYS:CD	1:A:34:TYR:CD1	0.68	2.77	18	2
1:A:35:VAL:HG13	1:A:37:LEU:HD11	0.68	1.65	1	1
1:A:65:LEU:HD21	1:B:37:LEU:HG	0.68	1.64	16	3
1:B:32:LEU:HD12	1:B:32:LEU:N	0.67	2.03	28	2
1:A:28:LEU:HD11	1:A:30:GLU:HG3	0.67	1.65	10	2
1:B:6:ILE:HD13	1:B:56:TYR:HB3	0.67	1.65	13	17
1:B:7:LYS:CD	1:B:34:TYR:CD1	0.67	2.77	18	2
1:B:48:THR:HG22	1:B:48:THR:O	0.67	1.89	25	1
1:B:29:ASN:OD1	1:B:29:ASN:N	0.67	2.28	13	7
1:B:35:VAL:HG12	1:B:37:LEU:HG	0.67	1.67	23	4
1:A:28:LEU:HD12	1:A:29:ASN:O	0.67	1.90	2	2
1:A:61:TYR:CD2	1:A:83:LEU:HD23	0.67	2.25	26	3
1:B:28:LEU:HD12	1:B:29:ASN:O	0.67	1.90	2	1
1:B:7:LYS:CD	1:B:34:TYR:CD2	0.66	2.79	11	15
1:B:29:ASN:N	1:B:29:ASN:OD1	0.66	2.28	22	9
1:B:37:LEU:HD23	1:B:37:LEU:O	0.66	1.90	13	3
1:A:28:LEU:C	1:A:28:LEU:HD12	0.66	2.10	10	1
1:A:37:LEU:O	1:A:37:LEU:HD23	0.66	1.90	13	4
1:A:65:LEU:HD23	1:A:68:PHE:HD2	0.66	1.47	9	1
1:B:65:LEU:CB	1:B:68:PHE:CD2	0.66	2.79	30	20
1:B:37:LEU:HD12	1:B:37:LEU:N	0.66	2.06	17	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASN:N	1:A:29:ASN:OD1	0.66	2.28	13	7
1:A:35:VAL:HG12	1:A:37:LEU:HG	0.66	1.67	23	4
1:B:28:LEU:CD2	1:B:48:THR:HG22	0.66	2.21	1	3
1:A:32:LEU:CB	1:A:44:LEU:HD11	0.66	2.20	28	7
1:B:61:TYR:CD2	1:B:83:LEU:HD23	0.66	2.26	26	3
1:B:32:LEU:CB	1:B:44:LEU:HD11	0.66	2.20	28	7
1:A:7:LYS:CD	1:A:34:TYR:CD2	0.66	2.79	4	15
1:A:34:TYR:CE1	1:A:44:LEU:HD13	0.66	2.26	8	12
1:A:35:VAL:O	1:A:37:LEU:HD23	0.65	1.91	7	1
1:B:34:TYR:CE1	1:B:44:LEU:HD13	0.65	2.27	8	12
1:A:37:LEU:HD22	1:B:69:LYS:HA	0.65	1.69	17	1
1:A:65:LEU:CB	1:A:68:PHE:CD2	0.65	2.79	30	20
1:A:43:VAL:O	1:A:43:VAL:HG23	0.65	1.92	18	17
1:A:28:LEU:CD2	1:A:48:THR:HG22	0.65	2.21	1	3
1:B:36:ASP:C	1:B:37:LEU:HD23	0.65	2.11	7	1
1:A:37:LEU:HD12	1:A:37:LEU:N	0.65	2.05	17	1
1:A:37:LEU:HD21	1:B:69:LYS:HA	0.65	1.67	13	7
1:B:35:VAL:O	1:B:37:LEU:HD23	0.65	1.91	7	1
1:B:4:VAL:CG1	1:B:83:LEU:HD11	0.65	2.21	29	1
1:A:65:LEU:HB2	1:A:68:PHE:CD2	0.64	2.26	19	27
1:B:47:ILE:CG2	1:B:56:TYR:CE1	0.64	2.79	15	19
1:A:36:ASP:C	1:A:37:LEU:HD23	0.64	2.11	7	1
1:B:65:LEU:HB2	1:B:68:PHE:CD2	0.64	2.27	27	27
1:B:43:VAL:HG23	1:B:43:VAL:O	0.64	1.92	18	15
1:A:4:VAL:CG1	1:A:83:LEU:HD11	0.64	2.21	29	1
1:B:2:ILE:HB	1:B:63:VAL:HG23	0.64	1.68	8	3
1:A:13:PHE:CD2	1:A:49:LEU:CD1	0.64	2.81	4	8
1:B:7:LYS:HD3	1:B:34:TYR:CD2	0.64	2.28	26	18
1:A:37:LEU:HD21	1:B:70:VAL:HG22	0.64	1.69	17	3
1:A:2:ILE:HB	1:A:63:VAL:HG23	0.64	1.68	8	4
1:A:49:LEU:O	1:A:49:LEU:HD13	0.64	1.93	6	1
1:B:13:PHE:CD2	1:B:49:LEU:CD1	0.64	2.80	26	8
1:A:49:LEU:HD21	1:A:55:ALA:HA	0.64	1.70	29	13
1:A:4:VAL:HG11	1:A:83:LEU:CD1	0.64	2.23	29	1
1:B:68:PHE:N	1:B:68:PHE:CD1	0.64	2.64	28	16
1:A:68:PHE:N	1:A:68:PHE:CD1	0.64	2.65	19	17
1:A:70:VAL:HG11	1:B:45:VAL:HG12	0.64	1.69	30	4
1:A:81:LEU:HD13	1:B:76:LEU:HD22	0.64	1.68	23	1
1:A:7:LYS:HD3	1:A:34:TYR:CD2	0.64	2.28	19	18
1:B:43:VAL:HG23	1:B:45:VAL:HG23	0.64	1.70	15	2
1:B:4:VAL:HG11	1:B:83:LEU:CD1	0.64	2.23	29	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:PHE:CE1	1:A:29:ASN:ND2	0.64	2.67	9	12
1:A:13:PHE:CD2	1:A:55:ALA:HB2	0.64	2.28	10	27
1:B:59:GLY:O	1:B:61:TYR:CD1	0.64	2.51	1	5
1:B:35:VAL:O	1:B:43:VAL:HG13	0.64	1.93	3	4
1:A:68:PHE:CD1	1:A:68:PHE:N	0.63	2.65	20	13
1:B:49:LEU:HD13	1:B:49:LEU:O	0.63	1.93	6	1
1:A:10:GLN:NE2	1:A:32:LEU:HD12	0.63	2.08	20	1
1:A:76:LEU:HD22	1:B:81:LEU:HD13	0.63	1.68	23	1
1:B:13:PHE:CD1	1:B:29:ASN:CB	0.63	2.81	19	20
1:A:13:PHE:CD1	1:A:29:ASN:CB	0.63	2.81	19	20
1:A:59:GLY:O	1:A:61:TYR:CD1	0.63	2.52	1	5
1:A:43:VAL:HG11	1:B:70:VAL:HG21	0.63	1.70	14	3
1:B:10:GLN:NE2	1:B:32:LEU:HD12	0.63	2.08	20	1
1:B:56:TYR:CE2	1:B:83:LEU:CB	0.63	2.81	26	19
1:B:40:GLU:O	1:B:41:HIS:CG	0.63	2.52	22	12
1:B:13:PHE:CE1	1:B:29:ASN:ND2	0.63	2.67	5	12
1:A:56:TYR:CE2	1:A:83:LEU:CB	0.63	2.82	26	19
1:A:43:VAL:HG23	1:A:45:VAL:HG23	0.63	1.70	15	2
1:B:68:PHE:CD1	1:B:68:PHE:N	0.63	2.65	19	14
1:A:37:LEU:H	1:A:37:LEU:HD13	0.63	1.54	1	1
1:A:40:GLU:O	1:A:41:HIS:CG	0.63	2.52	22	12
1:B:56:TYR:CE2	1:B:83:LEU:HB3	0.63	2.29	26	28
1:A:81:LEU:HD23	1:A:81:LEU:O	0.63	1.94	9	15
1:A:13:PHE:CD2	1:A:29:ASN:CB	0.63	2.82	8	3
1:B:13:PHE:CD2	1:B:29:ASN:CB	0.63	2.82	8	3
1:B:68:PHE:CE1	1:B:78:ILE:CG1	0.63	2.82	4	10
1:B:49:LEU:HD21	1:B:55:ALA:HA	0.62	1.71	14	12
1:A:43:VAL:HG23	1:A:43:VAL:O	0.62	1.93	17	12
1:A:68:PHE:CE1	1:A:78:ILE:CG1	0.62	2.82	4	10
1:A:31:GLN:CB	1:A:47:ILE:HG22	0.62	2.24	5	18
1:B:32:LEU:HD12	1:B:44:LEU:HG	0.62	1.72	19	1
1:B:32:LEU:HD22	1:B:44:LEU:HD21	0.62	1.71	10	3
1:B:13:PHE:CD2	1:B:55:ALA:HB2	0.62	2.29	10	27
1:A:69:LYS:HA	1:B:37:LEU:HD21	0.62	1.70	13	7
1:A:56:TYR:CE2	1:A:83:LEU:HB3	0.62	2.29	26	28
1:B:37:LEU:HD13	1:B:37:LEU:H	0.62	1.54	1	1
1:A:81:LEU:N	1:A:81:LEU:HD23	0.62	2.10	3	3
1:A:45:VAL:HG12	1:B:70:VAL:CG1	0.62	2.25	20	3
1:A:76:LEU:HD11	1:B:37:LEU:HD22	0.62	1.70	20	1
1:B:43:VAL:O	1:B:43:VAL:HG23	0.62	1.95	12	14
1:A:32:LEU:N	1:A:32:LEU:HD12	0.62	2.10	1	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:32:LEU:N	1:B:32:LEU:HD12	0.62	2.10	1	3
1:A:76:LEU:HD23	1:A:76:LEU:C	0.62	2.15	15	2
1:A:28:LEU:HD13	1:A:48:THR:HG23	0.62	1.72	17	1
1:A:35:VAL:O	1:A:43:VAL:HG13	0.62	1.94	3	4
1:A:37:LEU:HD22	1:B:76:LEU:HD11	0.61	1.71	20	1
1:B:76:LEU:HD23	1:B:76:LEU:C	0.61	2.15	15	2
1:A:6:ILE:HD11	1:A:83:LEU:CD2	0.61	2.26	22	3
1:B:81:LEU:O	1:B:81:LEU:HD23	0.61	1.96	6	8
1:A:72:GLN:N	1:A:72:GLN:NE2	0.61	2.48	13	2
1:A:32:LEU:HD12	1:A:44:LEU:HG	0.61	1.72	19	1
1:A:70:VAL:CG1	1:B:45:VAL:CG2	0.61	2.79	9	10
1:B:63:VAL:HG11	1:B:81:LEU:HD12	0.61	1.73	18	5
1:B:4:VAL:HG13	1:B:61:TYR:C	0.61	2.16	6	12
1:A:70:VAL:CG1	1:B:45:VAL:HG12	0.61	2.25	20	4
1:B:6:ILE:HD11	1:B:83:LEU:CD2	0.61	2.25	22	3
1:A:13:PHE:CG	1:A:49:LEU:HD12	0.61	2.31	6	4
1:A:32:LEU:HD22	1:A:44:LEU:HD21	0.61	1.71	10	3
1:B:7:LYS:HD2	1:B:34:TYR:CE2	0.61	2.31	20	5
1:A:60:LEU:HB3	1:A:86:ALA:HB3	0.61	1.72	22	18
1:A:45:VAL:HG12	1:B:70:VAL:HG11	0.61	1.70	30	5
1:A:69:LYS:HA	1:B:37:LEU:HD22	0.61	1.72	17	1
1:B:68:PHE:CE1	1:B:78:ILE:HG12	0.61	2.31	11	30
1:A:47:ILE:CD1	1:A:56:TYR:CE2	0.61	2.84	10	6
1:B:28:LEU:HD13	1:B:48:THR:HG23	0.61	1.72	17	1
1:A:76:LEU:CD1	1:B:37:LEU:HD21	0.61	2.25	3	2
1:B:81:LEU:HD23	1:B:81:LEU:N	0.61	2.10	3	4
1:B:65:LEU:HD23	1:B:68:PHE:HD2	0.61	1.48	9	1
1:A:13:PHE:CD1	1:A:29:ASN:HB3	0.60	2.31	10	25
1:B:72:GLN:NE2	1:B:72:GLN:N	0.60	2.48	13	2
1:A:47:ILE:HD12	1:A:56:TYR:CE1	0.60	2.31	29	3
1:A:13:PHE:CD2	1:A:49:LEU:HD12	0.60	2.31	18	5
1:B:28:LEU:HD11	1:B:30:GLU:CG	0.60	2.27	17	1
1:B:31:GLN:CB	1:B:47:ILE:HG22	0.60	2.24	5	18
1:A:37:LEU:CB	1:B:65:LEU:HD21	0.60	2.26	21	1
1:B:13:PHE:CG	1:B:49:LEU:HD12	0.60	2.31	6	4
1:B:10:GLN:NE2	1:B:32:LEU:HD22	0.60	2.12	27	1
1:A:76:LEU:C	1:A:76:LEU:HD23	0.60	2.16	17	2
1:B:13:PHE:CD2	1:B:49:LEU:HD12	0.60	2.31	18	6
1:A:68:PHE:CE1	1:A:78:ILE:HG12	0.60	2.31	11	30
1:B:47:ILE:HG21	1:B:56:TYR:CD1	0.60	2.31	27	19
1:A:45:VAL:CG2	1:B:70:VAL:CG1	0.60	2.80	18	11

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:ILE:HG12	1:B:56:TYR:CE2	0.60	2.32	9	4
1:A:45:VAL:CG1	1:B:70:VAL:CG1	0.60	2.79	14	5
1:B:40:GLU:O	1:B:41:HIS:CB	0.60	2.49	22	4
1:A:47:ILE:CG2	1:A:56:TYR:CE1	0.60	2.80	15	18
1:B:68:PHE:HB3	1:B:76:LEU:HD21	0.60	1.73	13	4
1:A:4:VAL:HG13	1:A:61:TYR:C	0.60	2.17	29	12
1:B:78:ILE:CG2	1:B:81:LEU:N	0.60	2.65	18	3
1:A:6:ILE:HG22	1:A:6:ILE:O	0.60	1.96	14	10
1:B:6:ILE:O	1:B:6:ILE:HG22	0.60	1.96	14	12
1:B:47:ILE:HD12	1:B:56:TYR:CE1	0.60	2.31	29	3
1:A:35:VAL:HG11	1:B:76:LEU:HD12	0.60	1.73	11	1
1:B:13:PHE:CD1	1:B:29:ASN:HB3	0.60	2.31	10	25
1:A:78:ILE:CD1	1:B:78:ILE:CD1	0.60	2.79	20	18
1:A:10:GLN:OE1	1:A:32:LEU:HD12	0.60	1.97	17	2
1:A:70:VAL:HG22	1:B:37:LEU:HD21	0.60	1.73	17	3
1:A:78:ILE:CG2	1:A:81:LEU:N	0.60	2.65	18	3
1:A:7:LYS:HD2	1:A:34:TYR:CE2	0.60	2.31	20	5
1:A:39:ASN:O	1:A:41:HIS:CE1	0.60	2.55	27	3
1:A:10:GLN:NE2	1:A:32:LEU:HD22	0.60	2.12	27	1
1:A:47:ILE:HG21	1:A:56:TYR:CD1	0.59	2.33	27	19
1:A:65:LEU:HD21	1:B:2:ILE:CG1	0.59	2.27	9	2
1:A:2:ILE:CG1	1:B:65:LEU:HD21	0.59	2.27	9	2
1:A:13:PHE:HD2	1:A:55:ALA:HB2	0.59	1.57	26	20
1:B:10:GLN:OE1	1:B:32:LEU:HD12	0.59	1.97	17	2
1:A:65:LEU:HD23	1:A:68:PHE:CE2	0.59	2.32	13	2
1:B:47:ILE:CD1	1:B:56:TYR:CE2	0.59	2.85	10	6
1:A:40:GLU:O	1:A:41:HIS:CB	0.59	2.49	23	4
1:B:60:LEU:HB3	1:B:86:ALA:HB3	0.59	1.72	22	18
1:B:34:TYR:HE1	1:B:44:LEU:HD13	0.59	1.57	8	11
1:A:37:LEU:HA	1:B:65:LEU:HD13	0.59	1.74	3	1
1:A:65:LEU:HD21	1:B:37:LEU:CB	0.59	2.27	21	1
1:A:2:ILE:HD13	1:A:63:VAL:HB	0.59	1.74	18	7
1:B:28:LEU:HD22	1:B:48:THR:HG22	0.59	1.74	11	2
1:A:29:ASN:CB	1:A:49:LEU:CB	0.59	2.81	2	3
1:A:70:VAL:HG11	1:B:45:VAL:HG23	0.59	1.74	26	1
1:B:39:ASN:O	1:B:41:HIS:CE1	0.59	2.56	27	3
1:A:72:GLN:O	1:A:73:PHE:CG	0.59	2.55	28	2
1:A:39:ASN:HD22	1:A:43:VAL:HG11	0.59	1.57	27	2
1:B:45:VAL:CG1	1:B:46:LYS:N	0.59	2.66	13	11
1:B:29:ASN:CB	1:B:49:LEU:CB	0.59	2.81	15	3
1:A:31:GLN:HE21	1:A:55:ALA:HB1	0.59	1.58	21	3

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:VAL:CG1	1:B:45:VAL:CG1	0.59	2.80	14	5
1:A:28:LEU:HD11	1:A:30:GLU:CG	0.59	2.27	17	1
1:B:31:GLN:HE21	1:B:55:ALA:HB1	0.59	1.58	21	3
1:B:37:LEU:CD2	1:B:38:GLY:N	0.59	2.65	1	2
1:A:28:LEU:HD22	1:A:48:THR:HG22	0.59	1.74	11	2
1:A:47:ILE:HG12	1:A:56:TYR:CE2	0.59	2.33	9	4
1:B:7:LYS:HD3	1:B:34:TYR:CD1	0.59	2.33	18	2
1:A:78:ILE:CD1	1:B:78:ILE:HD12	0.59	2.28	2	18
1:A:37:LEU:HD23	1:A:37:LEU:O	0.59	1.98	15	1
1:A:63:VAL:HG11	1:A:81:LEU:HD12	0.59	1.73	18	5
1:A:37:LEU:CD2	1:A:38:GLY:N	0.59	2.65	1	2
1:A:70:VAL:CG1	1:B:43:VAL:HG21	0.59	2.27	4	2
1:A:68:PHE:HB3	1:A:76:LEU:HD21	0.59	1.74	13	3
1:B:76:LEU:O	1:B:76:LEU:HD23	0.59	1.98	23	1
1:A:34:TYR:CD1	1:A:42:PRO:HB2	0.58	2.33	14	16
1:A:45:VAL:CG1	1:A:46:LYS:N	0.58	2.66	22	11
1:B:34:TYR:CD1	1:B:42:PRO:HB2	0.58	2.33	23	16
1:A:10:GLN:OE1	1:A:44:LEU:HD13	0.58	1.99	13	1
1:A:65:LEU:CD2	1:B:2:ILE:CG1	0.58	2.81	13	1
1:B:2:ILE:HD13	1:B:63:VAL:HB	0.58	1.73	18	8
1:B:39:ASN:HD22	1:B:43:VAL:HG11	0.58	1.57	27	2
1:A:29:ASN:OD1	1:A:29:ASN:N	0.58	2.37	27	9
1:B:4:VAL:CG2	1:B:5:GLU:N	0.58	2.67	26	19
1:A:65:LEU:HD22	1:B:2:ILE:HG13	0.58	1.75	4	3
1:A:2:ILE:CG1	1:B:65:LEU:CD2	0.58	2.81	13	1
1:B:6:ILE:CD1	1:B:61:TYR:CD1	0.58	2.87	7	12
1:A:67:SER:CB	1:A:80:ARG:O	0.58	2.52	19	28
1:A:72:GLN:O	1:A:73:PHE:CB	0.58	2.51	28	8
1:A:37:LEU:HD11	1:B:69:LYS:HA	0.58	1.75	8	4
1:B:65:LEU:HD23	1:B:68:PHE:CE2	0.58	2.33	13	2
1:A:45:VAL:CG2	1:B:75:SER:N	0.58	2.66	16	1
1:A:7:LYS:HD3	1:A:34:TYR:CD1	0.58	2.33	18	2
1:A:2:ILE:N	1:B:65:LEU:CD2	0.58	2.66	30	1
1:B:72:GLN:O	1:B:73:PHE:CG	0.58	2.56	28	2
1:B:72:GLN:O	1:B:73:PHE:CB	0.58	2.51	28	8
1:A:2:ILE:HG13	1:B:65:LEU:HD22	0.58	1.76	4	3
1:A:34:TYR:CD2	1:A:42:PRO:HB2	0.58	2.33	22	14
1:A:6:ILE:CD1	1:A:61:TYR:CD1	0.58	2.86	7	12
1:A:65:LEU:HD13	1:B:2:ILE:HG12	0.58	1.75	25	1
1:A:2:ILE:CG2	1:B:65:LEU:HD13	0.58	2.24	21	5
1:A:2:ILE:CG2	1:A:63:VAL:CG2	0.58	2.82	5	10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:HD12	1:B:35:VAL:HG11	0.58	1.74	11	1
1:B:34:TYR:CD2	1:B:42:PRO:HB2	0.58	2.33	22	14
1:B:13:PHE:HD2	1:B:55:ALA:HB2	0.58	1.57	26	22
1:A:2:ILE:HG12	1:B:65:LEU:HD13	0.58	1.75	25	1
1:A:79:ASP:O	1:A:80:ARG:CB	0.58	2.52	9	7
1:B:4:VAL:CB	1:B:35:VAL:HG22	0.58	2.29	14	6
1:A:34:TYR:HE1	1:A:44:LEU:HD13	0.58	1.58	9	11
1:A:65:LEU:CD2	1:B:2:ILE:N	0.58	2.66	30	2
1:A:4:VAL:CG2	1:A:5:GLU:N	0.58	2.67	8	19
1:B:1:MET:O	1:B:37:LEU:HD22	0.58	1.98	21	1
1:A:28:LEU:HD22	1:A:50:ASP:HB3	0.58	1.76	6	1
1:A:39:ASN:OD1	1:A:41:HIS:CD2	0.58	2.57	8	1
1:B:10:GLN:OE1	1:B:44:LEU:HD13	0.58	1.99	13	1
1:B:7:LYS:HD2	1:B:34:TYR:CE1	0.57	2.34	28	1
1:B:29:ASN:O	1:B:49:LEU:N	0.57	2.37	10	21
1:B:37:LEU:O	1:B:37:LEU:HD23	0.57	1.99	15	2
1:A:65:LEU:HD13	1:B:2:ILE:CG2	0.57	2.24	21	4
1:A:29:ASN:O	1:A:49:LEU:N	0.57	2.37	10	20
1:B:67:SER:CB	1:B:80:ARG:O	0.57	2.52	7	28
1:B:2:ILE:CG2	1:B:63:VAL:CG2	0.57	2.82	5	10
1:A:65:LEU:HD13	1:B:37:LEU:HA	0.57	1.75	3	1
1:B:28:LEU:CD1	1:B:28:LEU:N	0.57	2.67	18	1
1:B:28:LEU:HD22	1:B:29:ASN:N	0.57	2.14	18	1
1:B:36:ASP:O	1:B:38:GLY:N	0.57	2.37	3	19
1:B:4:VAL:CG1	1:B:5:GLU:N	0.57	2.67	1	10
1:A:3:LYS:C	1:A:4:VAL:HG12	0.57	2.19	21	4
1:B:70:VAL:HG22	1:B:76:LEU:CD1	0.57	2.29	4	1
1:B:28:LEU:HD22	1:B:50:ASP:HB3	0.57	1.76	6	1
1:B:49:LEU:HD21	1:B:53:GLN:O	0.57	1.99	6	1
1:A:49:LEU:HD21	1:A:53:GLN:O	0.57	1.99	6	1
1:A:81:LEU:CD2	1:A:81:LEU:N	0.57	2.67	3	2
1:B:4:VAL:N	1:B:61:TYR:O	0.57	2.38	30	17
1:A:37:LEU:HD11	1:B:69:LYS:N	0.57	2.14	5	6
1:A:4:VAL:N	1:A:61:TYR:O	0.57	2.38	30	18
1:A:34:TYR:CE1	1:A:44:LEU:HB2	0.57	2.35	27	27
1:A:6:ILE:O	1:A:6:ILE:HG22	0.57	1.99	1	12
1:A:1:MET:O	1:A:37:LEU:HD22	0.57	1.99	21	1
1:B:3:LYS:C	1:B:4:VAL:HG12	0.57	2.20	21	4
1:A:68:PHE:O	1:B:37:LEU:HD11	0.57	1.99	6	2
1:B:31:GLN:HB2	1:B:49:LEU:HD23	0.57	1.76	29	2
1:A:45:VAL:HG23	1:B:70:VAL:HG11	0.57	1.77	26	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:40:GLU:O	1:B:41:HIS:ND1	0.57	2.38	23	10
1:A:70:VAL:HG22	1:A:76:LEU:CD1	0.57	2.30	4	1
1:A:28:LEU:CD1	1:A:28:LEU:N	0.57	2.67	18	1
1:A:4:VAL:CG1	1:A:5:GLU:N	0.57	2.67	1	10
1:A:32:LEU:HD23	1:A:46:LYS:HA	0.57	1.76	5	3
1:B:35:VAL:HG12	1:B:36:ASP:N	0.57	2.15	26	2
1:B:79:ASP:O	1:B:80:ARG:CB	0.57	2.53	8	7
1:A:4:VAL:CB	1:A:35:VAL:HG22	0.57	2.29	14	7
1:B:35:VAL:CG1	1:B:37:LEU:HD23	0.57	2.29	20	1
1:B:6:ILE:HG23	1:B:10:GLN:O	0.57	2.00	24	4
1:A:6:ILE:HG23	1:A:10:GLN:O	0.57	2.00	24	3
1:B:81:LEU:CD2	1:B:81:LEU:N	0.57	2.67	3	2
1:A:76:LEU:O	1:A:76:LEU:HD23	0.57	1.98	23	1
1:A:7:LYS:HD2	1:A:34:TYR:CE1	0.57	2.35	28	1
1:A:36:ASP:O	1:A:38:GLY:N	0.57	2.37	3	19
1:B:3:LYS:O	1:B:4:VAL:CG2	0.57	2.53	1	11
1:A:28:LEU:HD22	1:A:29:ASN:N	0.57	2.14	18	1
1:A:13:PHE:N	1:A:13:PHE:CD1	0.57	2.73	8	2
1:A:3:LYS:O	1:A:4:VAL:CG2	0.56	2.53	1	11
1:A:37:LEU:N	1:A:37:LEU:CD2	0.56	2.68	25	1
1:B:6:ILE:HG22	1:B:6:ILE:O	0.56	1.99	1	10
1:A:31:GLN:HB2	1:A:49:LEU:HD23	0.56	1.76	29	3
1:A:2:ILE:HG21	1:B:76:LEU:HD22	0.56	1.76	16	1
1:A:4:VAL:HG12	1:A:5:GLU:N	0.56	2.16	16	11
1:A:81:LEU:HD13	1:B:76:LEU:HB2	0.56	1.76	14	5
1:B:39:ASN:OD1	1:B:41:HIS:CD2	0.56	2.58	8	1
1:A:62:THR:HG23	1:A:86:ALA:HB2	0.56	1.78	28	10
1:A:40:GLU:O	1:A:41:HIS:ND1	0.56	2.38	23	10
1:B:47:ILE:HG21	1:B:56:TYR:OH	0.56	2.00	15	1
1:A:78:ILE:O	1:A:79:ASP:CB	0.56	2.53	19	5
1:A:65:LEU:HD21	1:B:2:ILE:HG23	0.56	1.77	11	1
1:B:64:HIS:CB	1:B:82:ARG:O	0.56	2.54	5	29
1:B:34:TYR:CE1	1:B:44:LEU:HB2	0.56	2.36	22	27
1:A:6:ILE:HG13	1:A:61:TYR:CE1	0.56	2.36	23	3
1:A:76:LEU:CD1	1:B:37:LEU:HD22	0.56	2.31	20	1
1:B:4:VAL:CG1	1:B:61:TYR:CB	0.56	2.81	8	3
1:A:43:VAL:HG21	1:B:70:VAL:CG1	0.56	2.28	4	2
1:A:35:VAL:CG1	1:A:37:LEU:HD23	0.56	2.30	20	1
1:B:13:PHE:CD1	1:B:13:PHE:N	0.56	2.73	8	2
1:B:47:ILE:HG12	1:B:56:TYR:CE1	0.56	2.36	4	16
1:B:37:LEU:CD2	1:B:37:LEU:N	0.56	2.68	25	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD11	1:B:68:PHE:O	0.56	2.00	6	2
1:A:65:LEU:HA	1:A:68:PHE:CD2	0.56	2.36	14	24
1:A:64:HIS:CB	1:A:82:ARG:O	0.56	2.54	5	29
1:A:45:VAL:HG12	1:A:46:LYS:N	0.56	2.16	5	10
1:A:65:LEU:HD12	1:B:37:LEU:HG	0.56	1.76	6	1
1:B:37:LEU:HD22	1:B:39:ASN:HD21	0.56	1.60	13	2
1:B:34:TYR:CZ	1:B:44:LEU:HD13	0.56	2.36	17	1
1:B:32:LEU:HD23	1:B:46:LYS:HA	0.56	1.76	5	3
1:B:6:ILE:HG12	1:B:61:TYR:CD1	0.56	2.36	10	2
1:B:3:LYS:H	1:B:37:LEU:HD12	0.56	1.56	1	1
1:A:4:VAL:HG13	1:A:61:TYR:HB3	0.56	1.76	13	2
1:A:37:LEU:HD22	1:B:76:LEU:CD1	0.56	2.30	20	1
1:B:4:VAL:HG12	1:B:5:GLU:N	0.55	2.16	1	11
1:A:47:ILE:HG12	1:A:56:TYR:CE1	0.55	2.35	4	16
1:A:34:TYR:CZ	1:A:44:LEU:HD13	0.55	2.35	17	1
1:A:78:ILE:HD12	1:B:78:ILE:CD1	0.55	2.30	2	14
1:A:72:GLN:O	1:A:73:PHE:CD2	0.55	2.59	28	1
1:B:81:LEU:CD2	1:B:81:LEU:O	0.55	2.55	15	14
1:B:4:VAL:HG13	1:B:61:TYR:HB3	0.55	1.76	13	1
1:A:76:LEU:HD22	1:B:2:ILE:HG21	0.55	1.79	16	1
1:A:39:ASN:O	1:A:41:HIS:CD2	0.55	2.59	27	1
1:A:7:LYS:CG	1:A:34:TYR:CE2	0.55	2.90	11	15
1:B:6:ILE:HG13	1:B:61:TYR:CE1	0.55	2.37	10	3
1:A:28:LEU:HD23	1:A:49:LEU:O	0.55	2.01	13	2
1:B:65:LEU:HA	1:B:68:PHE:CD2	0.55	2.37	14	24
1:A:81:LEU:CD2	1:A:81:LEU:O	0.55	2.55	2	12
1:B:72:GLN:O	1:B:73:PHE:CD2	0.55	2.59	28	1
1:B:45:VAL:HG12	1:B:46:LYS:N	0.55	2.16	5	10
1:B:6:ILE:O	1:B:6:ILE:CG2	0.55	2.55	21	4
1:B:72:GLN:N	1:B:72:GLN:NE2	0.55	2.55	21	1
1:A:1:MET:O	1:B:65:LEU:HD22	0.55	2.02	21	1
1:B:37:LEU:HD22	1:B:38:GLY:N	0.55	2.16	1	1
1:B:37:LEU:CD1	1:B:39:ASN:ND2	0.55	2.70	9	1
1:A:13:PHE:CD2	1:A:49:LEU:HG	0.55	2.37	7	24
1:A:43:VAL:O	1:A:43:VAL:CG2	0.55	2.55	25	14
1:A:63:VAL:HG13	1:A:81:LEU:CD1	0.55	2.31	18	5
1:A:6:ILE:HG12	1:A:61:TYR:CD1	0.55	2.36	10	2
1:B:78:ILE:O	1:B:79:ASP:CB	0.55	2.54	7	5
1:B:63:VAL:CG1	1:B:81:LEU:HB2	0.55	2.32	27	29
1:B:43:VAL:O	1:B:43:VAL:CG2	0.55	2.55	25	11
1:B:76:LEU:O	1:B:77:MET:CG	0.55	2.55	3	18

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD22	1:A:38:GLY:N	0.55	2.17	1	1
1:A:65:LEU:CD1	1:B:37:LEU:O	0.55	2.55	19	1
1:A:75:SER:N	1:B:45:VAL:CG2	0.55	2.70	16	1
1:A:6:ILE:O	1:A:6:ILE:CG2	0.55	2.55	21	4
1:A:2:ILE:CG2	1:A:63:VAL:HG21	0.55	2.31	5	3
1:A:69:LYS:N	1:B:37:LEU:HD11	0.55	2.17	5	6
1:B:37:LEU:N	1:B:37:LEU:HD22	0.55	2.17	1	1
1:B:28:LEU:HD23	1:B:49:LEU:O	0.55	2.02	13	2
1:A:37:LEU:O	1:B:65:LEU:CD1	0.55	2.55	19	2
1:A:2:ILE:CA	1:B:65:LEU:HD21	0.55	2.31	11	1
1:B:13:PHE:CD2	1:B:49:LEU:HG	0.55	2.37	7	24
1:A:65:LEU:HD11	1:B:37:LEU:CA	0.55	2.32	25	1
1:B:13:PHE:N	1:B:13:PHE:CD1	0.55	2.73	25	1
1:A:13:PHE:N	1:A:55:ALA:HB2	0.55	2.17	17	12
1:A:81:LEU:O	1:A:81:LEU:CD2	0.55	2.55	23	11
1:A:2:ILE:CA	1:B:65:LEU:HD13	0.55	2.32	10	4
1:A:2:ILE:HG23	1:B:65:LEU:HD21	0.55	1.78	11	1
1:B:62:THR:HG23	1:B:86:ALA:HB2	0.54	1.77	28	10
1:B:81:LEU:O	1:B:81:LEU:CD2	0.54	2.55	2	9
1:A:63:VAL:CG1	1:A:81:LEU:HB2	0.54	2.32	27	29
1:A:47:ILE:HG21	1:A:56:TYR:OH	0.54	2.00	15	1
1:A:37:LEU:HG	1:B:65:LEU:HD12	0.54	1.78	6	1
1:A:37:LEU:HD21	1:B:76:LEU:CD1	0.54	2.32	3	2
1:A:37:LEU:CD1	1:A:39:ASN:ND2	0.54	2.70	9	1
1:B:39:ASN:O	1:B:41:HIS:CD2	0.54	2.59	27	1
1:A:13:PHE:CD1	1:A:29:ASN:CG	0.54	2.81	30	10
1:A:13:PHE:CD1	1:A:13:PHE:N	0.54	2.73	25	1
1:A:37:LEU:CA	1:B:65:LEU:HD11	0.54	2.32	25	1
1:B:57:ALA:CB	1:B:58:PRO:CD	0.54	2.84	13	20
1:A:72:GLN:NE2	1:A:72:GLN:N	0.54	2.55	21	1
1:A:76:LEU:O	1:A:77:MET:CG	0.54	2.55	26	18
1:B:7:LYS:HG2	1:B:34:TYR:CE1	0.54	2.38	5	2
1:A:70:VAL:HG21	1:B:43:VAL:HG11	0.54	1.78	3	3
1:A:35:VAL:CG1	1:A:37:LEU:HD21	0.54	2.32	1	1
1:B:43:VAL:HG23	1:B:45:VAL:HG13	0.54	1.79	14	3
1:A:62:THR:O	1:A:84:VAL:CG2	0.54	2.56	13	17
1:A:29:ASN:CB	1:A:49:LEU:HB3	0.54	2.32	5	5
1:A:7:LYS:HG2	1:A:34:TYR:CE1	0.54	2.37	5	2
1:B:63:VAL:HG13	1:B:81:LEU:CD1	0.54	2.31	18	4
1:A:3:LYS:O	1:A:37:LEU:CD1	0.54	2.56	1	1
1:A:7:LYS:HG3	1:A:34:TYR:CD2	0.54	2.37	20	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:VAL:CG1	1:A:61:TYR:CB	0.54	2.82	8	3
1:B:10:GLN:O	1:B:31:GLN:NE2	0.54	2.41	22	28
1:B:13:PHE:CD1	1:B:29:ASN:CG	0.54	2.81	6	11
1:B:61:TYR:CD2	1:B:84:VAL:C	0.54	2.81	13	18
1:B:29:ASN:HB2	1:B:49:LEU:CB	0.54	2.32	15	3
1:A:29:ASN:HB2	1:A:49:LEU:CB	0.54	2.32	15	4
1:A:31:GLN:CB	1:A:47:ILE:CG2	0.54	2.86	8	12
1:B:2:ILE:CG2	1:B:63:VAL:HG21	0.54	2.31	5	2
1:A:43:VAL:HG23	1:A:45:VAL:HG13	0.54	1.78	14	3
1:B:7:LYS:HG2	1:B:34:TYR:CE2	0.54	2.37	11	15
1:B:13:PHE:N	1:B:55:ALA:HB2	0.54	2.17	17	12
1:A:3:LYS:H	1:A:37:LEU:HD12	0.54	1.55	1	1
1:A:35:VAL:HG12	1:A:36:ASP:N	0.54	2.15	26	2
1:A:37:LEU:HD22	1:A:39:ASN:HD21	0.54	1.60	13	2
1:A:7:LYS:HG3	1:A:34:TYR:CD1	0.54	2.38	28	1
1:B:31:GLN:HB3	1:B:47:ILE:CG2	0.54	2.33	29	27
1:A:7:LYS:HG2	1:A:34:TYR:CE2	0.54	2.38	23	15
1:A:69:LYS:HA	1:B:37:LEU:HD11	0.54	1.78	8	4
1:A:1:MET:C	1:B:65:LEU:HD22	0.54	2.22	18	5
1:B:4:VAL:HG21	1:B:83:LEU:HD11	0.54	1.79	22	2
1:A:37:LEU:HD22	1:A:37:LEU:N	0.54	2.16	1	1
1:A:70:VAL:CG1	1:B:45:VAL:HG21	0.54	2.32	9	4
1:A:32:LEU:N	1:A:32:LEU:CD2	0.54	2.70	9	2
1:B:48:THR:HG21	1:B:80:ARG:CZ	0.54	2.33	22	2
1:B:7:LYS:HG3	1:B:34:TYR:CD2	0.54	2.37	20	1
1:A:10:GLN:O	1:A:31:GLN:NE2	0.54	2.41	7	28
1:B:43:VAL:CG2	1:B:43:VAL:O	0.54	2.56	18	14
1:B:7:LYS:CG	1:B:34:TYR:CE2	0.54	2.90	11	15
1:B:6:ILE:CD1	1:B:61:TYR:CG	0.54	2.91	7	4
1:B:28:LEU:HD12	1:B:29:ASN:C	0.54	2.23	10	2
1:B:33:CYS:SG	1:B:47:ILE:CG1	0.54	2.96	15	3
1:B:68:PHE:CD1	1:B:78:ILE:HG13	0.54	2.38	4	1
1:A:72:GLN:CG	1:A:72:GLN:O	0.54	2.56	29	4
1:B:10:GLN:HE22	1:B:32:LEU:HD22	0.54	1.63	27	1
1:B:7:LYS:HG3	1:B:34:TYR:CD1	0.54	2.38	28	1
1:B:29:ASN:CB	1:B:49:LEU:HB3	0.54	2.32	5	5
1:A:65:LEU:HD22	1:B:1:MET:O	0.54	2.02	21	1
1:A:62:THR:HG23	1:A:86:ALA:HA	0.54	1.80	8	12
1:B:49:LEU:CD1	1:B:53:GLN:O	0.54	2.56	1	8
1:B:32:LEU:N	1:B:32:LEU:CD2	0.54	2.70	9	2
1:A:65:LEU:HD13	1:B:2:ILE:HG22	0.54	1.77	30	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HD21	1:B:2:ILE:CA	0.54	2.32	11	1
1:B:3:LYS:O	1:B:37:LEU:CD1	0.54	2.56	1	1
1:A:1:MET:O	1:A:3:LYS:N	0.53	2.41	24	12
1:A:61:TYR:CD2	1:A:84:VAL:C	0.53	2.81	13	18
1:A:29:ASN:O	1:A:49:LEU:CB	0.53	2.56	14	8
1:A:28:LEU:HD12	1:A:29:ASN:C	0.53	2.23	10	2
1:B:36:ASP:O	1:B:39:ASN:N	0.53	2.41	26	6
1:B:72:GLN:O	1:B:72:GLN:CG	0.53	2.56	29	2
1:A:38:GLY:O	1:A:39:ASN:CB	0.53	2.55	26	1
1:B:62:THR:O	1:B:84:VAL:CG2	0.53	2.56	13	16
1:B:62:THR:HG23	1:B:86:ALA:HA	0.53	1.80	2	12
1:A:65:LEU:CD1	1:B:37:LEU:HG	0.53	2.33	1	4
1:A:49:LEU:CD1	1:A:53:GLN:O	0.53	2.56	1	8
1:B:38:GLY:O	1:B:39:ASN:CB	0.53	2.55	26	1
1:B:1:MET:O	1:B:3:LYS:N	0.53	2.42	24	12
1:A:33:CYS:SG	1:A:47:ILE:CG1	0.53	2.96	15	3
1:A:43:VAL:CG2	1:A:43:VAL:O	0.53	2.56	18	10
1:A:4:VAL:HG21	1:A:83:LEU:HD11	0.53	1.79	22	2
1:A:81:LEU:HD23	1:A:81:LEU:N	0.53	2.18	18	2
1:B:68:PHE:CD1	1:B:78:ILE:HG12	0.53	2.37	13	1
1:B:62:THR:HG23	1:B:86:ALA:CA	0.53	2.34	8	16
1:A:47:ILE:HG13	1:A:56:TYR:CE2	0.53	2.38	2	5
1:B:29:ASN:O	1:B:49:LEU:CB	0.53	2.57	3	8
1:A:31:GLN:NE2	1:A:56:TYR:O	0.53	2.40	17	11
1:A:7:LYS:CD	1:A:34:TYR:CE2	0.53	2.92	11	4
1:B:72:GLN:CG	1:B:72:GLN:O	0.53	2.56	18	4
1:A:65:LEU:HD21	1:B:2:ILE:HG13	0.53	1.81	13	1
1:B:62:THR:HG23	1:B:86:ALA:CB	0.53	2.34	28	11
1:A:33:CYS:O	1:A:44:LEU:HD12	0.53	2.03	18	8
1:A:31:GLN:HB3	1:A:47:ILE:CG2	0.53	2.33	29	27
1:B:49:LEU:O	1:B:49:LEU:CD1	0.53	2.56	23	1
1:B:1:MET:O	1:B:1:MET:CG	0.53	2.56	9	1
1:B:65:LEU:HG	1:B:68:PHE:CD2	0.53	2.39	11	1
1:B:81:LEU:O	1:B:81:LEU:CG	0.53	2.57	16	15
1:B:31:GLN:CB	1:B:47:ILE:CG2	0.53	2.86	8	11
1:B:40:GLU:C	1:B:41:HIS:CG	0.53	2.80	7	4
1:B:67:SER:O	1:B:79:ASP:CB	0.53	2.57	9	2
1:A:48:THR:HG21	1:A:80:ARG:CZ	0.53	2.33	22	2
1:B:65:LEU:HD12	1:B:65:LEU:O	0.53	2.04	8	2
1:B:10:GLN:O	1:B:11:ALA:C	0.53	2.47	27	1
1:B:35:VAL:CG1	1:B:37:LEU:HG	0.53	2.34	28	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:33:CYS:O	1:B:44:LEU:HD12	0.53	2.04	15	8
1:B:81:LEU:CG	1:B:81:LEU:O	0.53	2.57	17	10
1:A:1:MET:SD	1:A:62:THR:CG2	0.53	2.97	2	4
1:B:65:LEU:HA	1:B:68:PHE:CG	0.53	2.39	3	18
1:B:69:LYS:CG	1:B:77:MET:O	0.53	2.57	7	1
1:A:45:VAL:HG21	1:B:70:VAL:CG1	0.53	2.33	9	3
1:A:72:GLN:O	1:A:72:GLN:CG	0.53	2.56	18	2
1:A:65:LEU:HG	1:A:68:PHE:CD2	0.53	2.38	11	1
1:A:62:THR:HG23	1:A:86:ALA:CA	0.53	2.34	8	16
1:A:81:LEU:O	1:A:81:LEU:CG	0.53	2.57	29	15
1:A:40:GLU:C	1:A:41:HIS:CG	0.53	2.80	7	4
1:B:47:ILE:HD12	1:B:56:TYR:CZ	0.53	2.39	29	4
1:B:35:VAL:CG1	1:B:37:LEU:HD21	0.53	2.33	1	1
1:A:56:TYR:CE1	1:A:83:LEU:HB3	0.53	2.39	8	1
1:A:10:GLN:O	1:A:12:GLN:N	0.53	2.42	27	1
1:A:37:LEU:C	1:A:37:LEU:HD12	0.53	2.23	28	1
1:B:7:LYS:CD	1:B:34:TYR:CE1	0.53	2.92	18	2
1:B:47:ILE:HG13	1:B:56:TYR:CE2	0.53	2.39	11	5
1:A:39:ASN:O	1:A:41:HIS:N	0.53	2.42	18	6
1:A:47:ILE:HD12	1:A:56:TYR:CZ	0.53	2.39	29	4
1:B:29:ASN:ND2	1:B:49:LEU:O	0.53	2.42	18	6
1:A:39:ASN:O	1:A:41:HIS:NE2	0.53	2.42	27	1
1:B:64:HIS:N	1:B:82:ARG:O	0.53	2.42	13	8
1:A:31:GLN:HB3	1:A:47:ILE:HG22	0.53	1.80	14	15
1:A:65:LEU:HD22	1:B:1:MET:C	0.53	2.23	18	5
1:B:1:MET:SD	1:B:62:THR:CG2	0.53	2.97	2	4
1:A:65:LEU:HA	1:A:68:PHE:CG	0.53	2.39	8	19
1:A:47:ILE:CG2	1:A:47:ILE:O	0.53	2.56	1	2
1:A:29:ASN:ND2	1:A:49:LEU:O	0.53	2.42	3	6
1:B:37:LEU:O	1:B:37:LEU:CD1	0.53	2.57	26	2
1:B:31:GLN:OE1	1:B:56:TYR:N	0.53	2.41	8	2
1:B:56:TYR:CE1	1:B:83:LEU:HB3	0.53	2.39	8	1
1:A:65:LEU:CD2	1:B:2:ILE:HG12	0.53	2.34	13	1
1:A:49:LEU:CD1	1:A:49:LEU:O	0.53	2.56	23	1
1:B:37:LEU:C	1:B:37:LEU:HD12	0.52	2.23	28	1
1:A:80:ARG:O	1:A:81:LEU:C	0.52	2.48	4	23
1:A:4:VAL:HG21	1:A:35:VAL:HG22	0.52	1.79	7	3
1:B:4:VAL:O	1:B:61:TYR:N	0.52	2.40	15	8
1:B:7:LYS:HE2	1:B:34:TYR:CD2	0.52	2.39	10	2
1:A:31:GLN:OE1	1:A:55:ALA:CB	0.52	2.55	7	2
1:A:37:LEU:C	1:A:37:LEU:CD1	0.52	2.78	29	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:39:ASN:O	1:B:41:HIS:ND1	0.52	2.42	19	1
1:A:10:GLN:HE22	1:A:32:LEU:HD22	0.52	1.63	27	1
1:A:47:ILE:CG2	1:A:48:THR:N	0.52	2.72	2	4
1:B:33:CYS:SG	1:B:47:ILE:CD1	0.52	2.97	9	5
1:B:39:ASN:O	1:B:41:HIS:N	0.52	2.43	9	6
1:B:31:GLN:HB3	1:B:47:ILE:HG22	0.52	1.80	14	16
1:A:7:LYS:HE2	1:A:34:TYR:CD2	0.52	2.39	10	2
1:B:72:GLN:C	1:B:73:PHE:CG	0.52	2.81	8	3
1:A:31:GLN:OE1	1:A:56:TYR:N	0.52	2.41	8	2
1:B:80:ARG:O	1:B:81:LEU:C	0.52	2.47	4	23
1:A:64:HIS:N	1:A:82:ARG:O	0.52	2.42	13	8
1:A:12:GLN:HA	1:A:55:ALA:HB3	0.52	1.82	17	4
1:B:7:LYS:CD	1:B:34:TYR:CE2	0.52	2.92	11	4
1:A:6:ILE:CD1	1:A:83:LEU:CD2	0.52	2.88	22	3
1:A:72:GLN:C	1:A:73:PHE:CG	0.52	2.81	8	3
1:A:62:THR:HG23	1:A:86:ALA:CB	0.52	2.34	28	13
1:A:65:LEU:HD12	1:A:65:LEU:O	0.52	2.04	8	4
1:A:81:LEU:CG	1:A:81:LEU:O	0.52	2.57	16	9
1:B:7:LYS:CG	1:B:34:TYR:CE1	0.52	2.92	18	2
1:B:31:GLN:OE1	1:B:55:ALA:CB	0.52	2.55	7	2
1:B:47:ILE:CG2	1:B:47:ILE:O	0.52	2.56	1	2
1:B:31:GLN:O	1:B:47:ILE:N	0.52	2.43	13	6
1:A:68:PHE:CD1	1:A:78:ILE:HG12	0.52	2.38	13	1
1:B:56:TYR:CE1	1:B:83:LEU:O	0.52	2.63	13	1
1:A:7:LYS:CD	1:A:34:TYR:CE1	0.52	2.92	18	2
1:A:37:LEU:CD1	1:A:37:LEU:O	0.52	2.57	26	2
1:A:36:ASP:OD1	1:A:36:ASP:N	0.52	2.43	14	4
1:B:35:VAL:O	1:B:37:LEU:CD2	0.52	2.57	7	1
1:A:69:LYS:CG	1:A:77:MET:O	0.52	2.57	7	1
1:A:70:VAL:HG13	1:A:76:LEU:HD12	0.52	1.82	18	1
1:A:2:ILE:HG13	1:B:65:LEU:HD21	0.52	1.81	13	1
1:A:2:ILE:HG12	1:B:65:LEU:CD2	0.52	2.35	13	1
1:A:39:ASN:O	1:A:40:GLU:C	0.52	2.48	15	15
1:B:47:ILE:CG2	1:B:48:THR:N	0.52	2.73	2	4
1:A:6:ILE:CD1	1:A:61:TYR:CG	0.52	2.92	7	3
1:A:68:PHE:CD1	1:A:78:ILE:HG13	0.52	2.40	4	1
1:B:3:LYS:N	1:B:37:LEU:CD1	0.52	2.64	1	1
1:A:37:LEU:HG	1:B:65:LEU:CD1	0.52	2.34	1	3
1:A:31:GLN:O	1:A:47:ILE:N	0.52	2.43	9	6
1:A:1:MET:O	1:A:1:MET:CG	0.52	2.56	9	1
1:B:10:GLN:O	1:B:12:GLN:N	0.52	2.42	27	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLN:O	1:A:11:ALA:C	0.52	2.47	27	1
1:A:35:VAL:CG1	1:A:37:LEU:HG	0.52	2.34	28	1
1:B:36:ASP:N	1:B:36:ASP:OD1	0.52	2.42	28	3
1:A:35:VAL:O	1:A:37:LEU:CD2	0.52	2.57	7	1
1:A:39:ASN:O	1:A:41:HIS:ND1	0.52	2.43	19	1
1:B:39:ASN:O	1:B:41:HIS:NE2	0.52	2.42	27	1
1:B:47:ILE:HG12	1:B:56:TYR:CZ	0.52	2.40	26	18
1:A:70:VAL:HG11	1:B:45:VAL:CG1	0.52	2.35	28	3
1:B:63:VAL:CG1	1:B:81:LEU:CD1	0.52	2.87	4	2
1:B:28:LEU:HD22	1:B:48:THR:CG2	0.52	2.35	4	4
1:B:6:ILE:CD1	1:B:83:LEU:CD2	0.52	2.88	22	3
1:A:76:LEU:HB2	1:B:81:LEU:HD13	0.52	1.79	14	5
1:B:72:GLN:NE2	1:B:72:GLN:O	0.52	2.43	18	3
1:A:33:CYS:SG	1:A:47:ILE:CD1	0.52	2.98	15	5
1:A:7:LYS:CG	1:A:34:TYR:CE1	0.52	2.93	18	2
1:A:62:THR:O	1:A:84:VAL:HG23	0.52	2.05	13	1
1:B:31:GLN:NE2	1:B:56:TYR:O	0.52	2.41	17	12
1:B:32:LEU:CD2	1:B:44:LEU:CD1	0.52	2.87	10	1
1:B:70:VAL:HG13	1:B:76:LEU:HD12	0.52	1.82	18	1
1:B:47:ILE:HG21	1:B:56:TYR:CE2	0.52	2.40	13	1
1:B:39:ASN:N	1:B:39:ASN:OD1	0.51	2.43	28	3
1:A:65:LEU:HA	1:A:68:PHE:CE2	0.51	2.41	5	21
1:A:36:ASP:O	1:A:39:ASN:N	0.51	2.41	26	6
1:B:6:ILE:CD1	1:B:33:CYS:SG	0.51	2.98	16	2
1:A:63:VAL:CG1	1:A:81:LEU:CD1	0.51	2.87	4	2
1:B:35:VAL:CG1	1:B:36:ASP:N	0.51	2.73	26	2
1:B:34:TYR:CE2	1:B:44:LEU:HB2	0.51	2.40	28	3
1:B:67:SER:OG	1:B:82:ARG:N	0.51	2.43	28	7
1:B:71:GLY:O	1:B:72:GLN:CG	0.51	2.59	28	1
1:B:81:LEU:N	1:B:81:LEU:HD23	0.51	2.21	5	1
1:A:67:SER:O	1:A:79:ASP:N	0.51	2.43	9	2
1:A:28:LEU:HD22	1:A:48:THR:CG2	0.51	2.35	4	4
1:A:65:LEU:CD1	1:B:37:LEU:CA	0.51	2.88	19	4
1:A:35:VAL:CG1	1:A:36:ASP:N	0.51	2.73	26	2
1:A:37:LEU:CD1	1:A:37:LEU:C	0.51	2.79	26	3
1:A:2:ILE:HG22	1:B:65:LEU:HD13	0.51	1.81	30	1
1:A:34:TYR:CE2	1:A:44:LEU:HB2	0.51	2.40	28	3
1:B:62:THR:N	1:B:84:VAL:O	0.51	2.39	26	25
1:A:34:TYR:CE2	1:A:44:LEU:CD1	0.51	2.92	17	1
1:A:37:LEU:HD22	1:B:65:LEU:CD2	0.51	2.35	21	1
1:B:81:LEU:C	1:B:81:LEU:CD1	0.51	2.78	8	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:ILE:HG21	1:B:56:TYR:CD2	0.51	2.41	13	2
1:A:2:ILE:HG22	1:A:37:LEU:CD2	0.51	2.36	28	1
1:A:65:LEU:HD13	1:B:2:ILE:CA	0.51	2.33	10	3
1:B:6:ILE:CG1	1:B:61:TYR:CE1	0.51	2.94	10	2
1:B:37:LEU:C	1:B:37:LEU:CD1	0.51	2.78	29	2
1:A:72:GLN:O	1:A:72:GLN:NE2	0.51	2.44	27	2
1:A:70:VAL:HG11	1:B:45:VAL:CG2	0.51	2.36	9	2
1:A:47:ILE:HG21	1:A:56:TYR:CE2	0.51	2.40	13	1
1:A:36:ASP:N	1:A:36:ASP:OD1	0.51	2.43	28	3
1:A:67:SER:OG	1:A:82:ARG:N	0.51	2.43	28	7
1:B:12:GLN:HA	1:B:55:ALA:HB3	0.51	1.82	17	5
1:A:35:VAL:O	1:A:43:VAL:CG2	0.51	2.57	14	8
1:A:2:ILE:HA	1:B:65:LEU:CD2	0.51	2.36	11	2
1:B:2:ILE:HG22	1:B:37:LEU:CD2	0.51	2.36	28	1
1:B:51:GLU:O	1:B:53:GLN:N	0.51	2.43	6	2
1:A:51:GLU:O	1:A:53:GLN:N	0.51	2.43	6	2
1:A:67:SER:O	1:A:79:ASP:CB	0.51	2.57	9	2
1:A:56:TYR:CE1	1:A:83:LEU:O	0.51	2.63	13	1
1:A:65:LEU:O	1:A:68:PHE:N	0.51	2.43	13	3
1:A:4:VAL:HB	1:A:61:TYR:CB	0.51	2.36	25	11
1:B:76:LEU:C	1:B:77:MET:CG	0.51	2.79	4	6
1:B:7:LYS:HE2	1:B:34:TYR:CE2	0.51	2.41	6	3
1:A:63:VAL:HG13	1:A:81:LEU:CG	0.51	2.36	4	1
1:B:37:LEU:CD1	1:B:37:LEU:C	0.51	2.79	16	2
1:A:65:LEU:HB2	1:A:68:PHE:CE2	0.51	2.41	25	2
1:B:76:LEU:C	1:B:76:LEU:HD23	0.51	2.26	25	2
1:A:57:ALA:CB	1:A:58:PRO:CD	0.51	2.88	15	21
1:A:4:VAL:O	1:A:61:TYR:N	0.51	2.43	2	8
1:A:7:LYS:HE2	1:A:34:TYR:CE2	0.51	2.41	6	3
1:A:37:LEU:HD23	1:A:39:ASN:OD1	0.51	2.06	4	1
1:A:47:ILE:HG21	1:A:56:TYR:CD2	0.51	2.41	13	2
1:A:56:TYR:CZ	1:A:83:LEU:HB3	0.51	2.41	13	1
1:B:65:LEU:O	1:B:68:PHE:N	0.51	2.43	13	3
1:A:7:LYS:HD2	1:A:34:TYR:CZ	0.51	2.41	28	2
1:B:54:PRO:O	1:B:55:ALA:C	0.51	2.48	8	30
1:B:4:VAL:HB	1:B:61:TYR:CB	0.51	2.36	25	11
1:A:29:ASN:ND2	1:A:50:ASP:O	0.51	2.43	11	6
1:A:6:ILE:CD1	1:A:33:CYS:SG	0.51	2.98	16	2
1:B:63:VAL:HG13	1:B:81:LEU:CG	0.51	2.36	4	1
1:A:37:LEU:CA	1:B:65:LEU:CD1	0.51	2.89	19	4
1:B:62:THR:O	1:B:84:VAL:HG23	0.51	2.06	13	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:2:ILE:HA	1:A:37:LEU:HD22	0.51	1.83	28	1
1:A:47:ILE:HG12	1:A:56:TYR:CZ	0.51	2.40	26	18
1:B:65:LEU:HA	1:B:68:PHE:CE2	0.51	2.41	5	19
1:B:29:ASN:ND2	1:B:50:ASP:O	0.51	2.43	11	6
1:B:67:SER:O	1:B:79:ASP:N	0.51	2.43	9	3
1:A:3:LYS:N	1:A:37:LEU:CD1	0.51	2.64	1	1
1:B:33:CYS:SG	1:B:45:VAL:CG1	0.51	2.99	1	1
1:B:36:ASP:OD1	1:B:36:ASP:N	0.51	2.43	19	3
1:A:40:GLU:O	1:A:41:HIS:HB3	0.51	2.06	8	1
1:A:39:ASN:N	1:A:39:ASN:OD1	0.50	2.42	28	5
1:A:65:LEU:CD2	1:B:1:MET:C	0.50	2.80	22	9
1:B:39:ASN:O	1:B:40:GLU:CB	0.50	2.59	4	2
1:A:32:LEU:CD2	1:A:44:LEU:CD1	0.50	2.87	10	1
1:A:32:LEU:HD22	1:A:44:LEU:HD11	0.50	1.81	10	2
1:A:35:VAL:HG12	1:A:37:LEU:CD2	0.50	2.36	1	1
1:A:54:PRO:O	1:A:55:ALA:C	0.50	2.48	8	29
1:A:37:LEU:HA	1:B:65:LEU:HD11	0.50	1.83	25	2
1:A:13:PHE:CB	1:A:30:GLU:O	0.50	2.60	12	4
1:A:37:LEU:HB3	1:B:65:LEU:HD21	0.50	1.81	21	1
1:B:72:GLN:O	1:B:72:GLN:NE2	0.50	2.43	27	2
1:B:37:LEU:HD23	1:B:39:ASN:OD1	0.50	2.06	4	1
1:B:13:PHE:CD2	1:B:29:ASN:HB2	0.50	2.41	11	3
1:A:65:LEU:CD2	1:B:37:LEU:HD22	0.50	2.36	21	1
1:A:65:LEU:HD21	1:B:37:LEU:HD22	0.50	1.82	21	1
1:A:33:CYS:SG	1:A:45:VAL:CG1	0.50	3.00	1	1
1:B:7:LYS:HD2	1:B:34:TYR:CZ	0.50	2.42	28	2
1:A:13:PHE:CD2	1:A:29:ASN:HB2	0.50	2.42	8	3
1:A:72:GLN:NE2	1:A:72:GLN:O	0.50	2.45	16	3
1:B:63:VAL:CG1	1:B:81:LEU:HG	0.50	2.37	4	1
1:A:29:ASN:HD22	1:A:49:LEU:HD12	0.50	1.67	1	1
1:B:49:LEU:CD1	1:B:50:ASP:O	0.50	2.59	24	2
1:A:64:HIS:HB2	1:A:82:ARG:O	0.50	2.07	2	22
1:B:65:LEU:HB2	1:B:68:PHE:CE2	0.50	2.41	25	1
1:A:76:LEU:C	1:A:77:MET:CG	0.50	2.79	4	6
1:A:13:PHE:CD1	1:A:29:ASN:HB2	0.50	2.41	17	6
1:B:35:VAL:O	1:B:43:VAL:CG2	0.50	2.58	23	8
1:A:37:LEU:HD22	1:B:65:LEU:HD21	0.50	1.82	21	1
1:B:7:LYS:HE2	1:B:34:TYR:CE1	0.50	2.42	5	1
1:A:1:MET:C	1:B:65:LEU:CD2	0.50	2.80	18	8
1:B:40:GLU:O	1:B:41:HIS:HB3	0.50	2.06	8	1
1:A:81:LEU:CD1	1:B:76:LEU:HD22	0.50	2.36	23	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:VAL:HG22	1:A:35:VAL:HG13	0.50	1.83	17	2
1:B:37:LEU:N	1:B:37:LEU:CD1	0.50	2.72	17	1
1:A:6:ILE:CG1	1:A:61:TYR:CE1	0.50	2.94	10	3
1:A:83:LEU:O	1:A:84:VAL:CG1	0.50	2.60	1	2
1:B:83:LEU:O	1:B:84:VAL:CG1	0.50	2.59	1	2
1:A:63:VAL:CG1	1:A:81:LEU:HG	0.50	2.37	4	1
1:A:28:LEU:CD2	1:A:48:THR:CG2	0.50	2.90	1	1
1:B:31:GLN:OE1	1:B:32:LEU:N	0.50	2.45	19	2
1:B:13:PHE:CB	1:B:30:GLU:O	0.50	2.59	12	4
1:A:1:MET:O	1:A:2:ILE:CB	0.50	2.60	26	5
1:A:6:ILE:CD1	1:A:56:TYR:CB	0.50	2.90	13	3
1:B:56:TYR:CZ	1:B:83:LEU:HB3	0.50	2.41	13	1
1:B:64:HIS:HB2	1:B:82:ARG:O	0.50	2.07	2	22
1:B:13:PHE:CD1	1:B:29:ASN:HB2	0.50	2.42	19	6
1:B:28:LEU:CD2	1:B:48:THR:CG2	0.50	2.90	1	1
1:A:55:ALA:O	1:A:57:ALA:N	0.49	2.45	12	6
1:A:45:VAL:CG1	1:B:70:VAL:HG11	0.49	2.37	28	3
1:B:4:VAL:HG22	1:B:35:VAL:HG13	0.49	1.83	17	2
1:B:63:VAL:HG12	1:B:64:HIS:N	0.49	2.22	5	10
1:B:6:ILE:CD1	1:B:56:TYR:CB	0.49	2.90	13	3
1:B:49:LEU:CD2	1:B:56:TYR:CE1	0.49	2.95	1	1
1:B:47:ILE:HD12	1:B:56:TYR:HE2	0.49	1.67	13	1
1:A:32:LEU:HD13	1:A:45:VAL:O	0.49	2.07	9	1
1:B:39:ASN:O	1:B:40:GLU:C	0.49	2.48	15	16
1:A:71:GLY:O	1:A:72:GLN:CG	0.49	2.59	28	1
1:B:6:ILE:CG2	1:B:6:ILE:O	0.49	2.60	1	1
1:B:38:GLY:O	1:B:39:ASN:ND2	0.49	2.45	26	1
1:A:29:ASN:CB	1:A:49:LEU:O	0.49	2.61	18	1
1:B:2:ILE:HA	1:B:37:LEU:HD22	0.49	1.83	28	1
1:B:4:VAL:HG21	1:B:35:VAL:HG22	0.49	1.79	7	3
1:B:49:LEU:CD2	1:B:55:ALA:HA	0.49	2.37	8	5
1:B:29:ASN:OD1	1:B:49:LEU:O	0.49	2.30	7	6
1:A:4:VAL:HA	1:A:34:TYR:O	0.49	2.08	20	24
1:A:37:LEU:CG	1:A:37:LEU:O	0.49	2.60	8	3
1:A:32:LEU:HD23	1:A:44:LEU:HD11	0.49	1.81	10	2
1:B:7:LYS:HB2	1:B:10:GLN:CG	0.49	2.38	26	3
1:B:60:LEU:O	1:B:85:PRO:HA	0.49	2.07	6	26
1:A:61:TYR:HB3	1:A:83:LEU:CD2	0.49	2.38	5	21
1:A:39:ASN:O	1:A:41:HIS:O	0.49	2.30	15	6
1:B:67:SER:O	1:B:78:ILE:O	0.49	2.31	7	4
1:A:70:VAL:HG13	1:B:45:VAL:CG2	0.49	2.37	22	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:THR:N	1:A:84:VAL:O	0.49	2.40	1	30
1:A:31:GLN:OE1	1:A:32:LEU:O	0.49	2.31	17	18
1:B:39:ASN:O	1:B:41:HIS:O	0.49	2.31	18	7
1:A:49:LEU:CD2	1:A:55:ALA:HA	0.49	2.38	8	7
1:A:65:LEU:HD21	1:B:37:LEU:HB3	0.49	1.83	21	1
1:B:10:GLN:O	1:B:31:GLN:OE1	0.49	2.30	16	8
1:A:7:LYS:HE2	1:A:34:TYR:CE1	0.49	2.42	5	1
1:A:67:SER:O	1:A:78:ILE:O	0.49	2.30	7	4
1:A:65:LEU:CB	1:B:2:ILE:HG12	0.49	2.38	1	8
1:A:49:LEU:CD2	1:A:56:TYR:CE1	0.49	2.95	1	1
1:A:63:VAL:HG12	1:A:64:HIS:N	0.49	2.23	9	10
1:A:79:ASP:O	1:A:80:ARG:HB3	0.49	2.08	18	3
1:A:39:ASN:O	1:A:40:GLU:CB	0.49	2.59	4	2
1:A:68:PHE:CE1	1:A:78:ILE:HG13	0.49	2.43	4	1
1:B:37:LEU:C	1:B:37:LEU:HD13	0.49	2.28	16	1
1:A:67:SER:HB3	1:A:80:ARG:C	0.49	2.28	13	19
1:A:6:ILE:HD13	1:A:61:TYR:CZ	0.49	2.43	2	7
1:A:12:GLN:HA	1:A:55:ALA:CB	0.49	2.38	17	2
1:A:7:LYS:HB2	1:A:10:GLN:CG	0.49	2.38	26	4
1:B:6:ILE:HD12	1:B:56:TYR:CB	0.49	2.38	23	3
1:A:7:LYS:HD3	1:A:34:TYR:CG	0.49	2.43	10	2
1:A:38:GLY:O	1:A:39:ASN:ND2	0.49	2.45	26	1
1:B:31:GLN:OE1	1:B:49:LEU:HD23	0.49	2.08	8	1
1:A:47:ILE:HD12	1:A:56:TYR:HE2	0.49	1.68	13	1
1:A:6:ILE:HD13	1:A:56:TYR:CB	0.49	2.36	13	1
1:B:6:ILE:HD13	1:B:56:TYR:CB	0.49	2.37	13	1
1:A:1:MET:C	1:A:2:ILE:CG1	0.49	2.81	9	1
1:A:60:LEU:O	1:A:85:PRO:HA	0.49	2.08	6	26
1:A:65:LEU:HD11	1:B:37:LEU:HA	0.49	1.83	25	2
1:B:34:TYR:CE2	1:B:44:LEU:CD1	0.49	2.93	17	1
1:A:47:ILE:HD11	1:A:83:LEU:HD12	0.49	1.83	24	3
1:B:68:PHE:CE1	1:B:78:ILE:HG13	0.49	2.42	4	1
1:B:78:ILE:HG22	1:B:79:ASP:N	0.49	2.23	19	4
1:B:29:ASN:CB	1:B:49:LEU:O	0.49	2.61	18	1
1:A:7:LYS:HG3	1:A:34:TYR:CE1	0.49	2.43	27	3
1:A:47:ILE:O	1:A:47:ILE:CG2	0.49	2.60	16	1
1:B:1:MET:O	1:B:2:ILE:CB	0.49	2.60	26	4
1:B:2:ILE:HG21	1:B:63:VAL:CG2	0.49	2.36	5	1
1:B:7:LYS:HD3	1:B:34:TYR:CG	0.49	2.43	24	2
1:B:61:TYR:CD2	1:B:83:LEU:CD2	0.49	2.96	8	4
1:A:37:LEU:HA	1:B:65:LEU:CD1	0.49	2.37	3	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:6:ILE:HD13	1:B:61:TYR:CZ	0.49	2.43	11	6
1:A:29:ASN:OD1	1:A:49:LEU:O	0.49	2.31	7	6
1:B:37:LEU:O	1:B:37:LEU:CG	0.49	2.60	8	4
1:A:45:VAL:CG2	1:B:70:VAL:HG13	0.49	2.38	22	2
1:A:32:LEU:HD23	1:A:44:LEU:CD1	0.49	2.37	10	1
1:A:6:ILE:HD12	1:A:56:TYR:CB	0.49	2.38	23	3
1:B:83:LEU:HG	1:B:84:VAL:N	0.49	2.23	29	4
1:B:47:ILE:HG23	1:B:56:TYR:CE1	0.49	2.43	1	4
1:B:7:LYS:HG3	1:B:34:TYR:CE1	0.49	2.43	8	3
1:A:47:ILE:CG2	1:A:56:TYR:CE2	0.49	2.96	13	2
1:B:32:LEU:HD13	1:B:45:VAL:O	0.49	2.07	9	1
1:B:5:GLU:N	1:B:34:TYR:O	0.48	2.46	28	3
1:A:33:CYS:O	1:A:44:LEU:HA	0.48	2.08	15	22
1:A:37:LEU:CD1	1:B:69:LYS:CA	0.48	2.90	5	3
1:A:67:SER:OG	1:A:80:ARG:O	0.48	2.31	20	20
1:A:6:ILE:CG1	1:A:61:TYR:CD1	0.48	2.96	23	2
1:B:29:ASN:HD22	1:B:49:LEU:HD12	0.48	1.67	1	1
1:B:35:VAL:HG12	1:B:37:LEU:CD2	0.48	2.38	1	1
1:A:65:LEU:CD1	1:B:37:LEU:HA	0.48	2.38	3	4
1:B:47:ILE:O	1:B:47:ILE:CG2	0.48	2.60	16	1
1:B:55:ALA:O	1:B:57:ALA:N	0.48	2.46	9	7
1:B:6:ILE:CG1	1:B:61:TYR:CD1	0.48	2.96	23	2
1:B:36:ASP:O	1:B:39:ASN:OD1	0.48	2.32	8	2
1:A:83:LEU:HG	1:A:84:VAL:N	0.48	2.22	29	4
1:B:47:ILE:CG2	1:B:56:TYR:CE2	0.48	2.96	13	2
1:B:61:TYR:HB3	1:B:83:LEU:CD2	0.48	2.38	5	21
1:A:49:LEU:C	1:A:49:LEU:HD13	0.48	2.29	6	4
1:B:67:SER:HB3	1:B:80:ARG:O	0.48	2.08	8	12
1:B:34:TYR:HB3	1:B:42:PRO:HB2	0.48	1.85	18	21
1:A:28:LEU:CD1	1:A:28:LEU:C	0.48	2.78	17	1
1:B:71:GLY:C	1:B:72:GLN:NE2	0.48	2.67	21	2
1:A:10:GLN:O	1:A:31:GLN:OE1	0.48	2.31	16	9
1:A:2:ILE:HG12	1:B:65:LEU:CB	0.48	2.38	1	9
1:B:47:ILE:CD1	1:B:56:TYR:OH	0.48	2.61	1	2
1:B:10:GLN:OE1	1:B:44:LEU:CD1	0.48	2.62	26	1
1:B:48:THR:OG1	1:B:80:ARG:CZ	0.48	2.62	18	1
1:B:1:MET:C	1:B:2:ILE:CG1	0.48	2.81	9	1
1:A:32:LEU:CD1	1:A:32:LEU:N	0.48	2.74	28	2
1:B:34:TYR:CZ	1:B:44:LEU:HB2	0.48	2.44	11	13
1:B:31:GLN:OE1	1:B:32:LEU:O	0.48	2.31	9	18
1:A:13:PHE:CD1	1:A:13:PHE:C	0.48	2.87	18	5

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:47:ILE:HD12	1:B:83:LEU:HD12	0.48	1.85	15	1
1:A:3:LYS:O	1:A:35:VAL:HG13	0.48	2.09	21	2
1:B:3:LYS:O	1:B:35:VAL:HG13	0.48	2.08	21	2
1:A:7:LYS:CE	1:A:34:TYR:CD2	0.48	2.97	24	2
1:B:82:ARG:NH1	1:B:82:ARG:HG3	0.48	2.24	1	1
1:A:41:HIS:HB3	1:A:42:PRO:HD2	0.48	1.86	7	1
1:B:41:HIS:HB3	1:B:42:PRO:HD2	0.48	1.86	7	1
1:A:48:THR:OG1	1:A:80:ARG:CZ	0.48	2.62	18	1
1:A:37:LEU:HD13	1:B:70:VAL:HG22	0.48	1.84	13	2
1:A:37:LEU:C	1:A:37:LEU:HD13	0.48	2.28	16	2
1:A:2:ILE:HG21	1:B:76:LEU:CD2	0.48	2.37	16	2
1:A:7:LYS:HG3	1:A:34:TYR:CZ	0.48	2.44	27	3
1:A:37:LEU:HD22	1:A:39:ASN:ND2	0.48	2.23	13	2
1:B:33:CYS:O	1:B:44:LEU:HA	0.48	2.08	15	20
1:A:11:ALA:O	1:A:55:ALA:HB3	0.48	2.09	15	3
1:A:2:ILE:CG1	1:B:65:LEU:HB3	0.48	2.39	4	2
1:B:32:LEU:HD23	1:B:44:LEU:CD1	0.48	2.38	10	1
1:B:72:GLN:NE2	1:B:72:GLN:HA	0.48	2.23	3	3
1:A:31:GLN:OE1	1:A:32:LEU:N	0.48	2.45	19	2
1:A:76:LEU:HD22	1:B:81:LEU:CD1	0.48	2.38	23	1
1:A:34:TYR:HB3	1:A:42:PRO:HB2	0.48	1.85	17	22
1:B:67:SER:HB3	1:B:80:ARG:C	0.48	2.29	13	19
1:A:6:ILE:O	1:A:7:LYS:O	0.48	2.32	2	16
1:A:37:LEU:HD22	1:B:69:LYS:CA	0.48	2.38	17	1
1:B:12:GLN:HA	1:B:55:ALA:CB	0.48	2.38	17	2
1:B:28:LEU:C	1:B:28:LEU:CD1	0.48	2.77	17	2
1:A:71:GLY:C	1:A:72:GLN:NE2	0.48	2.67	15	2
1:A:3:LYS:O	1:A:37:LEU:HD11	0.48	2.09	1	1
1:A:47:ILE:CD1	1:A:56:TYR:OH	0.48	2.62	1	2
1:A:39:ASN:ND2	1:A:43:VAL:CG1	0.48	2.76	29	1
1:A:31:GLN:OE1	1:A:49:LEU:HD23	0.48	2.08	8	1
1:A:38:GLY:O	1:A:39:ASN:OD1	0.48	2.32	16	2
1:B:79:ASP:O	1:B:80:ARG:HB3	0.48	2.08	18	3
1:A:47:ILE:HG23	1:A:56:TYR:CE1	0.48	2.44	1	3
1:B:3:LYS:O	1:B:37:LEU:HD11	0.48	2.09	1	1
1:B:80:ARG:CG	1:B:80:ARG:O	0.48	2.62	12	2
1:A:49:LEU:CD1	1:A:50:ASP:O	0.48	2.61	30	2
1:A:10:GLN:OE1	1:A:44:LEU:CD1	0.48	2.61	26	1
1:B:39:ASN:ND2	1:B:43:VAL:HG21	0.48	2.24	26	1
1:B:70:VAL:O	1:B:71:GLY:O	0.48	2.32	8	1
1:A:65:LEU:CB	1:B:2:ILE:HG23	0.48	2.38	30	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:GLU:N	1:A:34:TYR:O	0.48	2.47	28	4
1:B:32:LEU:N	1:B:32:LEU:CD1	0.48	2.74	28	2
1:B:29:ASN:O	1:B:49:LEU:HB2	0.48	2.09	25	6
1:B:4:VAL:HA	1:B:34:TYR:O	0.48	2.08	19	25
1:A:72:GLN:N	1:A:72:GLN:CD	0.48	2.67	15	1
1:A:37:LEU:CD1	1:B:69:LYS:HA	0.48	2.39	8	3
1:B:32:LEU:HD22	1:B:44:LEU:HD11	0.48	1.82	10	2
1:B:13:PHE:CG	1:B:29:ASN:HB2	0.48	2.44	1	1
1:A:65:LEU:CD2	1:B:2:ILE:HA	0.48	2.36	11	4
1:A:45:VAL:CG2	1:B:75:SER:CA	0.48	2.92	16	1
1:A:2:ILE:HG23	1:B:65:LEU:CB	0.48	2.39	30	1
1:A:67:SER:HB3	1:A:80:ARG:O	0.48	2.09	24	14
1:A:12:GLN:CA	1:A:55:ALA:CB	0.48	2.92	27	2
1:B:72:GLN:CD	1:B:72:GLN:N	0.48	2.67	15	1
1:B:49:LEU:HD13	1:B:49:LEU:C	0.48	2.29	6	1
1:A:6:ILE:CD1	1:A:56:TYR:HB3	0.48	2.39	14	10
1:A:65:LEU:HB3	1:B:2:ILE:CG1	0.48	2.39	4	2
1:A:36:ASP:O	1:A:39:ASN:OD1	0.47	2.32	8	2
1:A:13:PHE:CG	1:A:29:ASN:HB2	0.47	2.44	1	1
1:A:78:ILE:HG22	1:A:79:ASP:N	0.47	2.24	24	4
1:A:74:GLY:O	1:A:75:SER:OG	0.47	2.32	9	2
1:B:32:LEU:HB3	1:B:44:LEU:CD1	0.47	2.39	20	6
1:B:6:ILE:O	1:B:7:LYS:O	0.47	2.31	2	16
1:A:79:ASP:O	1:A:80:ARG:HB2	0.47	2.08	12	7
1:B:12:GLN:CA	1:B:55:ALA:CB	0.47	2.92	27	2
1:B:7:LYS:HD3	1:B:34:TYR:CE2	0.47	2.45	22	3
1:B:81:LEU:N	1:B:81:LEU:CD2	0.47	2.77	27	2
1:B:6:ILE:CD1	1:B:56:TYR:HB3	0.47	2.39	14	12
1:B:32:LEU:HD23	1:B:44:LEU:HD11	0.47	1.82	10	2
1:A:73:PHE:CG	1:A:73:PHE:O	0.47	2.67	10	1
1:A:72:GLN:HA	1:A:72:GLN:NE2	0.47	2.23	3	1
1:A:31:GLN:C	1:A:32:LEU:HD22	0.47	2.30	9	2
1:A:81:LEU:C	1:A:81:LEU:CD1	0.47	2.78	8	1
1:B:13:PHE:C	1:B:13:PHE:CD1	0.47	2.87	18	3
1:B:62:THR:CG2	1:B:86:ALA:HA	0.47	2.40	8	11
1:B:7:LYS:CE	1:B:34:TYR:CD2	0.47	2.97	24	2
1:B:67:SER:CB	1:B:80:ARG:C	0.47	2.83	1	5
1:A:68:PHE:CE1	1:A:78:ILE:HG23	0.47	2.45	13	1
1:B:7:LYS:HG3	1:B:34:TYR:CZ	0.47	2.44	27	2
1:A:31:GLN:C	1:A:32:LEU:HD12	0.47	2.30	23	1
1:A:3:LYS:C	1:A:4:VAL:HG23	0.47	2.30	25	10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:49:LEU:C	1:B:49:LEU:HD13	0.47	2.30	30	4
1:A:80:ARG:NH1	1:A:80:ARG:HG3	0.47	2.24	18	2
1:B:38:GLY:O	1:B:39:ASN:OD1	0.47	2.32	16	2
1:B:79:ASP:O	1:B:80:ARG:HB2	0.47	2.09	12	4
1:B:83:LEU:O	1:B:84:VAL:HG13	0.47	2.10	1	1
1:A:45:VAL:CG2	1:B:70:VAL:HG11	0.47	2.39	9	3
1:A:28:LEU:HD13	1:A:28:LEU:N	0.47	2.24	18	1
1:A:6:ILE:HD12	1:A:56:TYR:HB2	0.47	1.85	8	2
1:A:47:ILE:CD1	1:A:83:LEU:HB2	0.47	2.39	12	6
1:B:6:ILE:HG21	1:B:57:ALA:O	0.47	2.10	16	5
1:A:56:TYR:O	1:A:57:ALA:O	0.47	2.33	12	7
1:A:63:VAL:CG1	1:A:81:LEU:HD11	0.47	2.40	4	1
1:B:65:LEU:HA	1:B:68:PHE:CD1	0.47	2.44	30	8
1:A:61:TYR:CB	1:A:83:LEU:HD21	0.47	2.39	22	3
1:B:61:TYR:CB	1:B:83:LEU:HD21	0.47	2.39	22	4
1:A:61:TYR:CD2	1:A:83:LEU:CD2	0.47	2.97	8	4
1:B:15:THR:HG23	1:B:28:LEU:C	0.47	2.30	29	1
1:B:6:ILE:HD12	1:B:61:TYR:CD1	0.47	2.45	7	2
1:A:81:LEU:HD12	1:A:83:LEU:N	0.47	2.25	8	1
1:B:39:ASN:OD1	1:B:41:HIS:O	0.47	2.32	8	1
1:B:65:LEU:O	1:B:67:SER:N	0.47	2.48	2	3
1:B:3:LYS:C	1:B:4:VAL:HG23	0.47	2.30	25	10
1:B:50:ASP:CB	1:B:53:GLN:HB2	0.47	2.40	16	9
1:B:11:ALA:O	1:B:55:ALA:HB3	0.47	2.09	15	3
1:B:73:PHE:CG	1:B:73:PHE:O	0.47	2.67	10	1
1:A:82:ARG:HG3	1:A:82:ARG:NH1	0.47	2.24	1	2
1:A:39:ASN:ND2	1:A:43:VAL:HG21	0.47	2.24	26	1
1:B:36:ASP:CB	1:B:41:HIS:O	0.47	2.63	14	1
1:B:56:TYR:CD1	1:B:61:TYR:CE2	0.47	3.03	13	1
1:B:36:ASP:O	1:B:37:LEU:C	0.47	2.53	19	11
1:A:65:LEU:CD1	1:B:37:LEU:HB2	0.47	2.40	20	2
1:B:67:SER:OG	1:B:80:ARG:O	0.47	2.33	3	20
1:A:37:LEU:HD12	1:A:38:GLY:H	0.47	1.69	17	1
1:A:7:LYS:HD3	1:A:34:TYR:CE2	0.47	2.44	22	3
1:A:46:LYS:O	1:B:74:GLY:O	0.47	2.33	5	2
1:A:76:LEU:CD2	1:B:2:ILE:HG21	0.47	2.39	16	2
1:B:33:CYS:SG	1:B:83:LEU:HD12	0.47	2.50	1	1
1:A:75:SER:N	1:B:45:VAL:HG23	0.47	2.25	29	1
1:A:82:ARG:NH1	1:A:82:ARG:HG2	0.47	2.25	7	2
1:B:81:LEU:HD12	1:B:83:LEU:N	0.47	2.25	8	1
1:B:37:LEU:HD22	1:B:39:ASN:ND2	0.47	2.24	13	2

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:60:LEU:O	1:B:86:ALA:N	0.47	2.43	23	1
1:A:34:TYR:CZ	1:A:44:LEU:HB2	0.47	2.45	28	13
1:A:29:ASN:O	1:A:49:LEU:HB2	0.47	2.09	25	6
1:A:47:ILE:HD12	1:A:83:LEU:HD12	0.47	1.85	15	1
1:B:39:ASN:O	1:B:40:GLU:HB2	0.47	2.10	4	1
1:A:28:LEU:C	1:A:28:LEU:CD1	0.47	2.79	10	1
1:A:83:LEU:O	1:A:84:VAL:HG13	0.47	2.10	1	1
1:B:33:CYS:SG	1:B:45:VAL:HG13	0.47	2.50	1	1
1:B:31:GLN:C	1:B:32:LEU:HD22	0.47	2.30	9	2
1:A:56:TYR:CD1	1:A:61:TYR:CE2	0.47	3.03	13	1
1:A:81:LEU:N	1:A:81:LEU:CD2	0.47	2.77	27	2
1:B:78:ILE:HG23	1:B:81:LEU:CA	0.47	2.40	18	3
1:A:62:THR:CG2	1:A:86:ALA:HA	0.47	2.40	2	10
1:A:35:VAL:CG1	1:A:37:LEU:HD11	0.47	2.37	1	1
1:A:37:LEU:HD22	1:A:38:GLY:H	0.47	1.70	1	1
1:A:10:GLN:OE1	1:A:34:TYR:CD2	0.47	2.68	26	1
1:A:39:ASN:OD1	1:A:41:HIS:O	0.47	2.32	8	1
1:A:32:LEU:HB3	1:A:44:LEU:CD1	0.47	2.40	23	6
1:A:39:ASN:O	1:A:40:GLU:HB2	0.47	2.10	4	1
1:B:10:GLN:NE2	1:B:33:CYS:HA	0.47	2.25	10	1
1:A:47:ILE:CD1	1:A:56:TYR:CZ	0.47	2.98	29	2
1:B:7:LYS:HA	1:B:7:LYS:CE	0.47	2.40	13	3
1:A:70:VAL:O	1:A:71:GLY:O	0.47	2.32	8	1
1:A:80:ARG:O	1:A:80:ARG:CG	0.47	2.62	12	1
1:B:47:ILE:HG23	1:B:48:THR:N	0.47	2.25	2	2
1:A:50:ASP:CB	1:A:53:GLN:HB2	0.46	2.40	16	9
1:B:60:LEU:O	1:B:61:TYR:CD1	0.46	2.68	2	3
1:A:63:VAL:HG12	1:A:64:HIS:H	0.46	1.70	24	8
1:A:80:ARG:O	1:A:81:LEU:O	0.46	2.33	4	1
1:A:2:ILE:CG2	1:A:37:LEU:CD2	0.46	2.94	28	1
1:A:37:LEU:HD13	1:B:65:LEU:HD13	0.46	1.81	28	1
1:A:36:ASP:O	1:A:37:LEU:C	0.46	2.53	19	11
1:B:80:ARG:NH1	1:B:80:ARG:HG3	0.46	2.24	18	2
1:A:68:PHE:O	1:A:69:LYS:CG	0.46	2.63	9	2
1:B:68:PHE:O	1:B:69:LYS:CG	0.46	2.63	9	2
1:A:33:CYS:SG	1:A:83:LEU:HD12	0.46	2.50	1	1
1:A:67:SER:CB	1:A:80:ARG:C	0.46	2.83	1	6
1:B:39:ASN:ND2	1:B:43:VAL:CG1	0.46	2.76	29	1
1:A:15:THR:HG23	1:A:28:LEU:C	0.46	2.29	29	1
1:A:4:VAL:HG22	1:A:5:GLU:N	0.46	2.25	8	3
1:A:70:VAL:HG22	1:B:37:LEU:HD13	0.46	1.86	13	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:63:VAL:CG1	1:B:81:LEU:HD11	0.46	2.40	4	1
1:A:65:LEU:HA	1:A:68:PHE:CD1	0.46	2.44	30	9
1:A:7:LYS:HA	1:A:7:LYS:CE	0.46	2.40	13	2
1:B:31:GLN:C	1:B:32:LEU:HD12	0.46	2.30	23	1
1:B:47:ILE:CD1	1:B:83:LEU:HB2	0.46	2.39	23	7
1:A:60:LEU:O	1:A:61:TYR:CD1	0.46	2.68	2	3
1:B:80:ARG:O	1:B:81:LEU:O	0.46	2.33	4	1
1:A:47:ILE:HD13	1:A:48:THR:N	0.46	2.26	1	1
1:B:47:ILE:CD1	1:B:56:TYR:CZ	0.46	2.98	29	2
1:B:10:GLN:OE1	1:B:34:TYR:CD2	0.46	2.68	26	1
1:B:28:LEU:HD13	1:B:28:LEU:N	0.46	2.24	18	1
1:A:36:ASP:CB	1:A:41:HIS:O	0.46	2.63	14	1
1:B:54:PRO:O	1:B:55:ALA:O	0.46	2.33	13	1
1:B:78:ILE:HG21	1:B:81:LEU:HB3	0.46	1.87	18	4
1:B:36:ASP:HA	1:B:41:HIS:O	0.46	2.11	6	11
1:B:82:ARG:NH1	1:B:82:ARG:CG	0.46	2.78	9	4
1:B:6:ILE:HD12	1:B:56:TYR:HB2	0.46	1.85	8	2
1:A:37:LEU:HB3	1:B:65:LEU:CD1	0.46	2.40	30	1
1:A:37:LEU:HB2	1:B:65:LEU:CD1	0.46	2.41	20	2
1:A:37:LEU:CD2	1:B:69:LYS:HA	0.46	2.40	15	7
1:A:73:PHE:CD1	1:A:73:PHE:N	0.46	2.84	8	3
1:A:78:ILE:HG23	1:A:81:LEU:CA	0.46	2.40	18	3
1:B:56:TYR:O	1:B:57:ALA:O	0.46	2.33	7	5
1:A:37:LEU:CD2	1:A:37:LEU:C	0.46	2.84	1	1
1:B:37:LEU:HD22	1:B:38:GLY:H	0.46	1.70	1	1
1:A:82:ARG:CG	1:A:82:ARG:NH1	0.46	2.79	24	6
1:B:78:ILE:O	1:B:79:ASP:C	0.46	2.54	8	3
1:A:35:VAL:HG12	1:A:37:LEU:N	0.46	2.26	8	1
1:B:35:VAL:HG12	1:B:37:LEU:N	0.46	2.26	8	1
1:A:65:LEU:HG	1:A:68:PHE:CE2	0.46	2.46	11	1
1:B:80:ARG:NH1	1:B:80:ARG:CG	0.46	2.78	18	2
1:A:72:GLN:NE2	1:A:72:GLN:HA	0.46	2.25	22	2
1:A:69:LYS:HA	1:B:37:LEU:CD1	0.46	2.41	8	2
1:A:78:ILE:O	1:A:79:ASP:HB3	0.46	2.11	7	5
1:A:6:ILE:HD12	1:A:61:TYR:CD1	0.46	2.45	7	2
1:B:68:PHE:CE1	1:B:78:ILE:HG23	0.46	2.45	13	1
1:B:1:MET:O	1:B:2:ILE:C	0.46	2.54	30	1
1:A:71:GLY:N	1:A:77:MET:SD	0.46	2.89	27	1
1:B:48:THR:O	1:B:48:THR:CG2	0.46	2.61	25	1
1:B:76:LEU:O	1:B:77:MET:HG2	0.46	2.11	19	11
1:A:6:ILE:HG21	1:A:57:ALA:O	0.46	2.11	13	4

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:35:VAL:HG13	1:B:37:LEU:CD1	0.46	2.38	1	1
1:B:4:VAL:HG22	1:B:5:GLU:N	0.46	2.25	8	4
1:B:32:LEU:N	1:B:32:LEU:HD22	0.46	2.25	9	1
1:B:71:GLY:N	1:B:77:MET:SD	0.46	2.89	27	1
1:B:2:ILE:CG2	1:B:37:LEU:CD2	0.46	2.94	28	1
1:A:32:LEU:C	1:A:33:CYS:SG	0.46	2.94	18	23
1:A:31:GLN:OE1	1:A:33:CYS:SG	0.46	2.74	15	1
1:A:36:ASP:HA	1:A:41:HIS:O	0.46	2.11	6	11
1:A:67:SER:HG	1:A:80:ARG:C	0.46	2.13	4	1
1:A:33:CYS:SG	1:A:45:VAL:HG13	0.46	2.51	1	1
1:B:1:MET:CG	1:B:62:THR:HB	0.46	2.41	16	3
1:A:1:MET:CG	1:A:62:THR:HB	0.46	2.41	16	3
1:B:82:ARG:NH1	1:B:82:ARG:HG2	0.46	2.25	7	1
1:A:32:LEU:N	1:A:32:LEU:HD22	0.46	2.24	9	1
1:A:65:LEU:CD2	1:B:2:ILE:CG2	0.46	2.85	9	1
1:B:1:MET:C	1:B:2:ILE:HG13	0.46	2.32	9	1
1:B:31:GLN:OE1	1:B:33:CYS:SG	0.46	2.74	15	1
1:A:36:ASP:O	1:A:39:ASN:CG	0.46	2.54	15	5
1:A:78:ILE:CG2	1:A:81:LEU:HB3	0.46	2.41	3	3
1:A:47:ILE:HG23	1:A:48:THR:N	0.46	2.25	2	2
1:A:83:LEU:C	1:A:84:VAL:HG13	0.46	2.32	1	2
1:B:37:LEU:C	1:B:37:LEU:CD2	0.46	2.84	1	1
1:A:45:VAL:CG1	1:B:75:SER:HA	0.46	2.41	13	1
1:B:37:LEU:CD1	1:B:38:GLY:N	0.45	2.64	28	1
1:B:32:LEU:C	1:B:33:CYS:SG	0.45	2.94	21	21
1:A:81:LEU:HG	1:A:81:LEU:O	0.45	2.11	29	12
1:A:7:LYS:CB	1:A:8:PRO:HD2	0.45	2.42	11	10
1:B:81:LEU:O	1:B:81:LEU:HG	0.45	2.11	17	13
1:A:10:GLN:O	1:A:31:GLN:CD	0.45	2.54	29	7
1:B:37:LEU:HD23	1:B:37:LEU:C	0.45	2.31	6	1
1:A:78:ILE:CD1	1:B:78:ILE:HG13	0.45	2.40	13	2
1:A:78:ILE:HG21	1:A:81:LEU:HB3	0.45	1.87	18	2
1:B:82:ARG:HG3	1:B:82:ARG:NH1	0.45	2.26	12	1
1:A:76:LEU:O	1:A:77:MET:HG2	0.45	2.11	9	11
1:B:37:LEU:HD12	1:B:38:GLY:H	0.45	1.69	17	1
1:B:36:ASP:O	1:B:39:ASN:CG	0.45	2.55	15	5
1:A:2:ILE:CD1	1:A:63:VAL:HB	0.45	2.41	11	8
1:B:29:ASN:CG	1:B:49:LEU:O	0.45	2.55	22	1
1:A:33:CYS:SG	1:A:83:LEU:CD1	0.45	3.04	1	1
1:A:35:VAL:HG13	1:A:37:LEU:CD1	0.45	2.38	1	1
1:A:74:GLY:O	1:B:46:LYS:N	0.45	2.49	24	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:13:PHE:HD2	1:A:49:LEU:HD12	0.45	1.71	8	1
1:A:54:PRO:O	1:A:55:ALA:O	0.45	2.33	13	1
1:B:13:PHE:HB2	1:B:30:GLU:O	0.45	2.12	12	1
1:A:76:LEU:O	1:A:77:MET:SD	0.45	2.74	12	1
1:A:1:MET:C	1:A:2:ILE:HG13	0.45	2.31	9	1
1:A:65:LEU:O	1:A:67:SER:N	0.45	2.49	2	3
1:A:29:ASN:HB2	1:A:49:LEU:HB3	0.45	1.88	15	6
1:A:37:LEU:CD1	1:A:37:LEU:N	0.45	2.72	17	1
1:B:51:GLU:O	1:B:52:GLY:C	0.45	2.53	6	3
1:B:4:VAL:HG13	1:B:61:TYR:O	0.45	2.10	23	3
1:B:10:GLN:O	1:B:31:GLN:CD	0.45	2.54	29	7
1:A:13:PHE:CD2	1:A:49:LEU:CG	0.45	2.99	26	5
1:A:10:GLN:NE2	1:A:33:CYS:HA	0.45	2.26	10	1
1:A:31:GLN:CA	1:A:47:ILE:HG22	0.45	2.42	22	3
1:B:59:GLY:O	1:B:60:LEU:C	0.45	2.55	13	2
1:A:49:LEU:HD13	1:A:49:LEU:C	0.45	2.32	24	1
1:A:28:LEU:C	1:A:28:LEU:CD2	0.45	2.78	18	1
1:B:7:LYS:HD2	1:B:34:TYR:CD1	0.45	2.45	18	1
1:A:13:PHE:HB2	1:A:30:GLU:O	0.45	2.12	12	1
1:B:40:GLU:C	1:B:41:HIS:ND1	0.45	2.69	2	1
1:B:13:PHE:CD2	1:B:49:LEU:CG	0.45	2.99	26	5
1:B:40:GLU:O	1:B:41:HIS:HB2	0.45	2.11	23	3
1:A:35:VAL:CG1	1:A:37:LEU:CD2	0.45	2.94	1	1
1:A:59:GLY:O	1:A:60:LEU:C	0.45	2.55	13	2
1:A:39:ASN:HB3	1:A:41:HIS:NE2	0.45	2.27	19	1
1:A:37:LEU:O	1:A:37:LEU:CD2	0.45	2.63	13	1
1:B:2:ILE:O	1:B:62:THR:HA	0.45	2.12	28	5
1:A:36:ASP:OD2	1:A:42:PRO:CA	0.45	2.65	19	2
1:A:4:VAL:HG23	1:A:34:TYR:O	0.45	2.12	15	8
1:A:6:ILE:HG13	1:A:33:CYS:CB	0.45	2.42	15	2
1:A:65:LEU:C	1:A:67:SER:N	0.45	2.69	2	11
1:A:29:ASN:CG	1:A:49:LEU:O	0.45	2.55	22	1
1:B:35:VAL:CG1	1:B:37:LEU:HD11	0.45	2.38	1	1
1:B:78:ILE:O	1:B:79:ASP:HB3	0.45	2.10	7	5
1:A:70:VAL:CG1	1:B:45:VAL:HG11	0.45	2.42	23	1
1:A:40:GLU:C	1:A:41:HIS:ND1	0.45	2.69	2	1
1:A:2:ILE:O	1:A:62:THR:HA	0.45	2.11	30	4
1:A:34:TYR:HB3	1:A:42:PRO:CB	0.45	2.42	14	9
1:B:4:VAL:HG23	1:B:34:TYR:O	0.45	2.12	15	8
1:A:72:GLN:O	1:A:73:PHE:HB2	0.45	2.11	7	7
1:B:4:VAL:HG21	1:B:83:LEU:CD1	0.45	2.41	22	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:CD1	1:B:37:LEU:CG	0.45	2.95	1	1
1:B:13:PHE:HD2	1:B:49:LEU:HD12	0.45	1.72	8	1
1:A:45:VAL:HG11	1:B:70:VAL:CG1	0.45	2.42	23	1
1:A:32:LEU:O	1:A:33:CYS:SG	0.45	2.74	30	2
1:A:45:VAL:CG2	1:B:74:GLY:C	0.45	2.85	16	1
1:B:65:LEU:HG	1:B:68:PHE:CE2	0.45	2.46	11	1
1:B:81:LEU:HG	1:B:81:LEU:O	0.45	2.11	1	9
1:B:6:ILE:HG13	1:B:33:CYS:SG	0.45	2.52	15	1
1:B:65:LEU:C	1:B:67:SER:N	0.45	2.70	11	10
1:B:74:GLY:O	1:B:75:SER:OG	0.45	2.32	9	3
1:B:38:GLY:C	1:B:39:ASN:OD1	0.45	2.55	9	2
1:A:37:LEU:O	1:A:39:ASN:OD1	0.45	2.35	18	1
1:B:76:LEU:O	1:B:77:MET:SD	0.45	2.75	12	1
1:A:56:TYR:CD1	1:A:56:TYR:N	0.45	2.85	9	1
1:B:69:LYS:HB2	1:B:69:LYS:NZ	0.45	2.27	30	1
1:A:72:GLN:CD	1:A:72:GLN:O	0.45	2.55	11	2
1:B:48:THR:O	1:B:49:LEU:C	0.45	2.55	25	3
1:B:80:ARG:HG2	1:B:80:ARG:NH1	0.45	2.27	17	1
1:A:68:PHE:O	1:B:37:LEU:HD21	0.45	2.11	27	3
1:A:37:LEU:HD21	1:B:68:PHE:O	0.45	2.11	27	3
1:A:3:LYS:N	1:A:37:LEU:HD11	0.45	2.27	21	1
1:B:63:VAL:HG12	1:B:64:HIS:H	0.45	1.71	24	8
1:B:73:PHE:CD1	1:B:73:PHE:N	0.45	2.84	21	2
1:B:78:ILE:CG2	1:B:81:LEU:HB3	0.45	2.42	18	3
1:A:4:VAL:HG13	1:A:61:TYR:O	0.45	2.11	23	3
1:B:70:VAL:HG22	1:B:76:LEU:HD12	0.45	1.88	4	1
1:A:37:LEU:O	1:A:37:LEU:CG	0.45	2.64	27	4
1:B:82:ARG:CG	1:B:82:ARG:NH1	0.45	2.78	24	4
1:A:36:ASP:O	1:A:37:LEU:HG	0.45	2.12	7	1
1:B:72:GLN:CD	1:B:72:GLN:O	0.45	2.55	2	1
1:A:49:LEU:O	1:A:50:ASP:O	0.45	2.34	11	1
1:B:3:LYS:HD3	1:B:60:LEU:HD21	0.45	1.89	28	1
1:A:76:LEU:HG	1:A:77:MET:N	0.45	2.27	28	1
1:B:7:LYS:CB	1:B:8:PRO:HD2	0.45	2.42	11	10
1:A:6:ILE:HG13	1:A:33:CYS:SG	0.45	2.52	15	2
1:A:29:ASN:HB3	1:A:49:LEU:CB	0.45	2.42	2	2
1:B:36:ASP:O	1:B:37:LEU:CB	0.45	2.65	29	4
1:A:78:ILE:HG13	1:B:78:ILE:CD1	0.45	2.42	24	2
1:A:13:PHE:HA	1:A:31:GLN:CG	0.45	2.42	8	1
1:B:2:ILE:HB	1:B:63:VAL:CG2	0.45	2.41	8	3
1:B:13:PHE:HA	1:B:31:GLN:CG	0.45	2.42	8	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:37:LEU:CG	1:B:37:LEU:O	0.45	2.65	27	2
1:B:49:LEU:O	1:B:50:ASP:O	0.45	2.34	11	1
1:A:55:ALA:O	1:A:56:TYR:C	0.45	2.56	8	9
1:B:65:LEU:O	1:B:65:LEU:HD12	0.45	2.12	17	2
1:A:80:ARG:CG	1:A:80:ARG:NH1	0.45	2.79	28	2
1:B:34:TYR:HB3	1:B:42:PRO:CB	0.45	2.41	14	7
1:A:56:TYR:CE2	1:A:83:LEU:HB2	0.45	2.46	10	3
1:A:40:GLU:O	1:A:41:HIS:HB2	0.45	2.11	23	3
1:B:33:CYS:SG	1:B:83:LEU:CD1	0.45	3.04	1	1
1:B:47:ILE:HD13	1:B:48:THR:N	0.45	2.26	1	1
1:A:38:GLY:C	1:A:39:ASN:OD1	0.45	2.55	9	2
1:A:74:GLY:O	1:B:46:LYS:CB	0.45	2.65	24	1
1:B:7:LYS:HD3	1:B:34:TYR:CE1	0.45	2.47	18	1
1:B:31:GLN:OE1	1:B:55:ALA:HA	0.45	2.12	8	1
1:A:69:LYS:NZ	1:A:69:LYS:HB2	0.45	2.27	30	1
1:A:65:LEU:HD13	1:B:37:LEU:HD22	0.44	1.87	28	1
1:A:69:LYS:CA	1:B:37:LEU:CD1	0.44	2.95	5	3
1:A:86:ALA:O	1:A:87:LYS:CB	0.44	2.65	17	1
1:B:6:ILE:HG13	1:B:33:CYS:CB	0.44	2.42	15	2
1:B:31:GLN:CA	1:B:47:ILE:HG22	0.44	2.42	22	3
1:B:35:VAL:CG1	1:B:37:LEU:CD2	0.44	2.95	1	1
1:B:1:MET:O	1:B:2:ILE:HB	0.44	2.12	26	3
1:B:67:SER:O	1:B:79:ASP:HB2	0.44	2.12	9	1
1:B:55:ALA:O	1:B:56:TYR:C	0.44	2.56	8	8
1:B:4:VAL:HB	1:B:61:TYR:HB2	0.44	1.89	16	11
1:A:69:LYS:HA	1:B:37:LEU:CD2	0.44	2.41	15	5
1:A:77:MET:O	1:A:78:ILE:C	0.44	2.54	27	7
1:B:13:PHE:CG	1:B:49:LEU:CD1	0.44	2.99	6	1
1:A:37:LEU:HD23	1:A:37:LEU:C	0.44	2.30	6	1
1:A:63:VAL:HG13	1:A:81:LEU:HG	0.44	1.88	4	1
1:A:67:SER:O	1:A:79:ASP:HB2	0.44	2.12	9	1
1:A:2:ILE:CG2	1:B:76:LEU:HD13	0.44	2.42	11	1
1:A:2:ILE:HA	1:B:65:LEU:CD1	0.44	2.39	10	3
1:A:51:GLU:O	1:A:52:GLY:C	0.44	2.55	23	3
1:B:83:LEU:C	1:B:84:VAL:HG13	0.44	2.32	1	2
1:A:82:ARG:NH1	1:A:82:ARG:CG	0.44	2.79	11	2
1:B:39:ASN:HB3	1:B:41:HIS:NE2	0.44	2.26	19	1
1:B:76:LEU:HD23	1:B:77:MET:H	0.44	1.66	9	1
1:A:3:LYS:HD3	1:A:60:LEU:HD21	0.44	1.89	28	1
1:A:81:LEU:O	1:A:81:LEU:HG	0.44	2.11	17	10
1:B:2:ILE:CD1	1:B:63:VAL:HB	0.44	2.41	11	8

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:HD12	1:A:56:TYR:CE2	0.44	2.47	10	1
1:A:37:LEU:HB3	1:A:39:ASN:ND2	0.44	2.27	8	2
1:B:36:ASP:O	1:B:37:LEU:HG	0.44	2.12	7	1
1:A:1:MET:O	1:A:2:ILE:HB	0.44	2.12	26	3
1:A:78:ILE:O	1:A:79:ASP:C	0.44	2.55	8	3
1:B:56:TYR:CD1	1:B:56:TYR:N	0.44	2.85	9	2
1:A:79:ASP:O	1:A:79:ASP:OD1	0.44	2.35	26	1
1:B:13:PHE:HA	1:B:31:GLN:HG3	0.44	1.89	8	1
1:B:10:GLN:CB	1:B:32:LEU:HB2	0.44	2.42	13	1
1:A:2:ILE:H	1:B:65:LEU:HD11	0.44	1.73	9	1
1:B:65:LEU:O	1:B:66:SER:C	0.44	2.56	11	3
1:B:72:GLN:O	1:B:72:GLN:CD	0.44	2.55	11	1
1:B:71:GLY:O	1:B:72:GLN:CB	0.44	2.66	28	2
1:A:80:ARG:HG2	1:A:80:ARG:NH1	0.44	2.28	17	1
1:A:4:VAL:CA	1:A:34:TYR:O	0.44	2.65	20	5
1:A:36:ASP:O	1:A:39:ASN:ND2	0.44	2.51	15	1
1:B:3:LYS:N	1:B:37:LEU:HD11	0.44	2.28	21	1
1:A:28:LEU:CD2	1:A:50:ASP:HB3	0.44	2.43	6	1
1:B:47:ILE:HD12	1:B:56:TYR:CE2	0.44	2.48	10	1
1:A:47:ILE:O	1:A:47:ILE:HG23	0.44	2.13	1	1
1:B:81:LEU:HD12	1:B:82:ARG:N	0.44	2.28	8	1
1:A:1:MET:O	1:A:2:ILE:C	0.44	2.54	30	1
1:B:29:ASN:HB2	1:B:49:LEU:HB3	0.44	1.89	25	7
1:B:7:LYS:CB	1:B:8:PRO:CD	0.44	2.95	11	5
1:A:6:ILE:CG1	1:A:33:CYS:SG	0.44	3.06	30	2
1:B:29:ASN:HB3	1:B:49:LEU:CB	0.44	2.42	15	2
1:B:72:GLN:O	1:B:73:PHE:HB2	0.44	2.13	1	7
1:A:65:LEU:HB3	1:B:2:ILE:HG12	0.44	1.90	1	7
1:B:65:LEU:CA	1:B:68:PHE:CD2	0.44	3.01	14	10
1:A:65:LEU:CD1	1:B:37:LEU:HB3	0.44	2.41	30	2
1:A:74:GLY:O	1:B:45:VAL:HG22	0.44	2.13	24	1
1:B:62:THR:CG2	1:B:86:ALA:CB	0.44	2.96	11	3
1:B:32:LEU:O	1:B:33:CYS:SG	0.44	2.74	30	2
1:A:48:THR:O	1:A:49:LEU:C	0.44	2.55	11	4
1:A:69:LYS:CA	1:B:37:LEU:HD22	0.44	2.42	17	1
1:A:7:LYS:CB	1:A:8:PRO:CD	0.44	2.96	5	8
1:B:6:ILE:CG1	1:B:33:CYS:SG	0.44	3.06	30	2
1:B:4:VAL:CA	1:B:34:TYR:O	0.44	2.66	20	4
1:B:37:LEU:O	1:B:37:LEU:CD2	0.44	2.66	15	1
1:A:65:LEU:CD1	1:B:2:ILE:HA	0.44	2.40	10	1
1:B:13:PHE:CA	1:B:30:GLU:O	0.44	2.66	12	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD23	1:B:65:LEU:CD1	0.44	2.42	1	1
1:B:4:VAL:CG1	1:B:33:CYS:HB2	0.44	2.43	1	1
1:A:2:ILE:HG12	1:B:65:LEU:HB3	0.44	1.88	1	5
1:A:37:LEU:HD22	1:B:65:LEU:HD13	0.44	1.88	28	1
1:B:39:ASN:OD1	1:B:39:ASN:N	0.44	2.51	20	3
1:B:28:LEU:CD2	1:B:49:LEU:O	0.44	2.66	7	1
1:A:7:LYS:HD3	1:A:34:TYR:CE1	0.44	2.47	18	1
1:A:80:ARG:NH1	1:A:80:ARG:CG	0.44	2.78	18	1
1:B:37:LEU:O	1:B:39:ASN:OD1	0.44	2.35	18	1
1:B:41:HIS:N	1:B:41:HIS:ND1	0.44	2.64	28	1
1:B:34:TYR:HA	1:B:43:VAL:O	0.44	2.13	20	5
1:A:36:ASP:O	1:A:37:LEU:CB	0.44	2.66	11	3
1:B:77:MET:O	1:B:78:ILE:C	0.44	2.56	14	8
1:B:51:GLU:HG2	1:B:52:GLY:N	0.44	2.28	1	1
1:B:36:ASP:C	1:B:37:LEU:CD1	0.44	2.83	3	1
1:B:68:PHE:CD1	1:B:78:ILE:HA	0.44	2.48	8	2
1:A:68:PHE:CD1	1:A:78:ILE:HA	0.44	2.47	8	2
1:A:76:LEU:CB	1:B:81:LEU:HD13	0.44	2.43	13	2
1:A:10:GLN:CB	1:A:32:LEU:HB2	0.44	2.43	13	1
1:A:2:ILE:HG13	1:A:63:VAL:CB	0.44	2.43	30	1
1:B:80:ARG:CG	1:B:80:ARG:NH1	0.43	2.78	17	1
1:A:56:TYR:N	1:A:56:TYR:CD1	0.43	2.86	5	2
1:B:56:TYR:N	1:B:56:TYR:CD1	0.43	2.86	5	1
1:A:70:VAL:HG22	1:A:76:LEU:HD12	0.43	1.88	4	1
1:A:4:VAL:HG21	1:A:83:LEU:CD1	0.43	2.42	22	2
1:B:49:LEU:HD11	1:B:54:PRO:C	0.43	2.34	1	1
1:A:74:GLY:O	1:B:46:LYS:HB3	0.43	2.13	16	1
1:B:36:ASP:OD2	1:B:42:PRO:CA	0.43	2.66	19	2
1:A:4:VAL:HB	1:A:61:TYR:HB2	0.43	1.90	11	9
1:A:13:PHE:HA	1:A:30:GLU:O	0.43	2.13	15	13
1:B:13:PHE:HA	1:B:30:GLU:O	0.43	2.13	15	12
1:A:65:LEU:HA	1:A:68:PHE:CZ	0.43	2.48	17	4
1:A:62:THR:O	1:A:63:VAL:O	0.43	2.36	11	3
1:A:13:PHE:CG	1:A:49:LEU:CD1	0.43	2.99	6	1
1:A:65:LEU:CA	1:A:68:PHE:CD2	0.43	3.01	14	11
1:B:56:TYR:CE2	1:B:83:LEU:HB2	0.43	2.49	2	3
1:A:65:LEU:CD1	1:B:37:LEU:HD23	0.43	2.42	1	1
1:B:79:ASP:O	1:B:79:ASP:OD1	0.43	2.35	26	1
1:A:36:ASP:OD2	1:A:41:HIS:C	0.43	2.57	14	1
1:A:75:SER:HA	1:B:45:VAL:CG1	0.43	2.43	13	1
1:B:6:ILE:CG2	1:B:57:ALA:O	0.43	2.66	16	2

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:3:LYS:C	1:B:4:VAL:CG2	0.43	2.86	30	1
1:B:15:THR:HG23	1:B:29:ASN:OD1	0.43	2.13	2	1
1:B:12:GLN:CG	1:B:12:GLN:O	0.43	2.66	27	1
1:B:65:LEU:HA	1:B:68:PHE:CZ	0.43	2.48	25	3
1:A:37:LEU:CD2	1:A:37:LEU:O	0.43	2.65	15	1
1:B:36:ASP:O	1:B:39:ASN:ND2	0.43	2.51	15	1
1:A:33:CYS:SG	1:A:47:ILE:HG12	0.43	2.54	10	3
1:B:47:ILE:CG1	1:B:83:LEU:HB2	0.43	2.43	1	1
1:B:47:ILE:HD11	1:B:56:TYR:OH	0.43	2.13	1	1
1:A:46:LYS:CB	1:B:74:GLY:O	0.43	2.66	24	1
1:A:28:LEU:CD2	1:A:49:LEU:O	0.43	2.66	7	1
1:B:2:ILE:HG13	1:B:63:VAL:CB	0.43	2.43	30	1
1:A:15:THR:HG23	1:A:29:ASN:OD1	0.43	2.13	2	1
1:A:41:HIS:N	1:A:41:HIS:ND1	0.43	2.65	28	1
1:A:34:TYR:HA	1:A:43:VAL:O	0.43	2.13	20	6
1:A:45:VAL:HG22	1:B:74:GLY:C	0.43	2.33	16	2
1:A:29:ASN:HB3	1:A:49:LEU:HB2	0.43	1.90	15	2
1:A:13:PHE:CA	1:A:30:GLU:O	0.43	2.66	12	2
1:B:37:LEU:HB3	1:B:39:ASN:ND2	0.43	2.27	8	2
1:A:65:LEU:CD1	1:B:37:LEU:CB	0.43	2.96	20	2
1:A:65:LEU:HD13	1:B:37:LEU:CB	0.43	2.44	20	1
1:B:31:GLN:NE2	1:B:56:TYR:HB2	0.43	2.28	26	2
1:A:68:PHE:O	1:A:69:LYS:HG2	0.43	2.13	8	1
1:A:6:ILE:CG2	1:A:57:ALA:O	0.43	2.66	16	2
1:B:47:ILE:HD11	1:B:83:LEU:HD12	0.43	1.89	15	4
1:A:31:GLN:NE2	1:A:56:TYR:HB2	0.43	2.29	26	2
1:A:45:VAL:HG23	1:B:75:SER:N	0.43	2.28	29	1
1:A:46:LYS:N	1:B:74:GLY:O	0.43	2.51	24	1
1:A:45:VAL:HG22	1:B:74:GLY:O	0.43	2.14	24	1
1:A:36:ASP:O	1:A:37:LEU:CD1	0.43	2.56	3	1
1:A:45:VAL:HG22	1:B:75:SER:N	0.43	2.29	26	1
1:B:71:GLY:O	1:B:72:GLN:C	0.43	2.55	26	1
1:B:75:SER:O	1:B:76:LEU:O	0.43	2.37	18	1
1:A:31:GLN:OE1	1:A:55:ALA:HA	0.43	2.13	8	1
1:B:38:GLY:O	1:B:39:ASN:CG	0.43	2.57	16	1
1:A:75:SER:O	1:A:76:LEU:C	0.43	2.57	19	4
1:B:73:PHE:O	1:B:75:SER:OG	0.43	2.34	21	1
1:A:4:VAL:CG1	1:A:33:CYS:HB2	0.43	2.43	1	1
1:A:47:ILE:CG1	1:A:83:LEU:HB2	0.43	2.43	1	1
1:A:2:ILE:CG2	1:A:63:VAL:HG23	0.43	2.44	13	1
1:A:7:LYS:HB3	1:A:8:PRO:HD2	0.43	1.91	9	7

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:7:LYS:NZ	1:B:7:LYS:HA	0.43	2.29	19	3
1:A:76:LEU:C	1:A:77:MET:HG3	0.43	2.34	20	3
1:B:81:LEU:HD21	1:B:83:LEU:HG	0.43	1.90	4	1
1:B:7:LYS:HA	1:B:7:LYS:NZ	0.43	2.29	2	4
1:A:47:ILE:HD11	1:A:56:TYR:OH	0.43	2.13	1	1
1:A:37:LEU:CB	1:B:65:LEU:CD1	0.43	2.97	20	2
1:A:37:LEU:CB	1:B:65:LEU:HD13	0.43	2.44	20	1
1:B:1:MET:SD	1:B:62:THR:HB	0.43	2.54	29	8
1:B:4:VAL:HG21	1:B:33:CYS:HB2	0.43	1.90	29	2
1:A:36:ASP:C	1:A:37:LEU:CD1	0.43	2.83	3	1
1:B:36:ASP:O	1:B:37:LEU:CD1	0.43	2.56	3	1
1:B:86:ALA:O	1:B:87:LYS:C	0.43	2.57	18	1
1:A:13:PHE:HA	1:A:31:GLN:HG3	0.43	1.89	8	1
1:A:75:SER:CA	1:B:45:VAL:CG2	0.43	2.96	16	1
1:A:2:ILE:CB	1:B:65:LEU:HD21	0.43	2.44	11	1
1:A:78:ILE:HD11	1:B:78:ILE:HG13	0.43	1.90	28	1
1:A:74:GLY:C	1:A:75:SER:OG	0.43	2.57	25	2
1:A:4:VAL:HG22	1:A:35:VAL:CB	0.43	2.43	7	2
1:B:29:ASN:HB2	1:B:49:LEU:O	0.43	2.13	23	2
1:B:6:ILE:O	1:B:7:LYS:C	0.43	2.56	8	4
1:B:13:PHE:CD1	1:B:13:PHE:C	0.43	2.90	10	8
1:A:47:ILE:CG1	1:A:56:TYR:CE2	0.43	3.02	2	4
1:A:49:LEU:HD11	1:A:54:PRO:C	0.43	2.34	1	1
1:A:4:VAL:CG1	1:A:83:LEU:HD21	0.43	2.44	20	1
1:A:62:THR:CG2	1:A:86:ALA:CB	0.43	2.96	11	3
1:A:6:ILE:O	1:A:7:LYS:C	0.43	2.56	8	1
1:A:81:LEU:HD12	1:A:82:ARG:N	0.43	2.28	8	1
1:A:81:LEU:HD13	1:B:76:LEU:CB	0.43	2.44	13	1
1:B:36:ASP:OD1	1:B:37:LEU:N	0.43	2.52	12	1
1:A:49:LEU:HD13	1:A:50:ASP:N	0.43	2.29	30	1
1:B:31:GLN:HB2	1:B:47:ILE:HG22	0.43	1.90	2	1
1:A:37:LEU:CD1	1:A:38:GLY:N	0.43	2.64	28	1
1:B:49:LEU:O	1:B:50:ASP:C	0.43	2.57	28	2
1:B:28:LEU:CD2	1:B:50:ASP:HB3	0.43	2.43	6	1
1:B:50:ASP:O	1:B:51:GLU:CB	0.43	2.65	6	1
1:A:5:GLU:O	1:A:34:TYR:HB2	0.43	2.14	7	14
1:A:29:ASN:HB2	1:A:49:LEU:O	0.43	2.14	23	3
1:A:37:LEU:CG	1:B:65:LEU:CD1	0.43	2.96	1	1
1:B:82:ARG:HG2	1:B:82:ARG:NH1	0.43	2.29	24	2
1:B:2:ILE:CG2	1:B:63:VAL:HG23	0.43	2.44	13	1
1:B:3:LYS:HB3	1:B:36:ASP:OD2	0.43	2.14	12	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:1:MET:HG3	1:B:62:THR:CG2	0.43	2.43	17	3
1:B:5:GLU:O	1:B:34:TYR:HB2	0.43	2.14	6	14
1:A:10:GLN:OE1	1:A:32:LEU:HB2	0.43	2.14	15	1
1:A:7:LYS:NZ	1:A:7:LYS:HA	0.43	2.29	19	4
1:A:50:ASP:O	1:A:51:GLU:CB	0.43	2.65	6	1
1:B:47:ILE:HG23	1:B:47:ILE:O	0.43	2.13	1	2
1:A:6:ILE:HG12	1:A:56:TYR:CB	0.43	2.44	26	1
1:A:3:LYS:C	1:A:4:VAL:CG2	0.43	2.86	30	1
1:A:76:LEU:HD13	1:B:2:ILE:CG2	0.43	2.43	11	1
1:A:65:LEU:HD13	1:B:37:LEU:HD13	0.42	1.82	28	1
1:A:7:LYS:HA	1:A:7:LYS:NZ	0.42	2.29	2	4
1:B:76:LEU:CD2	1:B:76:LEU:C	0.42	2.86	17	2
1:A:13:PHE:C	1:A:13:PHE:CD1	0.42	2.91	10	7
1:B:63:VAL:HG13	1:B:81:LEU:HG	0.42	1.88	4	1
1:B:4:VAL:CG1	1:B:83:LEU:HD21	0.42	2.44	20	1
1:B:56:TYR:O	1:B:57:ALA:C	0.42	2.57	7	2
1:A:43:VAL:CG1	1:B:70:VAL:HG21	0.42	2.44	14	1
1:A:81:LEU:HD11	1:A:83:LEU:HB2	0.42	1.91	8	1
1:A:65:LEU:HD11	1:B:2:ILE:H	0.42	1.73	9	1
1:A:7:LYS:CB	1:A:10:GLN:HG2	0.42	2.44	2	1
1:B:7:LYS:CB	1:B:10:GLN:HG2	0.42	2.44	2	1
1:B:76:LEU:HG	1:B:77:MET:N	0.42	2.27	28	1
1:B:68:PHE:O	1:B:69:LYS:HG3	0.42	2.14	17	1
1:B:4:VAL:HG22	1:B:35:VAL:CB	0.42	2.43	7	2
1:B:86:ALA:O	1:B:87:LYS:CB	0.42	2.65	17	1
1:A:1:MET:SD	1:A:62:THR:HB	0.42	2.54	29	8
1:A:37:LEU:HD21	1:A:43:VAL:HG11	0.42	1.91	7	1
1:A:39:ASN:ND2	1:A:43:VAL:CG2	0.42	2.82	26	1
1:B:56:TYR:CD2	1:B:83:LEU:HD22	0.42	2.49	26	1
1:A:7:LYS:HD2	1:A:34:TYR:CD1	0.42	2.46	18	1
1:A:86:ALA:O	1:A:87:LYS:C	0.42	2.57	18	1
1:B:49:LEU:HD13	1:B:50:ASP:N	0.42	2.29	30	1
1:A:78:ILE:HG13	1:B:78:ILE:HD11	0.42	1.90	28	1
1:B:75:SER:O	1:B:76:LEU:C	0.42	2.57	19	3
1:B:1:MET:O	1:B:37:LEU:CD2	0.42	2.67	21	1
1:B:3:LYS:HA	1:B:61:TYR:O	0.42	2.14	21	1
1:B:47:ILE:CG1	1:B:56:TYR:CE2	0.42	3.02	2	4
1:A:2:ILE:CG2	1:B:65:LEU:CD2	0.42	2.86	9	1
1:A:31:GLN:HB2	1:A:47:ILE:HG22	0.42	1.90	2	1
1:A:65:LEU:HD22	1:B:37:LEU:HB3	0.42	1.91	11	1
1:B:41:HIS:HB2	1:B:42:PRO:HD2	0.42	1.91	27	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:VAL:O	1:B:5:GLU:HG3	0.42	2.14	27	3
1:A:1:MET:HG3	1:A:62:THR:CG2	0.42	2.44	15	4
1:B:10:GLN:OE1	1:B:32:LEU:HB2	0.42	2.15	15	2
1:A:2:ILE:CB	1:B:65:LEU:HD13	0.42	2.44	10	2
1:A:63:VAL:HG13	1:A:81:LEU:HD11	0.42	1.90	4	1
1:B:63:VAL:HG13	1:B:81:LEU:HD11	0.42	1.90	4	1
1:A:36:ASP:HB2	1:A:39:ASN:O	0.42	2.14	3	1
1:A:6:ILE:HD11	1:A:56:TYR:HD2	0.42	1.74	26	1
1:B:47:ILE:HD13	1:B:48:THR:H	0.42	1.74	19	1
1:A:38:GLY:O	1:A:39:ASN:CG	0.42	2.57	16	1
1:B:7:LYS:HB3	1:B:8:PRO:HD2	0.42	1.91	9	7
1:A:65:LEU:HD13	1:B:2:ILE:CB	0.42	2.44	10	2
1:A:81:LEU:HD21	1:A:83:LEU:HG	0.42	1.89	4	1
1:A:29:ASN:ND2	1:A:49:LEU:HB3	0.42	2.30	13	2
1:A:4:VAL:HG21	1:A:33:CYS:HB2	0.42	1.90	29	1
1:A:69:LYS:HG2	1:A:77:MET:O	0.42	2.14	7	1
1:B:6:ILE:HG12	1:B:56:TYR:CB	0.42	2.44	26	1
1:A:28:LEU:O	1:A:29:ASN:C	0.42	2.58	27	2
1:B:68:PHE:N	1:B:68:PHE:HD1	0.42	2.12	18	2
1:B:28:LEU:CD2	1:B:28:LEU:C	0.42	2.78	18	1
1:A:75:SER:O	1:A:76:LEU:O	0.42	2.37	18	1
1:A:2:ILE:HB	1:A:63:VAL:CG2	0.42	2.41	8	3
1:A:47:ILE:HG23	1:A:47:ILE:O	0.42	2.13	23	2
1:A:12:GLN:CG	1:A:12:GLN:O	0.42	2.67	27	1
1:B:76:LEU:C	1:B:77:MET:HG3	0.42	2.34	20	3
1:B:62:THR:O	1:B:63:VAL:O	0.42	2.37	5	3
1:A:82:ARG:HG2	1:A:82:ARG:NH1	0.42	2.29	24	1
1:B:6:ILE:O	1:B:58:PRO:HA	0.42	2.14	7	1
1:B:36:ASP:HB2	1:B:39:ASN:O	0.42	2.14	3	1
1:A:71:GLY:O	1:A:72:GLN:C	0.42	2.55	26	1
1:A:47:ILE:HD13	1:A:48:THR:H	0.42	1.75	19	1
1:B:7:LYS:HD2	1:B:7:LYS:N	0.42	2.29	19	1
1:A:13:PHE:CA	1:A:31:GLN:HG3	0.42	2.44	8	1
1:B:4:VAL:CG1	1:B:61:TYR:O	0.42	2.68	23	1
1:A:65:LEU:HD21	1:B:2:ILE:CB	0.42	2.45	11	1
1:A:41:HIS:HB2	1:A:42:PRO:HD2	0.42	1.91	27	1
1:A:49:LEU:O	1:A:50:ASP:C	0.42	2.57	9	2
1:A:13:PHE:H	1:A:55:ALA:HB2	0.42	1.75	17	4
1:A:13:PHE:CE1	1:A:29:ASN:CG	0.42	2.93	26	2
1:B:33:CYS:SG	1:B:47:ILE:HG12	0.42	2.54	10	3
1:A:56:TYR:CD2	1:A:83:LEU:HD22	0.42	2.50	26	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:ASN:O	1:A:49:LEU:O	0.42	2.38	18	1
1:A:36:ASP:OD1	1:A:37:LEU:N	0.42	2.52	12	1
1:A:3:LYS:HA	1:A:61:TYR:O	0.42	2.14	21	1
1:A:51:GLU:HG2	1:A:52:GLY:N	0.42	2.28	1	1
1:B:72:GLN:O	1:B:72:GLN:HG2	0.42	2.14	29	1
1:B:36:ASP:OD2	1:B:41:HIS:C	0.42	2.57	14	1
1:A:41:HIS:O	1:A:41:HIS:CD2	0.42	2.73	8	1
1:B:68:PHE:O	1:B:69:LYS:HG2	0.42	2.15	8	1
1:B:81:LEU:HD11	1:B:83:LEU:HB2	0.42	1.91	8	1
1:B:29:ASN:ND2	1:B:49:LEU:HB3	0.42	2.30	13	1
1:A:37:LEU:HD11	1:B:69:LYS:C	0.42	2.35	13	1
1:A:31:GLN:N	1:A:47:ILE:O	0.42	2.46	23	1
1:A:63:VAL:HA	1:A:83:LEU:HD12	0.42	1.92	27	1
1:A:62:THR:O	1:A:63:VAL:C	0.42	2.58	9	4
1:B:62:THR:O	1:B:63:VAL:C	0.42	2.57	9	5
1:B:65:LEU:HG	1:B:65:LEU:O	0.42	2.13	2	2
1:A:76:LEU:HD11	1:B:37:LEU:HD12	0.42	1.92	10	1
1:B:6:ILE:HD11	1:B:83:LEU:HD23	0.42	1.92	29	1
1:B:69:LYS:HG2	1:B:77:MET:O	0.42	2.14	7	1
1:A:69:LYS:HG3	1:A:77:MET:O	0.42	2.15	7	1
1:A:50:ASP:HB2	1:A:53:GLN:NE2	0.42	2.30	7	1
1:A:37:LEU:HG	1:B:65:LEU:CD2	0.42	2.45	26	1
1:A:37:LEU:HD12	1:A:37:LEU:O	0.42	2.14	26	1
1:A:36:ASP:HB3	1:A:41:HIS:O	0.42	2.15	14	1
1:B:41:HIS:O	1:B:41:HIS:CD2	0.42	2.73	8	1
1:A:37:LEU:HD12	1:B:76:LEU:HD11	0.42	1.90	12	1
1:A:4:VAL:HG23	1:A:34:TYR:C	0.42	2.35	2	1
1:A:49:LEU:HA	1:A:49:LEU:HD22	0.42	1.69	17	4
1:B:29:ASN:HB3	1:B:49:LEU:HB2	0.42	1.90	15	2
1:A:6:ILE:HB	1:A:57:ALA:O	0.42	2.15	10	1
1:A:37:LEU:HG	1:A:37:LEU:O	0.42	2.15	22	1
1:A:28:LEU:HD13	1:A:28:LEU:O	0.42	2.14	18	1
1:A:6:ILE:CG2	1:A:6:ILE:O	0.42	2.68	2	1
1:A:68:PHE:O	1:A:69:LYS:HG3	0.41	2.15	17	1
1:B:1:MET:HG3	1:B:1:MET:O	0.41	2.15	5	1
1:A:10:GLN:HG3	1:A:10:GLN:O	0.41	2.14	10	1
1:A:50:ASP:O	1:A:51:GLU:C	0.41	2.57	1	1
1:A:56:TYR:O	1:A:57:ALA:C	0.41	2.57	7	2
1:B:50:ASP:HB2	1:B:53:GLN:NE2	0.41	2.30	7	1
1:A:2:ILE:CG1	1:B:65:LEU:HD22	0.41	2.45	3	1
1:B:13:PHE:CE1	1:B:29:ASN:CG	0.41	2.93	26	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:73:PHE:N	1:B:73:PHE:CD1	0.41	2.84	8	1
1:A:49:LEU:HD21	1:A:54:PRO:C	0.41	2.36	23	1
1:B:4:VAL:HG23	1:B:34:TYR:C	0.41	2.36	2	1
1:A:2:ILE:CG2	1:A:37:LEU:HD22	0.41	2.46	28	1
1:A:33:CYS:SG	1:A:47:ILE:HG13	0.41	2.55	20	3
1:B:74:GLY:C	1:B:75:SER:OG	0.41	2.57	25	2
1:B:49:LEU:HA	1:B:49:LEU:HD22	0.41	1.71	12	2
1:A:38:GLY:C	1:A:39:ASN:CG	0.41	2.79	16	2
1:A:73:PHE:O	1:A:74:GLY:C	0.41	2.59	26	3
1:A:1:MET:O	1:A:1:MET:HG3	0.41	2.15	5	1
1:A:2:ILE:CG1	1:B:65:LEU:HB2	0.41	2.46	5	1
1:B:36:ASP:O	1:B:37:LEU:HB3	0.41	2.15	6	2
1:A:6:ILE:HG13	1:A:61:TYR:CZ	0.41	2.50	10	1
1:B:4:VAL:CG1	1:B:61:TYR:HB2	0.41	2.45	1	1
1:B:15:THR:CG2	1:B:28:LEU:O	0.41	2.59	29	1
1:B:39:ASN:ND2	1:B:43:VAL:CG2	0.41	2.82	26	1
1:B:28:LEU:O	1:B:28:LEU:HD13	0.41	2.14	18	1
1:A:47:ILE:HG13	1:A:56:TYR:CD2	0.41	2.50	13	1
1:A:60:LEU:O	1:A:86:ALA:N	0.41	2.45	13	1
1:A:3:LYS:HB3	1:A:36:ASP:OD2	0.41	2.14	12	1
1:B:47:ILE:O	1:B:47:ILE:HG23	0.41	2.14	16	1
1:B:68:PHE:HD1	1:B:68:PHE:N	0.41	2.13	9	1
1:A:65:LEU:HG	1:A:65:LEU:O	0.41	2.13	2	1
1:A:69:LYS:O	1:A:77:MET:HG3	0.41	2.15	27	1
1:A:71:GLY:O	1:A:72:GLN:CB	0.41	2.66	28	1
1:A:6:ILE:HB	1:A:61:TYR:CE1	0.41	2.51	13	2
1:A:10:GLN:OE1	1:A:34:TYR:CE2	0.41	2.74	26	1
1:B:63:VAL:HG22	1:B:83:LEU:HD12	0.41	1.91	13	1
1:A:13:PHE:CG	1:A:29:ASN:HB3	0.41	2.50	30	1
1:A:65:LEU:HD21	1:B:2:ILE:CG2	0.41	2.44	11	1
1:B:33:CYS:SG	1:B:47:ILE:HG13	0.41	2.55	20	3
1:A:1:MET:O	1:A:37:LEU:CD2	0.41	2.67	21	1
1:B:38:GLY:C	1:B:39:ASN:CG	0.41	2.79	16	2
1:A:4:VAL:HB	1:A:35:VAL:HA	0.41	1.92	5	1
1:A:4:VAL:CG1	1:A:61:TYR:HB2	0.41	2.45	1	1
1:B:76:LEU:O	1:B:77:MET:HG3	0.41	2.16	1	1
1:A:6:ILE:HD11	1:A:83:LEU:HD23	0.41	1.92	29	1
1:B:10:GLN:OE1	1:B:34:TYR:CE2	0.41	2.74	26	1
1:A:32:LEU:HA	1:A:45:VAL:O	0.41	2.16	9	2
1:A:53:GLN:OE1	1:A:82:ARG:NH2	0.41	2.54	8	1
1:B:69:LYS:O	1:B:77:MET:HG3	0.41	2.15	27	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:LEU:CD2	1:A:76:LEU:C	0.41	2.85	15	1
1:A:3:LYS:C	1:A:4:VAL:CG1	0.41	2.89	21	1
1:A:67:SER:OG	1:A:80:ARG:C	0.41	2.59	4	1
1:A:4:VAL:HB	1:A:35:VAL:CG2	0.41	2.42	12	2
1:B:37:LEU:HG	1:B:37:LEU:O	0.41	2.15	22	1
1:A:73:PHE:CD1	1:A:73:PHE:O	0.41	2.74	29	1
1:A:86:ALA:O	1:A:87:LYS:O	0.41	2.38	26	1
1:A:49:LEU:HG	1:A:55:ALA:HA	0.41	1.92	18	1
1:B:29:ASN:O	1:B:49:LEU:O	0.41	2.38	18	1
1:A:7:LYS:N	1:A:7:LYS:HD2	0.41	2.29	19	1
1:A:4:VAL:CG1	1:A:61:TYR:HB3	0.41	2.44	13	1
1:A:68:PHE:N	1:A:68:PHE:HD1	0.41	2.13	13	1
1:A:76:LEU:O	1:A:77:MET:HG3	0.41	2.16	11	1
1:B:2:ILE:CG2	1:B:37:LEU:HD22	0.41	2.46	28	1
1:A:4:VAL:O	1:A:5:GLU:HG3	0.41	2.14	27	2
1:A:36:ASP:C	1:A:38:GLY:N	0.41	2.74	8	2
1:A:36:ASP:O	1:A:37:LEU:HB3	0.41	2.15	6	2
1:B:6:ILE:HG13	1:B:61:TYR:CZ	0.41	2.49	10	1
1:A:6:ILE:O	1:A:58:PRO:HA	0.41	2.15	7	1
1:B:32:LEU:HA	1:B:45:VAL:O	0.41	2.16	26	2
1:B:6:ILE:HD11	1:B:56:TYR:HD2	0.41	1.76	26	1
1:A:36:ASP:OD2	1:A:42:PRO:N	0.41	2.53	19	1
1:B:2:ILE:HG22	1:B:35:VAL:CG1	0.41	2.46	23	1
1:B:13:PHE:CG	1:B:29:ASN:HB3	0.41	2.50	30	1
1:A:2:ILE:CG2	1:B:65:LEU:HD21	0.41	2.44	11	1
1:A:7:LYS:CE	1:A:7:LYS:HA	0.41	2.46	27	1
1:A:2:ILE:HG21	1:B:76:LEU:HD13	0.41	1.92	11	2
1:B:4:VAL:HB	1:B:35:VAL:HA	0.41	1.92	5	1
1:A:13:PHE:HB3	1:A:49:LEU:HG	0.41	1.93	1	2
1:B:4:VAL:HG11	1:B:33:CYS:HB2	0.41	1.93	1	1
1:B:50:ASP:O	1:B:51:GLU:C	0.41	2.57	1	1
1:B:65:LEU:HA	1:B:68:PHE:CE1	0.41	2.50	18	1
1:B:49:LEU:HG	1:B:55:ALA:HA	0.41	1.92	18	1
1:A:63:VAL:HG22	1:A:83:LEU:HD12	0.41	1.92	13	1
1:A:37:LEU:HB3	1:B:65:LEU:HD22	0.41	1.91	11	1
1:B:28:LEU:O	1:B:29:ASN:C	0.41	2.58	27	1
1:B:71:GLY:CA	1:B:77:MET:SD	0.41	3.09	27	1
1:B:36:ASP:HA	1:B:39:ASN:OD1	0.41	2.16	28	1
1:A:48:THR:O	1:A:48:THR:CG2	0.41	2.61	25	1
1:B:13:PHE:H	1:B:55:ALA:HB2	0.41	1.76	11	4
1:A:70:VAL:HG13	1:B:45:VAL:HG21	0.41	1.93	6	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:63:VAL:CG1	1:B:81:LEU:CG	0.41	2.99	4	1
1:B:6:ILE:HB	1:B:57:ALA:O	0.41	2.16	10	1
1:A:39:ASN:OD1	1:A:39:ASN:N	0.41	2.54	29	1
1:B:73:PHE:CD1	1:B:73:PHE:O	0.41	2.74	29	1
1:B:69:LYS:HG3	1:B:77:MET:O	0.41	2.14	7	1
1:B:13:PHE:N	1:B:55:ALA:CB	0.41	2.84	26	1
1:A:49:LEU:HD22	1:A:49:LEU:HA	0.41	1.75	18	1
1:B:36:ASP:C	1:B:38:GLY:N	0.41	2.74	25	4
1:A:74:GLY:O	1:B:46:LYS:O	0.41	2.39	5	1
1:A:32:LEU:HD23	1:A:45:VAL:O	0.41	2.16	4	1
1:B:67:SER:OG	1:B:80:ARG:C	0.41	2.59	4	1
1:A:72:GLN:O	1:A:72:GLN:HG2	0.41	2.14	29	1
1:B:78:ILE:HG23	1:B:81:LEU:N	0.41	2.31	3	1
1:A:36:ASP:O	1:A:39:ASN:O	0.41	2.38	26	1
1:B:72:GLN:HG2	1:B:72:GLN:O	0.41	2.16	18	1
1:B:36:ASP:OD2	1:B:42:PRO:N	0.41	2.54	19	1
1:B:53:GLN:OE1	1:B:82:ARG:NH2	0.41	2.54	8	1
1:B:13:PHE:CA	1:B:31:GLN:HG3	0.41	2.45	8	1
1:A:35:VAL:HG11	1:B:76:LEU:HD11	0.41	1.91	13	1
1:B:68:PHE:HB3	1:B:76:LEU:CD2	0.41	2.44	13	1
1:B:37:LEU:CD2	1:B:37:LEU:O	0.41	2.64	13	1
1:A:65:LEU:O	1:A:66:SER:C	0.41	2.56	11	2
1:A:35:VAL:HG11	1:B:76:LEU:HD13	0.41	1.93	30	1
1:B:37:LEU:HD13	1:B:37:LEU:C	0.41	2.35	30	1
1:B:7:LYS:N	1:B:7:LYS:HD2	0.41	2.30	25	1
1:B:65:LEU:O	1:B:65:LEU:HG	0.41	2.16	21	1
1:B:10:GLN:O	1:B:10:GLN:HG3	0.41	2.14	10	1
1:A:60:LEU:C	1:A:61:TYR:CD1	0.41	2.95	10	1
1:B:37:LEU:HD21	1:B:43:VAL:HG11	0.41	1.91	7	1
1:A:28:LEU:CD1	1:A:28:LEU:H	0.41	2.29	18	1
1:B:81:LEU:CD1	1:B:83:LEU:N	0.41	2.84	8	1
1:A:38:GLY:O	1:A:39:ASN:HB3	0.40	2.16	26	1
1:B:86:ALA:O	1:B:87:LYS:O	0.40	2.39	26	1
1:B:1:MET:SD	1:B:62:THR:CB	0.40	3.09	23	1
1:A:71:GLY:CA	1:A:77:MET:SD	0.40	3.09	27	1
1:B:75:SER:O	1:B:77:MET:HG3	0.40	2.16	4	1
1:A:12:GLN:O	1:A:31:GLN:HG2	0.40	2.16	22	1
1:B:36:ASP:O	1:B:39:ASN:O	0.40	2.38	26	1
1:A:1:MET:SD	1:A:62:THR:CB	0.40	3.09	23	1
1:A:4:VAL:CG1	1:A:61:TYR:O	0.40	2.69	23	1
1:A:76:LEU:HD23	1:A:77:MET:H	0.40	1.67	9	1

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:74:GLY:O	1:B:75:SER:CB	0.40	2.68	30	1
1:B:71:GLY:O	1:B:75:SER:O	0.40	2.39	6	1
1:A:1:MET:HG3	1:A:62:THR:HB	0.40	1.92	22	1
1:A:37:LEU:CD2	1:B:65:LEU:CD1	0.40	2.99	1	1
1:B:13:PHE:HB3	1:B:49:LEU:HG	0.40	1.93	14	2
1:B:62:THR:OG1	1:B:84:VAL:HG23	0.40	2.16	26	1
1:A:72:GLN:HG2	1:A:72:GLN:O	0.40	2.16	16	1
1:A:4:VAL:HG22	1:A:35:VAL:CG1	0.40	2.46	7	2
1:A:67:SER:HB2	1:A:82:ARG:N	0.40	2.31	5	1
1:B:7:LYS:HE2	1:B:34:TYR:CD1	0.40	2.52	5	1
1:A:35:VAL:CG1	1:A:37:LEU:CD1	0.40	2.99	1	1
1:B:47:ILE:HG13	1:B:56:TYR:CD2	0.40	2.50	13	1
1:A:2:ILE:HG22	1:A:35:VAL:CG1	0.40	2.46	23	1
1:A:74:GLY:C	1:B:45:VAL:HG22	0.40	2.37	16	1
1:B:6:ILE:HB	1:B:61:TYR:CE1	0.40	2.51	21	2
1:A:63:VAL:CG1	1:A:81:LEU:CG	0.40	2.99	4	1
1:A:65:LEU:HD22	1:B:2:ILE:CG1	0.40	2.47	4	1
1:B:71:GLY:O	1:B:75:SER:N	0.40	2.41	7	1
1:A:35:VAL:O	1:A:42:PRO:HA	0.40	2.17	26	1
1:A:32:LEU:HD23	1:A:44:LEU:CG	0.40	2.47	8	1
1:A:14:THR:O	1:A:29:ASN:HA	0.40	2.17	12	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	73/87 (84%)	55±3 (76±3%)	13±2 (17±3%)	5±2 (7±2%)	3	18
1	B	73/87 (84%)	55±3 (76±4%)	13±2 (17±3%)	5±2 (7±2%)	3	17
All	All	4380/5220 (84%)	3319 (76%)	752 (17%)	309 (7%)	3	17

All 48 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	80	ARG	24
1	B	80	ARG	24
1	A	2	ILE	21
1	B	2	ILE	21
1	A	7	LYS	16
1	B	7	LYS	16
1	B	56	TYR	14
1	A	63	VAL	13
1	A	56	TYR	13
1	B	63	VAL	13
1	B	55	ALA	11
1	A	37	LEU	9
1	B	37	LEU	9
1	A	55	ALA	9
1	B	57	ALA	6
1	A	57	ALA	6
1	B	76	LEU	5
1	A	51	GLU	5
1	B	51	GLU	5
1	A	76	LEU	5
1	B	38	GLY	5
1	B	40	GLU	5
1	A	40	GLU	5
1	A	38	GLY	5
1	B	4	VAL	4
1	A	4	VAL	4
1	A	41	HIS	4
1	B	41	HIS	4
1	A	39	ASN	3
1	B	39	ASN	3
1	A	81	LEU	2
1	B	81	LEU	2
1	A	52	GLY	2
1	B	52	GLY	2
1	A	11	ALA	1
1	B	11	ALA	1
1	B	73	PHE	1
1	B	71	GLY	1
1	A	72	GLN	1
1	A	71	GLY	1
1	A	78	ILE	1
1	B	72	GLN	1
1	A	73	PHE	1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	50	ASP	1
1	B	50	ASP	1
1	B	78	ILE	1
1	B	29	ASN	1
1	A	29	ASN	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	66/76 (87%)	43±3 (65±4%)	23±3 (35±4%)	1	9
1	B	66/76 (87%)	43±3 (64±4%)	23±3 (36±4%)	1	9
All	All	3960/4560 (87%)	2554 (64%)	1406 (36%)	1	9

All 99 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	15	THR	29
1	B	15	THR	29
1	B	28	LEU	28
1	A	28	LEU	28
1	B	47	ILE	27
1	B	6	ILE	27
1	A	31	GLN	27
1	B	31	GLN	27
1	A	47	ILE	27
1	A	6	ILE	27
1	B	65	LEU	26
1	A	65	LEU	26
1	A	81	LEU	24
1	B	82	ARG	24
1	B	83	LEU	24
1	A	83	LEU	24
1	A	72	GLN	24
1	B	81	LEU	24
1	B	72	GLN	24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	82	ARG	24
1	A	37	LEU	23
1	B	37	LEU	23
1	B	70	VAL	21
1	A	70	VAL	21
1	A	33	CYS	20
1	B	33	CYS	20
1	A	87	LYS	20
1	B	87	LYS	20
1	B	49	LEU	19
1	B	4	VAL	19
1	A	4	VAL	19
1	A	49	LEU	19
1	A	46	LYS	18
1	A	50	ASP	18
1	B	50	ASP	18
1	A	29	ASN	18
1	B	46	LYS	18
1	B	29	ASN	18
1	B	1	MET	18
1	B	53	GLN	17
1	A	53	GLN	17
1	B	7	LYS	17
1	A	1	MET	17
1	A	7	LYS	17
1	A	80	ARG	16
1	B	60	LEU	16
1	B	80	ARG	16
1	A	60	LEU	16
1	B	76	LEU	14
1	A	76	LEU	14
1	B	73	PHE	14
1	A	69	LYS	14
1	B	69	LYS	14
1	A	73	PHE	14
1	B	9	SER	13
1	A	48	THR	13
1	A	9	SER	13
1	B	48	THR	13
1	B	3	LYS	12
1	A	75	SER	12
1	B	75	SER	12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	3	LYS	12
1	A	51	GLU	11
1	B	51	GLU	11
1	B	66	SER	9
1	A	66	SER	9
1	A	39	ASN	9
1	B	39	ASN	9
1	A	12	GLN	8
1	B	12	GLN	8
1	A	36	ASP	8
1	B	36	ASP	8
1	A	79	ASP	7
1	B	79	ASP	7
1	A	30	GLU	6
1	B	30	GLU	6
1	B	67	SER	5
1	B	41	HIS	5
1	A	41	HIS	5
1	A	67	SER	5
1	A	32	LEU	4
1	A	2	ILE	4
1	B	32	LEU	4
1	B	2	ILE	4
1	B	13	PHE	3
1	A	40	GLU	3
1	B	40	GLU	3
1	A	13	PHE	3
1	B	77	MET	2
1	A	45	VAL	2
1	A	14	THR	2
1	B	14	THR	2
1	A	10	GLN	2
1	B	10	GLN	2
1	B	45	VAL	2
1	A	77	MET	2
1	A	5	GLU	1
1	B	5	GLU	1
1	B	78	ILE	1

### 6.3.3 RNA ⓘ

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