



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:43 AM BST

PDB ID : 2N7H
Title : Hybrid structure of the Type 1 Pilus of Uropathogenic E.coli
Authors : Habenstein, B.; Loquet, A.; Giller, K.; Vasa, S.; Becker, S.; Habeck, M.; Lange, A.
Deposited on : 2015-09-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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

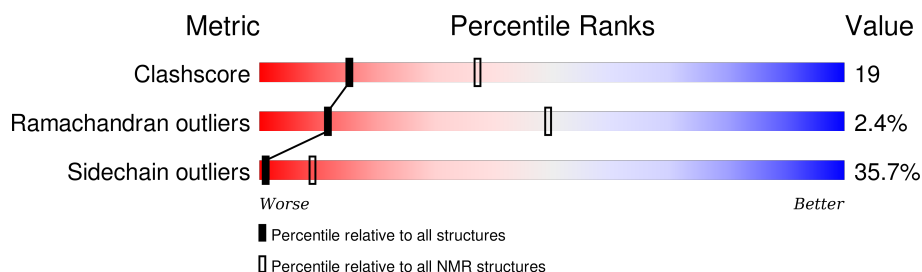
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 8%.

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 ≥ 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	160	 41% 54% . .
1	B	160	 38% 57% 5% .
1	C	160	 37% 58% . .
1	D	160	 36% 60% . .
1	E	160	 34% 61% . .
1	F	160	 41% 54% . .

2 Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:159, B:1-B:159, C:1-C:159, D:1-D:159, E:1-E:159, F:1-F:159 (953)	0.52	3

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

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

The models can be grouped into 2 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 8, 10
2	7, 9
Single-model clusters	5; 6

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13074 atoms, of which 6402 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FimA.

Mol	Chain	Residues	Atoms						Trace
1	A	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	B	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	C	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	D	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	E	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	
1	F	159	Total	C	H	N	O	S	0
			2179	680	1067	196	234	2	

There are 6 discrepancies between the modelled and reference sequences:

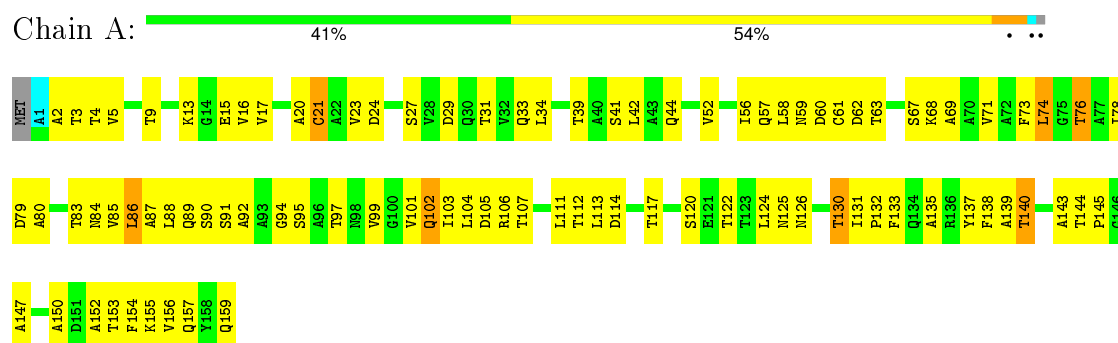
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q547G4
B	0	MET	-	EXPRESSION TAG	UNP Q547G4
C	0	MET	-	EXPRESSION TAG	UNP Q547G4
D	0	MET	-	EXPRESSION TAG	UNP Q547G4
E	0	MET	-	EXPRESSION TAG	UNP Q547G4
F	0	MET	-	EXPRESSION TAG	UNP Q547G4

4 Residue-property plots [i](#)

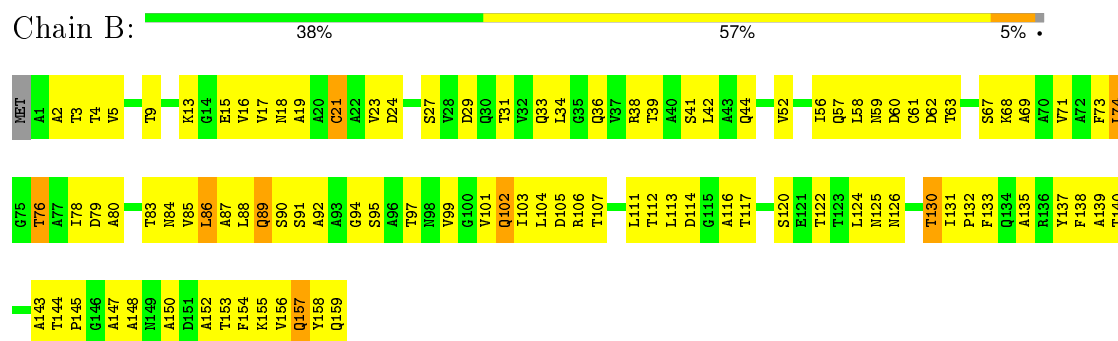
4.1 Average score per residue in the NMR ensemble

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

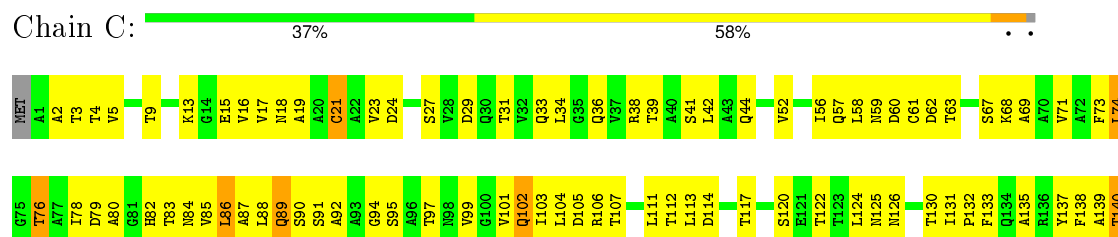
• Molecule 1: FimA



• Molecule 1: FimA

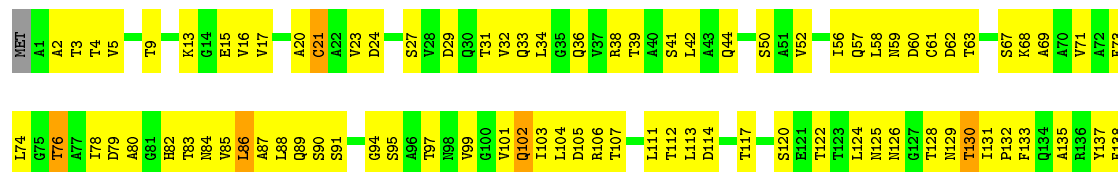


• Molecule 1: FimA

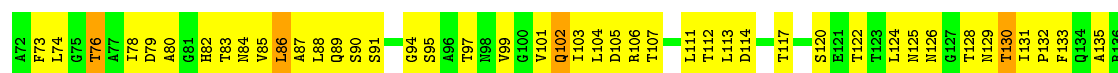
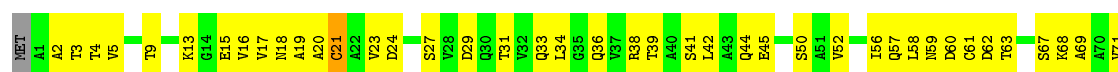
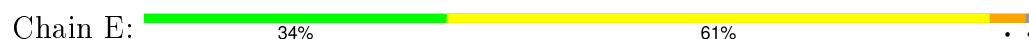




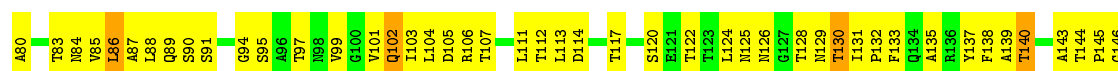
• Molecule 1: FimA



• Molecule 1: FimA



• Molecule 1: FimA

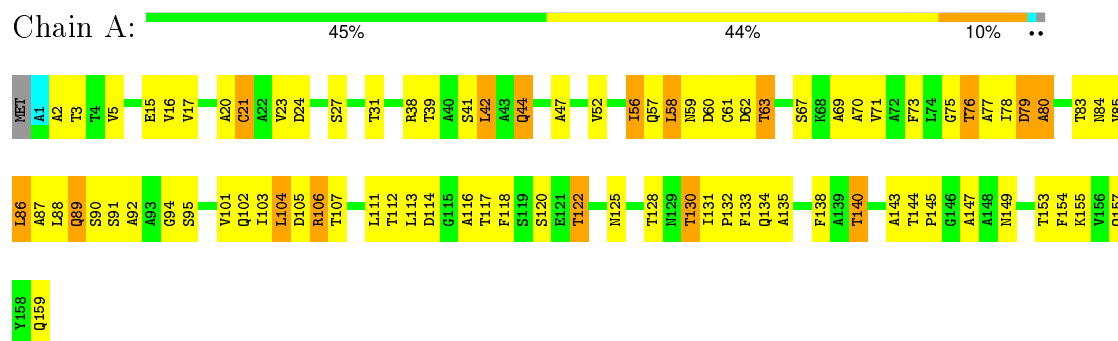


4.2 Scores per residue for each member of the ensemble

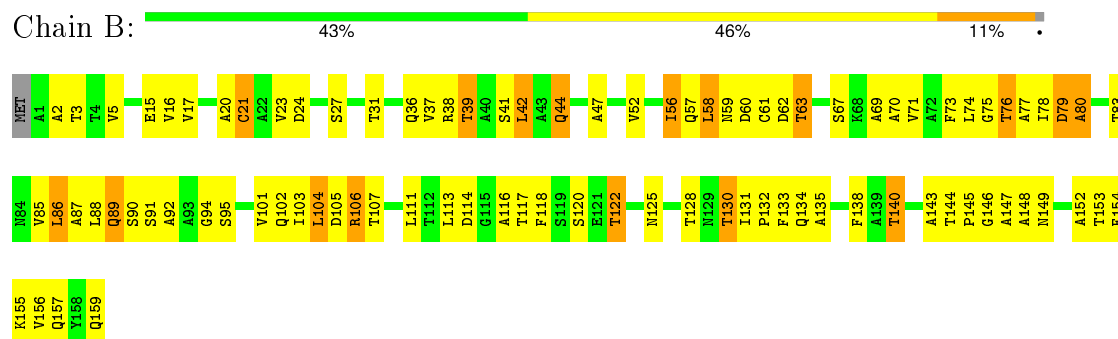
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

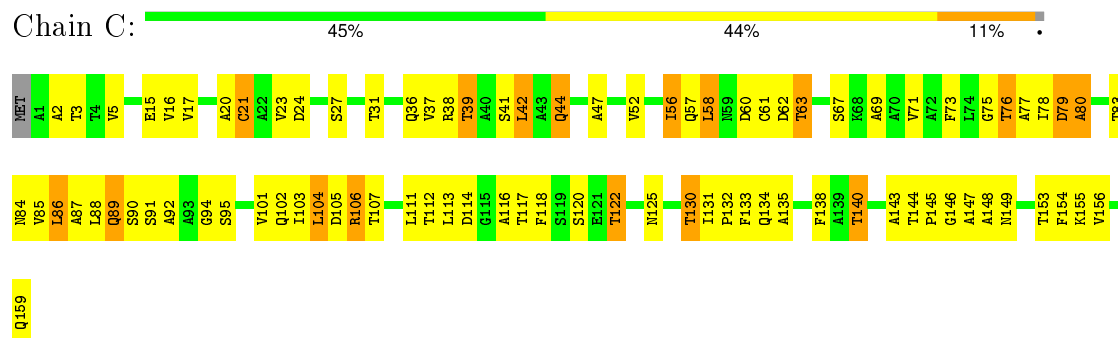
• Molecule 1: FimA



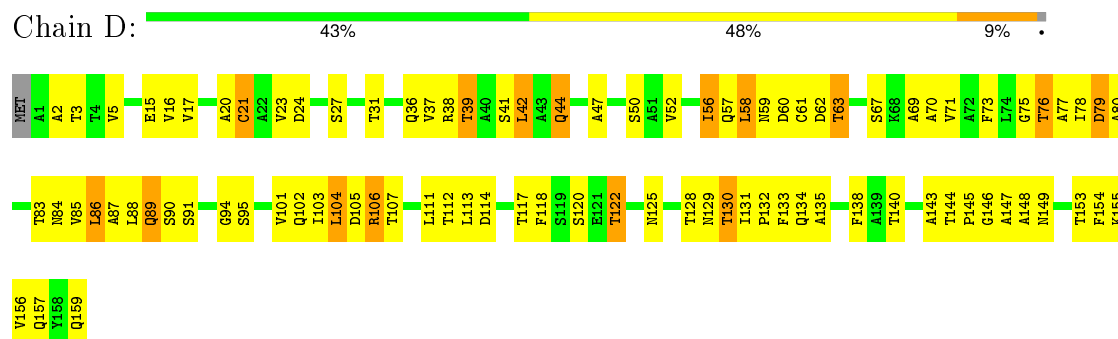
- Molecule 1: FimA



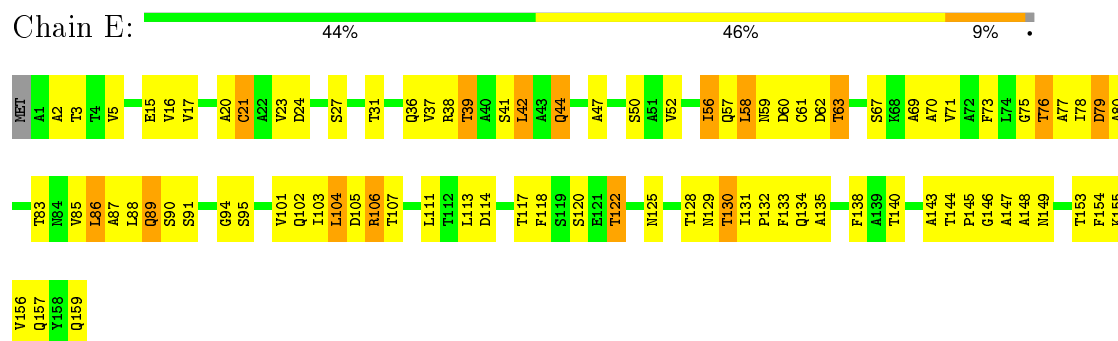
- Molecule 1: FimA



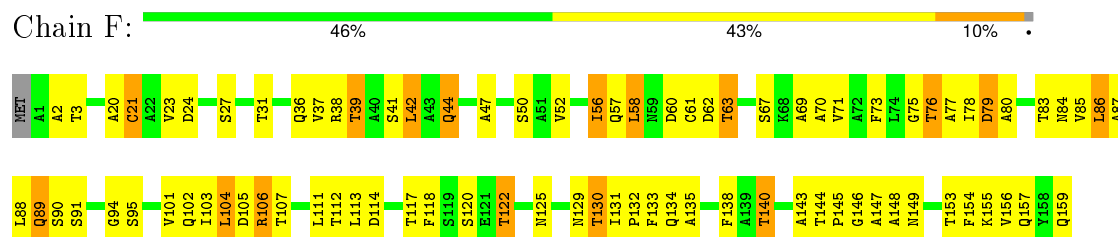
- Molecule 1: FimA



- Molecule 1: FimA

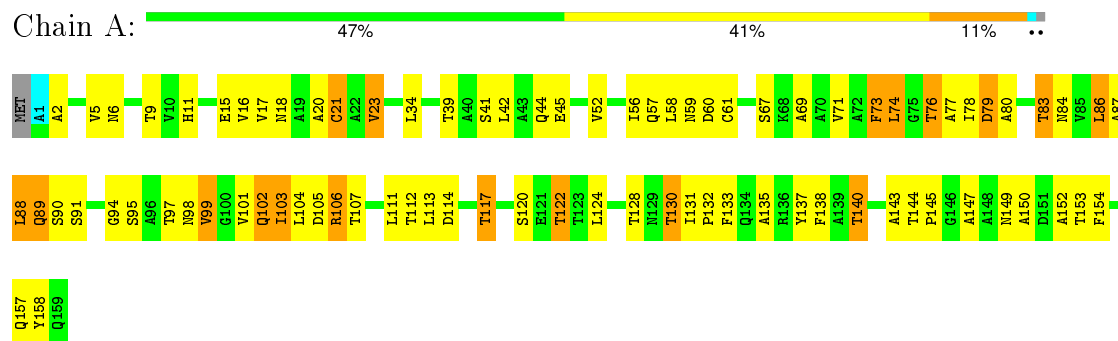


- Molecule 1: FimA

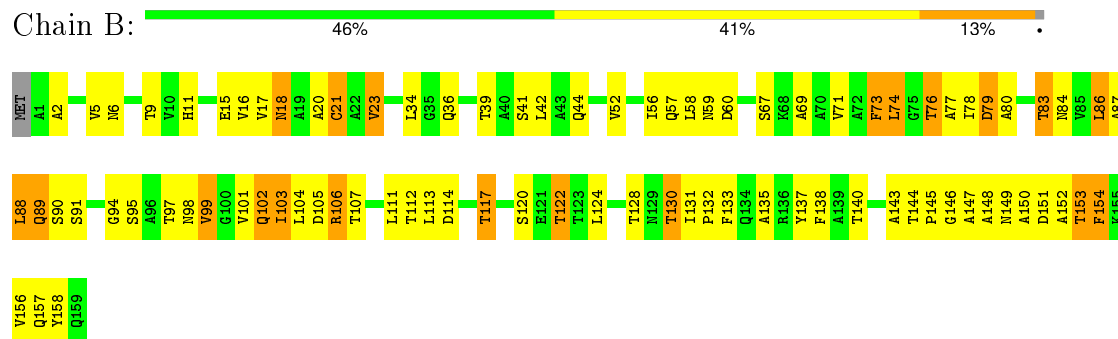


4.2.2 Score per residue for model 2

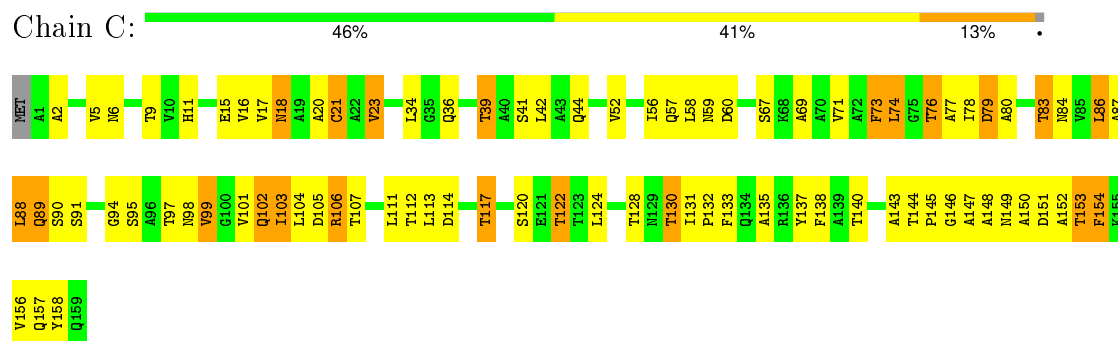
- Molecule 1: FimA



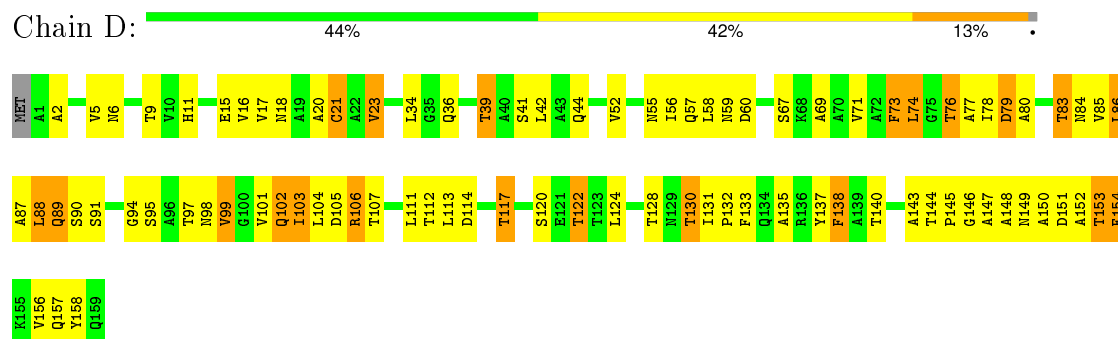
- Molecule 1: FimA



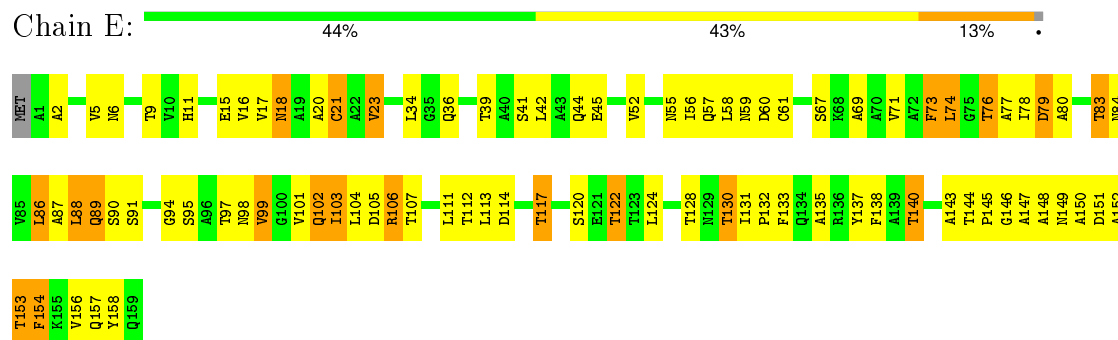
- Molecule 1: FimA



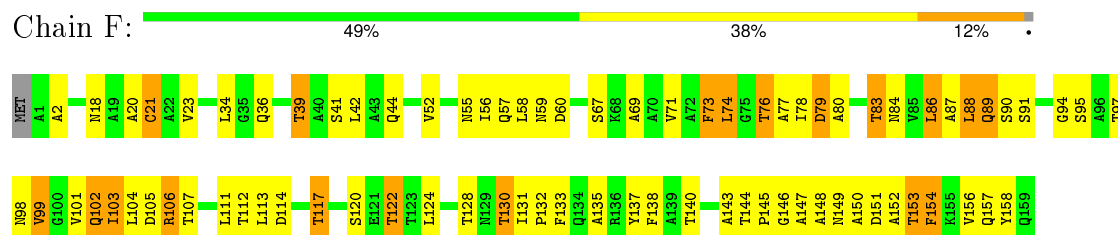
- Molecule 1: FimA



- Molecule 1: FimA

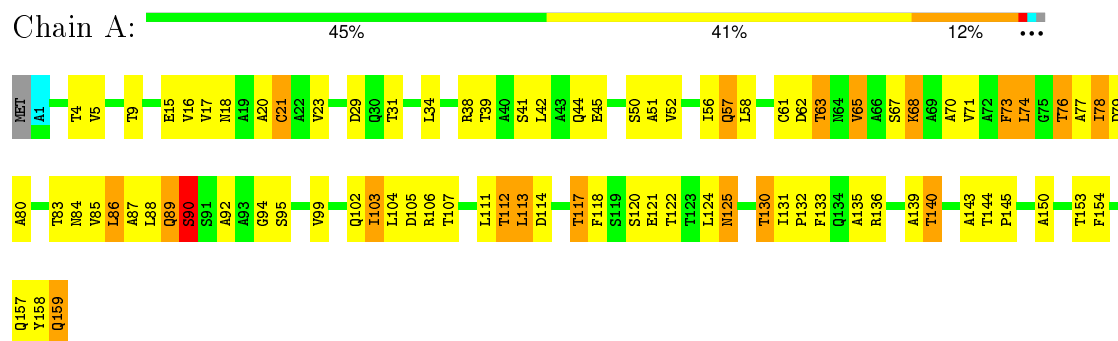


- Molecule 1: FimA

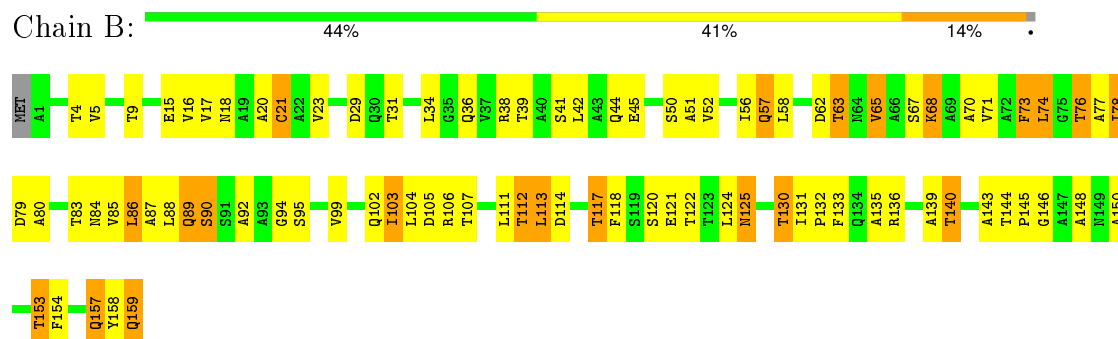


4.2.3 Score per residue for model 3 (medoid)

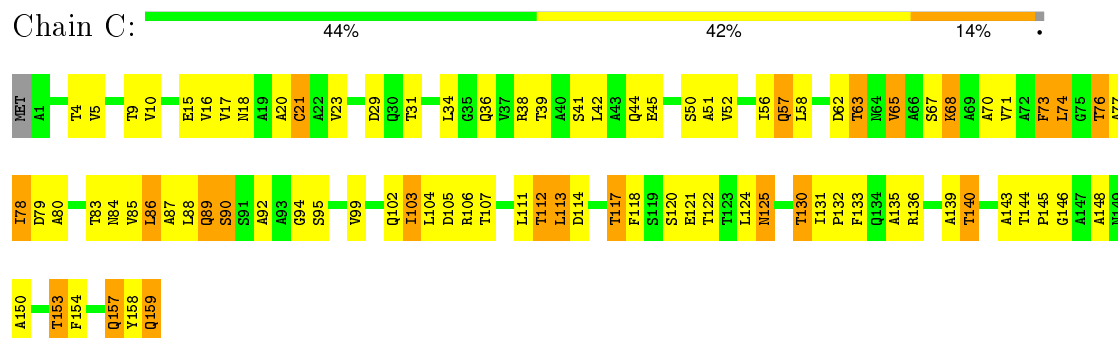
- Molecule 1: FimA



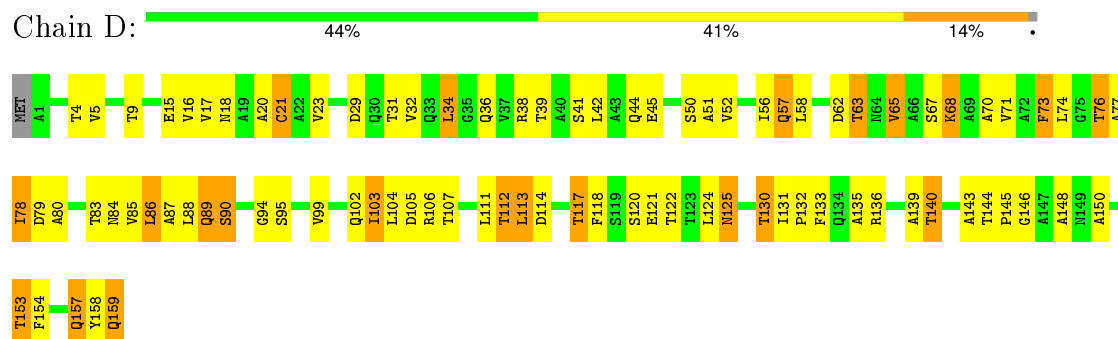
- Molecule 1: FimA



- Molecule 1: FimA

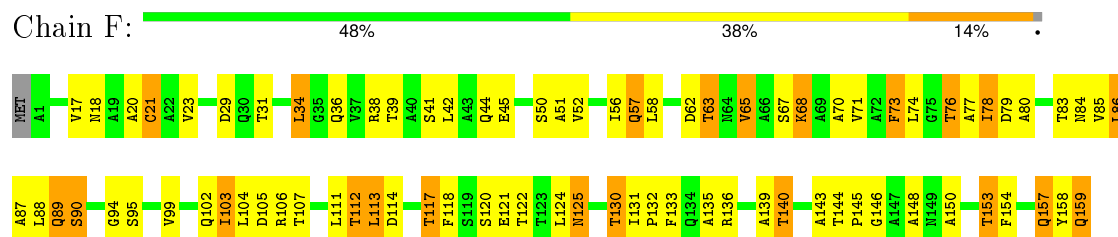


- Molecule 1: FimA



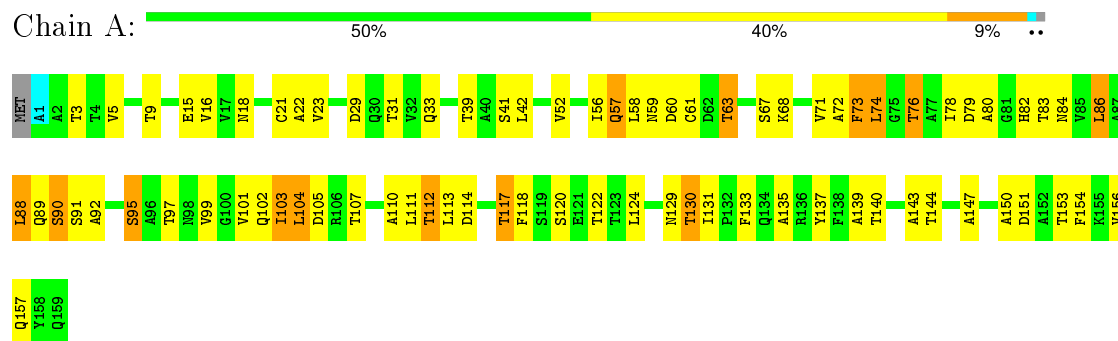
- Molecule 1: FimA

- Molecule 1: FimA

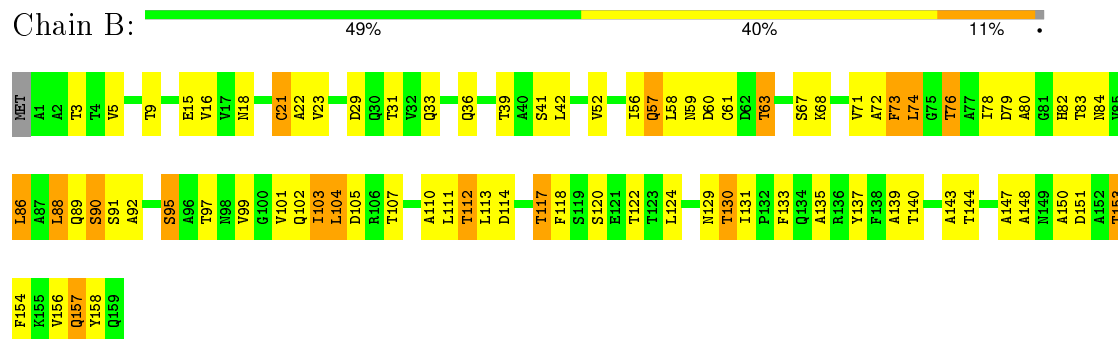


4.2.4 Score per residue for model 4

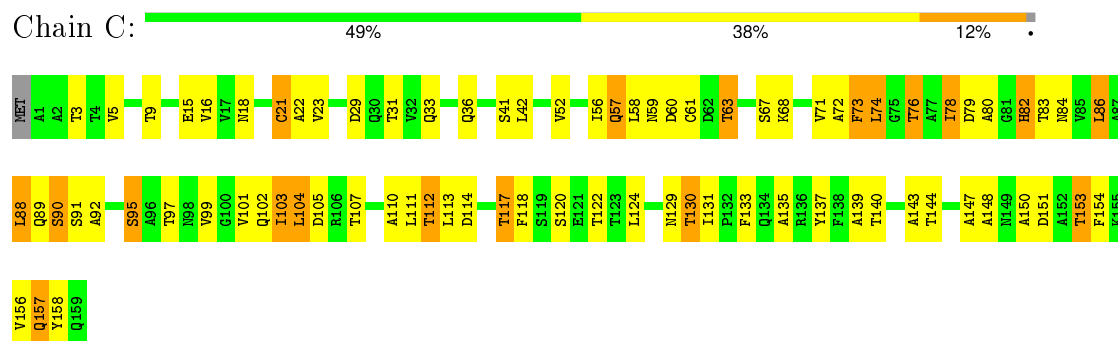
- Molecule 1: FimA



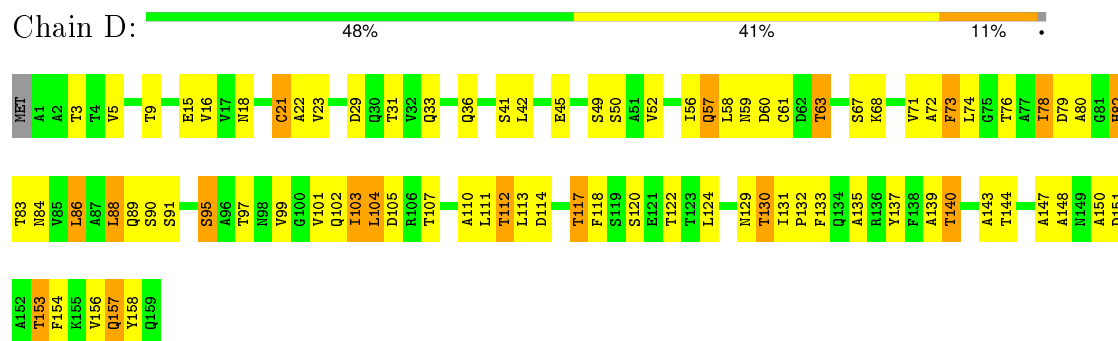
- Molecule 1: FimA



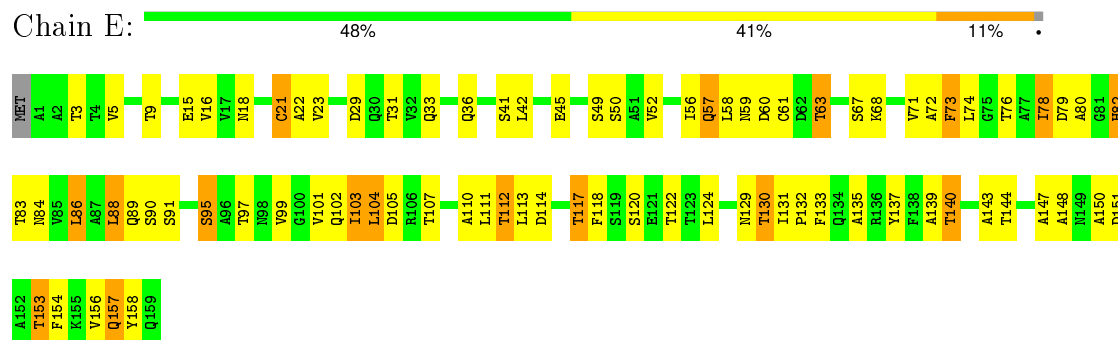
- Molecule 1: FimA



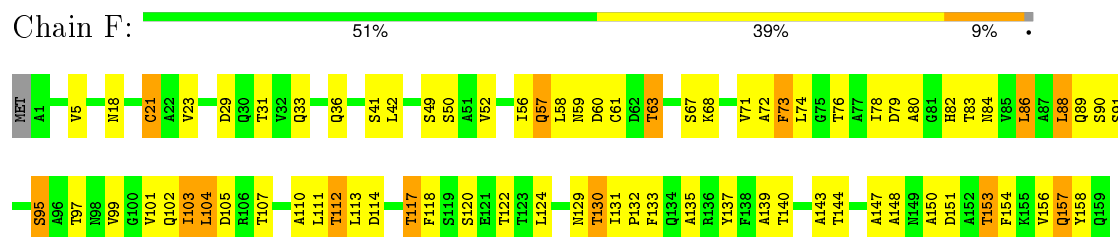
- Molecule 1: FimA



- Molecule 1: FimA

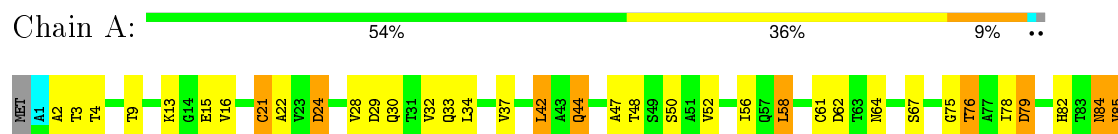


- Molecule 1: FimA

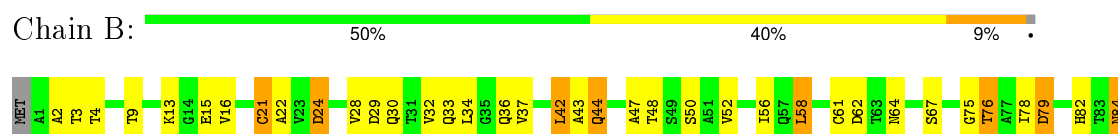


4.2.5 Score per residue for model 5

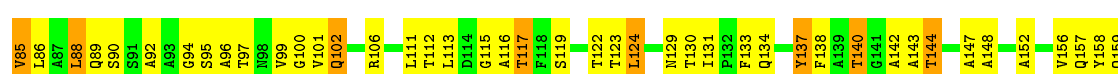
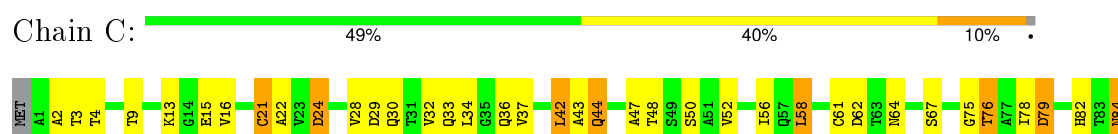
- Molecule 1: FimA



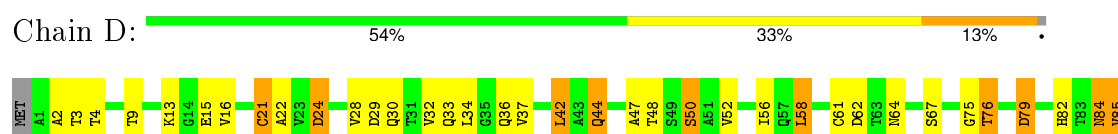
• Molecule 1: FimA



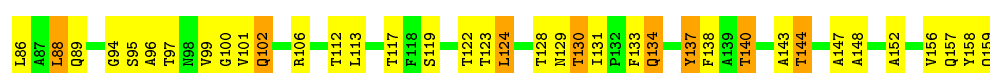
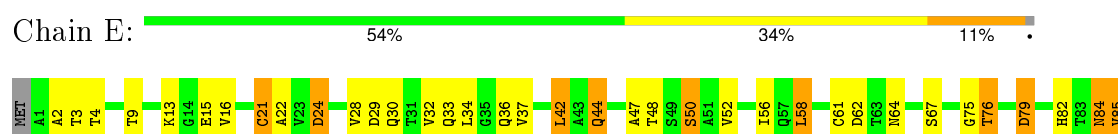
• Molecule 1: FimA



• Molecule 1: FimA

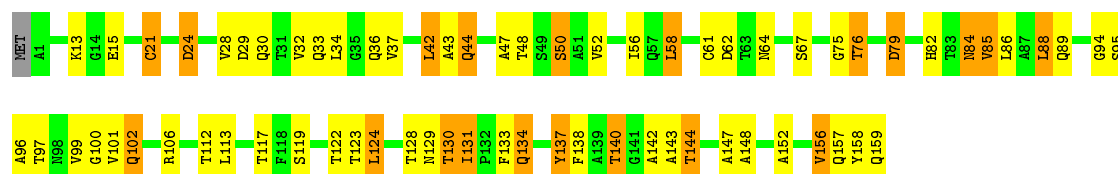


• Molecule 1: FimA



• Molecule 1: FimA

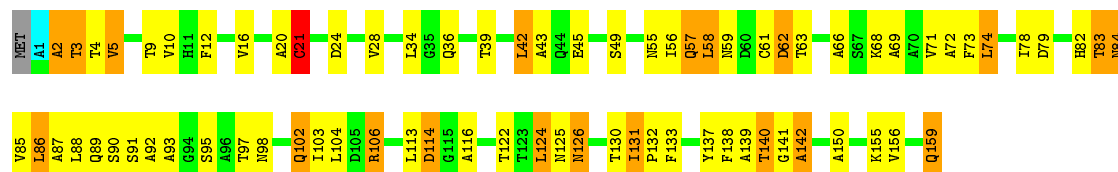




4.2.6 Score per residue for model 6

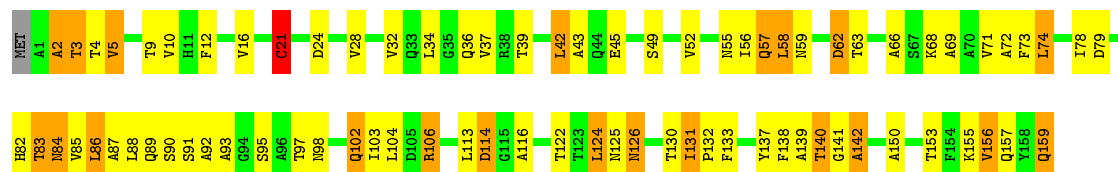
- Molecule 1: FimA

Chain A: 51% 34% 13% ...



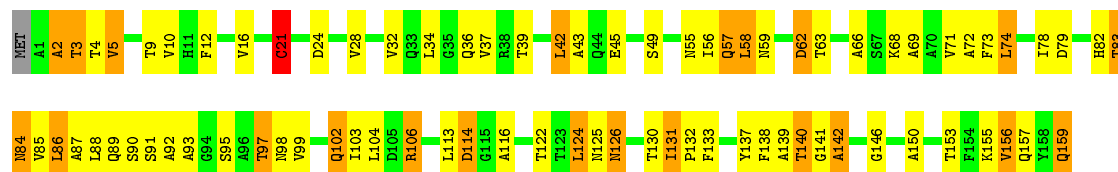
- Molecule 1: FimA

Chain B: 50% 36% 13% ..



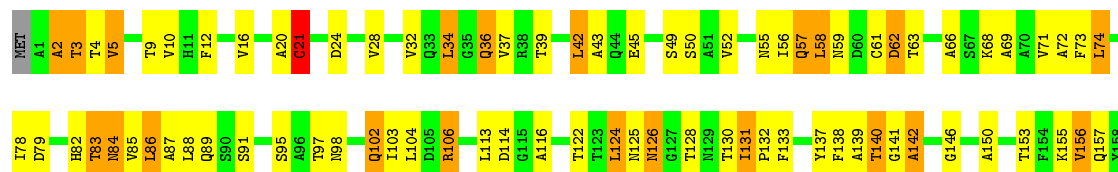
- Molecule 1: FimA

Chain C: 49% 36% 14% ..



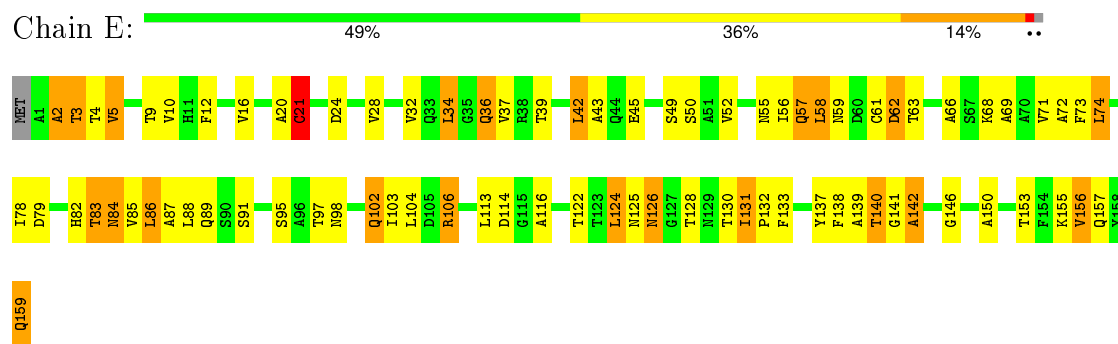
- Molecule 1: FimA

Chain D: 49% 36% 14% ..

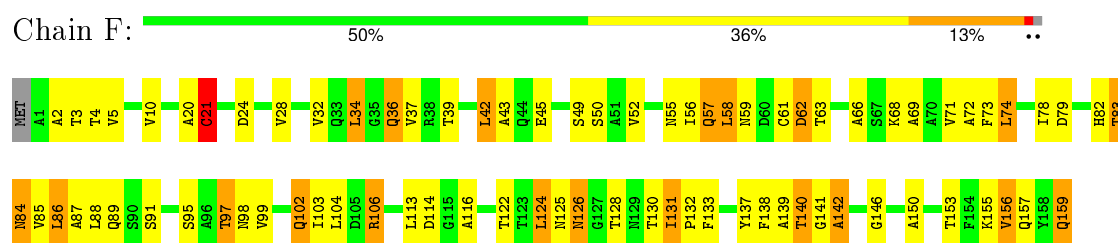


Q159

- Molecule 1: FimA

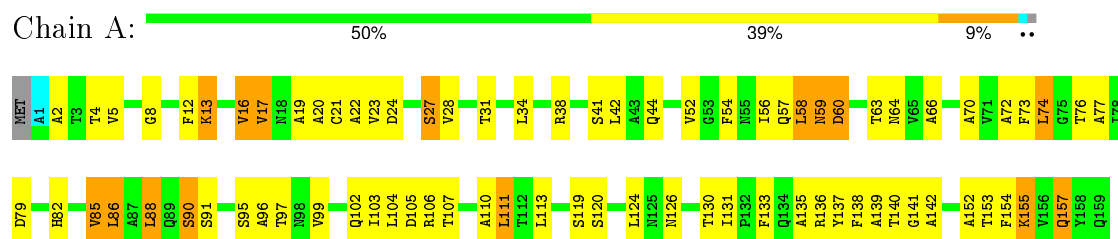


- Molecule 1: FimA

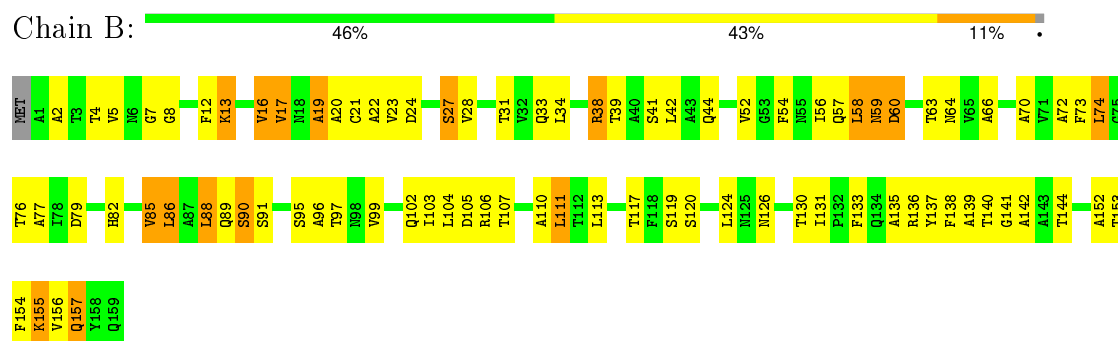


4.2.7 Score per residue for model 7

- Molecule 1: FimA

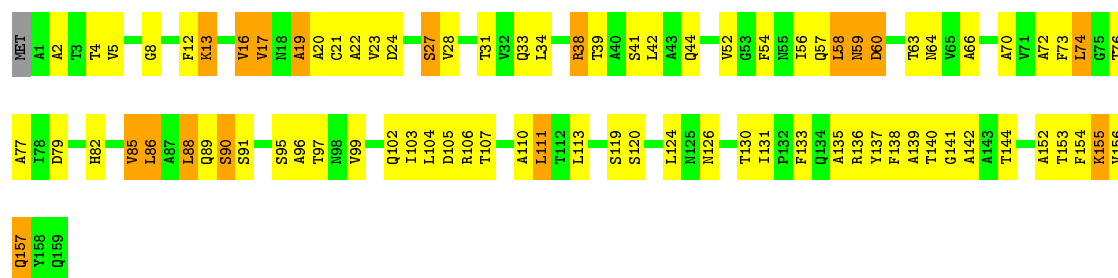


- Molecule 1: FimA



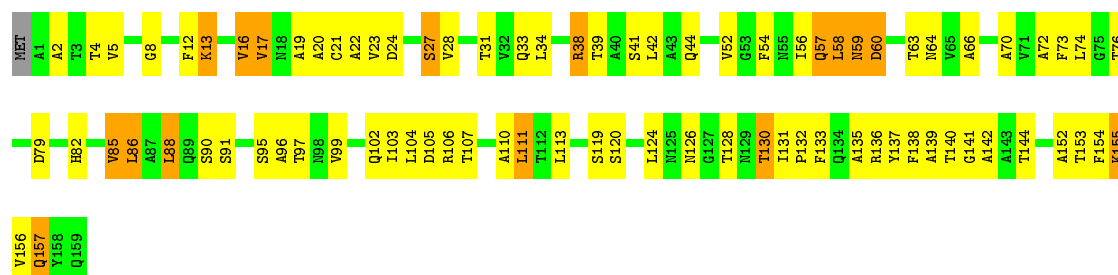
- Molecule 1: FimA





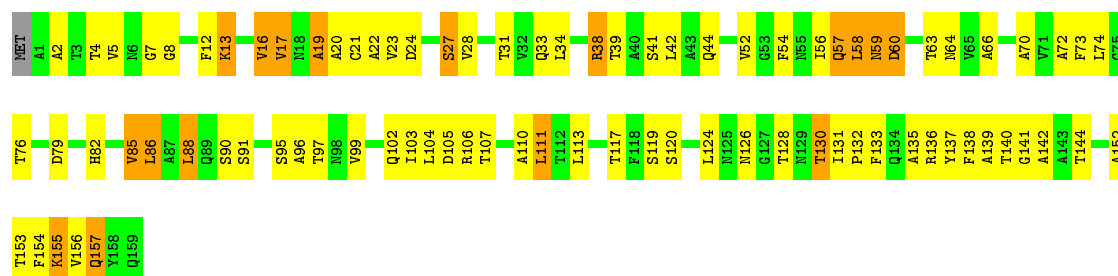
- Molecule 1: FimA

Chain D: 48% 42% 10%



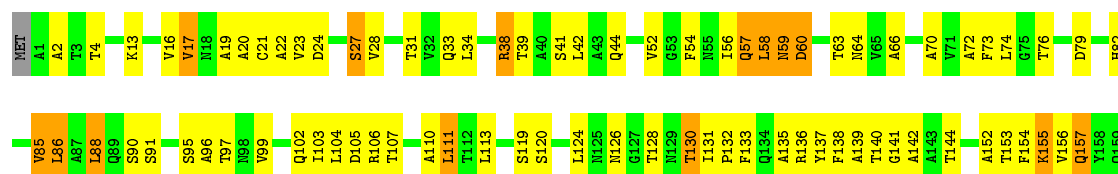
- Molecule 1: FimA

Chain E: 46% 43% 11%



- Molecule 1: FimA

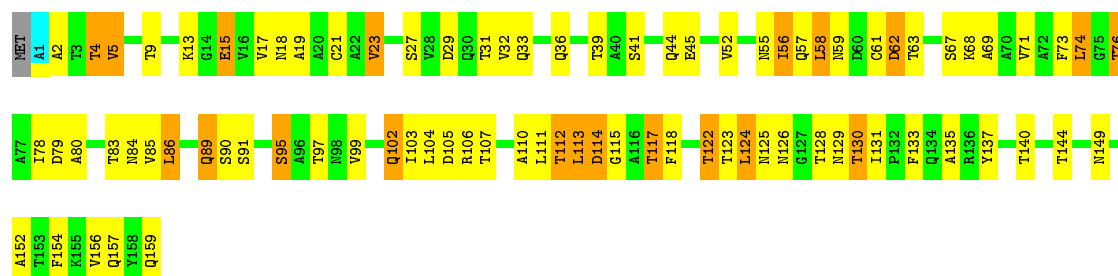
Chain F: 49% 41% 9%



4.2.8 Score per residue for model 8

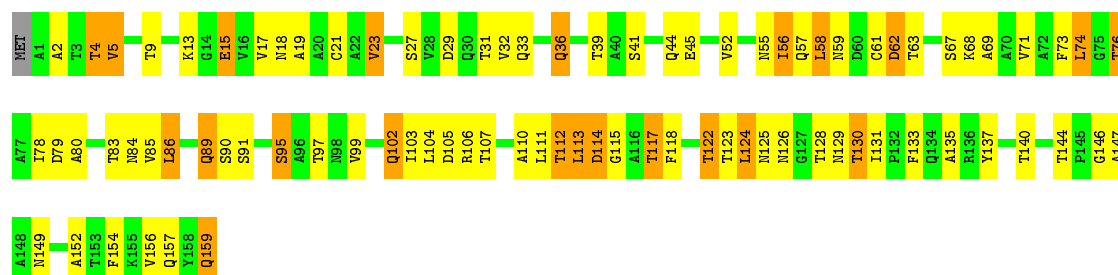
- Molecule 1: FimA

Chain A: 46% 40% 13%



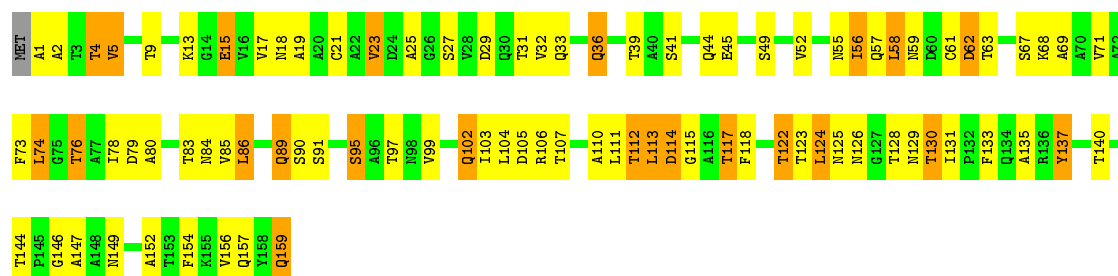
- Molecule 1: FimA

Chain B: 46% 40% 14%



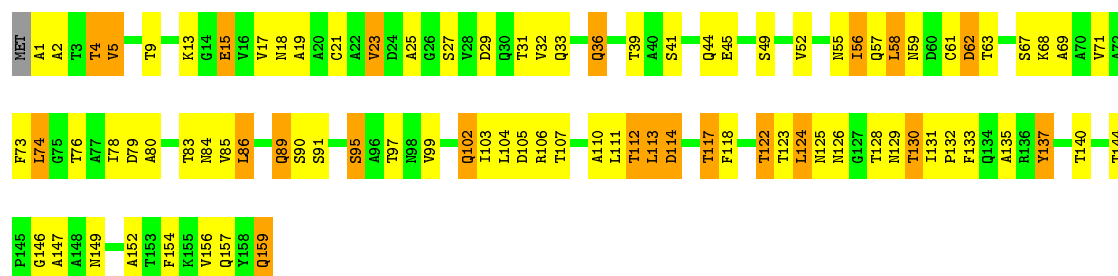
- Molecule 1: FimA

Chain C: 44% 41% 14%



- Molecule 1: FimA

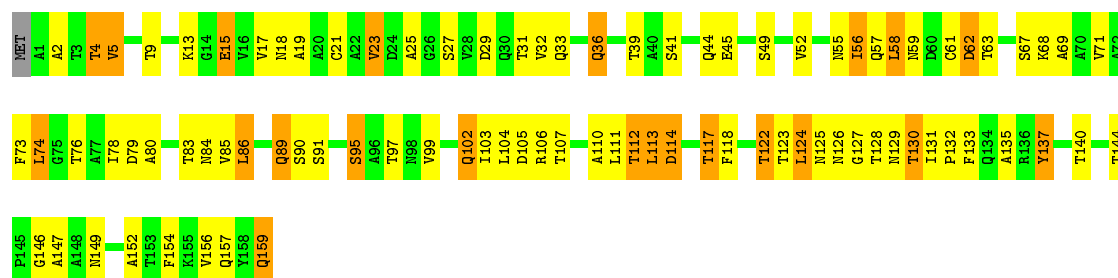
Chain D: 44% 42% 14%



- Molecule 1: FimA

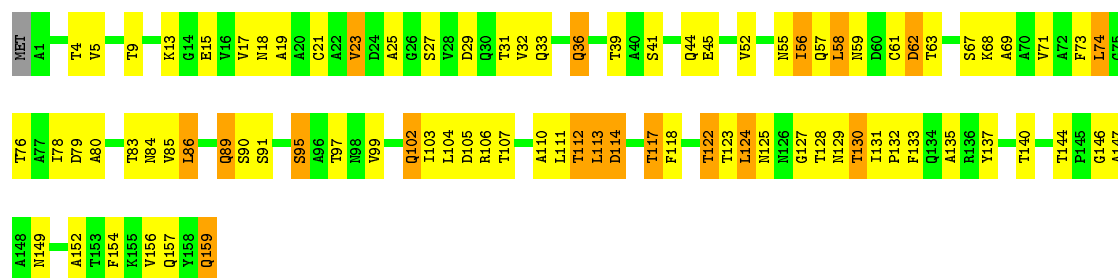
Chain E: 44% 42% 14%





• Molecule 1: FimA

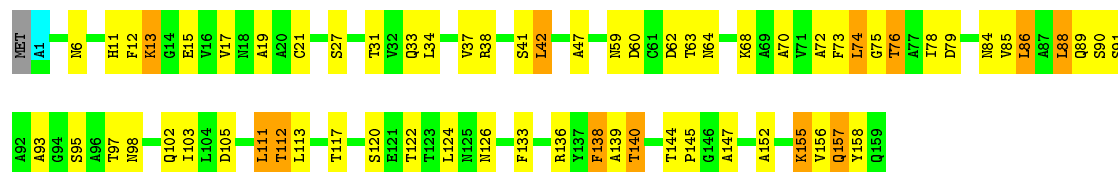
Chain F: 



4.2.9 Score per residue for model 9

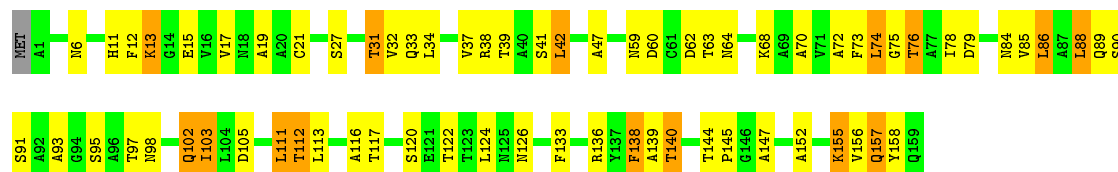
• Molecule 1: FimA

Chain A: 



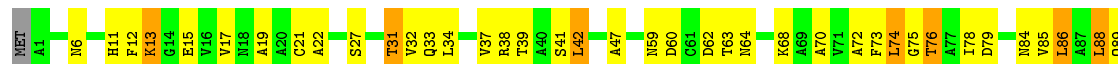
• Molecule 1: FimA

Chain B: 



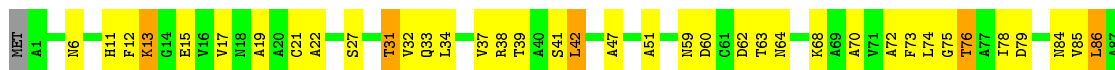
• Molecule 1: FimA

Chain C: 

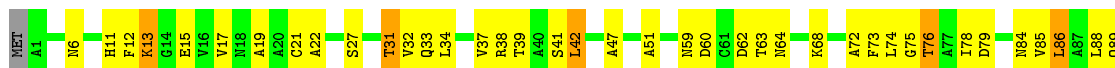




• Molecule 1: FimA



• Molecule 1: FimA

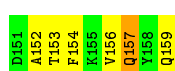
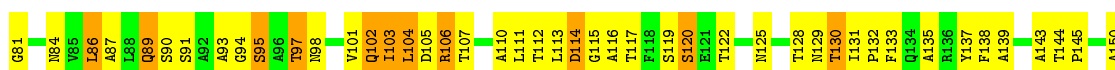
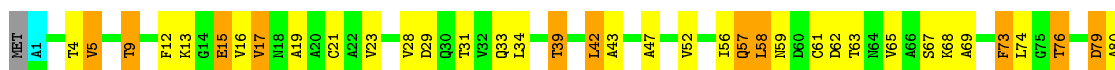


• Molecule 1: FimA



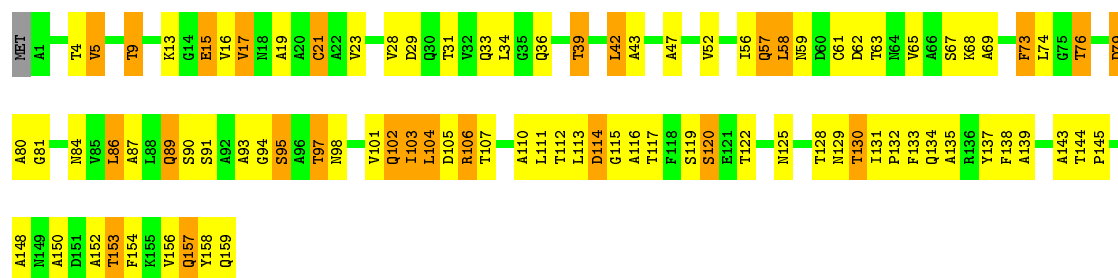
4.2.10 Score per residue for model 10

• Molecule 1: FimA

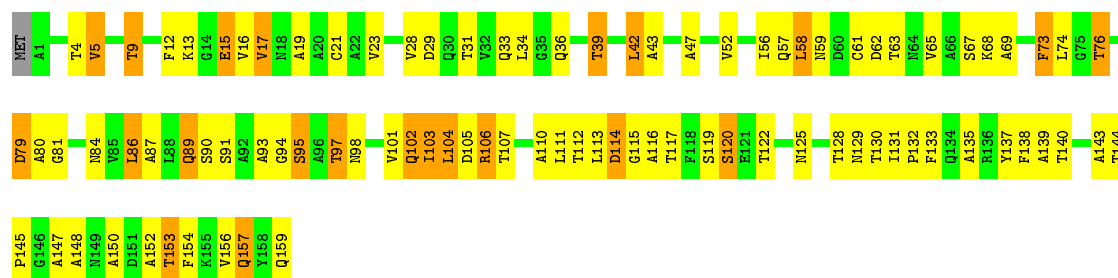


• Molecule 1: FimA

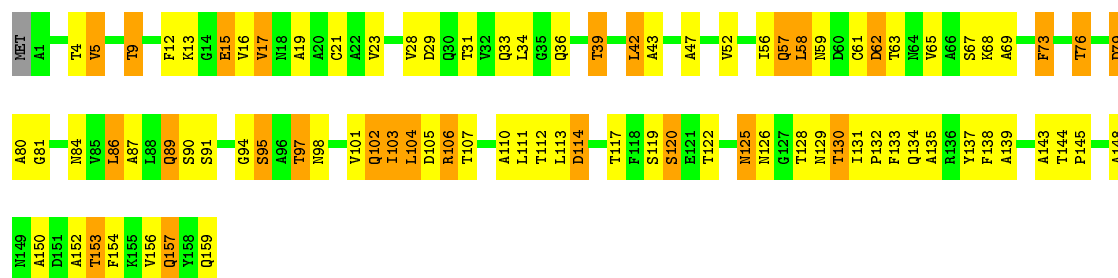




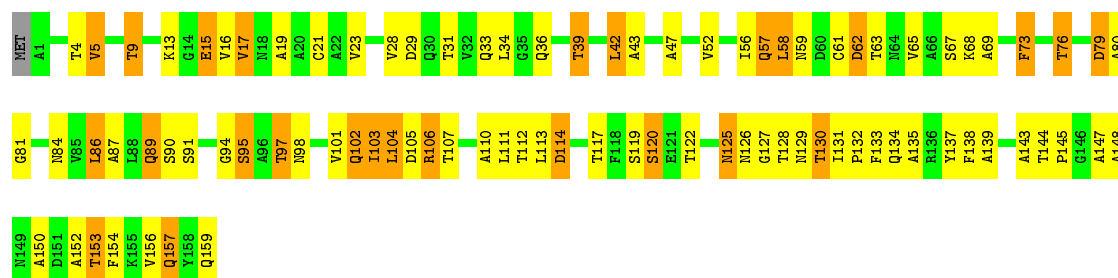
- Molecule 1: FimA



- Molecule 1: FimA

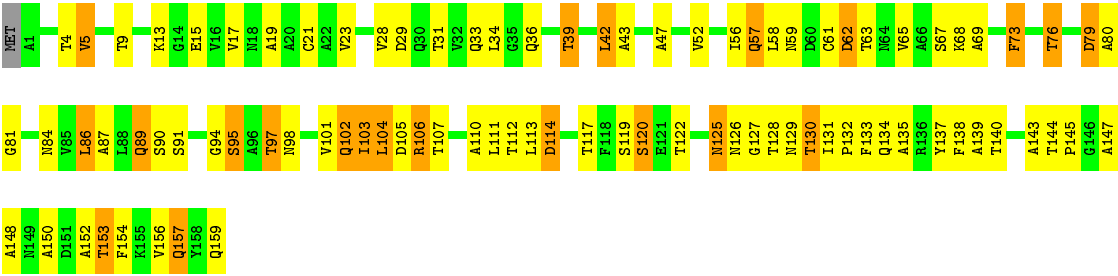


- Molecule 1: FimA



- Molecule 1: FimA





5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 1100 calculated structures, 10 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
ISD	refinement	

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

Chemical shift file(s)	2n7h_cs.str
Number of chemical shift lists	1
Total number of shifts	800
Number of shifts mapped to atoms	800
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	8%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	1107	1062	1070	46±10
1	B	1112	1067	1077	56±11
1	C	1112	1067	1077	56±11
1	D	1112	1067	1077	56±12
1	E	1112	1067	1077	56±12
1	F	1112	1067	1077	46±9
All	All	66670	63970	64526	2537

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:112:THR:HG23	1:B:117:THR:HG21	0.90	1.44	4	3
1:A:112:THR:HG23	1:A:117:THR:HG21	0.89	1.44	4	3
1:A:21:CYS:HG	1:A:61:CYS:HG	0.88	0.97	6	3
1:C:112:THR:HG23	1:C:117:THR:HG21	0.88	1.44	4	3
1:E:112:THR:HG23	1:E:117:THR:HG21	0.87	1.45	4	3
1:F:112:THR:HG23	1:F:117:THR:HG21	0.87	1.44	4	3
1:C:9:THR:HG22	1:D:153:THR:HG23	0.87	1.46	3	3
1:D:9:THR:HG22	1:E:153:THR:HG23	0.85	1.46	3	3
1:D:112:THR:HG23	1:D:117:THR:HG21	0.85	1.44	4	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:21:CYS:HG	1:C:61:CYS:HG	0.85	0.99	1	1
1:E:9:THR:HG22	1:F:153:THR:HG23	0.84	1.46	3	3
1:A:9:THR:HG22	1:B:153:THR:HG23	0.84	1.46	3	3
1:B:86:LEU:HD22	1:B:150:ALA:HB1	0.83	1.50	6	5
1:E:86:LEU:HD22	1:E:150:ALA:HB1	0.83	1.50	6	5
1:F:86:LEU:HD22	1:F:150:ALA:HB1	0.83	1.50	6	5
1:A:86:LEU:HD22	1:A:150:ALA:HB1	0.83	1.50	6	5
1:E:21:CYS:HG	1:E:61:CYS:HG	0.83	0.95	1	2
1:B:9:THR:HG22	1:C:153:THR:HG23	0.83	1.46	3	3
1:C:86:LEU:HD22	1:C:150:ALA:HB1	0.83	1.50	6	5
1:B:21:CYS:HG	1:B:61:CYS:HG	0.81	0.92	1	1
1:D:21:CYS:HG	1:D:61:CYS:HG	0.81	0.95	1	1
1:D:86:LEU:HD22	1:D:150:ALA:HB1	0.80	1.50	6	5
1:A:74:LEU:HD21	1:D:130:THR:HG21	0.80	1.53	4	3
1:B:74:LEU:HD21	1:E:130:THR:HG21	0.79	1.53	4	3
1:C:79:ASP:CB	1:C:140:THR:HG21	0.79	2.08	5	1
1:F:79:ASP:CB	1:F:140:THR:HG21	0.78	2.08	5	1
1:D:79:ASP:CB	1:D:140:THR:HG21	0.78	2.08	5	1
1:A:79:ASP:CB	1:A:140:THR:HG21	0.78	2.08	5	1
1:C:74:LEU:HD21	1:F:130:THR:HG21	0.78	1.53	4	3
1:F:79:ASP:HB3	1:F:140:THR:HG21	0.77	1.56	5	1
1:E:79:ASP:CB	1:E:140:THR:HG21	0.77	2.08	5	1
1:B:79:ASP:CB	1:B:140:THR:HG21	0.77	2.08	5	1
1:C:79:ASP:HB3	1:C:140:THR:HG21	0.77	1.56	5	1
1:E:104:LEU:HD12	1:E:110:ALA:HB2	0.77	1.56	8	2
1:B:104:LEU:HD12	1:B:110:ALA:HB2	0.77	1.56	8	2
1:D:79:ASP:HB3	1:D:140:THR:HG21	0.77	1.56	5	1
1:D:104:LEU:HD12	1:D:110:ALA:HB2	0.77	1.56	8	1
1:A:79:ASP:HB3	1:A:140:THR:HG21	0.77	1.56	5	1
1:E:112:THR:CG2	1:E:117:THR:HG21	0.76	2.10	4	3
1:B:112:THR:CG2	1:B:117:THR:HG21	0.76	2.10	4	3
1:E:79:ASP:HB3	1:E:140:THR:HG21	0.76	1.56	5	1
1:A:112:THR:CG2	1:A:117:THR:HG21	0.76	2.10	4	3
1:C:104:LEU:HD12	1:C:110:ALA:HB2	0.76	1.56	8	2
1:F:104:LEU:HD12	1:F:110:ALA:HB2	0.76	1.56	8	1
1:F:112:THR:CG2	1:F:117:THR:HG21	0.75	2.10	4	2
1:D:112:THR:CG2	1:D:117:THR:HG21	0.75	2.10	4	3
1:B:5:VAL:HG21	1:C:17:VAL:HG12	0.75	1.58	3	2
1:E:5:VAL:HG21	1:F:17:VAL:HG12	0.75	1.57	3	2
1:A:104:LEU:HD12	1:A:110:ALA:HB2	0.75	1.56	8	2
1:C:112:THR:CG2	1:C:117:THR:HG21	0.75	2.10	4	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:86:LEU:HD12	1:B:113:LEU:HD22	0.75	1.59	10	1
1:E:86:LEU:HD12	1:E:113:LEU:HD22	0.75	1.59	10	1
1:B:79:ASP:HB3	1:B:140:THR:HG21	0.74	1.56	5	1
1:C:5:VAL:HG21	1:D:17:VAL:HG12	0.74	1.58	3	2
1:D:5:VAL:HG21	1:E:17:VAL:HG12	0.74	1.58	3	2
1:F:86:LEU:HD12	1:F:113:LEU:HD22	0.74	1.59	10	1
1:D:69:ALA:HB2	1:D:124:LEU:HD13	0.74	1.60	8	1
1:C:86:LEU:HD12	1:C:113:LEU:HD22	0.73	1.59	10	1
1:A:5:VAL:HG21	1:B:17:VAL:HG12	0.73	1.58	3	2
1:E:69:ALA:HB2	1:E:124:LEU:HD13	0.73	1.60	8	1
1:A:90:SER:HA	1:D:52:VAL:HG13	0.73	1.60	6	1
1:F:144:THR:CG2	1:F:145:PRO:CD	0.73	2.67	2	4
1:E:144:THR:CG2	1:E:145:PRO:CD	0.73	2.67	2	4
1:D:86:LEU:HD12	1:D:113:LEU:HD22	0.73	1.59	10	1
1:A:69:ALA:HB2	1:A:124:LEU:HD13	0.73	1.60	8	1
1:B:144:THR:CG2	1:B:145:PRO:CD	0.72	2.67	2	4
1:B:69:ALA:HB2	1:B:124:LEU:HD13	0.72	1.60	8	1
1:A:86:LEU:HD12	1:A:113:LEU:HD22	0.72	1.59	10	1
1:A:144:THR:CG2	1:A:145:PRO:CD	0.72	2.67	2	4
1:F:21:CYS:HG	1:F:61:CYS:HG	0.72	0.73	1	1
1:F:69:ALA:HB2	1:F:124:LEU:HD13	0.72	1.60	8	1
1:C:69:ALA:HB2	1:C:124:LEU:HD13	0.72	1.60	8	1
1:C:90:SER:HA	1:F:52:VAL:HG13	0.72	1.60	6	1
1:D:144:THR:CG2	1:D:145:PRO:CD	0.72	2.67	2	4
1:C:144:THR:CG2	1:C:145:PRO:CD	0.71	2.67	2	4
1:B:90:SER:HA	1:E:52:VAL:HG13	0.71	1.60	6	1
1:D:84:ASN:HA	1:D:112:THR:HA	0.70	1.64	8	6
1:F:84:ASN:HA	1:F:112:THR:HA	0.70	1.64	8	6
1:A:84:ASN:HA	1:A:112:THR:HA	0.70	1.64	8	6
1:C:84:ASN:HA	1:C:112:THR:HA	0.70	1.64	8	6
1:E:16:VAL:HG23	1:F:148:ALA:HB2	0.69	1.64	4	5
1:B:16:VAL:HG23	1:C:148:ALA:HB2	0.69	1.64	4	5
1:B:15:GLU:CG	1:C:146:GLY:O	0.69	2.41	3	3
1:E:15:GLU:CG	1:F:146:GLY:O	0.69	2.41	3	3
1:C:16:VAL:HG23	1:D:148:ALA:HB2	0.68	1.65	4	5
1:A:57:GLN:HA	1:A:130:THR:HG23	0.68	1.65	4	5
1:A:16:VAL:HG23	1:B:148:ALA:HB2	0.68	1.65	4	5
1:D:16:VAL:HG23	1:E:148:ALA:HB2	0.68	1.64	4	5
1:F:72:ALA:HB3	1:F:155:LYS:HB3	0.68	1.66	7	2
1:C:15:GLU:CG	1:D:146:GLY:O	0.68	2.41	3	3
1:D:15:GLU:CG	1:E:146:GLY:O	0.68	2.41	3	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLU:CG	1:B:146:GLY:O	0.68	2.41	3	3
1:E:84:ASN:HA	1:E:112:THR:HA	0.67	1.64	8	5
1:F:57:GLN:HA	1:F:130:THR:HG23	0.67	1.65	4	4
1:D:57:GLN:HA	1:D:130:THR:HG23	0.67	1.65	4	4
1:C:72:ALA:HB3	1:C:155:LYS:HB3	0.67	1.66	7	2
1:C:57:GLN:HA	1:C:130:THR:HG23	0.67	1.65	4	4
1:B:84:ASN:HA	1:B:112:THR:HA	0.67	1.64	8	5
1:D:93:ALA:HB1	1:F:22:ALA:HB1	0.67	1.67	9	1
1:D:144:THR:CG2	1:D:145:PRO:HD2	0.67	2.20	2	4
1:C:93:ALA:HB1	1:E:22:ALA:HB1	0.67	1.67	9	1
1:C:144:THR:CG2	1:C:145:PRO:HD2	0.67	2.20	2	4
1:A:144:THR:CG2	1:A:145:PRO:HD2	0.67	2.20	2	4
1:A:93:ALA:HB1	1:C:22:ALA:HB1	0.67	1.67	9	1
1:F:42:LEU:O	1:F:143:ALA:HB2	0.67	1.90	10	4
1:B:42:LEU:O	1:B:143:ALA:HB2	0.66	1.90	10	4
1:E:42:LEU:O	1:E:143:ALA:HB2	0.66	1.90	10	4
1:B:57:GLN:HA	1:B:130:THR:HG23	0.66	1.65	4	5
1:E:57:GLN:HA	1:E:130:THR:HG23	0.66	1.65	4	4
1:C:42:LEU:O	1:C:143:ALA:HB2	0.66	1.90	10	4
1:F:105:ASP:HB3	1:F:107:THR:HG22	0.66	1.68	2	6
1:C:105:ASP:HB3	1:C:107:THR:HG22	0.66	1.68	2	6
1:C:21:CYS:SG	1:C:58:LEU:HB3	0.66	2.31	5	2
1:B:21:CYS:SG	1:B:58:LEU:HB3	0.66	2.31	5	2
1:F:144:THR:CG2	1:F:145:PRO:HD2	0.66	2.20	2	4
1:E:21:CYS:SG	1:E:58:LEU:HB3	0.66	2.31	5	2
1:F:21:CYS:SG	1:F:58:LEU:HB3	0.66	2.31	5	2
1:A:105:ASP:HB3	1:A:107:THR:HG22	0.66	1.68	2	6
1:B:52:VAL:HG22	1:B:135:ALA:O	0.65	1.91	1	4
1:B:93:ALA:HB1	1:D:22:ALA:HB1	0.65	1.67	9	1
1:D:105:ASP:HB3	1:D:107:THR:HG22	0.65	1.68	2	6
1:B:144:THR:CG2	1:B:145:PRO:HD2	0.65	2.20	2	4
1:B:72:ALA:HB3	1:B:155:LYS:HB3	0.65	1.66	7	2
1:E:144:THR:CG2	1:E:145:PRO:HD2	0.65	2.20	2	4
1:C:52:VAL:HG22	1:C:135:ALA:O	0.65	1.91	1	4
1:A:21:CYS:SG	1:A:58:LEU:HB3	0.65	2.31	5	2
1:A:17:VAL:O	1:B:39:THR:HG22	0.65	1.92	1	1
1:C:17:VAL:O	1:D:39:THR:HG22	0.65	1.92	1	1
1:A:52:VAL:HG22	1:A:135:ALA:O	0.65	1.91	1	4
1:D:72:ALA:HB3	1:D:155:LYS:HB3	0.65	1.66	7	2
1:F:71:VAL:HG11	1:F:131:ILE:HG21	0.65	1.69	1	5
1:A:42:LEU:O	1:A:143:ALA:HB2	0.65	1.91	10	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:21:CYS:SG	1:D:58:LEU:HB3	0.65	2.31	5	2
1:E:72:ALA:HB3	1:E:155:LYS:HB3	0.65	1.66	7	2
1:A:72:ALA:HB3	1:A:155:LYS:HB3	0.65	1.66	7	2
1:E:52:VAL:HG22	1:E:135:ALA:O	0.65	1.91	1	4
1:F:52:VAL:HG22	1:F:135:ALA:O	0.65	1.91	1	4
1:D:17:VAL:O	1:E:39:THR:HG22	0.65	1.92	1	1
1:E:105:ASP:HB3	1:E:107:THR:HG22	0.64	1.68	2	6
1:E:144:THR:HG23	1:E:145:PRO:CD	0.64	2.22	2	3
1:B:71:VAL:HG11	1:B:131:ILE:HG21	0.64	1.69	1	5
1:B:105:ASP:HB3	1:B:107:THR:HG22	0.64	1.68	2	6
1:F:144:THR:HG23	1:F:145:PRO:CD	0.64	2.23	2	3
1:D:52:VAL:HG22	1:D:135:ALA:O	0.64	1.91	1	4
1:C:144:THR:HG23	1:C:145:PRO:CD	0.64	2.23	2	3
1:A:44:GLN:HG3	1:A:47:ALA:HB2	0.64	1.70	5	1
1:A:71:VAL:HG11	1:A:131:ILE:HG21	0.64	1.70	3	3
1:B:144:THR:HG23	1:B:145:PRO:CD	0.64	2.23	2	3
1:C:71:VAL:HG11	1:C:131:ILE:HG21	0.64	1.69	1	3
1:D:42:LEU:O	1:D:143:ALA:HB2	0.64	1.90	10	4
1:E:17:VAL:O	1:F:39:THR:HG22	0.64	1.92	1	1
1:B:44:GLN:HG3	1:B:47:ALA:HB2	0.64	1.70	5	1
1:A:95:SER:HA	1:A:147:ALA:HB3	0.64	1.69	1	5
1:F:44:GLN:HG3	1:F:47:ALA:HB2	0.64	1.70	5	1
1:B:15:GLU:O	1:C:36:GLN:HA	0.64	1.93	2	6
1:A:56:ILE:HB	1:A:131:ILE:HD12	0.64	1.70	7	1
1:E:71:VAL:HG11	1:E:131:ILE:HG21	0.64	1.69	3	5
1:D:71:VAL:HG11	1:D:131:ILE:HG21	0.64	1.69	1	4
1:A:144:THR:HG23	1:A:145:PRO:CD	0.64	2.23	2	3
1:E:44:GLN:HG3	1:E:47:ALA:HB2	0.64	1.70	5	1
1:A:69:ALA:HB2	1:A:124:LEU:HD12	0.64	1.70	6	1
1:D:15:GLU:O	1:E:36:GLN:HA	0.64	1.93	2	6
1:B:69:ALA:HB2	1:B:124:LEU:HD12	0.64	1.71	6	1
1:E:95:SER:HA	1:E:147:ALA:HB3	0.63	1.69	1	5
1:B:17:VAL:O	1:C:39:THR:HG22	0.63	1.92	1	1
1:C:95:SER:HA	1:C:147:ALA:HB3	0.63	1.69	1	5
1:D:69:ALA:HB2	1:D:124:LEU:HD12	0.63	1.71	6	1
1:E:69:ALA:HB2	1:E:124:LEU:HD12	0.63	1.70	6	1
1:C:9:THR:HG23	1:D:153:THR:HG23	0.63	1.69	10	1
1:D:9:THR:HG23	1:E:153:THR:HG23	0.63	1.69	10	1
1:D:95:SER:HA	1:D:147:ALA:HB3	0.63	1.69	1	5
1:F:69:ALA:HB2	1:F:124:LEU:HD12	0.63	1.70	6	1
1:E:15:GLU:O	1:F:36:GLN:HA	0.63	1.93	2	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:95:SER:HA	1:B:147:ALA:HB3	0.63	1.69	1	5
1:D:44:GLN:HG3	1:D:47:ALA:HB2	0.63	1.70	5	1
1:C:44:GLN:HG3	1:C:47:ALA:HB2	0.63	1.70	5	1
1:A:9:THR:HG23	1:B:153:THR:HG23	0.63	1.69	10	1
1:B:9:THR:HG23	1:C:153:THR:HG23	0.63	1.69	10	1
1:A:15:GLU:O	1:B:36:GLN:HA	0.63	1.93	2	6
1:A:82:HIS:HB3	1:A:85:VAL:HB	0.63	1.70	6	1
1:C:69:ALA:HB2	1:C:124:LEU:HD12	0.63	1.71	6	1
1:C:63:THR:HG23	1:C:124:LEU:O	0.63	1.94	4	1
1:D:82:HIS:HB3	1:D:85:VAL:HB	0.62	1.70	6	1
1:C:56:ILE:HB	1:C:131:ILE:HD12	0.62	1.70	7	1
1:E:9:THR:HG23	1:F:153:THR:HG23	0.62	1.69	10	1
1:C:15:GLU:O	1:D:36:GLN:HA	0.62	1.93	2	6
1:F:95:SER:HA	1:F:147:ALA:HB3	0.62	1.69	1	5
1:D:56:ILE:HB	1:D:131:ILE:HD12	0.62	1.70	7	1
1:C:12:PHE:HB3	1:D:34:LEU:HD21	0.62	1.70	7	1
1:B:12:PHE:HB3	1:C:34:LEU:HD21	0.62	1.70	7	1
1:C:82:HIS:HB3	1:C:85:VAL:HB	0.62	1.70	6	1
1:C:15:GLU:HG3	1:D:146:GLY:O	0.62	1.94	3	4
1:B:56:ILE:HB	1:B:131:ILE:HD12	0.62	1.70	7	1
1:B:15:GLU:HG3	1:C:146:GLY:O	0.62	1.94	3	4
1:E:102:GLN:O	1:E:135:ALA:HA	0.62	1.94	4	5
1:B:102:GLN:O	1:B:135:ALA:HA	0.62	1.95	4	5
1:C:102:GLN:O	1:C:135:ALA:HA	0.62	1.95	4	5
1:C:75:GLY:HA3	1:C:113:LEU:HD22	0.62	1.72	1	1
1:C:88:LEU:HD12	1:F:51:ALA:O	0.62	1.95	9	1
1:A:104:LEU:HA	1:A:110:ALA:HA	0.62	1.72	4	4
1:A:12:PHE:HB3	1:B:34:LEU:HD21	0.62	1.70	7	1
1:F:56:ILE:HB	1:F:131:ILE:HD12	0.62	1.70	7	1
1:D:63:THR:HG23	1:D:124:LEU:O	0.62	1.94	4	1
1:D:12:PHE:HB3	1:E:34:LEU:HD21	0.62	1.70	7	1
1:A:102:GLN:O	1:A:135:ALA:HA	0.62	1.94	4	5
1:D:75:GLY:HA3	1:D:113:LEU:HD22	0.62	1.72	1	1
1:B:63:THR:HG23	1:B:124:LEU:O	0.62	1.94	4	1
1:F:63:THR:HG23	1:F:124:LEU:O	0.62	1.94	4	1
1:A:63:THR:HG23	1:A:124:LEU:O	0.62	1.94	4	1
1:E:56:ILE:HB	1:E:131:ILE:HD12	0.62	1.70	7	1
1:C:17:VAL:HG11	1:D:36:GLN:NE2	0.62	2.10	2	3
1:F:75:GLY:HA3	1:F:113:LEU:HD22	0.62	1.72	1	1
1:D:144:THR:HG23	1:D:145:PRO:CD	0.62	2.23	2	3
1:A:17:VAL:O	1:B:39:THR:HG23	0.62	1.95	7	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:12:PHE:HB3	1:F:34:LEU:HD21	0.62	1.70	7	1
1:D:17:VAL:HG11	1:E:36:GLN:NE2	0.62	2.10	2	3
1:E:63:THR:HG23	1:E:124:LEU:O	0.61	1.94	4	1
1:A:17:VAL:HG11	1:B:36:GLN:NE2	0.61	2.10	2	3
1:A:75:GLY:HA3	1:A:113:LEU:HD22	0.61	1.72	1	1
1:B:82:HIS:HB3	1:B:85:VAL:HB	0.61	1.70	6	1
1:D:15:GLU:HG3	1:E:146:GLY:O	0.61	1.94	3	4
1:E:17:VAL:O	1:F:39:THR:HG23	0.61	1.95	7	2
1:D:104:LEU:HA	1:D:110:ALA:HA	0.61	1.72	4	4
1:E:82:HIS:HB3	1:E:85:VAL:HB	0.61	1.70	6	1
1:A:88:LEU:HD12	1:D:51:ALA:O	0.61	1.95	9	1
1:B:61:CYS:SG	1:B:129:ASN:HB2	0.61	2.35	4	3
1:B:17:VAL:HG11	1:C:36:GLN:NE2	0.61	2.10	2	3
1:D:102:GLN:O	1:D:135:ALA:HA	0.61	1.94	4	5
1:E:75:GLY:HA3	1:E:113:LEU:HD22	0.61	1.72	1	1
1:E:15:GLU:HG3	1:F:146:GLY:O	0.61	1.94	3	4
1:B:17:VAL:O	1:C:39:THR:HG23	0.61	1.95	7	2
1:A:61:CYS:SG	1:A:129:ASN:HB2	0.61	2.36	4	3
1:A:15:GLU:HG3	1:B:146:GLY:O	0.61	1.94	3	4
1:B:88:LEU:HD12	1:E:51:ALA:O	0.61	1.95	9	1
1:F:61:CYS:SG	1:F:129:ASN:HB2	0.61	2.36	4	3
1:B:112:THR:HG22	1:B:117:THR:HG21	0.61	1.73	10	1
1:E:112:THR:HG22	1:E:117:THR:HG21	0.61	1.73	10	1
1:D:16:VAL:HG13	1:E:37:VAL:HG13	0.61	1.73	1	1
1:E:104:LEU:HA	1:E:110:ALA:HA	0.61	1.72	4	3
1:B:104:LEU:HA	1:B:110:ALA:HA	0.61	1.72	4	3
1:F:82:HIS:HB3	1:F:85:VAL:HB	0.61	1.70	6	1
1:A:42:LEU:CB	1:A:139:ALA:HB2	0.61	2.26	6	1
1:D:61:CYS:SG	1:D:129:ASN:HB2	0.61	2.36	4	3
1:E:17:VAL:HG11	1:F:36:GLN:NE2	0.61	2.10	2	3
1:D:42:LEU:CB	1:D:139:ALA:HB2	0.60	2.26	6	1
1:E:16:VAL:CG1	1:F:144:THR:O	0.60	2.49	3	2
1:F:102:GLN:O	1:F:135:ALA:HA	0.60	1.95	4	5
1:B:55:ASN:HA	1:B:131:ILE:O	0.60	1.96	6	1
1:C:42:LEU:CB	1:C:139:ALA:HB2	0.60	2.26	6	1
1:C:61:CYS:SG	1:C:129:ASN:HB2	0.60	2.36	4	3
1:E:55:ASN:HA	1:E:131:ILE:O	0.60	1.96	6	1
1:D:17:VAL:O	1:E:39:THR:HG23	0.60	1.95	7	2
1:E:5:VAL:HG21	1:F:17:VAL:CG1	0.60	2.26	3	1
1:C:16:VAL:CG1	1:D:144:THR:O	0.60	2.50	3	2
1:B:16:VAL:CG1	1:C:144:THR:O	0.60	2.49	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:104:LEU:HA	1:C:110:ALA:HA	0.60	1.72	4	3
1:E:91:SER:HB2	1:E:95:SER:HB2	0.60	1.73	10	2
1:B:5:VAL:HG21	1:C:17:VAL:CG1	0.60	2.27	3	1
1:A:16:VAL:CG1	1:B:144:THR:O	0.60	2.49	3	2
1:D:55:ASN:HA	1:D:131:ILE:O	0.60	1.96	6	1
1:B:42:LEU:CB	1:B:139:ALA:HB2	0.60	2.26	6	1
1:C:5:VAL:HG21	1:D:17:VAL:CG1	0.60	2.27	3	1
1:E:61:CYS:SG	1:E:129:ASN:HB2	0.60	2.36	4	3
1:C:90:SER:HA	1:F:52:VAL:HB	0.60	1.74	4	1
1:B:75:GLY:HA3	1:B:113:LEU:HD22	0.60	1.72	1	1
1:F:42:LEU:CB	1:F:139:ALA:HB2	0.60	2.26	6	1
1:B:91:SER:HB2	1:B:95:SER:HB2	0.60	1.73	10	2
1:C:17:VAL:O	1:D:39:THR:HG23	0.60	1.95	7	2
1:B:90:SER:HA	1:E:52:VAL:HB	0.60	1.74	4	1
1:F:55:ASN:HA	1:F:131:ILE:O	0.59	1.96	6	1
1:F:104:LEU:HA	1:F:110:ALA:HA	0.59	1.72	4	3
1:A:91:SER:HB2	1:A:95:SER:HB2	0.59	1.73	10	2
1:A:5:VAL:HG21	1:B:17:VAL:CG1	0.59	2.27	3	1
1:D:16:VAL:CG1	1:E:144:THR:O	0.59	2.50	3	2
1:E:42:LEU:CB	1:E:139:ALA:HB2	0.59	2.26	6	1
1:D:91:SER:HB2	1:D:95:SER:HB2	0.59	1.72	10	2
1:F:91:SER:HB2	1:F:95:SER:HB2	0.59	1.73	10	2
1:A:16:VAL:HG13	1:B:37:VAL:HG13	0.59	1.73	1	1
1:A:55:ASN:HA	1:A:131:ILE:O	0.59	1.96	6	1
1:E:97:THR:H	1:E:144:THR:HB	0.59	1.58	4	2
1:F:112:THR:HG22	1:F:117:THR:HG21	0.59	1.73	10	1
1:D:5:VAL:HG21	1:E:17:VAL:CG1	0.59	2.27	3	1
1:E:86:LEU:HG	1:E:113:LEU:HD13	0.59	1.75	2	3
1:A:97:THR:H	1:A:144:THR:HB	0.59	1.58	4	2
1:C:91:SER:HB2	1:C:95:SER:HB2	0.59	1.73	10	2
1:B:86:LEU:HG	1:B:113:LEU:HD13	0.59	1.75	2	3
1:C:55:ASN:HA	1:C:131:ILE:O	0.59	1.96	6	1
1:C:85:VAL:HA	1:C:102:GLN:HA	0.59	1.74	7	2
1:E:3:THR:O	1:F:157:GLN:HA	0.59	1.98	4	2
1:C:16:VAL:HG13	1:D:37:VAL:HG13	0.59	1.73	1	1
1:A:3:THR:O	1:B:157:GLN:HA	0.59	1.98	4	2
1:D:97:THR:H	1:D:144:THR:HB	0.59	1.58	4	2
1:B:97:THR:H	1:B:144:THR:HB	0.59	1.58	4	2
1:C:112:THR:HG22	1:C:117:THR:HG21	0.59	1.73	10	1
1:A:78:ILE:HB	1:A:87:ALA:HA	0.59	1.75	6	1
1:D:78:ILE:HB	1:D:87:ALA:HA	0.59	1.75	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:16:VAL:HG13	1:C:37:VAL:HG13	0.58	1.73	1	1
1:C:3:THR:O	1:D:157:GLN:HA	0.58	1.98	4	2
1:B:5:VAL:HG23	1:C:156:VAL:HG23	0.58	1.75	10	5
1:D:85:VAL:HA	1:D:102:GLN:HA	0.58	1.74	7	2
1:F:85:VAL:HA	1:F:102:GLN:HA	0.58	1.74	7	2
1:A:112:THR:HG22	1:A:117:THR:HG21	0.58	1.73	10	1
1:C:77:ALA:O	1:C:87:ALA:HB2	0.58	1.98	1	3
1:A:85:VAL:HA	1:A:102:GLN:HA	0.58	1.74	7	2
1:E:86:LEU:HD21	1:E:152:ALA:HB2	0.58	1.75	9	2
1:C:97:THR:H	1:C:144:THR:HB	0.58	1.58	4	2
1:F:86:LEU:HG	1:F:113:LEU:HD13	0.58	1.75	2	3
1:F:77:ALA:O	1:F:87:ALA:HB2	0.58	1.98	1	3
1:B:77:ALA:O	1:B:87:ALA:HB2	0.58	1.98	1	3
1:B:144:THR:HG23	1:B:145:PRO:HD2	0.58	1.76	2	3
1:C:144:THR:HG23	1:C:145:PRO:HD2	0.58	1.76	2	3
1:D:3:THR:O	1:E:157:GLN:HA	0.58	1.98	4	2
1:B:3:THR:O	1:C:157:GLN:HA	0.58	1.98	4	2
1:A:86:LEU:HD21	1:A:152:ALA:HB2	0.58	1.75	9	2
1:D:112:THR:HG22	1:D:117:THR:HG21	0.58	1.73	10	1
1:E:16:VAL:HG13	1:F:37:VAL:HG13	0.58	1.73	1	1
1:E:78:ILE:HB	1:E:87:ALA:HA	0.58	1.75	6	1
1:E:5:VAL:HG23	1:F:156:VAL:HG23	0.58	1.75	10	5
1:D:86:LEU:HD21	1:D:152:ALA:HB2	0.58	1.75	9	2
1:C:42:LEU:HD23	1:C:99:VAL:HG13	0.58	1.75	2	1
1:D:77:ALA:O	1:D:87:ALA:HB2	0.58	1.98	1	3
1:B:86:LEU:HD21	1:B:152:ALA:HB2	0.58	1.75	9	2
1:D:42:LEU:HD23	1:D:99:VAL:HG13	0.58	1.75	2	1
1:E:77:ALA:O	1:E:87:ALA:HB2	0.58	1.99	1	3
1:C:86:LEU:HG	1:C:113:LEU:HD13	0.58	1.75	2	3
1:A:90:SER:HA	1:D:52:VAL:HB	0.58	1.74	4	2
1:A:42:LEU:HD23	1:A:99:VAL:HG13	0.58	1.75	2	1
1:D:23:VAL:HA	1:D:58:LEU:HG	0.58	1.76	8	3
1:D:144:THR:HG23	1:D:145:PRO:HD2	0.58	1.76	2	3
1:B:78:ILE:HB	1:B:87:ALA:HA	0.58	1.75	6	1
1:F:52:VAL:HG22	1:F:135:ALA:HB3	0.58	1.76	4	3
1:C:111:LEU:HD21	1:C:117:THR:O	0.58	1.99	8	2
1:A:77:ALA:O	1:A:87:ALA:HB2	0.57	1.98	1	3
1:C:73:PHE:HD2	1:C:103:ILE:HD13	0.57	1.59	10	1
1:B:73:PHE:HD2	1:B:103:ILE:HD13	0.57	1.59	10	1
1:F:73:PHE:HD2	1:F:103:ILE:HD13	0.57	1.59	10	1
1:F:42:LEU:HD23	1:F:99:VAL:HG13	0.57	1.75	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:VAL:HA	1:A:58:LEU:HG	0.57	1.76	8	3
1:F:97:THR:H	1:F:144:THR:HB	0.57	1.58	4	2
1:E:52:VAL:HG22	1:E:135:ALA:HB3	0.57	1.76	4	3
1:E:73:PHE:HD2	1:E:103:ILE:HD13	0.57	1.59	10	1
1:E:23:VAL:HA	1:E:58:LEU:HG	0.57	1.76	8	3
1:A:86:LEU:HG	1:A:113:LEU:HD13	0.57	1.75	2	3
1:D:86:LEU:HG	1:D:113:LEU:HD13	0.57	1.75	2	3
1:B:85:VAL:HA	1:B:102:GLN:HA	0.57	1.74	7	2
1:A:111:LEU:HD21	1:A:117:THR:O	0.57	1.99	8	2
1:A:73:PHE:HD2	1:A:103:ILE:HD13	0.57	1.59	10	1
1:E:42:LEU:HD23	1:E:99:VAL:HG13	0.57	1.75	2	1
1:B:42:LEU:HD23	1:B:99:VAL:HG13	0.57	1.75	2	1
1:D:76:THR:O	1:D:86:LEU:HA	0.57	2.00	10	5
1:C:5:VAL:HG23	1:D:156:VAL:HG23	0.57	1.75	10	5
1:A:5:VAL:HG23	1:B:156:VAL:HG23	0.57	1.75	10	5
1:F:111:LEU:HD21	1:F:117:THR:O	0.57	1.99	8	2
1:E:16:VAL:HG11	1:F:144:THR:O	0.57	2.00	5	4
1:E:106:ARG:HG3	1:E:132:PRO:HG2	0.57	1.77	2	4
1:B:52:VAL:HG22	1:B:135:ALA:HB3	0.57	1.77	4	3
1:B:111:LEU:HD21	1:B:117:THR:O	0.57	1.99	8	2
1:A:4:THR:HG21	1:E:127:GLY:HA2	0.57	1.75	8	2
1:B:23:VAL:HA	1:B:58:LEU:HG	0.57	1.76	8	3
1:B:106:ARG:HG3	1:B:132:PRO:HG2	0.57	1.77	2	4
1:A:144:THR:HG23	1:A:145:PRO:HD2	0.57	1.76	2	3
1:D:52:VAL:HG22	1:D:135:ALA:HB3	0.57	1.76	4	3
1:E:13:LYS:HG2	1:F:33:GLN:HA	0.57	1.77	7	1
1:D:73:PHE:HD2	1:D:103:ILE:HD13	0.57	1.59	10	1
1:D:106:ARG:HG3	1:D:132:PRO:HG2	0.57	1.77	2	4
1:E:144:THR:HG23	1:E:145:PRO:HD2	0.57	1.76	2	3
1:E:85:VAL:HA	1:E:102:GLN:HA	0.57	1.74	7	2
1:B:74:LEU:HD11	1:E:57:GLN:HG2	0.57	1.77	7	1
1:A:13:LYS:HG2	1:B:33:GLN:HA	0.57	1.77	7	1
1:E:111:LEU:HD21	1:E:117:THR:O	0.57	1.99	8	2
1:F:23:VAL:HA	1:F:58:LEU:HG	0.56	1.76	8	3
1:A:16:VAL:HG11	1:B:144:THR:O	0.56	2.00	5	4
1:A:76:THR:O	1:A:86:LEU:HA	0.56	2.00	10	5
1:A:106:ARG:HG3	1:A:132:PRO:HG2	0.56	1.77	2	4
1:C:78:ILE:HB	1:C:87:ALA:HA	0.56	1.75	6	1
1:C:23:VAL:HA	1:C:58:LEU:HG	0.56	1.77	8	3
1:C:74:LEU:HD11	1:F:57:GLN:HG2	0.56	1.77	7	1
1:A:88:LEU:HG	1:A:95:SER:HB3	0.56	1.78	4	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:144:THR:HG23	1:F:145:PRO:HD2	0.56	1.76	2	3
1:C:86:LEU:HD21	1:C:152:ALA:HB2	0.56	1.75	9	2
1:D:111:LEU:HD21	1:D:117:THR:O	0.56	1.99	8	2
1:C:16:VAL:HG11	1:D:144:THR:O	0.56	2.00	5	4
1:F:78:ILE:HB	1:F:87:ALA:HA	0.56	1.75	6	1
1:D:13:LYS:HG2	1:E:33:GLN:HA	0.56	1.77	7	1
1:C:86:LEU:HD11	1:C:152:ALA:HB2	0.56	1.78	8	1
1:B:4:THR:HG21	1:F:127:GLY:HA2	0.56	1.75	8	2
1:D:16:VAL:HG11	1:E:144:THR:O	0.56	2.00	5	4
1:B:45:GLU:HA	1:B:140:THR:O	0.56	2.01	8	2
1:D:88:LEU:HG	1:D:95:SER:HB3	0.56	1.78	4	4
1:D:5:VAL:HG23	1:E:156:VAL:HG23	0.56	1.75	10	5
1:F:86:LEU:HD21	1:F:152:ALA:HB2	0.56	1.75	9	2
1:C:74:LEU:HD12	1:F:130:THR:OG1	0.56	2.01	9	2
1:F:86:LEU:HD11	1:F:152:ALA:HB2	0.56	1.78	8	1
1:A:45:GLU:HA	1:A:140:THR:O	0.56	2.01	8	2
1:A:76:THR:HA	1:D:132:PRO:HB3	0.56	1.77	4	4
1:C:52:VAL:HG22	1:C:135:ALA:HB3	0.56	1.76	4	3
1:C:23:VAL:HG12	1:D:36:GLN:HB2	0.56	1.78	2	1
1:E:76:THR:O	1:E:86:LEU:HA	0.56	2.00	10	5
1:B:76:THR:O	1:B:86:LEU:HA	0.56	2.00	10	5
1:C:76:THR:O	1:C:86:LEU:HA	0.56	2.00	10	5
1:F:45:GLU:HA	1:F:140:THR:O	0.56	2.01	8	2
1:D:45:GLU:HA	1:D:140:THR:O	0.56	2.01	8	3
1:F:76:THR:O	1:F:86:LEU:HA	0.56	2.00	10	5
1:A:74:LEU:HD12	1:D:130:THR:OG1	0.56	2.01	9	2
1:B:13:LYS:HG2	1:C:33:GLN:HA	0.56	1.77	7	1
1:C:45:GLU:HA	1:C:140:THR:O	0.56	2.01	8	2
1:A:74:LEU:HD11	1:A:155:LYS:HG2	0.56	1.78	6	1
1:C:74:LEU:HD11	1:C:155:LYS:HG2	0.56	1.78	6	1
1:B:16:VAL:HG11	1:C:144:THR:O	0.56	2.00	5	4
1:D:74:LEU:HD11	1:D:155:LYS:HG2	0.56	1.78	6	1
1:A:74:LEU:HD11	1:D:57:GLN:HG2	0.56	1.77	7	1
1:D:88:LEU:HD22	1:D:96:ALA:O	0.56	2.01	7	1
1:E:88:LEU:HG	1:E:95:SER:HB3	0.55	1.78	4	4
1:F:74:LEU:HD11	1:F:155:LYS:HG2	0.55	1.78	6	1
1:B:74:LEU:HD12	1:E:130:THR:OG1	0.55	2.01	9	2
1:F:88:LEU:HD22	1:F:96:ALA:O	0.55	2.01	7	1
1:C:56:ILE:HG23	1:C:56:ILE:O	0.55	2.02	4	3
1:C:13:LYS:HG2	1:D:33:GLN:HA	0.55	1.77	7	1
1:B:88:LEU:HD22	1:B:96:ALA:O	0.55	2.01	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:106:ARG:HG3	1:C:132:PRO:HG2	0.55	1.77	2	4
1:E:45:GLU:HA	1:E:140:THR:O	0.55	2.01	8	3
1:F:56:ILE:O	1:F:56:ILE:HG23	0.55	2.02	4	3
1:C:88:LEU:HG	1:C:95:SER:HB3	0.55	1.78	4	4
1:B:88:LEU:HG	1:B:95:SER:HB3	0.55	1.78	4	4
1:B:76:THR:HA	1:E:132:PRO:HB3	0.55	1.77	4	4
1:F:104:LEU:HD13	1:F:134:GLN:NE2	0.55	2.17	1	1
1:B:56:ILE:O	1:B:56:ILE:HG23	0.55	2.02	4	1
1:E:88:LEU:HD22	1:E:96:ALA:O	0.55	2.01	7	1
1:A:52:VAL:HG22	1:A:135:ALA:HB3	0.55	1.76	4	3
1:D:86:LEU:HD11	1:D:152:ALA:HB2	0.55	1.78	8	1
1:A:9:THR:HG22	1:B:153:THR:CG2	0.55	2.30	2	1
1:D:4:THR:HG23	1:E:157:GLN:HG3	0.55	1.79	8	2
1:E:56:ILE:O	1:E:56:ILE:HG23	0.55	2.02	4	3
1:D:84:ASN:HA	1:D:113:LEU:HD13	0.55	1.79	9	1
1:F:106:ARG:HG3	1:F:132:PRO:HG2	0.55	1.77	2	4
1:F:88:LEU:HG	1:F:95:SER:HB3	0.55	1.78	4	4
1:C:104:LEU:HD13	1:C:134:GLN:NE2	0.55	2.17	1	1
1:B:104:LEU:HD13	1:B:134:GLN:NE2	0.55	2.17	1	1
1:B:74:LEU:HD11	1:B:155:LYS:HG2	0.55	1.78	6	1
1:A:84:ASN:HA	1:A:113:LEU:HD13	0.55	1.79	9	1
1:A:86:LEU:HD11	1:A:152:ALA:HB2	0.55	1.78	8	1
1:B:4:THR:HG23	1:C:157:GLN:HG3	0.55	1.79	8	2
1:A:104:LEU:HD13	1:A:134:GLN:NE2	0.55	2.17	1	1
1:E:74:LEU:HD11	1:E:155:LYS:HG2	0.55	1.79	6	1
1:B:84:ASN:HA	1:B:113:LEU:HD13	0.55	1.79	9	1
1:B:9:THR:HG22	1:C:153:THR:CG2	0.55	2.31	2	1
1:E:23:VAL:HG12	1:F:36:GLN:HB2	0.55	1.78	2	1
1:E:104:LEU:HD13	1:E:134:GLN:NE2	0.54	2.17	1	1
1:E:84:ASN:HA	1:E:113:LEU:HD13	0.54	1.79	9	1
1:A:88:LEU:HD22	1:A:96:ALA:O	0.54	2.01	7	1
1:C:88:LEU:HD22	1:C:96:ALA:O	0.54	2.01	7	1
1:E:42:LEU:HD23	1:E:139:ALA:HB2	0.54	1.79	4	2
1:A:4:THR:HG23	1:B:157:GLN:HG3	0.54	1.79	8	2
1:C:76:THR:HA	1:F:132:PRO:HB3	0.54	1.77	4	4
1:D:104:LEU:HD13	1:D:134:GLN:NE2	0.54	2.17	1	1
1:B:23:VAL:HG12	1:C:36:GLN:HB2	0.54	1.78	2	1
1:D:42:LEU:HD23	1:D:139:ALA:HB2	0.54	1.79	4	2
1:E:70:ALA:HB3	1:E:157:GLN:HB3	0.54	1.80	7	2
1:A:56:ILE:HG21	1:A:154:PHE:CZ	0.54	2.38	7	1
1:A:23:VAL:HG12	1:B:36:GLN:HB2	0.54	1.78	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:78:ILE:CG2	1:C:85:VAL:HB	0.54	2.33	3	2
1:C:4:THR:HG23	1:D:157:GLN:HG3	0.54	1.79	8	2
1:D:56:ILE:HG21	1:D:154:PHE:CZ	0.54	2.38	7	1
1:D:23:VAL:HG12	1:E:36:GLN:HB2	0.54	1.78	2	1
1:E:4:THR:HG23	1:F:157:GLN:HG3	0.54	1.79	8	2
1:D:73:PHE:CD2	1:D:103:ILE:HD13	0.54	2.38	10	1
1:D:70:ALA:HB3	1:D:157:GLN:HB3	0.54	1.80	7	3
1:C:56:ILE:HG21	1:C:154:PHE:CZ	0.54	2.38	7	1
1:F:56:ILE:HG21	1:F:154:PHE:CZ	0.54	2.38	7	1
1:E:131:ILE:HD11	1:E:156:VAL:HG12	0.54	1.80	10	2
1:F:78:ILE:CG2	1:F:85:VAL:HB	0.54	2.33	3	2
1:A:113:LEU:N	1:A:113:LEU:HD12	0.54	2.18	7	1
1:B:86:LEU:HD11	1:B:152:ALA:HB2	0.54	1.78	8	1
1:D:59:ASN:HA	1:D:128:THR:HA	0.54	1.80	8	3
1:A:73:PHE:CD2	1:A:103:ILE:HD13	0.54	2.38	10	1
1:F:42:LEU:HD23	1:F:139:ALA:HB2	0.54	1.79	4	2
1:B:80:ALA:HB1	1:E:105:ASP:O	0.54	2.03	1	1
1:B:43:ALA:HA	1:B:142:ALA:HA	0.54	1.80	6	2
1:B:113:LEU:HD12	1:B:113:LEU:N	0.54	2.18	7	1
1:B:78:ILE:CG2	1:B:85:VAL:HB	0.54	2.33	3	2
1:E:78:ILE:CG2	1:E:85:VAL:HB	0.54	2.33	3	2
1:B:42:LEU:HD23	1:B:139:ALA:HB2	0.54	1.79	4	2
1:B:70:ALA:HB3	1:B:157:GLN:HB3	0.54	1.80	7	3
1:D:43:ALA:HA	1:D:142:ALA:HA	0.54	1.80	6	1
1:F:113:LEU:HD12	1:F:113:LEU:N	0.54	2.18	7	1
1:C:59:ASN:HA	1:C:128:THR:HA	0.54	1.80	8	3
1:E:86:LEU:HD11	1:E:152:ALA:HB2	0.54	1.78	8	1
1:D:78:ILE:CG2	1:D:85:VAL:HB	0.54	2.33	3	2
1:A:42:LEU:HD23	1:A:139:ALA:HB2	0.54	1.79	4	2
1:C:84:ASN:HA	1:C:113:LEU:HD13	0.54	1.79	9	1
1:D:56:ILE:O	1:D:56:ILE:HG23	0.54	2.02	4	1
1:C:42:LEU:HD23	1:C:139:ALA:HB2	0.53	1.79	4	2
1:A:56:ILE:O	1:A:56:ILE:HG23	0.53	2.02	4	4
1:A:80:ALA:HB1	1:D:105:ASP:O	0.53	2.03	1	1
1:A:70:ALA:HB3	1:A:157:GLN:HB3	0.53	1.80	7	3
1:F:84:ASN:HA	1:F:113:LEU:HD13	0.53	1.79	9	1
1:D:113:LEU:N	1:D:113:LEU:HD12	0.53	2.18	7	1
1:D:131:ILE:HD11	1:D:156:VAL:HG12	0.53	1.80	10	2
1:E:59:ASN:HA	1:E:128:THR:HA	0.53	1.80	8	3
1:E:20:ALA:HB1	1:E:124:LEU:CD2	0.53	2.34	3	1
1:B:90:SER:HA	1:E:52:VAL:CG1	0.53	2.33	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:42:LEU:HB3	1:E:143:ALA:HB2	0.53	1.80	4	1
1:B:72:ALA:HB3	1:B:155:LYS:CB	0.53	2.33	7	1
1:E:73:PHE:CD2	1:E:103:ILE:HD13	0.53	2.38	10	1
1:D:9:THR:HG22	1:E:153:THR:CG2	0.53	2.30	2	1
1:B:11:HIS:HA	1:C:151:ASP:OD1	0.53	2.03	2	1
1:C:80:ALA:HB1	1:F:105:ASP:O	0.53	2.03	1	1
1:C:90:SER:HA	1:F:52:VAL:CG1	0.53	2.33	6	1
1:A:82:HIS:O	1:A:84:ASN:N	0.53	2.42	6	1
1:B:82:HIS:O	1:B:84:ASN:N	0.53	2.42	6	1
1:F:72:ALA:HB3	1:F:155:LYS:CB	0.53	2.33	7	1
1:D:82:HIS:O	1:D:84:ASN:N	0.53	2.42	6	1
1:D:72:ALA:HB3	1:D:155:LYS:CB	0.53	2.33	7	1
1:E:72:ALA:HB3	1:E:155:LYS:CB	0.53	2.33	7	1
1:A:72:ALA:HB3	1:A:155:LYS:CB	0.53	2.33	7	1
1:B:56:ILE:HG21	1:B:154:PHE:CZ	0.53	2.38	7	1
1:E:56:ILE:HG21	1:E:154:PHE:CZ	0.53	2.38	7	1
1:C:73:PHE:CD2	1:C:103:ILE:HD13	0.53	2.38	10	1
1:B:73:PHE:CD2	1:B:103:ILE:HD13	0.53	2.38	10	1
1:F:73:PHE:CD2	1:F:103:ILE:HD13	0.53	2.38	10	1
1:F:69:ALA:HB3	1:F:122:THR:O	0.53	2.04	2	1
1:D:20:ALA:HB1	1:D:124:LEU:CD2	0.53	2.34	3	1
1:A:20:ALA:HB1	1:A:124:LEU:CD2	0.53	2.34	3	1
1:D:102:GLN:HB2	1:D:138:PHE:CD1	0.53	2.39	5	1
1:A:155:LYS:NZ	1:D:128:THR:HG21	0.53	2.19	7	1
1:B:20:ALA:HB1	1:B:124:LEU:CD2	0.53	2.34	3	1
1:F:70:ALA:HB3	1:F:157:GLN:HB3	0.53	1.80	7	3
1:C:72:ALA:HB3	1:C:155:LYS:CB	0.53	2.33	7	1
1:C:113:LEU:N	1:C:113:LEU:HD12	0.53	2.18	7	1
1:A:78:ILE:CG2	1:A:85:VAL:HB	0.53	2.33	3	2
1:B:102:GLN:HB2	1:B:138:PHE:CD1	0.53	2.39	5	1
1:E:102:GLN:HB2	1:E:138:PHE:CD1	0.53	2.39	5	1
1:E:82:HIS:O	1:E:84:ASN:N	0.53	2.42	6	1
1:D:42:LEU:HB3	1:D:143:ALA:HB2	0.53	1.80	4	1
1:B:19:ALA:O	1:B:65:VAL:HG21	0.53	2.04	10	1
1:B:69:ALA:HB3	1:B:122:THR:O	0.53	2.04	2	1
1:B:116:ALA:HB2	1:E:129:ASN:HA	0.53	1.80	5	1
1:E:43:ALA:HA	1:E:142:ALA:HA	0.53	1.80	6	1
1:C:155:LYS:NZ	1:F:128:THR:HG21	0.53	2.19	7	1
1:E:19:ALA:O	1:E:65:VAL:HG21	0.53	2.04	10	1
1:C:69:ALA:HB3	1:C:122:THR:O	0.53	2.04	2	1
1:A:11:HIS:HA	1:B:151:ASP:OD1	0.53	2.03	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:116:ALA:HB2	1:F:129:ASN:HA	0.53	1.80	5	1
1:F:102:GLN:HB2	1:F:138:PHE:CD1	0.53	2.39	5	1
1:F:43:ALA:HA	1:F:142:ALA:HA	0.53	1.80	6	2
1:C:43:ALA:HA	1:C:142:ALA:HA	0.53	1.80	6	2
1:C:70:ALA:HB3	1:C:157:GLN:HB3	0.53	1.80	7	2
1:C:42:LEU:HB3	1:C:143:ALA:HB2	0.53	1.80	4	1
1:B:59:ASN:HA	1:B:128:THR:HA	0.53	1.80	8	3
1:E:11:HIS:HA	1:F:151:ASP:OD1	0.53	2.03	2	1
1:C:19:ALA:HA	1:D:38:ARG:HG2	0.52	1.80	7	1
1:D:19:ALA:HA	1:E:38:ARG:HG2	0.52	1.80	7	1
1:E:113:LEU:N	1:E:113:LEU:HD12	0.52	2.18	7	1
1:A:102:GLN:HB2	1:A:138:PHE:CD1	0.52	2.39	5	1
1:A:42:LEU:HB3	1:A:143:ALA:HB2	0.52	1.80	4	1
1:A:131:ILE:HD11	1:A:156:VAL:HG12	0.52	1.80	10	2
1:C:9:THR:HG22	1:D:153:THR:CG2	0.52	2.30	2	1
1:E:69:ALA:HB3	1:E:122:THR:O	0.52	2.04	2	1
1:D:70:ALA:HB1	1:D:118:PHE:HB3	0.52	1.81	3	1
1:A:85:VAL:HB	1:A:100:GLY:HA3	0.52	1.82	5	1
1:C:102:GLN:HB2	1:C:138:PHE:CD1	0.52	2.39	5	1
1:A:90:SER:HA	1:D:52:VAL:CG1	0.52	2.33	6	1
1:A:43:ALA:HA	1:A:142:ALA:HA	0.52	1.80	6	1
1:B:155:LYS:NZ	1:E:128:THR:HG21	0.52	2.19	7	1
1:F:131:ILE:HD11	1:F:156:VAL:HG12	0.52	1.80	10	1
1:C:11:HIS:HA	1:D:151:ASP:OD1	0.52	2.03	2	1
1:D:11:HIS:HA	1:E:151:ASP:OD1	0.52	2.04	2	1
1:C:70:ALA:HB1	1:C:118:PHE:HB3	0.52	1.81	3	1
1:B:19:ALA:HA	1:C:38:ARG:HG2	0.52	1.80	7	1
1:E:71:VAL:CG1	1:E:131:ILE:HG21	0.52	2.35	1	1
1:A:78:ILE:O	1:D:134:GLN:HG2	0.52	2.05	5	1
1:A:70:ALA:HB1	1:A:118:PHE:HB3	0.52	1.81	3	1
1:D:56:ILE:HG23	1:D:56:ILE:O	0.52	2.05	3	4
1:F:82:HIS:O	1:F:84:ASN:N	0.52	2.42	6	1
1:C:6:ASN:HA	1:D:155:LYS:HE2	0.52	1.81	9	1
1:B:42:LEU:HB3	1:B:143:ALA:HB2	0.52	1.80	4	1
1:A:59:ASN:HA	1:A:128:THR:HA	0.52	1.80	8	3
1:A:19:ALA:O	1:A:65:VAL:HG21	0.52	2.04	10	1
1:E:9:THR:HG22	1:F:153:THR:CG2	0.52	2.30	2	1
1:A:69:ALA:HB3	1:A:122:THR:O	0.52	2.04	2	1
1:E:19:ALA:HA	1:F:38:ARG:HG2	0.52	1.80	7	1
1:A:19:ALA:HA	1:B:38:ARG:HG2	0.52	1.81	7	1
1:C:19:ALA:O	1:C:65:VAL:HG21	0.52	2.04	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:19:ALA:O	1:F:65:VAL:HG21	0.52	2.04	10	1
1:D:69:ALA:HB3	1:D:122:THR:O	0.52	2.04	2	1
1:C:20:ALA:HB1	1:C:124:LEU:CD2	0.52	2.34	3	1
1:B:71:VAL:CG1	1:B:131:ILE:HG21	0.52	2.35	1	1
1:A:116:ALA:HB2	1:D:129:ASN:HA	0.52	1.80	5	1
1:B:78:ILE:O	1:E:134:GLN:HG2	0.52	2.05	5	1
1:C:82:HIS:O	1:C:84:ASN:N	0.52	2.42	6	1
1:A:6:ASN:HA	1:B:155:LYS:HE2	0.52	1.81	9	1
1:B:131:ILE:HD11	1:B:156:VAL:HG12	0.52	1.80	10	2
1:D:39:THR:HA	1:D:143:ALA:HB3	0.52	1.82	3	1
1:C:131:ILE:HD11	1:C:156:VAL:HG12	0.52	1.80	10	1
1:D:19:ALA:O	1:D:65:VAL:HG21	0.52	2.04	10	1
1:F:20:ALA:HB1	1:F:124:LEU:CD2	0.52	2.34	3	1
1:C:101:VAL:HG22	1:C:137:TYR:CE1	0.52	2.41	5	1
1:F:42:LEU:HB3	1:F:143:ALA:HB2	0.52	1.80	4	1
1:F:71:VAL:CG1	1:F:131:ILE:HG21	0.51	2.35	1	1
1:C:71:VAL:CG1	1:C:131:ILE:HG21	0.51	2.35	1	1
1:F:59:ASN:HA	1:F:128:THR:HA	0.51	1.80	8	3
1:E:85:VAL:HB	1:E:100:GLY:HA3	0.51	1.82	5	1
1:D:101:VAL:HG22	1:D:137:TYR:CE1	0.51	2.41	5	1
1:F:70:ALA:HB1	1:F:118:PHE:HB3	0.51	1.81	3	1
1:B:88:LEU:HB3	1:B:148:ALA:HA	0.51	1.83	5	1
1:B:83:THR:HG21	1:B:114:ASP:OD1	0.51	2.05	8	1
1:A:71:VAL:CG1	1:A:131:ILE:HG21	0.51	2.35	1	1
1:A:101:VAL:HG22	1:A:137:TYR:CE1	0.51	2.40	5	1
1:C:78:ILE:O	1:F:134:GLN:HG2	0.51	2.05	5	1
1:C:85:VAL:HB	1:C:100:GLY:HA3	0.51	1.82	5	1
1:C:83:THR:HG21	1:C:114:ASP:OD1	0.51	2.05	8	1
1:C:86:LEU:HD23	1:C:87:ALA:N	0.51	2.21	10	1
1:E:39:THR:HA	1:E:143:ALA:HB3	0.51	1.81	3	1
1:B:56:ILE:HG23	1:B:56:ILE:O	0.51	2.05	3	4
1:F:101:VAL:HG22	1:F:137:TYR:CE1	0.51	2.41	5	1
1:F:24:ASP:O	1:F:28:VAL:HG23	0.51	2.06	6	3
1:A:24:ASP:O	1:A:28:VAL:HG23	0.51	2.06	6	3
1:F:39:THR:HA	1:F:143:ALA:HB3	0.51	1.82	3	1
1:D:48:THR:HA	1:D:137:TYR:O	0.51	2.06	5	1
1:B:48:THR:HA	1:B:137:TYR:O	0.51	2.06	5	1
1:D:6:ASN:HA	1:E:155:LYS:HE2	0.51	1.82	9	1
1:F:83:THR:HG21	1:F:114:ASP:OD1	0.51	2.05	8	1
1:C:56:ILE:O	1:C:56:ILE:HG23	0.51	2.05	3	2
1:D:71:VAL:CG1	1:D:131:ILE:HG21	0.51	2.35	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:VAL:HG23	1:C:156:VAL:HG22	0.51	1.83	1	1
1:E:101:VAL:HG22	1:E:137:TYR:CE1	0.51	2.41	5	1
1:F:112:THR:HB	1:F:117:THR:HG21	0.51	1.82	9	1
1:E:15:GLU:HB3	1:F:36:GLN:HG3	0.51	1.83	8	1
1:C:124:LEU:HG	1:C:129:ASN:ND2	0.51	2.21	5	1
1:A:48:THR:HA	1:A:137:TYR:O	0.51	2.06	5	1
1:B:85:VAL:HB	1:B:100:GLY:HA3	0.51	1.82	5	1
1:F:85:VAL:HB	1:F:100:GLY:HA3	0.51	1.82	5	1
1:E:88:LEU:HB3	1:E:148:ALA:HA	0.51	1.83	5	1
1:E:6:ASN:HA	1:F:155:LYS:HE2	0.51	1.81	9	1
1:D:83:THR:HG21	1:D:114:ASP:OD1	0.51	2.05	8	1
1:E:83:THR:HG21	1:E:114:ASP:OD1	0.51	2.05	8	1
1:C:144:THR:HG22	1:C:145:PRO:CD	0.51	2.36	2	1
1:E:70:ALA:HB1	1:E:118:PHE:HB3	0.51	1.81	3	1
1:B:90:SER:O	1:E:52:VAL:HG22	0.51	2.06	5	1
1:D:24:ASP:O	1:D:28:VAL:HG23	0.51	2.06	6	3
1:B:6:ASN:HA	1:C:155:LYS:HE2	0.51	1.82	9	1
1:A:112:THR:HB	1:A:117:THR:HG21	0.51	1.82	9	1
1:B:112:THR:HB	1:B:117:THR:HG21	0.51	1.82	9	1
1:A:83:THR:HG21	1:A:114:ASP:OD1	0.51	2.05	8	1
1:D:91:SER:HA	1:F:25:ALA:HB2	0.51	1.83	8	1
1:E:86:LEU:HD23	1:E:87:ALA:N	0.51	2.21	10	1
1:E:91:SER:O	1:E:95:SER:HB2	0.50	2.06	4	3
1:E:124:LEU:HG	1:E:129:ASN:ND2	0.50	2.21	5	1
1:C:22:ALA:HA	1:D:36:GLN:HB2	0.50	1.84	5	1
1:D:85:VAL:HB	1:D:100:GLY:HA3	0.50	1.82	5	1
1:C:90:SER:O	1:F:52:VAL:HG22	0.50	2.06	5	1
1:B:114:ASP:O	1:E:130:THR:O	0.50	2.28	6	1
1:C:45:GLU:N	1:C:141:GLY:HA2	0.50	2.22	6	1
1:A:91:SER:HA	1:C:25:ALA:HB2	0.50	1.83	8	1
1:D:86:LEU:HD23	1:D:87:ALA:N	0.50	2.21	10	1
1:D:144:THR:HG22	1:D:145:PRO:CD	0.50	2.36	2	1
1:B:62:ASP:OD2	1:B:65:VAL:HG23	0.50	2.07	3	1
1:B:39:THR:HA	1:B:143:ALA:HB3	0.50	1.81	3	1
1:E:45:GLU:N	1:E:141:GLY:HA2	0.50	2.22	6	1
1:C:112:THR:HB	1:C:117:THR:HG21	0.50	1.82	9	1
1:B:86:LEU:HD23	1:B:87:ALA:N	0.50	2.21	10	1
1:A:114:ASP:O	1:D:130:THR:O	0.50	2.28	6	1
1:C:114:ASP:O	1:F:130:THR:O	0.50	2.28	6	1
1:F:69:ALA:CB	1:F:124:LEU:HD13	0.50	2.36	8	1
1:A:86:LEU:HD23	1:A:87:ALA:N	0.50	2.21	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:124:LEU:HG	1:D:129:ASN:ND2	0.50	2.21	5	1
1:B:101:VAL:HG22	1:B:137:TYR:CE1	0.50	2.41	5	1
1:E:48:THR:HA	1:E:137:TYR:O	0.50	2.06	5	1
1:B:15:GLU:HB3	1:C:36:GLN:HG3	0.50	1.83	8	2
1:F:86:LEU:HD23	1:F:87:ALA:N	0.50	2.21	10	1
1:C:91:SER:O	1:C:95:SER:HB2	0.50	2.06	4	3
1:B:24:ASP:O	1:B:28:VAL:HG23	0.50	2.06	6	3
1:D:45:GLU:N	1:D:141:GLY:HA2	0.50	2.22	6	1
1:D:112:THR:HB	1:D:117:THR:HG21	0.50	1.82	9	1
1:B:15:GLU:HG2	1:C:146:GLY:O	0.50	2.07	3	1
1:C:39:THR:HA	1:C:143:ALA:HB3	0.50	1.81	3	1
1:A:91:SER:O	1:A:95:SER:HB2	0.50	2.07	4	3
1:A:124:LEU:HG	1:A:129:ASN:ND2	0.50	2.21	5	1
1:F:48:THR:HA	1:F:137:TYR:O	0.50	2.06	5	1
1:E:112:THR:HB	1:E:117:THR:HG21	0.50	1.82	9	1
1:A:39:THR:HA	1:A:143:ALA:HB3	0.50	1.81	3	1
1:D:62:ASP:OD2	1:D:65:VAL:HG23	0.50	2.07	3	1
1:A:5:VAL:HG23	1:B:156:VAL:HG22	0.50	1.83	1	1
1:C:88:LEU:HB3	1:C:148:ALA:HA	0.50	1.83	5	1
1:A:45:GLU:N	1:A:141:GLY:HA2	0.50	2.22	6	1
1:E:62:ASP:OD2	1:E:65:VAL:HG23	0.50	2.07	3	1
1:E:5:VAL:HG23	1:F:156:VAL:HG22	0.50	1.83	1	1
1:A:22:ALA:HA	1:B:36:GLN:HB2	0.50	1.83	5	1
1:A:15:GLU:HB3	1:B:36:GLN:HG3	0.50	1.83	8	1
1:B:91:SER:HA	1:D:25:ALA:HB2	0.50	1.83	8	1
1:B:91:SER:O	1:B:95:SER:HB2	0.50	2.07	4	2
1:B:124:LEU:HG	1:B:129:ASN:ND2	0.50	2.21	5	1
1:F:124:LEU:HG	1:F:129:ASN:ND2	0.50	2.21	5	1
1:D:22:ALA:HA	1:E:36:GLN:HB2	0.50	1.83	5	1
1:C:24:ASP:O	1:C:28:VAL:HG23	0.49	2.06	6	3
1:C:91:SER:HA	1:E:25:ALA:HB2	0.49	1.83	8	1
1:A:9:THR:CG2	1:B:153:THR:HG23	0.49	2.31	3	1
1:F:91:SER:O	1:F:95:SER:HB2	0.49	2.06	4	3
1:C:48:THR:HA	1:C:137:TYR:O	0.49	2.06	5	1
1:E:22:ALA:HA	1:F:36:GLN:HB2	0.49	1.83	5	1
1:D:88:LEU:HB3	1:D:148:ALA:HA	0.49	1.83	5	1
1:A:90:SER:O	1:D:52:VAL:HG22	0.49	2.06	5	1
1:E:24:ASP:O	1:E:28:VAL:HG23	0.49	2.06	6	3
1:F:39:THR:HA	1:F:42:LEU:HD12	0.49	1.84	6	1
1:A:17:VAL:HG21	1:A:21:CYS:O	0.49	2.07	7	1
1:B:4:THR:HG21	1:F:127:GLY:CA	0.49	2.37	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:69:ALA:HA	1:F:157:GLN:O	0.49	2.08	10	1
1:F:144:THR:HG22	1:F:145:PRO:CD	0.49	2.36	2	1
1:B:144:THR:HG22	1:B:145:PRO:CD	0.49	2.36	2	1
1:D:42:LEU:HD21	1:D:137:TYR:HB3	0.49	1.83	2	1
1:E:42:LEU:HD21	1:E:137:TYR:HB3	0.49	1.83	2	1
1:B:42:LEU:HD21	1:B:137:TYR:HB3	0.49	1.83	2	1
1:C:9:THR:CG2	1:D:153:THR:HG23	0.49	2.31	3	1
1:E:15:GLU:HG2	1:F:146:GLY:O	0.49	2.07	3	1
1:B:70:ALA:HB1	1:B:118:PHE:HB3	0.49	1.81	3	1
1:C:39:THR:HA	1:C:42:LEU:HD12	0.49	1.85	6	1
1:C:19:ALA:O	1:C:62:ASP:HB2	0.49	2.08	8	1
1:D:69:ALA:HA	1:D:157:GLN:O	0.49	2.08	10	1
1:A:69:ALA:HA	1:A:157:GLN:O	0.49	2.08	10	1
1:F:21:CYS:HB2	1:F:158:TYR:CE1	0.49	2.43	2	3
1:E:21:CYS:HB2	1:E:158:TYR:CE1	0.49	2.43	2	3
1:E:5:VAL:HG23	1:F:156:VAL:CG2	0.49	2.38	1	1
1:D:57:GLN:HA	1:D:130:THR:HG22	0.49	1.84	6	1
1:F:45:GLU:N	1:F:141:GLY:HA2	0.49	2.22	6	1
1:D:73:PHE:HB2	1:D:111:LEU:HD11	0.49	1.84	7	1
1:B:69:ALA:HA	1:B:157:GLN:O	0.49	2.08	10	1
1:D:9:THR:CG2	1:E:153:THR:HG23	0.49	2.31	3	1
1:A:62:ASP:OD2	1:A:65:VAL:HG23	0.49	2.07	3	1
1:A:5:VAL:HG23	1:B:156:VAL:CG2	0.49	2.38	1	1
1:F:88:LEU:HB3	1:F:148:ALA:HA	0.49	1.83	5	1
1:B:45:GLU:N	1:B:141:GLY:HA2	0.49	2.22	6	1
1:D:72:ALA:HB1	1:D:116:ALA:HA	0.49	1.85	6	1
1:C:71:VAL:O	1:C:118:PHE:HA	0.49	2.08	4	1
1:E:17:VAL:HG21	1:E:21:CYS:O	0.49	2.07	7	1
1:C:17:VAL:HG21	1:C:21:CYS:O	0.49	2.07	7	1
1:F:19:ALA:O	1:F:62:ASP:HB2	0.49	2.08	8	1
1:F:42:LEU:HD21	1:F:137:TYR:HB3	0.49	1.83	2	1
1:C:62:ASP:OD2	1:C:65:VAL:HG23	0.49	2.07	3	1
1:C:5:VAL:HG23	1:D:156:VAL:CG2	0.49	2.38	1	1
1:F:71:VAL:O	1:F:118:PHE:HA	0.49	2.08	4	1
1:E:71:VAL:O	1:E:118:PHE:HA	0.49	2.08	4	1
1:D:19:ALA:O	1:D:62:ASP:HB2	0.49	2.08	8	1
1:C:69:ALA:HA	1:C:157:GLN:O	0.49	2.08	10	1
1:C:15:GLU:HG2	1:D:146:GLY:O	0.49	2.07	3	1
1:B:21:CYS:HB2	1:B:158:TYR:CE1	0.49	2.43	2	3
1:F:62:ASP:OD2	1:F:65:VAL:HG23	0.49	2.07	3	1
1:B:22:ALA:HA	1:C:36:GLN:HB2	0.49	1.83	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:72:ALA:HB1	1:B:116:ALA:HA	0.49	1.84	6	1
1:C:57:GLN:HA	1:C:130:THR:HG22	0.49	1.84	6	1
1:D:71:VAL:O	1:D:118:PHE:HA	0.49	2.08	4	1
1:A:73:PHE:HB2	1:A:111:LEU:HD11	0.49	1.84	7	1
1:E:69:ALA:CB	1:E:124:LEU:HD13	0.49	2.36	8	1
1:B:56:ILE:HG21	1:B:131:ILE:HD12	0.49	1.85	10	1
1:E:56:ILE:HG21	1:E:131:ILE:HD12	0.49	1.85	10	1
1:E:69:ALA:HA	1:E:157:GLN:O	0.49	2.08	10	1
1:C:21:CYS:HB2	1:C:158:TYR:CE1	0.49	2.43	2	3
1:C:5:VAL:HG23	1:D:156:VAL:HG22	0.49	1.83	1	1
1:B:56:ILE:O	1:B:58:LEU:HD12	0.49	2.08	5	1
1:E:56:ILE:O	1:E:58:LEU:HD12	0.49	2.08	5	1
1:A:39:THR:HA	1:A:42:LEU:HD12	0.49	1.85	6	1
1:D:39:THR:HA	1:D:42:LEU:HD12	0.49	1.85	6	1
1:D:56:ILE:O	1:D:130:THR:HA	0.49	2.08	6	1
1:D:69:ALA:CB	1:D:124:LEU:HD13	0.49	2.36	8	1
1:D:15:GLU:HB3	1:E:36:GLN:HG3	0.49	1.83	8	1
1:A:144:THR:HG22	1:A:145:PRO:CD	0.49	2.36	2	1
1:D:91:SER:O	1:D:95:SER:HB2	0.49	2.07	4	3
1:B:5:VAL:HG23	1:C:156:VAL:CG2	0.49	2.38	1	1
1:B:69:ALA:HB3	1:B:122:THR:HB	0.49	1.85	1	2
1:D:5:VAL:HG23	1:E:156:VAL:CG2	0.49	2.38	1	1
1:A:88:LEU:HB3	1:A:148:ALA:HA	0.49	1.83	5	1
1:A:56:ILE:O	1:A:130:THR:HA	0.49	2.08	6	1
1:A:19:ALA:O	1:A:62:ASP:HB2	0.49	2.08	8	1
1:E:19:ALA:O	1:E:62:ASP:HB2	0.49	2.08	8	1
1:A:79:ASP:O	1:A:81:GLY:N	0.49	2.46	10	1
1:C:79:ASP:O	1:C:81:GLY:N	0.49	2.46	10	1
1:E:144:THR:HG22	1:E:145:PRO:CD	0.49	2.36	2	1
1:A:42:LEU:HD21	1:A:137:TYR:HB3	0.49	1.83	2	1
1:A:21:CYS:HB2	1:A:158:TYR:CE1	0.48	2.43	2	2
1:C:42:LEU:HB2	1:C:139:ALA:HB2	0.48	1.84	6	1
1:A:56:ILE:HG23	1:A:56:ILE:O	0.48	2.08	8	1
1:A:15:GLU:HG2	1:B:146:GLY:O	0.48	2.07	3	1
1:A:20:ALA:O	1:A:124:LEU:HD21	0.48	2.08	3	2
1:B:20:ALA:O	1:B:124:LEU:HD21	0.48	2.08	3	2
1:A:103:ILE:HD12	1:A:111:LEU:HB3	0.48	1.86	3	1
1:A:56:ILE:O	1:A:58:LEU:HD12	0.48	2.08	5	1
1:F:57:GLN:HA	1:F:130:THR:HG22	0.48	1.84	6	1
1:C:15:GLU:HB3	1:D:36:GLN:HG3	0.48	1.83	8	2
1:F:56:ILE:HG21	1:F:131:ILE:HD12	0.48	1.85	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:79:ASP:O	1:F:81:GLY:N	0.48	2.46	10	1
1:B:79:ASP:O	1:B:81:GLY:N	0.48	2.46	10	1
1:D:15:GLU:HG2	1:E:146:GLY:O	0.48	2.07	3	1
1:D:5:VAL:HG23	1:E:156:VAL:HG22	0.48	1.83	1	1
1:E:56:ILE:HG23	1:E:56:ILE:O	0.48	2.08	8	2
1:D:56:ILE:O	1:D:58:LEU:HD12	0.48	2.08	5	1
1:C:56:ILE:O	1:C:58:LEU:HD12	0.48	2.08	5	1
1:D:42:LEU:HB2	1:D:139:ALA:HB2	0.48	1.84	6	1
1:D:16:VAL:HA	1:E:37:VAL:O	0.48	2.09	6	1
1:C:16:VAL:HA	1:D:37:VAL:O	0.48	2.09	6	1
1:D:17:VAL:HG21	1:D:21:CYS:O	0.48	2.07	7	1
1:D:20:ALA:O	1:D:124:LEU:HD21	0.48	2.08	3	2
1:F:20:ALA:O	1:F:124:LEU:HD21	0.48	2.08	3	2
1:D:103:ILE:HD12	1:D:111:LEU:HB3	0.48	1.86	3	1
1:D:78:ILE:HG23	1:D:79:ASP:N	0.48	2.24	1	2
1:A:16:VAL:HA	1:B:37:VAL:O	0.48	2.09	6	1
1:B:71:VAL:O	1:B:118:PHE:HA	0.48	2.08	4	1
1:A:4:THR:HG21	1:E:127:GLY:CA	0.48	2.37	8	1
1:D:79:ASP:O	1:D:81:GLY:N	0.48	2.46	10	1
1:D:21:CYS:HB2	1:D:158:TYR:CE1	0.48	2.43	2	3
1:F:56:ILE:O	1:F:58:LEU:HD12	0.48	2.08	5	1
1:B:3:THR:OG1	1:C:158:TYR:HB2	0.48	2.09	5	1
1:B:42:LEU:HB2	1:B:139:ALA:HB2	0.48	1.84	6	1
1:C:56:ILE:O	1:C:130:THR:HA	0.48	2.08	6	1
1:E:144:THR:HB	1:E:145:PRO:CD	0.48	2.39	9	1
1:B:73:PHE:HB2	1:B:111:LEU:HD11	0.48	1.84	7	1
1:C:56:ILE:HG21	1:C:131:ILE:HD12	0.48	1.85	10	1
1:C:20:ALA:O	1:C:124:LEU:HD21	0.48	2.08	3	2
1:A:57:GLN:HA	1:A:130:THR:HG22	0.48	1.84	6	1
1:A:72:ALA:HB1	1:A:116:ALA:HA	0.48	1.85	6	1
1:C:144:THR:HB	1:C:145:PRO:CD	0.48	2.39	9	1
1:F:73:PHE:HB2	1:F:111:LEU:HD11	0.48	1.84	7	1
1:C:42:LEU:HD21	1:C:137:TYR:HB3	0.48	1.83	2	1
1:C:103:ILE:HD12	1:C:111:LEU:HB3	0.48	1.86	3	1
1:E:78:ILE:HG23	1:E:79:ASP:N	0.48	2.24	1	2
1:A:69:ALA:HB3	1:A:122:THR:HB	0.48	1.85	1	2
1:A:42:LEU:HB2	1:A:139:ALA:HB2	0.48	1.84	6	1
1:E:39:THR:HA	1:E:42:LEU:HD12	0.48	1.84	6	1
1:E:57:GLN:HA	1:E:130:THR:HG22	0.48	1.84	6	1
1:C:72:ALA:HB1	1:C:116:ALA:HA	0.48	1.85	6	1
1:B:57:GLN:HA	1:B:130:THR:HG22	0.48	1.84	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:72:ALA:HB1	1:E:116:ALA:HA	0.48	1.84	6	1
1:F:144:THR:HB	1:F:145:PRO:CD	0.48	2.39	9	1
1:A:71:VAL:O	1:A:118:PHE:HA	0.48	2.08	4	1
1:B:17:VAL:HG21	1:B:21:CYS:O	0.48	2.07	7	1
1:F:17:VAL:HG21	1:F:21:CYS:O	0.48	2.07	7	1
1:C:3:THR:OG1	1:D:158:TYR:HB2	0.48	2.09	5	1
1:D:3:THR:OG1	1:E:158:TYR:HB2	0.48	2.09	5	1
1:B:39:THR:HA	1:B:42:LEU:HD12	0.48	1.84	6	1
1:E:20:ALA:O	1:E:124:LEU:HD21	0.48	2.08	3	2
1:C:12:PHE:HA	1:D:32:VAL:O	0.48	2.09	6	1
1:B:158:TYR:C	1:B:159:GLN:HG3	0.48	2.30	3	1
1:E:158:TYR:C	1:E:159:GLN:HG3	0.48	2.30	3	1
1:B:78:ILE:HG23	1:B:79:ASP:N	0.48	2.24	1	2
1:C:78:ILE:HG23	1:C:79:ASP:N	0.48	2.24	1	2
1:F:42:LEU:HB2	1:F:139:ALA:HB2	0.48	1.84	6	1
1:E:56:ILE:O	1:E:130:THR:HA	0.48	2.08	6	1
1:A:3:THR:HB	1:B:158:TYR:CD2	0.48	2.44	4	1
1:D:34:LEU:HD22	1:D:34:LEU:N	0.48	2.24	7	1
1:A:34:LEU:N	1:A:34:LEU:HD22	0.48	2.24	7	1
1:E:73:PHE:HB2	1:E:111:LEU:HD11	0.48	1.84	7	1
1:F:103:ILE:HD12	1:F:111:LEU:HB3	0.47	1.86	3	1
1:D:20:ALA:O	1:D:61:CYS:HA	0.47	2.09	1	2
1:F:56:ILE:O	1:F:130:THR:HA	0.47	2.08	6	1
1:E:16:VAL:HA	1:F:37:VAL:O	0.47	2.09	6	1
1:B:144:THR:HB	1:B:145:PRO:CD	0.47	2.39	9	1
1:B:19:ALA:O	1:B:62:ASP:HB2	0.47	2.08	8	1
1:B:74:LEU:O	1:B:152:ALA:HA	0.47	2.09	2	3
1:E:42:LEU:HB2	1:E:139:ALA:HB2	0.47	1.84	6	1
1:B:56:ILE:O	1:B:130:THR:HA	0.47	2.08	6	1
1:A:144:THR:HB	1:A:145:PRO:CD	0.47	2.39	9	1
1:B:3:THR:HB	1:C:158:TYR:CD2	0.47	2.45	4	1
1:E:79:ASP:O	1:E:81:GLY:N	0.47	2.46	10	1
1:A:23:VAL:HA	1:A:58:LEU:HA	0.47	1.86	3	1
1:F:56:ILE:HG23	1:F:56:ILE:O	0.47	2.09	1	2
1:A:3:THR:OG1	1:B:158:TYR:HB2	0.47	2.09	5	1
1:F:72:ALA:HB1	1:F:116:ALA:HA	0.47	1.85	6	1
1:C:73:PHE:HB2	1:C:111:LEU:HD11	0.47	1.84	7	1
1:A:74:LEU:O	1:A:152:ALA:HA	0.47	2.09	2	2
1:F:158:TYR:C	1:F:159:GLN:HG3	0.47	2.30	3	1
1:C:158:TYR:C	1:C:159:GLN:HG3	0.47	2.30	3	1
1:A:20:ALA:O	1:A:61:CYS:HA	0.47	2.09	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:3:THR:OG1	1:F:158:TYR:HB2	0.47	2.09	5	1
1:D:144:THR:HB	1:D:145:PRO:CD	0.47	2.39	9	1
1:F:74:LEU:O	1:F:152:ALA:HA	0.47	2.09	2	2
1:E:55:ASN:OD1	1:E:130:THR:HG21	0.47	2.10	8	1
1:A:47:ALA:HB3	1:A:139:ALA:HB3	0.47	1.86	10	1
1:A:155:LYS:HE2	1:D:128:THR:HG21	0.47	1.87	6	1
1:D:15:GLU:HG2	1:E:147:ALA:HA	0.47	1.87	9	1
1:E:71:VAL:HG21	1:E:131:ILE:CG2	0.47	2.40	8	1
1:A:71:VAL:HG21	1:A:131:ILE:CG2	0.47	2.40	8	1
1:F:71:VAL:HG21	1:F:131:ILE:CG2	0.47	2.40	8	1
1:D:23:VAL:HA	1:D:58:LEU:HA	0.47	1.86	3	1
1:E:103:ILE:HD12	1:E:111:LEU:HB3	0.47	1.86	3	1
1:D:12:PHE:HA	1:E:32:VAL:O	0.47	2.09	6	1
1:B:16:VAL:HA	1:C:37:VAL:O	0.47	2.09	6	1
1:D:74:LEU:O	1:D:152:ALA:HA	0.47	2.09	2	2
1:B:71:VAL:HG21	1:B:131:ILE:CG2	0.47	2.40	8	1
1:A:55:ASN:OD1	1:A:130:THR:HG21	0.47	2.10	8	1
1:D:47:ALA:HB3	1:D:139:ALA:HB3	0.47	1.86	10	1
1:B:9:THR:CG2	1:C:153:THR:HG23	0.47	2.31	3	1
1:A:158:TYR:C	1:A:159:GLN:HG3	0.47	2.30	3	1
1:B:20:ALA:O	1:B:61:CYS:HA	0.47	2.09	1	1
1:F:20:ALA:O	1:F:61:CYS:HA	0.47	2.09	1	2
1:F:78:ILE:HG23	1:F:79:ASP:N	0.47	2.24	1	2
1:E:118:PHE:CZ	1:E:155:LYS:HB3	0.47	2.45	1	1
1:E:69:ALA:HB3	1:E:122:THR:HB	0.47	1.85	1	2
1:C:3:THR:HB	1:D:158:TYR:CD2	0.47	2.44	4	1
1:B:52:VAL:HG13	1:B:135:ALA:O	0.47	2.10	4	2
1:C:52:VAL:HG13	1:C:135:ALA:O	0.47	2.10	10	2
1:A:52:VAL:HG13	1:A:135:ALA:O	0.47	2.10	10	2
1:D:52:VAL:HG13	1:D:135:ALA:O	0.47	2.10	4	2
1:C:34:LEU:N	1:C:34:LEU:HD22	0.47	2.24	7	1
1:E:34:LEU:HD22	1:E:34:LEU:N	0.47	2.24	7	1
1:C:71:VAL:HG21	1:C:131:ILE:CG2	0.47	2.40	8	1
1:C:85:VAL:HG22	1:C:102:GLN:HB2	0.47	1.87	8	1
1:F:85:VAL:HG22	1:F:102:GLN:HB2	0.47	1.87	8	1
1:A:56:ILE:HG21	1:A:131:ILE:HD12	0.47	1.85	10	1
1:E:23:VAL:CA	1:E:58:LEU:HG	0.47	2.40	3	2
1:A:78:ILE:HG23	1:A:79:ASP:N	0.47	2.24	1	2
1:C:69:ALA:HB3	1:C:122:THR:HB	0.47	1.85	1	2
1:B:118:PHE:CZ	1:B:155:LYS:HB3	0.47	2.45	1	1
1:E:12:PHE:HA	1:F:32:VAL:O	0.47	2.09	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:3:THR:HB	1:E:158:TYR:CD2	0.47	2.44	4	1
1:E:3:THR:HB	1:F:158:TYR:CD2	0.47	2.44	4	1
1:A:72:ALA:HA	1:A:111:LEU:HD21	0.47	1.86	4	1
1:E:5:VAL:CG2	1:F:17:VAL:HG12	0.47	2.40	8	1
1:D:56:ILE:HG21	1:D:131:ILE:HD12	0.47	1.85	10	1
1:E:97:THR:O	1:E:98:ASN:HB2	0.47	2.10	10	2
1:D:23:VAL:CA	1:D:58:LEU:HG	0.47	2.40	3	2
1:B:103:ILE:HD12	1:B:111:LEU:HB3	0.47	1.86	3	1
1:B:79:ASP:HB2	1:B:140:THR:HG21	0.47	1.86	5	2
1:B:116:ALA:HB3	1:E:129:ASN:OD1	0.47	2.10	1	1
1:C:32:VAL:HG11	1:C:52:VAL:HG11	0.47	1.87	5	1
1:F:37:VAL:CG1	1:F:42:LEU:HD21	0.47	2.40	5	1
1:B:2:ALA:HB2	1:C:159:GLN:HG3	0.47	1.87	6	1
1:E:52:VAL:HG13	1:E:135:ALA:O	0.47	2.10	4	2
1:F:82:HIS:NE2	1:F:139:ALA:O	0.47	2.48	7	1
1:E:74:LEU:O	1:E:152:ALA:HA	0.47	2.09	2	2
1:C:55:ASN:OD1	1:C:130:THR:HG21	0.47	2.10	8	1
1:B:97:THR:O	1:B:98:ASN:HB2	0.47	2.10	10	2
1:E:47:ALA:HB3	1:E:139:ALA:HB3	0.47	1.86	10	1
1:C:97:THR:O	1:C:98:ASN:HB2	0.47	2.10	10	2
1:B:6:ASN:OD1	1:C:154:PHE:O	0.47	2.33	2	1
1:E:6:ASN:OD1	1:F:154:PHE:O	0.47	2.33	2	1
1:A:23:VAL:CA	1:A:58:LEU:HG	0.47	2.40	3	2
1:B:23:VAL:CA	1:B:58:LEU:HG	0.47	2.40	3	2
1:E:23:VAL:HA	1:E:58:LEU:HA	0.47	1.86	3	1
1:E:44:GLN:CG	1:E:47:ALA:HB2	0.47	2.40	5	1
1:F:52:VAL:HG13	1:F:135:ALA:O	0.47	2.10	10	2
1:D:16:VAL:HB	1:E:144:THR:O	0.47	2.10	7	1
1:C:69:ALA:CB	1:C:124:LEU:HD13	0.47	2.36	8	1
1:B:5:VAL:CG2	1:C:17:VAL:HG12	0.47	2.40	8	1
1:E:97:THR:O	1:E:99:VAL:HG23	0.47	2.10	8	1
1:A:97:THR:O	1:A:99:VAL:HG23	0.47	2.10	8	1
1:F:55:ASN:OD1	1:F:130:THR:HG21	0.47	2.10	8	1
1:A:97:THR:O	1:A:98:ASN:HB2	0.47	2.10	10	2
1:F:97:THR:O	1:F:98:ASN:HB2	0.47	2.10	10	2
1:A:6:ASN:OD1	1:B:154:PHE:O	0.47	2.33	2	1
1:D:6:ASN:OD1	1:E:154:PHE:O	0.47	2.33	2	1
1:A:44:GLN:CG	1:A:47:ALA:HB2	0.46	2.40	5	1
1:D:44:GLN:CG	1:D:47:ALA:HB2	0.46	2.41	5	1
1:C:115:GLY:HA3	1:F:130:THR:OG1	0.46	2.10	5	3
1:C:2:ALA:HB2	1:D:159:GLN:HG3	0.46	1.87	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:GLU:HG2	1:B:147:ALA:HA	0.46	1.86	9	1
1:B:34:LEU:HD22	1:B:34:LEU:N	0.46	2.24	7	1
1:F:34:LEU:HD22	1:F:34:LEU:N	0.46	2.24	7	1
1:C:6:ASN:OD1	1:D:154:PHE:O	0.46	2.33	2	1
1:B:23:VAL:HA	1:B:58:LEU:HA	0.46	1.86	3	1
1:D:158:TYR:C	1:D:159:GLN:HG3	0.46	2.30	3	1
1:C:37:VAL:CG1	1:C:42:LEU:HD21	0.46	2.41	5	1
1:B:37:VAL:CG1	1:B:42:LEU:HD21	0.46	2.40	5	1
1:C:155:LYS:HE2	1:F:128:THR:HG21	0.46	1.87	6	1
1:D:2:ALA:HB2	1:E:159:GLN:HG3	0.46	1.87	6	1
1:B:68:LYS:HB3	1:B:159:GLN:HB3	0.46	1.87	6	1
1:B:12:PHE:HA	1:C:32:VAL:O	0.46	2.09	6	1
1:E:15:GLU:HG2	1:F:147:ALA:HA	0.46	1.87	9	1
1:C:72:ALA:HA	1:C:111:LEU:HD21	0.46	1.87	4	1
1:F:72:ALA:HA	1:F:111:LEU:HD21	0.46	1.87	4	1
1:A:82:HIS:NE2	1:A:139:ALA:O	0.46	2.48	7	1
1:D:5:VAL:CG2	1:E:17:VAL:HG12	0.46	2.40	8	1
1:B:55:ASN:OD1	1:B:130:THR:HG21	0.46	2.10	8	1
1:E:20:ALA:O	1:E:61:CYS:HA	0.46	2.09	1	2
1:F:69:ALA:HB3	1:F:122:THR:HB	0.46	1.85	1	2
1:B:44:GLN:CG	1:B:47:ALA:HB2	0.46	2.40	5	1
1:D:37:VAL:CG1	1:D:42:LEU:HD21	0.46	2.41	5	1
1:B:2:ALA:H	1:C:159:GLN:HA	0.46	1.70	6	3
1:A:12:PHE:HA	1:B:32:VAL:O	0.46	2.09	6	1
1:C:92:ALA:HB3	1:F:34:LEU:HD21	0.46	1.87	6	1
1:B:56:ILE:CB	1:B:131:ILE:HD12	0.46	2.40	7	1
1:E:82:HIS:NE2	1:E:139:ALA:O	0.46	2.48	7	1
1:D:55:ASN:OD1	1:D:130:THR:HG21	0.46	2.10	8	1
1:E:114:ASP:HB2	1:E:117:THR:OG1	0.46	2.11	10	1
1:B:47:ALA:HB3	1:B:139:ALA:HB3	0.46	1.86	10	1
1:D:97:THR:O	1:D:98:ASN:HB2	0.46	2.10	10	2
1:D:63:THR:HG23	1:D:125:ASN:HA	0.46	1.87	1	2
1:C:20:ALA:O	1:C:61:CYS:HA	0.46	2.09	1	1
1:E:79:ASP:HB2	1:E:140:THR:HG21	0.46	1.86	5	1
1:F:32:VAL:HG11	1:F:52:VAL:HG11	0.46	1.87	5	1
1:B:32:VAL:HG11	1:B:52:VAL:HG11	0.46	1.87	5	1
1:E:37:VAL:CG1	1:E:42:LEU:HD21	0.46	2.41	5	1
1:D:5:VAL:HG12	1:F:146:GLY:HA2	0.46	1.87	6	1
1:A:92:ALA:HA	1:D:50:SER:O	0.46	2.11	4	1
1:E:56:ILE:CB	1:E:131:ILE:HD12	0.46	2.40	7	1
1:C:5:VAL:CG2	1:D:17:VAL:HG12	0.46	2.40	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:85:VAL:HG22	1:D:102:GLN:HB2	0.46	1.87	8	1
1:A:63:THR:HG23	1:A:125:ASN:HA	0.46	1.87	1	2
1:C:116:ALA:HB3	1:F:129:ASN:OD1	0.46	2.10	1	1
1:F:118:PHE:CZ	1:F:155:LYS:HB3	0.46	2.45	1	1
1:D:69:ALA:HB3	1:D:122:THR:HB	0.46	1.85	1	2
1:A:37:VAL:CG1	1:A:42:LEU:HD21	0.46	2.41	5	1
1:E:68:LYS:HB3	1:E:159:GLN:HB3	0.46	1.87	6	1
1:C:5:VAL:HG12	1:E:146:GLY:HA2	0.46	1.87	6	1
1:A:16:VAL:HB	1:B:144:THR:O	0.46	2.10	7	1
1:C:118:PHE:CZ	1:C:155:LYS:HB3	0.46	2.45	1	1
1:A:116:ALA:HB3	1:D:129:ASN:OD1	0.46	2.10	1	1
1:A:115:GLY:HA3	1:D:130:THR:OG1	0.46	2.10	5	3
1:C:58:LEU:HD11	1:C:131:ILE:HG13	0.46	1.87	6	1
1:D:68:LYS:HB3	1:D:159:GLN:HB3	0.46	1.87	6	1
1:F:68:LYS:HB3	1:F:159:GLN:HB3	0.46	1.87	6	1
1:C:92:ALA:HA	1:F:50:SER:O	0.46	2.11	4	1
1:B:16:VAL:HB	1:C:144:THR:O	0.46	2.10	7	1
1:B:111:LEU:HD11	1:B:117:THR:HG22	0.46	1.88	8	1
1:E:111:LEU:HD11	1:E:117:THR:HG22	0.46	1.88	8	1
1:C:74:LEU:O	1:C:152:ALA:HA	0.46	2.09	2	2
1:D:71:VAL:HG21	1:D:131:ILE:CG2	0.46	2.40	8	1
1:A:5:VAL:CG2	1:B:17:VAL:HG12	0.46	2.40	8	1
1:A:21:CYS:HB3	1:A:58:LEU:HD23	0.46	1.88	3	1
1:C:21:CYS:HB3	1:C:58:LEU:HD23	0.46	1.88	3	1
1:A:21:CYS:SG	1:A:58:LEU:HB2	0.46	2.51	6	1
1:D:21:CYS:SG	1:D:58:LEU:HB2	0.46	2.51	6	1
1:A:103:ILE:HD12	1:A:113:LEU:HD11	0.46	1.88	6	1
1:B:34:LEU:HD21	1:B:101:VAL:CG2	0.46	2.41	10	1
1:B:21:CYS:HB3	1:B:58:LEU:HD23	0.46	1.88	3	1
1:F:21:CYS:HB3	1:F:58:LEU:HD23	0.46	1.88	3	1
1:E:21:CYS:HB3	1:E:58:LEU:HD23	0.46	1.88	3	1
1:F:44:GLN:CG	1:F:47:ALA:HB2	0.46	2.41	5	1
1:C:44:GLN:CG	1:C:47:ALA:HB2	0.46	2.40	5	1
1:F:58:LEU:HD11	1:F:131:ILE:HG13	0.46	1.87	6	1
1:E:2:ALA:HB2	1:F:159:GLN:HG3	0.46	1.87	6	1
1:B:15:GLU:HG2	1:C:147:ALA:HA	0.46	1.86	9	1
1:A:22:ALA:HB1	1:B:36:GLN:O	0.46	2.11	4	1
1:D:72:ALA:HA	1:D:111:LEU:HD21	0.46	1.86	4	1
1:E:16:VAL:HB	1:F:144:THR:O	0.46	2.10	7	1
1:D:82:HIS:NE2	1:D:139:ALA:O	0.46	2.48	7	1
1:A:114:ASP:HB2	1:A:117:THR:OG1	0.46	2.11	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HD21	1:A:101:VAL:CG2	0.46	2.41	10	1
1:C:23:VAL:CA	1:C:58:LEU:HG	0.46	2.40	3	2
1:C:63:THR:HG23	1:C:125:ASN:HA	0.46	1.87	1	2
1:B:16:VAL:CG2	1:C:148:ALA:HB2	0.46	2.41	10	2
1:F:21:CYS:SG	1:F:58:LEU:HB2	0.46	2.51	6	1
1:E:103:ILE:HD12	1:E:113:LEU:HD11	0.46	1.88	6	1
1:C:21:CYS:SG	1:C:58:LEU:HB2	0.46	2.51	6	1
1:F:97:THR:N	1:F:144:THR:HB	0.46	2.26	4	1
1:B:92:ALA:HA	1:E:50:SER:O	0.46	2.11	4	1
1:A:111:LEU:HD11	1:A:117:THR:HG22	0.46	1.88	8	1
1:D:111:LEU:HD11	1:D:117:THR:HG22	0.46	1.88	8	1
1:F:97:THR:O	1:F:99:VAL:HG23	0.46	2.10	8	1
1:C:114:ASP:HB2	1:C:117:THR:OG1	0.46	2.11	10	1
1:D:34:LEU:HD21	1:D:101:VAL:CG2	0.46	2.41	10	1
1:F:34:LEU:HD21	1:F:101:VAL:CG2	0.46	2.41	10	1
1:C:23:VAL:HA	1:C:58:LEU:HA	0.46	1.86	3	1
1:C:16:VAL:CG2	1:D:148:ALA:HB2	0.46	2.41	10	2
1:A:58:LEU:HD11	1:A:131:ILE:HG13	0.46	1.87	6	1
1:A:2:ALA:HB2	1:B:159:GLN:HG3	0.46	1.87	6	1
1:A:5:VAL:HG12	1:C:146:GLY:HA2	0.46	1.87	6	1
1:D:97:THR:O	1:D:99:VAL:HG23	0.46	2.10	8	1
1:A:39:THR:O	1:A:43:ALA:HB2	0.46	2.11	10	1
1:B:39:THR:O	1:B:43:ALA:HB2	0.46	2.11	10	1
1:E:34:LEU:HD21	1:E:101:VAL:CG2	0.46	2.41	10	1
1:D:39:THR:O	1:D:43:ALA:HB2	0.46	2.11	10	1
1:E:39:THR:O	1:E:43:ALA:HB2	0.46	2.11	10	1
1:F:39:THR:O	1:F:43:ALA:HB2	0.46	2.11	10	1
1:F:23:VAL:CA	1:F:58:LEU:HG	0.45	2.40	3	2
1:D:21:CYS:HB3	1:D:58:LEU:HD23	0.45	1.88	3	1
1:B:63:THR:HG23	1:B:125:ASN:HA	0.45	1.87	1	2
1:E:58:LEU:HD11	1:E:131:ILE:HG13	0.45	1.87	6	1
1:A:92:ALA:HB3	1:D:34:LEU:HD21	0.45	1.87	6	1
1:C:15:GLU:HG2	1:D:147:ALA:HA	0.45	1.87	9	1
1:B:114:ASP:HB2	1:B:117:THR:OG1	0.45	2.11	10	1
1:E:9:THR:CG2	1:F:153:THR:HG23	0.45	2.31	3	1
1:D:16:VAL:CG2	1:E:148:ALA:HB2	0.45	2.41	10	2
1:E:32:VAL:HG11	1:E:52:VAL:HG11	0.45	1.87	5	1
1:C:76:THR:H	1:C:86:LEU:HD12	0.45	1.71	5	1
1:D:58:LEU:HD11	1:D:131:ILE:HG13	0.45	1.87	6	1
1:E:86:LEU:HG	1:E:113:LEU:CD2	0.45	2.41	6	1
1:D:66:ALA:HB1	1:D:159:GLN:O	0.45	2.11	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:6:ASN:CA	1:F:155:LYS:HE2	0.45	2.41	9	1
1:C:13:LYS:HD3	1:D:31:THR:HG22	0.45	1.89	9	1
1:C:16:VAL:HB	1:D:144:THR:O	0.45	2.10	7	1
1:B:56:ILE:HG22	1:B:131:ILE:HB	0.45	1.89	8	1
1:A:85:VAL:HG22	1:A:102:GLN:HB2	0.45	1.87	8	1
1:B:97:THR:O	1:B:99:VAL:HG23	0.45	2.10	8	1
1:A:16:VAL:CG2	1:B:148:ALA:HB2	0.45	2.41	10	2
1:E:16:VAL:CG2	1:F:148:ALA:HB2	0.45	2.41	10	2
1:B:115:GLY:HA3	1:E:130:THR:OG1	0.45	2.10	5	3
1:B:155:LYS:HE2	1:E:128:THR:HG21	0.45	1.87	6	1
1:B:5:VAL:HG12	1:D:146:GLY:HA2	0.45	1.87	6	1
1:D:6:ASN:CA	1:E:155:LYS:HE2	0.45	2.41	9	1
1:D:13:LYS:HD3	1:E:31:THR:HG22	0.45	1.89	9	1
1:A:13:LYS:HD3	1:B:31:THR:HG22	0.45	1.89	9	1
1:E:22:ALA:HB1	1:F:36:GLN:O	0.45	2.11	4	1
1:B:72:ALA:HA	1:B:111:LEU:HD21	0.45	1.86	4	1
1:B:82:HIS:NE2	1:B:139:ALA:O	0.45	2.48	7	1
1:C:111:LEU:HD11	1:C:117:THR:HG22	0.45	1.88	8	1
1:F:111:LEU:HD11	1:F:117:THR:HG22	0.45	1.88	8	1
1:F:56:ILE:HG22	1:F:131:ILE:HB	0.45	1.89	8	1
1:C:97:THR:O	1:C:99:VAL:HG23	0.45	2.10	8	1
1:A:91:SER:CB	1:A:95:SER:HB2	0.45	2.42	10	1
1:F:114:ASP:HB2	1:F:117:THR:OG1	0.45	2.11	10	1
1:F:68:LYS:HE3	1:F:121:GLU:HB3	0.45	1.89	3	1
1:F:75:GLY:HA3	1:F:113:LEU:HD11	0.45	1.88	5	1
1:B:58:LEU:HD11	1:B:131:ILE:HG13	0.45	1.87	6	1
1:A:86:LEU:HG	1:A:113:LEU:CD2	0.45	2.42	6	1
1:D:86:LEU:HG	1:D:113:LEU:CD2	0.45	2.42	6	1
1:F:17:VAL:HG11	1:F:158:TYR:CE2	0.45	2.47	9	1
1:E:56:ILE:HG22	1:E:131:ILE:HB	0.45	1.89	8	1
1:D:91:SER:CB	1:D:95:SER:HB2	0.45	2.42	10	1
1:C:34:LEU:HD21	1:C:101:VAL:CG2	0.45	2.41	10	1
1:F:63:THR:HG23	1:F:125:ASN:HA	0.45	1.89	3	2
1:D:32:VAL:HG11	1:D:52:VAL:HG11	0.45	1.87	5	1
1:D:2:ALA:H	1:E:159:GLN:HA	0.45	1.70	6	3
1:B:86:LEU:HG	1:B:113:LEU:CD2	0.45	2.42	6	1
1:C:66:ALA:HB1	1:C:159:GLN:O	0.45	2.11	6	1
1:F:66:ALA:HB1	1:F:159:GLN:O	0.45	2.11	6	1
1:C:97:THR:N	1:C:144:THR:HB	0.45	2.26	4	1
1:C:52:VAL:HG23	1:C:54:PHE:CD1	0.45	2.47	7	1
1:C:56:ILE:HG22	1:C:131:ILE:HB	0.45	1.89	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:85:VAL:HG22	1:B:102:GLN:HB2	0.45	1.87	8	1
1:A:116:ALA:O	1:D:125:ASN:HB3	0.45	2.12	10	1
1:E:144:THR:HG22	1:E:145:PRO:HD2	0.45	1.88	2	1
1:F:23:VAL:HA	1:F:58:LEU:HA	0.45	1.86	3	1
1:D:68:LYS:HE3	1:D:121:GLU:HB3	0.45	1.89	3	1
1:A:75:GLY:HA3	1:A:113:LEU:HD11	0.45	1.88	5	1
1:E:2:ALA:H	1:F:159:GLN:HA	0.45	1.72	5	3
1:A:32:VAL:HG11	1:A:52:VAL:HG11	0.45	1.87	5	1
1:C:2:ALA:H	1:D:159:GLN:HA	0.45	1.70	6	3
1:A:68:LYS:HB3	1:A:159:GLN:HB3	0.45	1.87	6	1
1:A:66:ALA:HB1	1:A:159:GLN:O	0.45	2.11	6	1
1:C:6:ASN:CA	1:D:155:LYS:HE2	0.45	2.41	9	1
1:A:90:SER:O	1:D:52:VAL:HG12	0.45	2.12	7	1
1:D:52:VAL:HG23	1:D:54:PHE:CD1	0.45	2.47	7	1
1:D:144:THR:HG22	1:D:145:PRO:HD2	0.45	1.88	2	1
1:A:118:PHE:CZ	1:A:155:LYS:HB3	0.45	2.45	1	1
1:D:118:PHE:CZ	1:D:155:LYS:HB3	0.45	2.45	1	1
1:D:79:ASP:HB2	1:D:140:THR:HG21	0.45	1.86	5	1
1:B:98:ASN:HA	1:B:140:THR:HB	0.45	1.89	6	1
1:C:98:ASN:HA	1:C:140:THR:HB	0.45	1.88	6	1
1:E:13:LYS:HD3	1:F:31:THR:HG22	0.45	1.89	9	1
1:D:22:ALA:HB1	1:E:36:GLN:O	0.45	2.11	4	1
1:E:72:ALA:HA	1:E:111:LEU:HD21	0.45	1.87	4	1
1:E:85:VAL:HG22	1:E:102:GLN:HB2	0.45	1.87	8	1
1:C:47:ALA:HB3	1:C:139:ALA:HB3	0.45	1.86	10	1
1:F:103:ILE:HD12	1:F:113:LEU:HD11	0.45	1.88	6	1
1:C:68:LYS:HB3	1:C:159:GLN:HB3	0.45	1.87	6	1
1:F:98:ASN:HA	1:F:140:THR:HB	0.45	1.89	6	1
1:B:6:ASN:CA	1:C:155:LYS:HE2	0.45	2.41	9	1
1:C:47:ALA:O	1:C:138:PHE:HA	0.45	2.12	9	1
1:D:97:THR:N	1:D:144:THR:HB	0.45	2.26	4	1
1:C:22:ALA:HB1	1:D:36:GLN:O	0.45	2.11	4	1
1:D:8:GLY:N	1:E:154:PHE:CE1	0.45	2.85	7	1
1:A:52:VAL:HG23	1:A:54:PHE:CD1	0.45	2.47	7	1
1:C:39:THR:O	1:C:43:ALA:HB2	0.45	2.11	10	1
1:C:68:LYS:HE3	1:C:121:GLU:HB3	0.45	1.89	3	1
1:B:9:THR:HG23	1:C:152:ALA:O	0.45	2.12	5	1
1:C:86:LEU:HG	1:C:113:LEU:CD2	0.45	2.41	6	1
1:A:92:ALA:HA	1:D:50:SER:HB2	0.45	1.89	6	1
1:B:92:ALA:HB3	1:E:34:LEU:HD21	0.45	1.87	6	1
1:A:6:ASN:CA	1:B:155:LYS:HE2	0.45	2.41	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:13:LYS:HD3	1:C:31:THR:HG22	0.45	1.89	9	1
1:B:22:ALA:HB1	1:C:36:GLN:O	0.45	2.11	4	1
1:A:8:GLY:N	1:B:154:PHE:CE1	0.45	2.85	7	1
1:D:23:VAL:HG13	1:D:27:SER:HB3	0.45	1.89	7	1
1:C:105:ASP:OD2	1:C:111:LEU:HD22	0.45	2.12	8	1
1:A:105:ASP:OD2	1:A:111:LEU:HD22	0.45	2.12	8	1
1:F:47:ALA:HB3	1:F:139:ALA:HB3	0.45	1.86	10	1
1:E:85:VAL:HG11	1:E:138:PHE:HB3	0.45	1.89	1	1
1:E:9:THR:HG23	1:F:152:ALA:O	0.45	2.12	5	1
1:A:76:THR:H	1:A:86:LEU:HD12	0.45	1.71	5	1
1:A:2:ALA:H	1:B:159:GLN:HA	0.45	1.70	6	3
1:E:86:LEU:HG	1:E:113:LEU:HD21	0.45	1.89	6	1
1:D:103:ILE:HD12	1:D:113:LEU:HD11	0.45	1.88	6	1
1:B:66:ALA:HB1	1:B:159:GLN:O	0.45	2.11	6	1
1:E:17:VAL:HG11	1:E:158:TYR:CE2	0.45	2.46	9	1
1:F:52:VAL:HG23	1:F:54:PHE:CD1	0.45	2.47	7	1
1:B:90:SER:O	1:E:52:VAL:HG12	0.45	2.12	7	1
1:B:52:VAL:HG23	1:B:54:PHE:CD1	0.45	2.47	7	1
1:B:103:ILE:HG12	1:B:113:LEU:HG	0.45	1.89	8	2
1:B:44:GLN:HB2	1:B:47:ALA:HB2	0.44	1.89	1	1
1:D:44:GLN:HB2	1:D:47:ALA:HB2	0.44	1.89	1	1
1:D:85:VAL:HG11	1:D:138:PHE:HB3	0.44	1.89	1	1
1:C:75:GLY:HA3	1:C:113:LEU:HD11	0.44	1.88	5	1
1:D:9:THR:HG23	1:E:152:ALA:O	0.44	2.12	5	1
1:B:86:LEU:HG	1:B:113:LEU:HD21	0.44	1.89	6	1
1:F:86:LEU:HG	1:F:113:LEU:CD2	0.44	2.42	6	1
1:D:42:LEU:HB3	1:D:139:ALA:HB2	0.44	1.89	9	2
1:B:8:GLY:N	1:C:154:PHE:CE1	0.44	2.85	7	1
1:E:8:GLY:N	1:F:154:PHE:CE1	0.44	2.85	7	1
1:E:22:ALA:HB3	1:E:59:ASN:O	0.44	2.13	7	1
1:F:23:VAL:HG13	1:F:27:SER:HB3	0.44	1.89	7	1
1:B:69:ALA:CB	1:B:124:LEU:HD13	0.44	2.36	8	1
1:F:103:ILE:HG12	1:F:113:LEU:HG	0.44	1.89	8	2
1:D:56:ILE:HG22	1:D:131:ILE:HB	0.44	1.89	8	1
1:A:56:ILE:HG22	1:A:131:ILE:HB	0.44	1.89	8	1
1:B:91:SER:CB	1:B:95:SER:HB2	0.44	2.42	10	1
1:C:91:SER:CB	1:C:95:SER:HB2	0.44	2.42	10	1
1:F:144:THR:HG22	1:F:145:PRO:HD2	0.44	1.88	2	1
1:C:4:THR:HG22	1:D:157:GLN:HB2	0.44	1.90	5	1
1:B:103:ILE:HD12	1:B:113:LEU:HD11	0.44	1.88	6	1
1:E:66:ALA:HB1	1:E:159:GLN:O	0.44	2.11	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:VAL:HG11	1:A:158:TYR:CE2	0.44	2.47	9	1
1:B:17:VAL:HG11	1:B:158:TYR:CE2	0.44	2.47	9	1
1:B:11:HIS:O	1:C:32:VAL:HB	0.44	2.13	9	1
1:C:92:ALA:O	1:F:49:SER:HB3	0.44	2.13	4	1
1:C:8:GLY:N	1:D:154:PHE:CE1	0.44	2.85	7	1
1:F:56:ILE:CB	1:F:131:ILE:HD12	0.44	2.40	7	1
1:E:52:VAL:HG23	1:E:54:PHE:CD1	0.44	2.47	7	1
1:A:22:ALA:HB3	1:A:59:ASN:O	0.44	2.13	7	1
1:B:22:ALA:HB3	1:B:59:ASN:O	0.44	2.13	7	1
1:F:105:ASP:OD2	1:F:111:LEU:HD22	0.44	2.12	8	1
1:E:91:SER:CB	1:E:95:SER:HB2	0.44	2.42	10	1
1:D:114:ASP:HB2	1:D:117:THR:OG1	0.44	2.11	10	1
1:E:73:PHE:CB	1:E:103:ILE:HD13	0.44	2.42	2	1
1:A:44:GLN:HB2	1:A:47:ALA:HB2	0.44	1.89	1	1
1:B:85:VAL:HG11	1:B:138:PHE:HB3	0.44	1.89	1	1
1:E:44:GLN:HB2	1:E:47:ALA:HB2	0.44	1.89	1	1
1:F:44:GLN:HB2	1:F:47:ALA:HB2	0.44	1.89	1	1
1:E:76:THR:H	1:E:86:LEU:HD12	0.44	1.71	5	1
1:E:98:ASN:HA	1:E:140:THR:HB	0.44	1.89	6	1
1:C:42:LEU:HB3	1:C:139:ALA:HB2	0.44	1.89	9	2
1:F:47:ALA:O	1:F:138:PHE:HA	0.44	2.12	9	1
1:B:92:ALA:O	1:E:49:SER:HB3	0.44	2.12	4	1
1:D:56:ILE:CB	1:D:131:ILE:HD12	0.44	2.40	7	1
1:D:22:ALA:HB3	1:D:59:ASN:O	0.44	2.13	7	1
1:D:105:ASP:OD2	1:D:111:LEU:HD22	0.44	2.12	8	1
1:E:68:LYS:HE3	1:E:121:GLU:HB3	0.44	1.89	3	1
1:A:79:ASP:HB2	1:A:140:THR:HG21	0.44	1.86	5	2
1:C:44:GLN:HB2	1:C:47:ALA:HB2	0.44	1.89	1	1
1:D:76:THR:H	1:D:86:LEU:HD12	0.44	1.71	5	1
1:B:21:CYS:SG	1:B:58:LEU:HB2	0.44	2.51	6	1
1:C:11:HIS:O	1:D:32:VAL:HB	0.44	2.13	9	1
1:C:17:VAL:HG11	1:C:158:TYR:CE2	0.44	2.47	9	1
1:D:17:VAL:HG11	1:D:158:TYR:CE2	0.44	2.47	9	1
1:D:11:HIS:O	1:E:32:VAL:HB	0.44	2.13	9	1
1:E:23:VAL:HG13	1:E:27:SER:HB3	0.44	1.89	7	1
1:E:105:ASP:OD2	1:E:111:LEU:HD22	0.44	2.12	8	1
1:A:9:THR:HG23	1:B:152:ALA:O	0.44	2.12	5	1
1:B:76:THR:H	1:B:86:LEU:HD12	0.44	1.71	5	1
1:D:4:THR:HG22	1:E:157:GLN:HB2	0.44	1.90	5	1
1:D:75:GLY:HA3	1:D:113:LEU:HD11	0.44	1.88	5	1
1:F:86:LEU:HG	1:F:113:LEU:HD21	0.44	1.89	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:9:THR:HA	1:F:153:THR:HG22	0.44	1.90	6	1
1:D:47:ALA:O	1:D:138:PHE:HA	0.44	2.12	9	1
1:C:102:GLN:HG2	1:C:103:ILE:N	0.44	2.28	4	1
1:A:69:ALA:CB	1:A:124:LEU:HD13	0.44	2.36	8	1
1:C:73:PHE:CB	1:C:103:ILE:HD13	0.44	2.42	2	1
1:A:68:LYS:HE3	1:A:121:GLU:HB3	0.44	1.89	3	1
1:E:21:CYS:SG	1:E:58:LEU:HB2	0.44	2.51	6	1
1:A:98:ASN:HA	1:A:140:THR:HB	0.44	1.89	6	1
1:D:98:ASN:HA	1:D:140:THR:HB	0.44	1.89	6	1
1:B:102:GLN:HG2	1:B:103:ILE:N	0.44	2.28	4	1
1:E:102:GLN:HG2	1:E:103:ILE:N	0.44	2.28	4	1
1:A:102:GLN:HG2	1:A:103:ILE:N	0.44	2.28	4	1
1:D:102:GLN:HG2	1:D:103:ILE:N	0.44	2.28	4	1
1:A:92:ALA:O	1:D:49:SER:HB3	0.44	2.13	4	1
1:F:118:PHE:CD1	1:F:157:GLN:HB2	0.44	2.48	8	1
1:F:91:SER:CB	1:F:95:SER:HB2	0.44	2.42	10	1
1:B:116:ALA:O	1:E:125:ASN:HB3	0.44	2.12	10	1
1:F:73:PHE:CB	1:F:103:ILE:HD13	0.44	2.42	2	1
1:E:63:THR:HG23	1:E:125:ASN:HA	0.44	1.87	1	2
1:C:103:ILE:HD12	1:C:113:LEU:HD11	0.44	1.88	6	1
1:D:9:THR:HA	1:E:153:THR:HG22	0.44	1.90	6	1
1:A:42:LEU:HB3	1:A:139:ALA:HB2	0.44	1.89	9	2
1:E:47:ALA:O	1:E:138:PHE:HA	0.44	2.12	9	1
1:A:56:ILE:CB	1:A:131:ILE:HD12	0.44	2.40	7	1
1:C:90:SER:O	1:F:52:VAL:HG12	0.44	2.12	7	1
1:C:77:ALA:H	1:F:132:PRO:HB3	0.44	1.73	7	1
1:B:105:ASP:OD2	1:B:111:LEU:HD22	0.44	2.12	8	1
1:C:118:PHE:CD1	1:C:157:GLN:HB2	0.44	2.48	8	1
1:A:16:VAL:O	1:B:145:PRO:HA	0.44	2.13	10	1
1:C:16:VAL:O	1:D:145:PRO:HA	0.44	2.13	10	1
1:B:68:LYS:HE3	1:B:121:GLU:HB3	0.44	1.89	3	1
1:D:51:ALA:CA	1:D:136:ARG:HB3	0.44	2.43	3	1
1:C:86:LEU:HG	1:C:113:LEU:HD21	0.44	1.89	6	1
1:E:11:HIS:O	1:F:32:VAL:HB	0.44	2.13	9	1
1:F:73:PHE:CB	1:F:111:LEU:HD11	0.44	2.43	9	1
1:E:42:LEU:HB3	1:E:139:ALA:HB2	0.44	1.89	9	2
1:B:47:ALA:O	1:B:138:PHE:HA	0.44	2.12	9	1
1:D:118:PHE:CD1	1:D:157:GLN:HB2	0.44	2.48	8	1
1:A:118:PHE:CD1	1:A:157:GLN:HB2	0.44	2.48	8	1
1:F:89:GLN:CG	1:F:149:ASN:HB2	0.44	2.43	2	1
1:E:89:GLN:CG	1:E:149:ASN:HB2	0.44	2.43	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:89:GLN:CG	1:B:149:ASN:HB2	0.44	2.42	2	1
1:C:89:GLN:CG	1:C:149:ASN:HB2	0.44	2.43	2	1
1:D:51:ALA:HA	1:D:136:ARG:HB3	0.44	1.90	3	1
1:B:75:GLY:HA3	1:B:113:LEU:HD11	0.44	1.88	5	1
1:C:98:ASN:HA	1:C:140:THR:OG1	0.44	2.13	9	1
1:E:73:PHE:CB	1:E:111:LEU:HD11	0.44	2.43	9	1
1:A:11:HIS:O	1:B:32:VAL:HB	0.44	2.13	9	1
1:C:23:VAL:HG13	1:C:27:SER:HB3	0.44	1.89	7	1
1:C:116:ALA:O	1:F:125:ASN:HB3	0.44	2.12	10	1
1:D:89:GLN:CG	1:D:149:ASN:HB2	0.44	2.43	2	1
1:F:39:THR:OG1	1:F:143:ALA:O	0.43	2.33	3	1
1:A:4:THR:HG22	1:B:157:GLN:HB2	0.43	1.90	5	1
1:F:76:THR:H	1:F:86:LEU:HD12	0.43	1.71	5	1
1:A:93:ALA:HB3	1:D:36:GLN:O	0.43	2.13	6	2
1:B:93:ALA:HB3	1:E:36:GLN:O	0.43	2.13	10	2
1:A:98:ASN:HA	1:A:140:THR:OG1	0.43	2.13	9	1
1:C:73:PHE:CB	1:C:111:LEU:HD11	0.43	2.43	9	1
1:A:97:THR:N	1:A:144:THR:HB	0.43	2.26	4	1
1:A:103:ILE:HG12	1:A:113:LEU:HG	0.43	1.89	8	2
1:D:73:PHE:CB	1:D:103:ILE:HD13	0.43	2.42	2	1
1:E:51:ALA:HA	1:E:136:ARG:HB3	0.43	1.90	3	1
1:F:51:ALA:CA	1:F:136:ARG:HB3	0.43	2.43	3	1
1:A:51:ALA:CA	1:A:136:ARG:HB3	0.43	2.43	3	1
1:B:51:ALA:CA	1:B:136:ARG:HB3	0.43	2.43	3	1
1:F:105:ASP:HB2	1:F:111:LEU:HB2	0.43	1.91	1	2
1:C:9:THR:HG23	1:D:152:ALA:O	0.43	2.12	5	1
1:E:75:GLY:HA3	1:E:113:LEU:HD11	0.43	1.88	5	1
1:F:98:ASN:HA	1:F:140:THR:OG1	0.43	2.13	9	1
1:B:42:LEU:HB3	1:B:139:ALA:HB2	0.43	1.89	9	2
1:D:98:ASN:HA	1:D:140:THR:OG1	0.43	2.13	9	1
1:E:55:ASN:OD1	1:E:130:THR:CG2	0.43	2.66	8	1
1:C:61:CYS:HB3	1:C:125:ASN:O	0.43	2.13	8	1
1:B:16:VAL:O	1:C:145:PRO:HA	0.43	2.13	10	1
1:A:73:PHE:CB	1:A:103:ILE:HD13	0.43	2.42	2	2
1:D:105:ASP:HB2	1:D:111:LEU:HB2	0.43	1.91	1	2
1:C:105:ASP:HB2	1:C:111:LEU:HB2	0.43	1.91	1	2
1:F:85:VAL:HG11	1:F:138:PHE:HB3	0.43	1.89	1	1
1:C:85:VAL:HG11	1:C:138:PHE:HB3	0.43	1.89	1	1
1:B:92:ALA:HA	1:E:50:SER:HB2	0.43	1.89	6	1
1:C:93:ALA:HB3	1:F:36:GLN:O	0.43	2.13	6	2
1:B:9:THR:HA	1:C:153:THR:HG22	0.43	1.90	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:102:GLN:HG2	1:F:103:ILE:N	0.43	2.28	4	1
1:D:16:VAL:O	1:E:145:PRO:HA	0.43	2.13	10	1
1:E:16:VAL:O	1:F:145:PRO:HA	0.43	2.13	10	1
1:B:74:LEU:HD11	1:E:57:GLN:HG3	0.43	1.89	10	1
1:B:73:PHE:CB	1:B:103:ILE:HD13	0.43	2.42	2	1
1:C:5:VAL:CG1	1:E:146:GLY:HA2	0.43	2.44	6	1
1:B:73:PHE:CB	1:B:111:LEU:HD11	0.43	2.43	9	1
1:C:22:ALA:HB3	1:C:59:ASN:O	0.43	2.13	7	1
1:B:77:ALA:H	1:E:132:PRO:HB3	0.43	1.73	7	1
1:C:82:HIS:NE2	1:C:139:ALA:O	0.43	2.48	7	1
1:A:23:VAL:HG13	1:A:27:SER:HB3	0.43	1.89	7	1
1:B:77:ALA:HB2	1:B:83:THR:HG23	0.43	1.90	2	1
1:E:51:ALA:CA	1:E:136:ARG:HB3	0.43	2.43	3	1
1:A:51:ALA:HA	1:A:136:ARG:HB3	0.43	1.90	3	1
1:D:6:ASN:CB	1:E:155:LYS:HE2	0.43	2.44	9	1
1:A:47:ALA:O	1:A:138:PHE:HA	0.43	2.12	9	1
1:C:63:THR:HA	1:C:66:ALA:O	0.43	2.14	7	1
1:E:103:ILE:HG12	1:E:113:LEU:HG	0.43	1.89	8	2
1:E:61:CYS:HB3	1:E:125:ASN:O	0.43	2.13	8	1
1:A:61:CYS:HB3	1:A:125:ASN:O	0.43	2.13	8	1
1:C:73:PHE:CD1	1:C:152:ALA:HB1	0.43	2.49	2	1
1:A:73:PHE:CD1	1:A:152:ALA:HB1	0.43	2.49	2	1
1:E:77:ALA:HB2	1:E:83:THR:HG23	0.43	1.90	2	1
1:C:92:ALA:HA	1:F:50:SER:HB2	0.43	1.89	6	1
1:D:5:VAL:CG1	1:F:146:GLY:HA2	0.43	2.44	6	1
1:A:106:ARG:CZ	1:A:132:PRO:HG2	0.43	2.44	6	1
1:D:106:ARG:CZ	1:D:132:PRO:HG2	0.43	2.44	6	1
1:A:6:ASN:CB	1:B:155:LYS:HE2	0.43	2.44	9	1
1:F:42:LEU:HB3	1:F:139:ALA:HB2	0.43	1.89	9	2
1:B:98:ASN:HA	1:B:140:THR:OG1	0.43	2.13	9	1
1:A:77:ALA:H	1:D:132:PRO:HB3	0.43	1.73	7	1
1:B:23:VAL:HG13	1:B:27:SER:HB3	0.43	1.89	7	1
1:C:103:ILE:HG12	1:C:113:LEU:HG	0.43	1.89	8	2
1:A:55:ASN:OD1	1:A:130:THR:CG2	0.43	2.66	8	1
1:F:55:ASN:OD1	1:F:130:THR:CG2	0.43	2.66	8	1
1:B:55:ASN:OD1	1:B:130:THR:CG2	0.43	2.66	8	1
1:E:73:PHE:CD1	1:E:152:ALA:HB1	0.43	2.49	2	1
1:A:89:GLN:CG	1:A:149:ASN:HB2	0.43	2.43	2	1
1:B:84:ASN:HB3	1:B:102:GLN:HG2	0.43	1.91	5	1
1:E:99:VAL:HB	1:E:143:ALA:HB1	0.43	1.90	5	1
1:A:86:LEU:HG	1:A:113:LEU:HD21	0.43	1.89	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:F:63:THR:HA	1:F:66:ALA:O	0.43	2.14	7	1
1:C:55:ASN:OD1	1:C:130:THR:CG2	0.43	2.66	8	1
1:B:61:CYS:HB3	1:B:125:ASN:O	0.43	2.14	8	1
1:D:107:THR:HB	1:D:120:SER:HA	0.43	1.91	10	1
1:C:51:ALA:CA	1:C:136:ARG:HB3	0.43	2.43	3	1
1:A:85:VAL:HG11	1:A:138:PHE:HB3	0.43	1.89	1	1
1:D:86:LEU:HG	1:D:113:LEU:HD21	0.43	1.89	6	1
1:C:9:THR:HA	1:D:153:THR:HG22	0.43	1.90	6	1
1:A:74:LEU:HD11	1:D:57:GLN:HG3	0.43	1.89	10	1
1:E:107:THR:HB	1:E:120:SER:HA	0.43	1.91	10	1
1:F:73:PHE:CD1	1:F:152:ALA:HB1	0.43	2.49	2	1
1:D:73:PHE:CD1	1:D:152:ALA:HB1	0.43	2.49	2	1
1:A:105:ASP:HB2	1:A:111:LEU:HB2	0.43	1.91	1	2
1:B:99:VAL:HB	1:B:143:ALA:HB1	0.43	1.90	5	1
1:B:63:THR:HA	1:B:66:ALA:O	0.43	2.14	7	1
1:F:22:ALA:HB3	1:F:59:ASN:O	0.43	2.13	7	1
1:D:15:GLU:HG3	1:E:147:ALA:HA	0.43	1.91	8	2
1:C:74:LEU:HD11	1:F:57:GLN:HG3	0.43	1.89	10	1
1:A:107:THR:HB	1:A:120:SER:HA	0.43	1.91	10	1
1:C:17:VAL:HG11	1:D:36:GLN:HE21	0.43	1.74	2	1
1:B:73:PHE:CD1	1:B:152:ALA:HB1	0.43	2.49	2	1
1:B:92:ALA:HB3	1:E:34:LEU:HB3	0.43	1.91	3	1
1:E:106:ARG:CZ	1:E:132:PRO:HG2	0.43	2.44	6	1
1:A:9:THR:HA	1:B:153:THR:HG22	0.43	1.90	6	1
1:B:118:PHE:CD1	1:B:157:GLN:HB2	0.43	2.48	8	1
1:E:15:GLU:HG3	1:F:147:ALA:HA	0.43	1.91	8	2
1:C:59:ASN:CA	1:C:128:THR:HG23	0.43	2.44	8	1
1:D:55:ASN:OD1	1:D:130:THR:CG2	0.43	2.66	8	1
1:F:89:GLN:HG3	1:F:149:ASN:HB2	0.42	1.91	1	1
1:A:89:GLN:HG3	1:A:149:ASN:HB2	0.42	1.91	1	1
1:A:5:VAL:CG1	1:C:146:GLY:HA2	0.42	2.44	6	1
1:C:106:ARG:CZ	1:C:132:PRO:HG2	0.42	2.44	6	1
1:E:6:ASN:CB	1:F:155:LYS:HE2	0.42	2.44	9	1
1:B:97:THR:N	1:B:144:THR:HB	0.42	2.26	4	1
1:F:61:CYS:HB3	1:F:125:ASN:O	0.42	2.13	8	1
1:A:144:THR:HG22	1:A:145:PRO:HD2	0.42	1.88	2	1
1:B:74:LEU:HD21	1:E:55:ASN:OD1	0.42	2.14	2	1
1:C:77:ALA:HB2	1:C:83:THR:HG23	0.42	1.90	2	1
1:F:51:ALA:HA	1:F:136:ARG:HB3	0.42	1.90	3	1
1:B:92:ALA:O	1:E:50:SER:HB3	0.42	2.14	1	1
1:E:59:ASN:CA	1:E:128:THR:HG23	0.42	2.44	8	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:4:THR:HG22	1:C:157:GLN:HB2	0.42	1.90	5	1
1:F:106:ARG:CZ	1:F:132:PRO:HG2	0.42	2.44	6	1
1:B:106:ARG:CZ	1:B:132:PRO:HG2	0.42	2.44	6	1
1:D:73:PHE:CB	1:D:111:LEU:HD11	0.42	2.44	9	1
1:A:73:PHE:CB	1:A:111:LEU:HD11	0.42	2.44	9	1
1:D:17:VAL:HG13	1:E:36:GLN:HG2	0.42	1.91	8	1
1:D:56:ILE:CG2	1:D:131:ILE:HD12	0.42	2.44	10	1
1:A:74:LEU:HD21	1:D:55:ASN:OD1	0.42	2.14	2	1
1:B:51:ALA:HA	1:B:136:ARG:HB3	0.42	1.90	3	1
1:A:92:ALA:HB3	1:D:34:LEU:HB3	0.42	1.91	3	1
1:B:89:GLN:HG3	1:B:149:ASN:HB2	0.42	1.91	1	1
1:C:92:ALA:HA	1:F:50:SER:HB3	0.42	1.91	5	1
1:D:99:VAL:HB	1:D:143:ALA:HB1	0.42	1.91	5	1
1:F:62:ASP:HA	1:F:126:ASN:OD1	0.42	2.15	6	2
1:B:62:ASP:HA	1:B:126:ASN:OD1	0.42	2.15	6	2
1:B:6:ASN:CB	1:C:155:LYS:HE2	0.42	2.44	9	1
1:A:131:ILE:CD1	1:A:156:VAL:HG12	0.42	2.44	4	1
1:A:17:VAL:HG23	1:B:38:ARG:HA	0.42	1.92	7	1
1:B:17:VAL:HG23	1:C:38:ARG:HA	0.42	1.91	7	1
1:E:63:THR:HA	1:E:66:ALA:O	0.42	2.14	7	1
1:E:118:PHE:CD1	1:E:157:GLN:HB2	0.42	2.48	8	1
1:B:4:THR:O	1:B:5:VAL:HG13	0.42	2.14	10	1
1:B:144:THR:HG22	1:B:145:PRO:HD2	0.42	1.88	2	1
1:B:17:VAL:HG11	1:C:36:GLN:HE21	0.42	1.74	2	1
1:B:59:ASN:CA	1:B:128:THR:HG23	0.42	2.44	8	2
1:A:99:VAL:HB	1:A:143:ALA:HB1	0.42	1.90	5	1
1:B:92:ALA:HA	1:E:50:SER:HB3	0.42	1.91	5	1
1:E:97:THR:N	1:E:144:THR:HB	0.42	2.26	4	1
1:F:131:ILE:CD1	1:F:156:VAL:HG12	0.42	2.45	4	1
1:E:17:VAL:HG23	1:F:38:ARG:HA	0.42	1.92	7	1
1:C:15:GLU:HG3	1:D:147:ALA:HA	0.42	1.91	8	1
1:B:86:LEU:CD1	1:B:152:ALA:HB2	0.42	2.45	10	1
1:F:56:ILE:CG2	1:F:131:ILE:HD12	0.42	2.44	10	1
1:E:17:VAL:HG11	1:F:36:GLN:HE21	0.42	1.74	2	1
1:B:105:ASP:HB2	1:B:111:LEU:HB2	0.42	1.91	1	2
1:F:24:ASP:HB3	1:F:27:SER:HB2	0.42	1.92	1	1
1:C:84:ASN:HB3	1:C:102:GLN:HG2	0.42	1.91	5	1
1:C:99:VAL:HB	1:C:143:ALA:HB1	0.42	1.90	5	1
1:E:131:ILE:CD1	1:E:156:VAL:HG12	0.42	2.45	4	1
1:D:17:VAL:HG23	1:E:38:ARG:HA	0.42	1.92	7	1
1:C:86:LEU:HG	1:C:113:LEU:HD22	0.42	1.92	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:103:ILE:HG12	1:D:113:LEU:HG	0.42	1.89	8	2
1:D:61:CYS:HB3	1:D:125:ASN:O	0.42	2.13	8	1
1:C:92:ALA:HB3	1:F:34:LEU:HB3	0.42	1.91	3	1
1:C:89:GLN:HG3	1:C:149:ASN:HB2	0.42	1.91	1	1
1:F:84:ASN:HB3	1:F:102:GLN:HG2	0.42	1.91	5	1
1:C:6:ASN:CB	1:D:155:LYS:HE2	0.42	2.44	9	1
1:A:63:THR:HA	1:A:66:ALA:O	0.42	2.14	7	1
1:C:5:VAL:CB	1:D:17:VAL:HG12	0.42	2.45	8	1
1:A:56:ILE:CG2	1:A:131:ILE:HD12	0.42	2.44	10	1
1:B:107:THR:HB	1:B:120:SER:HA	0.42	1.91	10	1
1:D:73:PHE:HB2	1:D:103:ILE:HD13	0.42	1.92	3	1
1:C:51:ALA:HA	1:C:136:ARG:HB3	0.42	1.90	3	1
1:D:89:GLN:HG3	1:D:149:ASN:HB2	0.42	1.91	1	1
1:C:24:ASP:HB3	1:C:27:SER:HB2	0.42	1.92	1	1
1:A:62:ASP:HA	1:A:126:ASN:OD1	0.42	2.15	6	2
1:D:73:PHE:HB3	1:D:113:LEU:HD23	0.42	1.92	4	1
1:E:5:VAL:CB	1:F:17:VAL:HG12	0.42	2.45	8	1
1:E:86:LEU:CD1	1:E:152:ALA:HB2	0.42	2.45	10	1
1:A:4:THR:O	1:A:5:VAL:HG13	0.42	2.14	10	1
1:A:77:ALA:HB2	1:A:83:THR:HG23	0.42	1.90	2	1
1:A:73:PHE:HB2	1:A:103:ILE:HD13	0.42	1.92	3	2
1:A:92:ALA:O	1:D:50:SER:HB3	0.42	2.14	1	1
1:B:5:VAL:CG1	1:D:146:GLY:HA2	0.42	2.44	6	1
1:D:62:ASP:HA	1:D:126:ASN:OD1	0.42	2.15	6	3
1:C:131:ILE:CD1	1:C:156:VAL:HG12	0.42	2.45	4	1
1:F:86:LEU:HG	1:F:113:LEU:HD22	0.42	1.92	8	1
1:E:4:THR:O	1:E:5:VAL:HG13	0.42	2.14	10	1
1:E:17:VAL:HG21	1:F:36:GLN:HE21	0.42	1.75	3	1
1:B:17:VAL:HG21	1:C:36:GLN:HE21	0.42	1.75	3	1
1:C:73:PHE:HB2	1:C:103:ILE:HD13	0.42	1.92	3	1
1:B:116:ALA:HA	1:E:128:THR:O	0.42	2.15	5	1
1:E:84:ASN:HB3	1:E:102:GLN:HG2	0.42	1.91	5	1
1:F:99:VAL:HB	1:F:143:ALA:CB	0.42	2.45	5	1
1:F:73:PHE:HB3	1:F:113:LEU:HD23	0.42	1.92	4	1
1:A:15:GLU:HG3	1:B:147:ALA:HA	0.42	1.91	8	1
1:A:17:VAL:HG13	1:B:36:GLN:HG2	0.42	1.91	8	1
1:F:59:ASN:CA	1:F:128:THR:HG23	0.42	2.44	8	1
1:C:56:ILE:CG2	1:C:131:ILE:HD12	0.42	2.44	10	1
1:C:74:LEU:HD21	1:F:55:ASN:OD1	0.42	2.14	2	1
1:F:77:ALA:HB2	1:F:83:THR:HG23	0.42	1.90	2	1
1:E:39:THR:OG1	1:E:143:ALA:O	0.42	2.33	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:24:ASP:HB3	1:D:27:SER:HB2	0.42	1.92	1	1
1:A:59:ASN:CA	1:A:128:THR:HG23	0.42	2.44	8	2
1:A:116:ALA:HA	1:D:128:THR:O	0.42	2.15	5	1
1:E:98:ASN:HA	1:E:140:THR:OG1	0.42	2.13	9	1
1:E:73:PHE:HB3	1:E:113:LEU:HD23	0.42	1.92	4	1
1:D:131:ILE:CD1	1:D:156:VAL:HG12	0.42	2.45	4	1
1:D:86:LEU:HG	1:D:113:LEU:HD22	0.42	1.92	8	1
1:C:107:THR:HB	1:C:120:SER:HA	0.42	1.91	10	1
1:A:92:ALA:HA	1:D:50:SER:HB3	0.41	1.91	5	1
1:C:56:ILE:CB	1:C:131:ILE:HD12	0.41	2.40	7	1
1:B:5:VAL:CB	1:C:17:VAL:HG12	0.41	2.45	8	1
1:E:17:VAL:HG13	1:F:36:GLN:HG2	0.41	1.91	8	1
1:B:56:ILE:CG2	1:B:131:ILE:HD12	0.41	2.44	10	1
1:E:56:ILE:CG2	1:E:131:ILE:HD12	0.41	2.44	10	1
1:F:73:PHE:HB2	1:F:103:ILE:HD13	0.41	1.92	3	1
1:A:84:ASN:HB3	1:A:102:GLN:HG2	0.41	1.91	5	1
1:B:89:GLN:OE1	1:B:91:SER:HB3	0.41	2.16	9	1
1:E:89:GLN:OE1	1:E:91:SER:HB3	0.41	2.16	9	1
1:B:131:ILE:CD1	1:B:156:VAL:HG12	0.41	2.45	4	1
1:C:17:VAL:HG13	1:D:36:GLN:HG2	0.41	1.91	8	1
1:F:4:THR:O	1:F:5:VAL:HG13	0.41	2.14	10	1
1:E:73:PHE:HB2	1:E:103:ILE:HD13	0.41	1.92	2	2
1:D:84:ASN:HB3	1:D:102:GLN:HG2	0.41	1.91	5	1
1:A:22:ALA:HA	1:B:36:GLN:CB	0.41	2.46	5	1
1:F:99:VAL:HB	1:F:143:ALA:HB1	0.41	1.90	5	1
1:E:4:THR:HG22	1:F:157:GLN:HB2	0.41	1.90	5	1
1:A:73:PHE:HB3	1:A:113:LEU:HD23	0.41	1.92	4	1
1:D:63:THR:HA	1:D:66:ALA:O	0.41	2.14	7	1
1:A:5:VAL:CB	1:B:17:VAL:HG12	0.41	2.45	8	1
1:C:49:SER:HB2	1:C:137:TYR:HB2	0.41	1.93	8	1
1:E:86:LEU:HD23	1:E:87:ALA:H	0.41	1.75	10	1
1:C:86:LEU:CD1	1:C:152:ALA:HB2	0.41	2.45	10	1
1:D:77:ALA:HB2	1:D:83:THR:HG23	0.41	1.90	2	1
1:A:17:VAL:HG21	1:B:36:GLN:HE21	0.41	1.75	3	1
1:C:92:ALA:O	1:F:50:SER:HB3	0.41	2.14	1	1
1:D:88:LEU:HD13	1:D:96:ALA:O	0.41	2.16	5	1
1:C:99:VAL:HB	1:C:143:ALA:CB	0.41	2.45	5	1
1:C:62:ASP:HA	1:C:126:ASN:OD1	0.41	2.15	6	2
1:F:75:GLY:C	1:F:113:LEU:HD23	0.41	2.36	9	1
1:A:89:GLN:OE1	1:A:91:SER:HB3	0.41	2.16	9	1
1:A:86:LEU:HG	1:A:113:LEU:HD22	0.41	1.92	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:86:LEU:HD23	1:C:87:ALA:H	0.41	1.75	10	1
1:D:4:THR:O	1:D:5:VAL:HG13	0.41	2.14	10	1
1:F:101:VAL:CG2	1:F:135:ALA:HB1	0.41	2.46	1	1
1:B:24:ASP:HB3	1:B:27:SER:HB2	0.41	1.92	1	1
1:A:24:ASP:HB3	1:A:27:SER:HB2	0.41	1.92	1	1
1:D:59:ASN:CA	1:D:128:THR:HG23	0.41	2.44	8	2
1:C:116:ALA:HA	1:F:128:THR:O	0.41	2.15	5	1
1:B:88:LEU:HD13	1:B:96:ALA:O	0.41	2.16	5	1
1:F:56:ILE:O	1:F:56:ILE:CG2	0.41	2.69	4	1
1:D:5:VAL:CB	1:E:17:VAL:HG12	0.41	2.45	8	1
1:D:1:ALA:HA	1:E:159:GLN:HA	0.41	1.93	8	1
1:E:49:SER:HB2	1:E:137:TYR:HB2	0.41	1.93	8	1
1:F:86:LEU:CD1	1:F:152:ALA:HB2	0.41	2.45	10	1
1:F:86:LEU:HD23	1:F:87:ALA:H	0.41	1.75	10	1
1:D:86:LEU:CD1	1:D:152:ALA:HB2	0.41	2.45	10	1
1:C:4:THR:O	1:C:5:VAL:HG13	0.41	2.14	10	1
1:D:17:VAL:HG21	1:E:36:GLN:HE21	0.41	1.75	3	1
1:B:101:VAL:CG2	1:B:135:ALA:HB1	0.41	2.46	1	1
1:D:58:LEU:HB2	1:D:129:ASN:O	0.41	2.15	5	1
1:E:88:LEU:HD13	1:E:96:ALA:O	0.41	2.16	5	1
1:D:22:ALA:HA	1:E:36:GLN:CB	0.41	2.46	5	1
1:F:88:LEU:HD13	1:F:96:ALA:O	0.41	2.15	5	1
1:B:99:VAL:HB	1:B:143:ALA:CB	0.41	2.45	5	1
1:A:99:VAL:HB	1:A:143:ALA:CB	0.41	2.45	5	1
1:E:62:ASP:HA	1:E:126:ASN:OD1	0.41	2.15	6	3
1:D:75:GLY:C	1:D:113:LEU:HD23	0.41	2.36	9	1
1:E:75:GLY:C	1:E:113:LEU:HD23	0.41	2.36	9	1
1:C:75:GLY:C	1:C:113:LEU:HD23	0.41	2.36	9	1
1:C:73:PHE:HB3	1:C:113:LEU:HD23	0.41	1.92	4	1
1:B:15:GLU:HG3	1:C:147:ALA:HA	0.41	1.91	8	2
1:E:58:LEU:O	1:E:61:CYS:SG	0.41	2.79	10	1
1:A:86:LEU:CD1	1:A:152:ALA:HB2	0.41	2.45	10	1
1:A:39:THR:OG1	1:A:143:ALA:O	0.41	2.37	4	2
1:B:73:PHE:HB2	1:B:103:ILE:HD13	0.41	1.93	2	2
1:E:24:ASP:HB3	1:E:27:SER:HB2	0.41	1.92	1	1
1:C:58:LEU:HB2	1:C:129:ASN:O	0.41	2.15	5	1
1:F:84:ASN:HA	1:F:113:LEU:HB3	0.41	1.93	5	1
1:C:88:LEU:HD13	1:C:96:ALA:O	0.41	2.15	5	1
1:B:22:ALA:HA	1:C:36:GLN:CB	0.41	2.46	5	1
1:D:56:ILE:O	1:D:56:ILE:CG2	0.41	2.69	4	1
1:B:73:PHE:HB3	1:B:113:LEU:HD23	0.41	1.92	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:CYS:HB3	1:A:58:LEU:HD22	0.41	1.93	7	1
1:B:86:LEU:HD23	1:B:87:ALA:H	0.41	1.75	10	1
1:A:17:VAL:HG11	1:B:36:GLN:HE21	0.41	1.74	2	1
1:A:45:GLU:HG3	1:A:140:THR:O	0.41	2.16	2	1
1:C:101:VAL:CG2	1:C:135:ALA:HB1	0.41	2.46	1	1
1:E:101:VAL:CG2	1:E:135:ALA:HB1	0.41	2.46	1	1
1:D:101:VAL:CG2	1:D:135:ALA:HB1	0.41	2.46	1	1
1:E:105:ASP:HB2	1:E:111:LEU:HB2	0.41	1.91	1	2
1:E:89:GLN:HG3	1:E:149:ASN:HB2	0.41	1.91	1	1
1:E:58:LEU:HB2	1:E:129:ASN:O	0.41	2.15	5	1
1:C:84:ASN:HA	1:C:113:LEU:HB3	0.41	1.93	5	1
1:C:89:GLN:OE1	1:C:91:SER:HB3	0.41	2.16	9	1
1:B:86:LEU:HD11	1:B:151:ASP:C	0.41	2.36	4	1
1:E:21:CYS:HB3	1:E:58:LEU:HD22	0.41	1.93	7	1
1:B:89:GLN:O	1:E:52:VAL:HA	0.41	2.16	7	1
1:A:101:VAL:CG2	1:A:135:ALA:HB1	0.41	2.46	1	1
1:C:79:ASP:HB2	1:C:140:THR:HG21	0.41	1.93	10	2
1:E:22:ALA:HA	1:F:36:GLN:CB	0.41	2.46	5	1
1:A:88:LEU:HD13	1:A:96:ALA:O	0.41	2.16	5	1
1:E:99:VAL:HB	1:E:143:ALA:CB	0.41	2.45	5	1
1:C:85:VAL:HG22	1:C:102:GLN:HG3	0.41	1.93	9	1
1:B:85:VAL:HG22	1:B:102:GLN:HG3	0.41	1.93	9	1
1:F:89:GLN:OE1	1:F:91:SER:HB3	0.41	2.16	9	1
1:D:89:GLN:OE1	1:D:91:SER:HB3	0.41	2.16	9	1
1:C:86:LEU:HD11	1:C:151:ASP:C	0.41	2.36	4	1
1:B:21:CYS:HB3	1:B:58:LEU:HD22	0.41	1.93	7	1
1:D:21:CYS:HB3	1:D:58:LEU:HD22	0.41	1.93	7	1
1:C:52:VAL:HG23	1:C:54:PHE:HD1	0.41	1.76	7	1
1:A:58:LEU:O	1:A:61:CYS:SG	0.41	2.79	10	1
1:B:58:LEU:O	1:B:61:CYS:SG	0.41	2.79	10	1
1:F:107:THR:HB	1:F:120:SER:HA	0.41	1.90	10	1
1:D:32:VAL:CG1	1:D:52:VAL:HG11	0.41	2.46	6	1
1:C:84:ASN:O	1:C:103:ILE:HD12	0.41	2.16	9	1
1:B:17:VAL:HG13	1:C:36:GLN:HG2	0.41	1.91	8	1
1:C:1:ALA:HA	1:D:159:GLN:HA	0.41	1.93	8	1
1:D:49:SER:HB2	1:D:137:TYR:HB2	0.41	1.93	8	1
1:B:18:ASN:HA	1:C:39:THR:HG22	0.41	1.93	2	1
1:F:79:ASP:HB2	1:F:140:THR:HG21	0.40	1.93	1	2
1:A:58:LEU:HB2	1:A:129:ASN:O	0.40	2.15	5	1
1:D:99:VAL:HB	1:D:143:ALA:CB	0.40	2.45	5	1
1:C:111:LEU:HD11	1:C:117:THR:O	0.40	2.16	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:E:32:VAL:CG1	1:E:52:VAL:HG11	0.40	2.46	6	1
1:C:58:LEU:O	1:C:61:CYS:SG	0.40	2.79	10	1
1:A:144:THR:HG22	1:A:145:PRO:N	0.40	2.31	2	1
1:F:42:LEU:HD23	1:F:99:VAL:CG1	0.40	2.46	2	1
1:E:18:ASN:HA	1:F:39:THR:HG22	0.40	1.93	2	1
1:C:17:VAL:HG21	1:D:36:GLN:HE21	0.40	1.75	3	1
1:F:58:LEU:HB2	1:F:129:ASN:O	0.40	2.15	5	1
1:F:97:THR:O	1:F:99:VAL:HG12	0.40	2.17	6	1
1:F:84:ASN:O	1:F:103:ILE:HD12	0.40	2.17	9	1
1:D:85:VAL:HG22	1:D:102:GLN:HG3	0.40	1.93	9	1
1:B:7:GLY:HA3	1:C:154:PHE:CZ	0.40	2.51	7	1
1:C:89:GLN:O	1:F:52:VAL:HA	0.40	2.16	7	1
1:D:58:LEU:O	1:D:61:CYS:SG	0.40	2.79	10	1
1:B:21:CYS:HB3	1:B:158:TYR:OH	0.40	2.16	10	1
1:A:86:LEU:HD23	1:A:87:ALA:H	0.40	1.75	10	1
1:F:52:VAL:O	1:F:134:GLN:HA	0.40	2.16	10	1
1:B:52:VAL:O	1:B:134:GLN:HA	0.40	2.16	10	1
1:C:12:PHE:CD1	1:D:34:LEU:HD11	0.40	2.52	10	1
1:B:42:LEU:HD23	1:B:99:VAL:CG1	0.40	2.46	2	1
1:E:45:GLU:HG3	1:E:140:THR:O	0.40	2.16	2	1
1:B:58:LEU:HB2	1:B:129:ASN:O	0.40	2.15	5	1
1:B:155:LYS:CE	1:E:128:THR:HG21	0.40	2.47	6	1
1:B:32:VAL:CG1	1:B:52:VAL:HG11	0.40	2.46	6	1
1:B:75:GLY:C	1:B:113:LEU:HD23	0.40	2.36	9	1
1:E:85:VAL:HG22	1:E:102:GLN:HG3	0.40	1.93	9	1
1:B:116:ALA:HB3	1:E:125:ASN:HB3	0.40	1.94	9	1
1:A:86:LEU:HD11	1:A:151:ASP:C	0.40	2.36	4	1
1:D:86:LEU:HD11	1:D:151:ASP:C	0.40	2.36	4	1
1:C:56:ILE:CG2	1:C:56:ILE:O	0.40	2.69	4	1
1:E:78:ILE:HG22	1:E:82:HIS:HB3	0.40	1.94	4	1
1:C:17:VAL:HG23	1:D:38:ARG:HA	0.40	1.92	7	1
1:E:7:GLY:HA3	1:F:154:PHE:CZ	0.40	2.51	7	1
1:E:86:LEU:HG	1:E:113:LEU:HD22	0.40	1.92	8	1
1:D:12:PHE:CD1	1:E:34:LEU:HD11	0.40	2.52	10	1
1:C:144:THR:HG22	1:C:145:PRO:N	0.40	2.31	2	1
1:D:85:VAL:HG21	1:D:138:PHE:HB3	0.40	1.93	2	1
1:C:10:VAL:HG13	1:D:32:VAL:HG23	0.40	1.94	3	1
1:C:22:ALA:HA	1:D:36:GLN:CB	0.40	2.46	5	1
1:C:155:LYS:CE	1:F:128:THR:HG21	0.40	2.47	6	1
1:E:86:LEU:HD11	1:E:151:ASP:C	0.40	2.36	4	1
1:D:78:ILE:HG22	1:D:82:HIS:HB3	0.40	1.94	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:21:CYS:HB3	1:C:58:LEU:HD22	0.40	1.93	7	1
1:F:21:CYS:HB3	1:F:58:LEU:HD22	0.40	1.93	7	1
1:E:52:VAL:O	1:E:134:GLN:HA	0.40	2.16	10	1
1:A:12:PHE:CD1	1:B:34:LEU:HD11	0.40	2.51	10	1
1:F:144:THR:HG22	1:F:145:PRO:N	0.40	2.31	2	1
1:F:97:THR:HB	1:F:144:THR:OG1	0.40	2.17	2	1
1:E:144:THR:HG22	1:E:145:PRO:N	0.40	2.32	2	1
1:E:97:THR:HB	1:E:144:THR:OG1	0.40	2.17	2	1
1:D:131:ILE:HD13	1:D:156:VAL:HG11	0.40	1.94	5	1
1:F:131:ILE:HD13	1:F:156:VAL:HG11	0.40	1.93	5	1
1:C:97:THR:O	1:C:99:VAL:HG12	0.40	2.17	6	1
1:A:75:GLY:C	1:A:113:LEU:HD23	0.40	2.36	9	1
1:B:84:ASN:O	1:B:103:ILE:HD12	0.40	2.17	9	1
1:A:78:ILE:HG22	1:A:85:VAL:HB	0.40	1.93	9	1
1:F:86:LEU:HD11	1:F:151:ASP:C	0.40	2.36	4	1
1:B:39:THR:OG1	1:B:143:ALA:O	0.40	2.37	4	1
1:A:56:ILE:O	1:A:56:ILE:CG2	0.40	2.69	4	1
1:C:78:ILE:HG22	1:C:82:HIS:HB3	0.40	1.94	4	1
1:B:72:ALA:HA	1:B:117:THR:O	0.40	2.17	7	1
1:E:72:ALA:HA	1:E:117:THR:O	0.40	2.17	7	1
1:F:52:VAL:HG23	1:F:54:PHE:HD1	0.40	1.76	7	1
1:D:52:VAL:O	1:D:134:GLN:HA	0.40	2.16	10	1
1:C:97:THR:HB	1:C:144:THR:OG1	0.40	2.17	2	1
1:C:18:ASN:HA	1:D:39:THR:HG22	0.40	1.93	2	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	157/160 (98%)	135±4 (86±2%)	19±4 (12±3%)	4±2 (2±1%)	12	49
1	B	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	12	49
1	C	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	12	49
1	D	157/160 (98%)	135±4 (86±2%)	19±4 (12±3%)	4±2 (2±1%)	12	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	12	49
1	F	157/160 (98%)	135±4 (86±2%)	18±4 (12±3%)	4±2 (2±1%)	12	49
All	All	9420/9600 (98%)	8088 (86%)	1106 (12%)	226 (2%)	12	49

All 90 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	90	SER	6
1	C	80	ALA	6
1	E	80	ALA	6
1	E	90	SER	6
1	A	80	ALA	6
1	F	80	ALA	6
1	C	90	SER	6
1	B	80	ALA	6
1	B	90	SER	6
1	A	90	SER	6
1	F	90	SER	6
1	D	80	ALA	6
1	F	89	GLN	5
1	D	94	GLY	5
1	A	89	GLN	5
1	F	94	GLY	5
1	B	89	GLN	5
1	E	89	GLN	5
1	E	94	GLY	5
1	A	94	GLY	5
1	D	89	GLN	5
1	C	89	GLN	5
1	C	94	GLY	5
1	B	94	GLY	5
1	A	2	ALA	4
1	F	2	ALA	4
1	D	2	ALA	4
1	B	2	ALA	4
1	C	2	ALA	4
1	E	2	ALA	4
1	B	142	ALA	2
1	D	142	ALA	2
1	C	142	ALA	2
1	A	142	ALA	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	E	19	ALA	2
1	F	19	ALA	2
1	B	19	ALA	2
1	F	142	ALA	2
1	C	19	ALA	2
1	E	142	ALA	2
1	B	60	ASP	1
1	D	99	VAL	1
1	E	21	CYS	1
1	D	19	ALA	1
1	F	20	ALA	1
1	E	141	GLY	1
1	A	28	VAL	1
1	C	83	THR	1
1	D	20	ALA	1
1	D	141	GLY	1
1	B	28	VAL	1
1	D	60	ASP	1
1	D	65	VAL	1
1	E	60	ASP	1
1	C	65	VAL	1
1	A	83	THR	1
1	A	65	VAL	1
1	C	99	VAL	1
1	D	21	CYS	1
1	F	99	VAL	1
1	F	65	VAL	1
1	A	20	ALA	1
1	F	28	VAL	1
1	A	60	ASP	1
1	E	83	THR	1
1	E	99	VAL	1
1	A	21	CYS	1
1	F	60	ASP	1
1	F	83	THR	1
1	C	28	VAL	1
1	B	21	CYS	1
1	E	28	VAL	1
1	B	99	VAL	1
1	E	65	VAL	1
1	C	141	GLY	1
1	C	20	ALA	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	99	VAL	1
1	F	141	GLY	1
1	C	21	CYS	1
1	B	141	GLY	1
1	E	20	ALA	1
1	D	83	THR	1
1	A	19	ALA	1
1	F	21	CYS	1
1	A	141	GLY	1
1	D	28	VAL	1
1	B	65	VAL	1
1	C	60	ASP	1
1	B	20	ALA	1
1	B	83	THR	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	112/113 (99%)	72±4 (64±3%)	40±4 (36±3%)	1	9
1	B	112/113 (99%)	72±4 (64±3%)	40±4 (36±3%)	1	9
1	C	112/113 (99%)	72±4 (64±3%)	40±4 (36±3%)	1	9
1	D	112/113 (99%)	72±4 (64±3%)	40±4 (36±3%)	1	9
1	E	112/113 (99%)	72±4 (64±3%)	40±4 (36±3%)	1	9
1	F	112/113 (99%)	72±4 (64±3%)	40±4 (36±3%)	1	9
All	All	6720/6780 (99%)	4320 (64%)	2400 (36%)	1	9

All 564 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	B	133	PHE	10
1	A	133	PHE	10
1	D	133	PHE	10
1	E	79	ASP	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	79	ASP	10
1	D	79	ASP	10
1	E	133	PHE	10
1	F	133	PHE	10
1	F	79	ASP	10
1	A	79	ASP	10
1	B	79	ASP	10
1	C	133	PHE	10
1	E	76	THR	9
1	E	21	CYS	9
1	C	122	THR	9
1	D	86	LEU	9
1	D	21	CYS	9
1	D	122	THR	9
1	B	76	THR	9
1	B	21	CYS	9
1	A	122	THR	9
1	B	122	THR	9
1	E	122	THR	9
1	F	86	LEU	9
1	B	86	LEU	9
1	F	76	THR	9
1	C	86	LEU	9
1	F	21	CYS	9
1	D	76	THR	9
1	F	122	THR	9
1	C	21	CYS	9
1	A	21	CYS	9
1	E	86	LEU	9
1	C	76	THR	9
1	A	76	THR	9
1	A	86	LEU	9
1	B	130	THR	8
1	D	130	THR	8
1	E	130	THR	8
1	C	58	LEU	8
1	A	58	LEU	8
1	C	130	THR	8
1	E	140	THR	8
1	C	140	THR	8
1	E	58	LEU	8
1	A	140	THR	8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	F	140	THR	8
1	A	130	THR	8
1	F	58	LEU	8
1	B	58	LEU	8
1	D	140	THR	8
1	F	130	THR	8
1	B	140	THR	8
1	D	58	LEU	8
1	B	74	LEU	7
1	A	106	ARG	7
1	B	103	ILE	7
1	F	31	THR	7
1	C	120	SER	7
1	D	103	ILE	7
1	F	103	ILE	7
1	B	67	SER	7
1	D	74	LEU	7
1	C	114	ASP	7
1	D	63	THR	7
1	F	67	SER	7
1	E	106	ARG	7
1	D	41	SER	7
1	D	73	PHE	7
1	E	31	THR	7
1	A	67	SER	7
1	E	114	ASP	7
1	B	73	PHE	7
1	C	103	ILE	7
1	D	120	SER	7
1	B	63	THR	7
1	F	63	THR	7
1	C	67	SER	7
1	D	31	THR	7
1	E	120	SER	7
1	F	120	SER	7
1	F	73	PHE	7
1	A	73	PHE	7
1	E	103	ILE	7
1	E	41	SER	7
1	E	67	SER	7
1	A	74	LEU	7
1	F	74	LEU	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	F	41	SER	7
1	C	74	LEU	7
1	C	73	PHE	7
1	A	31	THR	7
1	B	120	SER	7
1	B	41	SER	7
1	A	114	ASP	7
1	C	31	THR	7
1	C	63	THR	7
1	A	63	THR	7
1	A	120	SER	7
1	B	31	THR	7
1	A	41	SER	7
1	E	63	THR	7
1	C	106	ARG	7
1	C	41	SER	7
1	D	106	ARG	7
1	A	103	ILE	7
1	D	67	SER	7
1	E	74	LEU	7
1	D	114	ASP	7
1	F	106	ARG	7
1	B	106	ARG	7
1	F	114	ASP	7
1	E	73	PHE	7
1	B	114	ASP	7
1	F	44	GLN	6
1	A	154	PHE	6
1	E	117	THR	6
1	F	102	GLN	6
1	F	117	THR	6
1	E	57	GLN	6
1	C	104	LEU	6
1	E	88	LEU	6
1	A	137	TYR	6
1	E	44	GLN	6
1	A	104	LEU	6
1	D	44	GLN	6
1	C	102	GLN	6
1	A	89	GLN	6
1	A	157	GLN	6
1	B	157	GLN	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	62	ASP	6
1	B	89	GLN	6
1	E	137	TYR	6
1	E	153	THR	6
1	E	62	ASP	6
1	D	157	GLN	6
1	D	62	ASP	6
1	D	89	GLN	6
1	C	89	GLN	6
1	D	153	THR	6
1	F	157	GLN	6
1	C	154	PHE	6
1	A	117	THR	6
1	F	89	GLN	6
1	F	88	LEU	6
1	F	104	LEU	6
1	D	102	GLN	6
1	C	157	GLN	6
1	A	88	LEU	6
1	C	137	TYR	6
1	B	88	LEU	6
1	D	104	LEU	6
1	E	157	GLN	6
1	A	153	THR	6
1	A	102	GLN	6
1	F	137	TYR	6
1	E	102	GLN	6
1	C	44	GLN	6
1	B	62	ASP	6
1	D	154	PHE	6
1	C	117	THR	6
1	B	104	LEU	6
1	D	117	THR	6
1	B	102	GLN	6
1	C	153	THR	6
1	C	88	LEU	6
1	A	44	GLN	6
1	F	153	THR	6
1	B	117	THR	6
1	D	57	GLN	6
1	B	137	TYR	6
1	F	154	PHE	6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	57	GLN	6
1	A	62	ASP	6
1	F	62	ASP	6
1	B	44	GLN	6
1	B	154	PHE	6
1	C	57	GLN	6
1	D	88	LEU	6
1	E	154	PHE	6
1	E	89	GLN	6
1	B	153	THR	6
1	F	57	GLN	6
1	E	104	LEU	6
1	A	57	GLN	6
1	D	137	TYR	6
1	B	60	ASP	5
1	A	42	LEU	5
1	A	97	THR	5
1	A	124	LEU	5
1	C	83	THR	5
1	D	29	ASP	5
1	B	138	PHE	5
1	F	42	LEU	5
1	A	83	THR	5
1	A	34	LEU	5
1	A	60	ASP	5
1	C	159	GLN	5
1	A	13	LYS	5
1	C	13	LYS	5
1	E	124	LEU	5
1	E	13	LYS	5
1	B	159	GLN	5
1	F	124	LEU	5
1	E	33	GLN	5
1	F	68	LYS	5
1	D	13	LYS	5
1	C	60	ASP	5
1	B	124	LEU	5
1	F	95	SER	5
1	E	97	THR	5
1	B	42	LEU	5
1	C	97	THR	5
1	B	34	LEU	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	F	29	ASP	5
1	D	34	LEU	5
1	D	60	ASP	5
1	C	29	ASP	5
1	D	124	LEU	5
1	A	68	LYS	5
1	E	83	THR	5
1	F	97	THR	5
1	E	95	SER	5
1	C	33	GLN	5
1	F	13	LYS	5
1	F	83	THR	5
1	B	97	THR	5
1	E	60	ASP	5
1	D	33	GLN	5
1	C	34	LEU	5
1	A	138	PHE	5
1	E	29	ASP	5
1	C	42	LEU	5
1	D	112	THR	5
1	B	112	THR	5
1	E	68	LYS	5
1	F	112	THR	5
1	C	112	THR	5
1	B	33	GLN	5
1	B	29	ASP	5
1	D	95	SER	5
1	D	138	PHE	5
1	A	29	ASP	5
1	F	34	LEU	5
1	A	95	SER	5
1	D	159	GLN	5
1	C	124	LEU	5
1	D	68	LYS	5
1	C	68	LYS	5
1	C	138	PHE	5
1	E	138	PHE	5
1	D	97	THR	5
1	B	95	SER	5
1	C	95	SER	5
1	A	112	THR	5
1	E	159	GLN	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	33	GLN	5
1	F	138	PHE	5
1	B	68	LYS	5
1	E	34	LEU	5
1	F	33	GLN	5
1	F	60	ASP	5
1	A	159	GLN	5
1	E	112	THR	5
1	D	42	LEU	5
1	E	42	LEU	5
1	D	83	THR	5
1	F	159	GLN	5
1	B	13	LYS	5
1	B	83	THR	5
1	A	59	ASN	4
1	B	5	VAL	4
1	F	23	VAL	4
1	B	18	ASN	4
1	C	18	ASN	4
1	E	38	ARG	4
1	F	59	ASN	4
1	B	59	ASN	4
1	E	39	THR	4
1	E	5	VAL	4
1	D	59	ASN	4
1	F	5	VAL	4
1	A	18	ASN	4
1	C	23	VAL	4
1	C	38	ARG	4
1	D	18	ASN	4
1	C	39	THR	4
1	F	18	ASN	4
1	A	23	VAL	4
1	A	38	ARG	4
1	A	39	THR	4
1	D	39	THR	4
1	E	18	ASN	4
1	D	23	VAL	4
1	D	5	VAL	4
1	F	38	ARG	4
1	C	5	VAL	4
1	C	59	ASN	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	39	THR	4
1	B	38	ARG	4
1	B	23	VAL	4
1	F	39	THR	4
1	D	38	ARG	4
1	E	59	ASN	4
1	E	23	VAL	4
1	A	5	VAL	4
1	A	119	SER	3
1	A	64	ASN	3
1	A	156	VAL	3
1	B	64	ASN	3
1	B	126	ASN	3
1	E	64	ASN	3
1	C	119	SER	3
1	B	156	VAL	3
1	E	15	GLU	3
1	C	126	ASN	3
1	F	27	SER	3
1	A	90	SER	3
1	C	64	ASN	3
1	E	126	ASN	3
1	C	91	SER	3
1	C	125	ASN	3
1	D	15	GLU	3
1	B	27	SER	3
1	D	64	ASN	3
1	A	126	ASN	3
1	D	90	SER	3
1	F	156	VAL	3
1	C	99	VAL	3
1	F	99	VAL	3
1	F	125	ASN	3
1	C	90	SER	3
1	B	15	GLU	3
1	E	119	SER	3
1	E	156	VAL	3
1	A	27	SER	3
1	D	125	ASN	3
1	A	125	ASN	3
1	F	126	ASN	3
1	E	125	ASN	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	D	156	VAL	3
1	A	4	THR	3
1	C	156	VAL	3
1	D	119	SER	3
1	E	78	ILE	3
1	D	99	VAL	3
1	E	90	SER	3
1	F	64	ASN	3
1	C	27	SER	3
1	F	4	THR	3
1	C	15	GLU	3
1	B	99	VAL	3
1	F	91	SER	3
1	A	78	ILE	3
1	A	99	VAL	3
1	B	90	SER	3
1	F	90	SER	3
1	D	78	ILE	3
1	D	126	ASN	3
1	F	15	GLU	3
1	E	27	SER	3
1	A	15	GLU	3
1	D	91	SER	3
1	D	4	THR	3
1	B	4	THR	3
1	C	4	THR	3
1	E	91	SER	3
1	B	125	ASN	3
1	C	78	ILE	3
1	B	78	ILE	3
1	F	78	ILE	3
1	E	99	VAL	3
1	B	119	SER	3
1	E	4	THR	3
1	A	91	SER	3
1	B	91	SER	3
1	F	119	SER	3
1	D	27	SER	3
1	B	56	ILE	2
1	C	123	THR	2
1	E	155	LYS	2
1	B	84	ASN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	D	85	VAL	2
1	C	82	HIS	2
1	C	131	ILE	2
1	D	9	THR	2
1	A	105	ASP	2
1	A	3	THR	2
1	B	155	LYS	2
1	A	113	LEU	2
1	D	84	ASN	2
1	C	9	THR	2
1	D	56	ILE	2
1	E	56	ILE	2
1	C	17	VAL	2
1	E	17	VAL	2
1	C	111	LEU	2
1	D	101	VAL	2
1	F	56	ILE	2
1	B	111	LEU	2
1	A	82	HIS	2
1	B	123	THR	2
1	B	50	SER	2
1	F	82	HIS	2
1	B	82	HIS	2
1	F	17	VAL	2
1	F	85	VAL	2
1	B	17	VAL	2
1	E	84	ASN	2
1	C	101	VAL	2
1	F	113	LEU	2
1	C	155	LYS	2
1	E	111	LEU	2
1	A	17	VAL	2
1	A	9	THR	2
1	E	131	ILE	2
1	D	136	ARG	2
1	D	105	ASP	2
1	D	50	SER	2
1	B	101	VAL	2
1	F	36	GLN	2
1	A	111	LEU	2
1	C	85	VAL	2
1	B	36	GLN	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	E	113	LEU	2
1	A	50	SER	2
1	C	113	LEU	2
1	C	50	SER	2
1	C	36	GLN	2
1	B	113	LEU	2
1	A	36	GLN	2
1	A	56	ILE	2
1	A	84	ASN	2
1	B	9	THR	2
1	F	105	ASP	2
1	E	82	HIS	2
1	A	155	LYS	2
1	E	36	GLN	2
1	D	113	LEU	2
1	A	123	THR	2
1	F	84	ASN	2
1	F	3	THR	2
1	C	136	ARG	2
1	A	131	ILE	2
1	E	123	THR	2
1	D	36	GLN	2
1	C	56	ILE	2
1	B	3	THR	2
1	D	82	HIS	2
1	F	136	ARG	2
1	F	50	SER	2
1	F	155	LYS	2
1	B	131	ILE	2
1	B	136	ARG	2
1	A	101	VAL	2
1	D	111	LEU	2
1	E	50	SER	2
1	E	105	ASP	2
1	C	84	ASN	2
1	A	85	VAL	2
1	B	85	VAL	2
1	D	155	LYS	2
1	E	3	THR	2
1	C	3	THR	2
1	E	101	VAL	2
1	F	123	THR	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	E	85	VAL	2
1	D	17	VAL	2
1	C	105	ASP	2
1	F	131	ILE	2
1	F	111	LEU	2
1	B	105	ASP	2
1	E	136	ARG	2
1	F	101	VAL	2
1	A	136	ARG	2
1	F	9	THR	2
1	E	9	THR	2
1	D	3	THR	2
1	D	131	ILE	2
1	D	123	THR	2
1	A	16	VAL	1
1	E	32	VAL	1
1	D	32	VAL	1
1	A	12	PHE	1
1	C	144	THR	1
1	A	134	GLN	1
1	A	30	GLN	1
1	A	71	VAL	1
1	C	49	SER	1
1	F	10	VAL	1
1	B	12	PHE	1
1	F	37	VAL	1
1	F	71	VAL	1
1	D	24	ASP	1
1	F	149	ASN	1
1	E	134	GLN	1
1	B	134	GLN	1
1	D	149	ASN	1
1	B	30	GLN	1
1	D	144	THR	1
1	B	61	CYS	1
1	A	107	THR	1
1	E	71	VAL	1
1	A	24	ASP	1
1	A	37	VAL	1
1	C	12	PHE	1
1	B	24	ASP	1
1	E	30	GLN	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	24	ASP	1
1	C	107	THR	1
1	C	37	VAL	1
1	D	37	VAL	1
1	E	144	THR	1
1	D	107	THR	1
1	B	32	VAL	1
1	D	30	GLN	1
1	B	71	VAL	1
1	D	49	SER	1
1	E	37	VAL	1
1	D	134	GLN	1
1	E	49	SER	1
1	F	24	ASP	1
1	A	32	VAL	1
1	D	16	VAL	1
1	F	49	SER	1
1	F	107	THR	1
1	E	24	ASP	1
1	C	71	VAL	1
1	B	37	VAL	1
1	F	30	GLN	1
1	C	16	VAL	1
1	F	61	CYS	1
1	E	16	VAL	1
1	A	144	THR	1
1	E	107	THR	1
1	C	10	VAL	1
1	C	30	GLN	1
1	A	61	CYS	1
1	C	61	CYS	1
1	E	12	PHE	1
1	C	134	GLN	1
1	A	10	VAL	1
1	E	149	ASN	1
1	D	71	VAL	1
1	E	10	VAL	1
1	F	134	GLN	1
1	B	49	SER	1
1	C	149	ASN	1
1	D	10	VAL	1
1	E	61	CYS	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	F	32	VAL	1
1	D	61	CYS	1
1	B	16	VAL	1
1	F	12	PHE	1
1	F	144	THR	1
1	D	12	PHE	1
1	A	149	ASN	1
1	A	49	SER	1
1	C	32	VAL	1
1	B	149	ASN	1
1	B	10	VAL	1
1	B	144	THR	1
1	F	16	VAL	1
1	B	107	THR	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 8% for the well-defined parts and 8% for the entire structure.

7.1 Chemical shift list 1

File name: 2n7h_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	800
Number of shifts mapped to atoms	800
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	159	0.24 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	143	-0.41 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}'$	159	0.53 ± 0.13	Should be applied
^{15}N	159	0.45 ± 0.48	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 8%, i.e. 764 atoms were assigned a chemical shift out of a possible 9905. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	472/4741 (10%)	0/1894 (0%)	316/1906 (17%)	156/941 (17%)
Sidechain	280/4606 (6%)	0/2597 (0%)	278/1811 (15%)	2/198 (1%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	12/558 (2%)	0/306 (0%)	12/240 (5%)	0/12 (0%)
Overall	764/9905 (8%)	0/4797 (0%)	606/3957 (15%)	158/1151 (14%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 768 atoms were assigned a chemical shift out of a possible 9912. 0 out of 150 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	475/4746 (10%)	0/1896 (0%)	318/1908 (17%)	157/942 (17%)
Sidechain	281/4608 (6%)	0/2598 (0%)	279/1812 (15%)	2/198 (1%)
Aromatic	12/558 (2%)	0/306 (0%)	12/240 (5%)	0/12 (0%)
Overall	768/9912 (8%)	0/4800 (0%)	609/3960 (15%)	159/1152 (14%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

