Full wwPDB NMR Structure Validation Report (i)

Jun 15, 2024 – 09:38 AM EDT

PDB ID	:	2JSF
Title	:	Solution structures of the envelope protein domain III from the dengue-2 virus
Authors	:	Huang, K.; Cheng, J.
Deposited on	:	2007-07-03

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

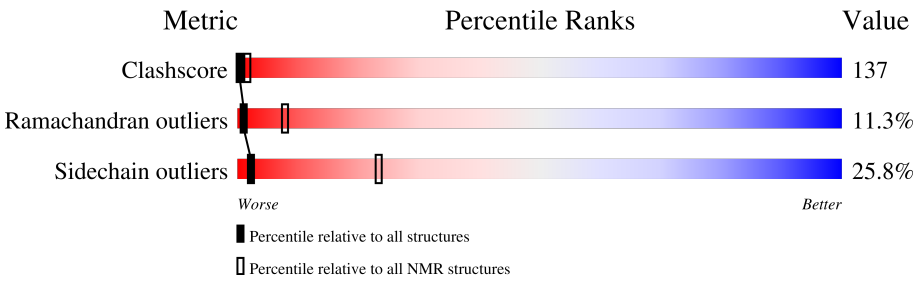
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	117	

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:14-A:51, A:61-A:84, A:89-A:103 (77)	0.41	17

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

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

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

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1868 atoms, of which 936 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called domain III of ENVELOPE PROTEIN E.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	117	1868	595	936	161	170	6	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	-	EXPRESSION TAG	UNP P18356
A	111	GLU	-	EXPRESSION TAG	UNP P18356
A	112	HIS	-	EXPRESSION TAG	UNP P18356
A	113	HIS	-	EXPRESSION TAG	UNP P18356
A	114	HIS	-	EXPRESSION TAG	UNP P18356
A	115	HIS	-	EXPRESSION TAG	UNP P18356
A	116	HIS	-	EXPRESSION TAG	UNP P18356
A	117	HIS	-	EXPRESSION TAG	UNP P18356

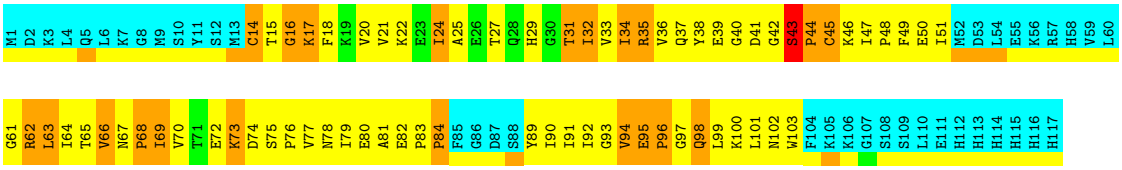
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: domain III of ENVELOPE PROTEIN E

Chain A: 5% 42% 18% • 34%



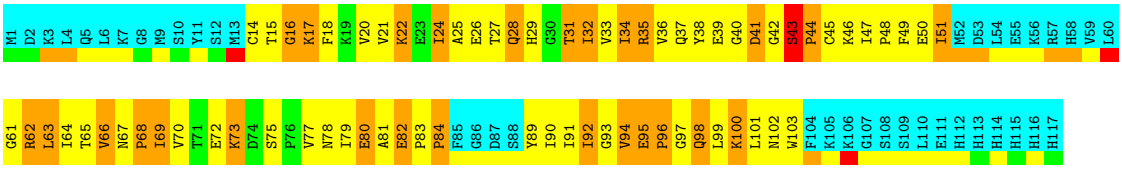
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: domain III of ENVELOPE PROTEIN E

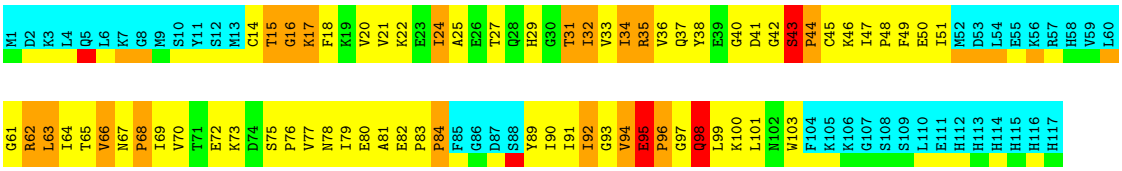
Chain A: 5% 37% 23% • 34%



4.2.2 Score per residue for model 2

• Molecule 1: domain III of ENVELOPE PROTEIN E

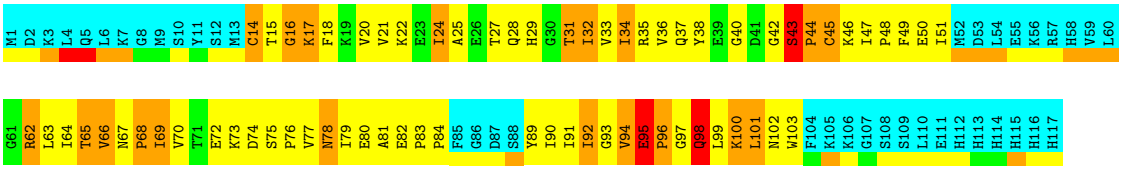
Chain A: 8% 41% 15% • 34%



4.2.3 Score per residue for model 3

- Molecule 1: domain III of ENVELOPE PROTEIN E

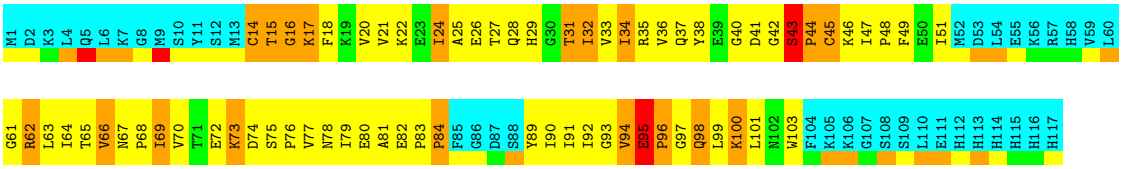
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A:



4.2.5 Score per residue for model 5

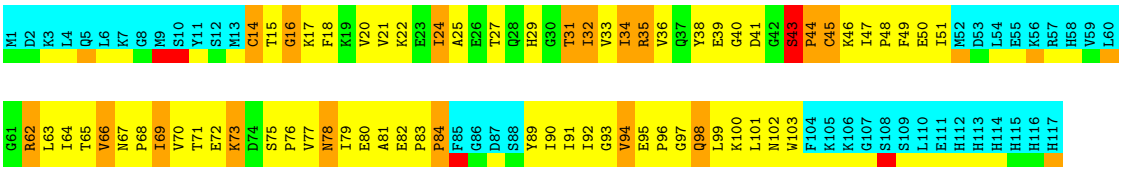
- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A:

4.2.6 Score per residue for model 6

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A:



4.2.7 Score per residue for model 7

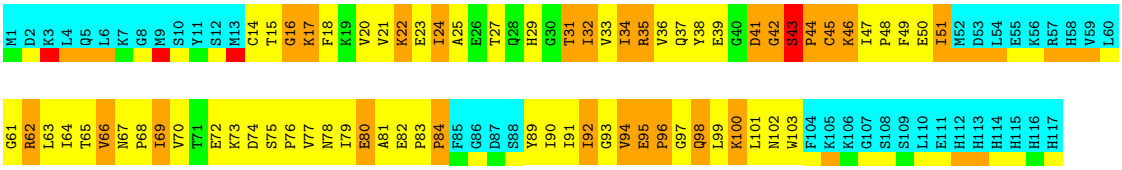
- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A:

4.2.8 Score per residue for model 8

- Molecule 1: domain III of ENVELOPE PROTEIN E

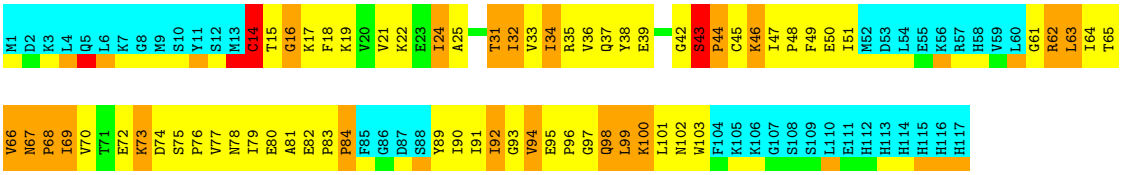
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A: 5% 39% 20% • 34%

M1 D2 K3 L4 Q5 L6 K7 G8 M9 S10 Y11 S12 M13 C14 T15 G16 K17 F18 K19 V20 V21 K22 E23 I24 A25 E26 T27 Q28 H29 G30 T31 I32 V33 I34 R35 V36 Q37 Y38 E39 G40 D41 G42 S43 P44 C45 K46 I47 P48 F49 E50 I51 M52 D53 L54 E55 K56 R57 H58 V59 L60

G61 R62 L63 I64 T65 V66 N67 P68 I69 V70 T71 E72 K73 D74 S75 P76 V77 N78 I79 E80 A81 E82 P83 P84 F85 G86 D87 S88 Y89 I90 I91 I92 G93 V94 E95 P96 G97 Q98 L99 K100 L101 N102 W103 F104 K105 K106 G107 S108 S109 L110 E111 H112 H113 H114 H115 H116 H117

4.2.11 Score per residue for model 11

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A: 9% 37% 18% • 34%

M1 D2 K3 L4 Q5 L6 K7 G8 M9 S10 Y11 S12 M13 C14 T15 G16 K17 F18 K19 V20 V21 K22 E23 I24 A25 E26 T27 T31 I32 V33 I34 R35 V36 Q37 Y38 E39 G40 D41 G42 S43 P44 C45 K46 I47 P48 F49 E50 I51 M52 D53 L54 E55 K56 R57 H58 V59 L60 G61 R62

L63 I64 T65 V66 N67 P68 I69 V70 T71 E72 K73 D74 S75 P76 V77 N78 I79 E80 A81 E82 P83 P84 F85 G86 D87 S88 Y89 I90 I91 I92 G93 V94 E95 P96 G97 Q98 L99 K100 L101 N102 W103 F104 K105 K106 G107 S108 S109 L110 E111 H112 H113 H114 H115 H116 H117

4.2.12 Score per residue for model 12

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A: 8% 39% 18% • 34%

M1 D2 K3 L4 Q5 L6 K7 G8 M9 S10 Y11 S12 M13 C14 T15 G16 K17 F18 K19 V20 V21 K22 E23 I24 A25 E26 T27 Q28 H29 G30 T31 I32 V33 I34 R35 V36 Q37 Y38 E39 G40 D41 G42 S43 P44 C45 K46 I47 P48 F49 E50 I51 M52 D53 L54 E55 K56 R57 H58 V59 L60

G61 R62 L63 I64 T65 V66 N67 P68 I69 V70 T71 E72 K73 P76 V77 N78 I79 E80 A81 E82 P83 P84 F85 G86 D87 S88 Y89 I90 I91 I92 G93 V94 E95 P96 G97 Q98 L99 K100 L101 N102 W103 F104 K105 K106 G107 S108 S109 L110 E111 H112 H113 H114 H115 H116 H117

4.2.13 Score per residue for model 13

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A: 7% 40% 18% • 34%

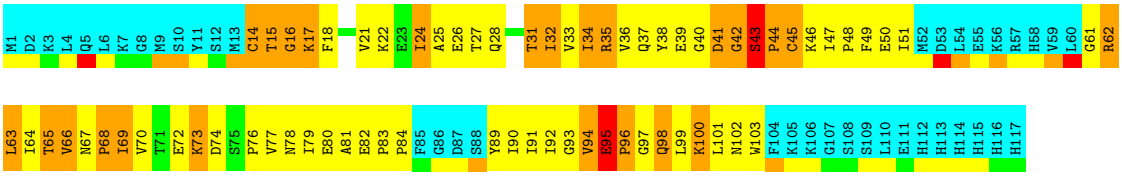
M1 D2 K3 L4 Q5 L6 K7 G8 M9 S10 Y11 S12 M13 C14 T15 G16 K17 F18 K19 V20 V21 K22 E23 I24 A25 E26 T27 Q28 H29 G30 T31 I32 V33 I34 R35 V36 Q37 Y38 E39 G40 D41 G42 S43 P44 C45 K46 I47 P48 F49 E50 I51 M52 D53 L54 E55 K56 R57 H58 V59 L60

G61 R62 L63 I64 T65 V66 N67 P68 I69 V70 T71 E72 K73 D74 S75 P76 V77 N78 I79 E80 A81 E82 P83 P84 F85 G86 D87 S88 Y89 I90 I91 I92 G93 V94 E95 P96 G97 Q98 L99 K100 L101 N102 W103 F104 K105 K106 G107 S108 S109 L110 E111 H112 H113 H114 H115 H116 H117

4.2.14 Score per residue for model 14

- Molecule 1: domain III of ENVELOPE PROTEIN E

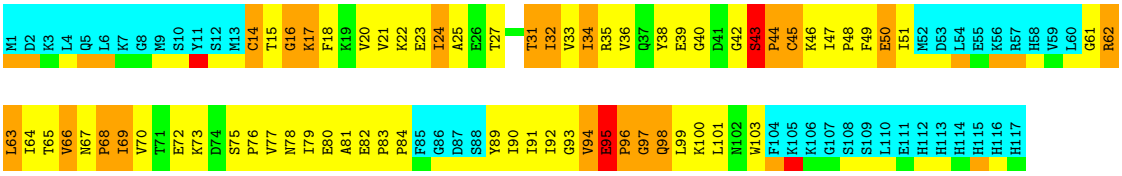
Chain A: 6% 38% 21% • 34%



4.2.15 Score per residue for model 15

- Molecule 1: domain III of ENVELOPE PROTEIN E

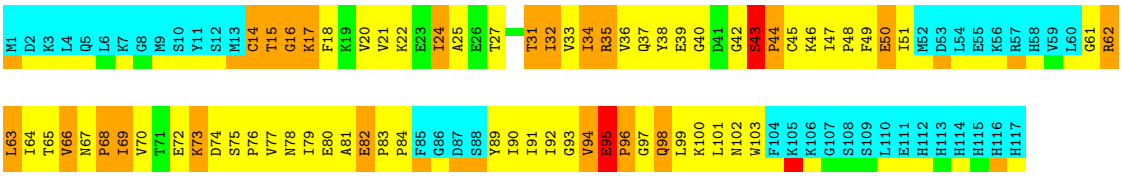
Chain A: 9% 39% 16% • 34%



4.2.16 Score per residue for model 16

- Molecule 1: domain III of ENVELOPE PROTEIN E

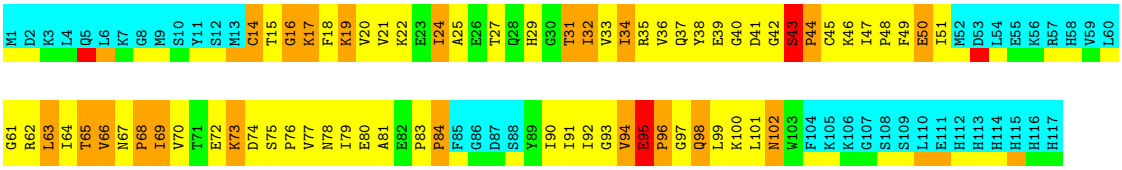
Chain A: 7% 39% 18% • 34%



4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: domain III of ENVELOPE PROTEIN E

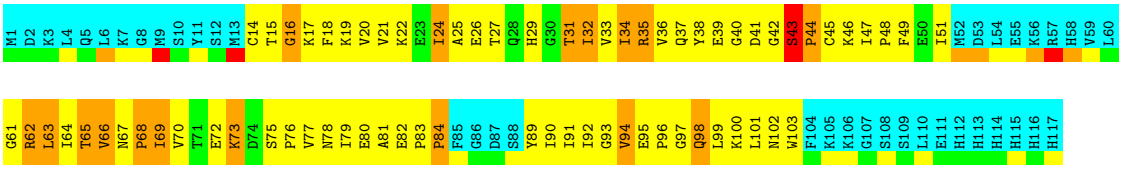
Chain A: 7% 39% 18% • 34%



4.2.18 Score per residue for model 18

- Molecule 1: domain III of ENVELOPE PROTEIN E

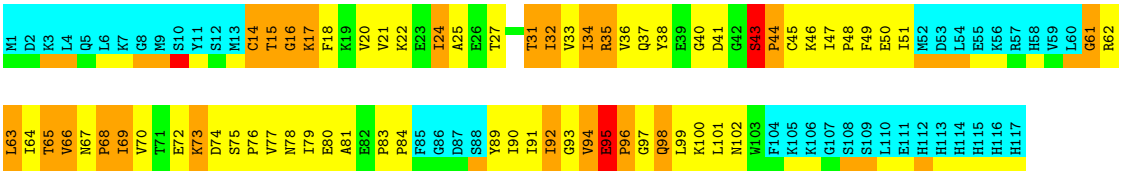
Chain A: 5% 45% 15% • 34%



4.2.19 Score per residue for model 19

- Molecule 1: domain III of ENVELOPE PROTEIN E

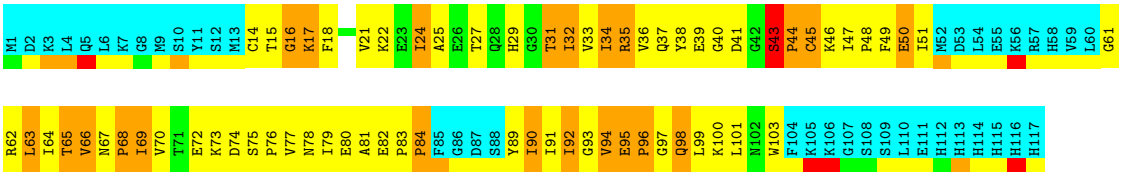
Chain A: 9% 37% 18% • 34%



4.2.20 Score per residue for model 20

- Molecule 1: domain III of ENVELOPE PROTEIN E

Chain A: 8% 38% 19% • 34%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
XPLOR-NIH	structure solution	
XPLOR-NIH	refinement	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.05±0.00	0±0/613 (0.0± 0.0%)	1.23±0.01	0±0/836 (0.0± 0.0%)
All	All	1.05	0/12260 (0.0%)	1.23	1/16720 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	37	GLN	N-CA-CB	-5.05	101.51	110.60	10	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	599	614	614	166±8
All	All	11980	12280	12280	3324

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 137.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:ILE:HD11	1:A:70:VAL:HG23	1.14	1.16	17	20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HG21	1:A:92:ILE:HD11	1.06	1.27	7	20
1:A:63:LEU:HD23	1:A:81:ALA:HB2	1.03	1.27	11	6
1:A:47:ILE:CD1	1:A:70:VAL:HG23	0.99	1.86	11	20
1:A:18:PHE:CE2	1:A:47:ILE:HG23	0.98	1.94	4	18
1:A:47:ILE:HD11	1:A:70:VAL:CG2	0.97	1.88	20	19
1:A:51:ILE:HD11	1:A:81:ALA:HB1	0.97	1.28	13	17
1:A:63:LEU:O	1:A:66:VAL:HG23	0.94	1.63	11	15
1:A:70:VAL:HG22	1:A:77:VAL:HG21	0.92	1.40	2	18
1:A:49:PHE:CE1	1:A:79:ILE:HG21	0.92	2.00	4	9
1:A:32:ILE:HD13	1:A:103:TRP:CD1	0.92	1.99	14	1
1:A:63:LEU:CD2	1:A:81:ALA:HB2	0.91	1.96	4	12
1:A:49:PHE:CZ	1:A:90:ILE:HG23	0.90	2.01	13	16
1:A:49:PHE:CD1	1:A:63:LEU:HD11	0.89	2.01	12	3
1:A:49:PHE:CE2	1:A:79:ILE:HG21	0.89	2.02	5	9
1:A:18:PHE:CE1	1:A:47:ILE:HG23	0.89	2.03	2	2
1:A:34:ILE:CG2	1:A:92:ILE:HD11	0.88	1.98	1	20
1:A:38:TYR:HB2	1:A:70:VAL:HG21	0.87	1.46	1	20
1:A:45:CYS:O	1:A:69:ILE:HG23	0.87	1.70	13	20
1:A:63:LEU:HD23	1:A:81:ALA:CB	0.87	2.00	4	6
1:A:68:PRO:CG	1:A:79:ILE:HD12	0.85	2.01	5	4
1:A:31:THR:HG22	1:A:81:ALA:C	0.85	1.92	8	20
1:A:27:THR:HG21	1:A:80:GLU:OE2	0.85	1.71	15	14
1:A:49:PHE:CG	1:A:63:LEU:HD11	0.85	2.07	12	3
1:A:27:THR:HG21	1:A:80:GLU:CD	0.85	1.91	11	16
1:A:25:ALA:HB3	1:A:33:VAL:HB	0.84	1.49	13	15
1:A:50:GLU:O	1:A:91:ILE:HD12	0.84	1.72	19	9
1:A:18:PHE:CZ	1:A:47:ILE:HG23	0.83	2.08	8	20
1:A:49:PHE:CD2	1:A:79:ILE:HG21	0.83	2.09	1	9
1:A:31:THR:HG21	1:A:64:ILE:CG1	0.83	2.04	18	20
1:A:31:THR:HG21	1:A:64:ILE:HG12	0.82	1.51	16	20
1:A:50:GLU:HG2	1:A:91:ILE:HD12	0.82	1.49	5	7
1:A:51:ILE:HG21	1:A:83:PRO:HB3	0.82	1.51	14	2
1:A:34:ILE:HD12	1:A:36:VAL:CG1	0.80	2.06	14	20
1:A:18:PHE:O	1:A:99:LEU:HD21	0.80	1.76	9	1
1:A:100:LYS:C	1:A:101:LEU:HD12	0.80	1.96	19	7
1:A:25:ALA:O	1:A:32:ILE:HG22	0.79	1.75	1	18
1:A:92:ILE:HD12	1:A:101:LEU:HD11	0.79	1.52	3	2
1:A:49:PHE:CD1	1:A:63:LEU:HD21	0.79	2.13	2	7
1:A:66:VAL:HG12	1:A:67:ASN:ND2	0.78	1.93	2	5
1:A:24:ILE:HG12	1:A:101:LEU:HD22	0.78	1.56	11	6
1:A:65:THR:HG22	1:A:65:THR:O	0.77	1.79	16	14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ILE:HD11	1:A:101:LEU:HD21	0.77	1.56	3	3
1:A:32:ILE:HD11	1:A:83:PRO:CG	0.77	2.08	20	3
1:A:21:VAL:HG21	1:A:76:PRO:HB3	0.76	1.58	7	6
1:A:63:LEU:HD22	1:A:81:ALA:HB2	0.75	1.56	7	13
1:A:63:LEU:HD12	1:A:66:VAL:N	0.75	1.97	13	13
1:A:63:LEU:HD12	1:A:65:THR:C	0.74	2.03	13	11
1:A:32:ILE:HD11	1:A:83:PRO:HG2	0.74	1.59	14	2
1:A:20:VAL:CG2	1:A:99:LEU:HD13	0.73	2.14	10	17
1:A:101:LEU:N	1:A:101:LEU:HD12	0.72	1.97	1	1
1:A:70:VAL:HG22	1:A:77:VAL:CG2	0.72	2.15	12	8
1:A:49:PHE:CD1	1:A:79:ILE:HG21	0.71	2.20	6	10
1:A:32:ILE:HD12	1:A:90:ILE:HD11	0.69	1.61	14	5
1:A:33:VAL:HG22	1:A:80:GLU:OE1	0.69	1.87	13	1
1:A:31:THR:HG22	1:A:81:ALA:O	0.69	1.87	8	19
1:A:90:ILE:O	1:A:101:LEU:HD12	0.69	1.88	17	6
1:A:49:PHE:CD2	1:A:63:LEU:HD21	0.68	2.23	19	9
1:A:51:ILE:HD11	1:A:81:ALA:CB	0.68	2.15	13	11
1:A:38:TYR:CB	1:A:70:VAL:HG21	0.68	2.18	1	8
1:A:34:ILE:CG1	1:A:101:LEU:HD22	0.68	2.19	1	3
1:A:51:ILE:HG22	1:A:51:ILE:O	0.67	1.90	7	2
1:A:32:ILE:CD1	1:A:90:ILE:HD11	0.66	2.20	16	18
1:A:63:LEU:HD22	1:A:81:ALA:CB	0.66	2.20	17	13
1:A:34:ILE:HD11	1:A:101:LEU:CD2	0.66	2.20	1	2
1:A:36:VAL:HG11	1:A:92:ILE:HD13	0.66	1.66	19	17
1:A:46:LYS:CG	1:A:69:ILE:HD11	0.66	2.21	17	11
1:A:49:PHE:CD2	1:A:63:LEU:HD23	0.66	2.26	13	3
1:A:20:VAL:HG23	1:A:99:LEU:HD13	0.65	1.67	6	12
1:A:46:LYS:HG3	1:A:69:ILE:HD11	0.65	1.67	18	14
1:A:49:PHE:CD1	1:A:63:LEU:CD2	0.65	2.79	15	6
1:A:14:CYS:SG	1:A:47:ILE:HD13	0.65	2.31	12	2
1:A:18:PHE:O	1:A:99:LEU:HD11	0.65	1.91	6	14
1:A:49:PHE:CE2	1:A:79:ILE:CG2	0.65	2.80	8	9
1:A:49:PHE:CE1	1:A:63:LEU:HD21	0.65	2.26	2	9
1:A:65:THR:CG2	1:A:65:THR:O	0.65	2.45	10	1
1:A:43:SER:CB	1:A:44:PRO:CD	0.64	2.75	16	20
1:A:18:PHE:HE2	1:A:47:ILE:HD12	0.64	1.52	14	14
1:A:65:THR:O	1:A:65:THR:CG2	0.64	2.46	17	19
1:A:32:ILE:HD11	1:A:83:PRO:HG3	0.64	1.67	10	3
1:A:68:PRO:HG3	1:A:79:ILE:HG23	0.64	1.69	15	6
1:A:49:PHE:CD2	1:A:63:LEU:CD2	0.64	2.80	19	7
1:A:31:THR:HG21	1:A:64:ILE:HG13	0.63	1.69	18	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:SER:O	1:A:77:VAL:HG23	0.63	1.92	16	15
1:A:49:PHE:CE2	1:A:63:LEU:CD2	0.63	2.81	13	7
1:A:49:PHE:CD2	1:A:63:LEU:HD11	0.63	2.28	3	2
1:A:68:PRO:HG3	1:A:79:ILE:HD12	0.62	1.69	12	2
1:A:51:ILE:HG21	1:A:83:PRO:CB	0.62	2.23	14	2
1:A:90:ILE:HG22	1:A:101:LEU:HB2	0.62	1.69	20	1
1:A:34:ILE:CD1	1:A:36:VAL:CG1	0.62	2.77	14	20
1:A:21:VAL:HG23	1:A:36:VAL:HA	0.62	1.71	10	16
1:A:64:ILE:HD12	1:A:64:ILE:N	0.62	2.08	5	4
1:A:34:ILE:HG13	1:A:101:LEU:HD13	0.62	1.70	9	2
1:A:49:PHE:CE2	1:A:63:LEU:HD23	0.61	2.30	13	2
1:A:64:ILE:CD1	1:A:64:ILE:N	0.61	2.63	4	11
1:A:49:PHE:CE1	1:A:79:ILE:CG2	0.61	2.81	4	3
1:A:64:ILE:N	1:A:64:ILE:CD1	0.61	2.63	5	2
1:A:89:TYR:CD1	1:A:89:TYR:N	0.61	2.68	15	10
1:A:34:ILE:O	1:A:78:ASN:HA	0.61	1.96	20	20
1:A:32:ILE:HD13	1:A:90:ILE:HD11	0.61	1.71	4	3
1:A:49:PHE:CZ	1:A:90:ILE:CG2	0.61	2.84	2	17
1:A:24:ILE:HG22	1:A:103:TRP:CE3	0.60	2.32	18	6
1:A:20:VAL:HG22	1:A:99:LEU:HD13	0.60	1.72	11	7
1:A:46:LYS:CG	1:A:69:ILE:CD1	0.60	2.79	9	11
1:A:49:PHE:CE2	1:A:63:LEU:HD21	0.60	2.31	10	9
1:A:68:PRO:CB	1:A:79:ILE:CD1	0.60	2.80	5	6
1:A:32:ILE:HG21	1:A:103:TRP:CE2	0.60	2.32	14	1
1:A:14:CYS:N	1:A:45:CYS:SG	0.60	2.75	3	10
1:A:31:THR:HG21	1:A:64:ILE:CD1	0.59	2.27	13	13
1:A:64:ILE:N	1:A:64:ILE:HD12	0.59	2.12	3	9
1:A:92:ILE:HG22	1:A:99:LEU:HD12	0.59	1.73	9	1
1:A:34:ILE:HG22	1:A:79:ILE:HB	0.59	1.73	7	20
1:A:66:VAL:CG1	1:A:67:ASN:ND2	0.59	2.66	1	3
1:A:72:GLU:O	1:A:73:LYS:CB	0.59	2.50	10	18
1:A:24:ILE:HG23	1:A:32:ILE:HG22	0.59	1.73	14	3
1:A:31:THR:CG2	1:A:64:ILE:CD1	0.59	2.81	6	13
1:A:32:ILE:HG21	1:A:103:TRP:NE1	0.59	2.13	14	3
1:A:25:ALA:O	1:A:33:VAL:N	0.58	2.34	20	20
1:A:50:GLU:CG	1:A:91:ILE:CG2	0.58	2.81	10	2
1:A:66:VAL:HG12	1:A:67:ASN:CG	0.58	2.19	16	3
1:A:24:ILE:HG13	1:A:90:ILE:HD13	0.58	1.74	13	4
1:A:89:TYR:CE2	1:A:102:ASN:ND2	0.58	2.72	6	1
1:A:66:VAL:HG12	1:A:67:ASN:HD22	0.58	1.58	7	1
1:A:18:PHE:HB2	1:A:99:LEU:HD11	0.58	1.73	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLU:O	1:A:51:ILE:HG23	0.58	1.99	1	1
1:A:34:ILE:HD12	1:A:36:VAL:HG11	0.58	1.76	7	20
1:A:90:ILE:CG2	1:A:101:LEU:HD13	0.58	2.28	20	1
1:A:49:PHE:CZ	1:A:90:ILE:HG21	0.58	2.33	9	2
1:A:95:GLU:O	1:A:97:GLY:N	0.58	2.36	8	16
1:A:14:CYS:SG	1:A:38:TYR:CE2	0.58	2.97	20	8
1:A:92:ILE:HG22	1:A:99:LEU:CD1	0.58	2.29	9	1
1:A:24:ILE:HD11	1:A:34:ILE:HB	0.58	1.76	10	20
1:A:24:ILE:O	1:A:103:TRP:CZ3	0.58	2.57	2	3
1:A:43:SER:OG	1:A:44:PRO:CD	0.58	2.52	10	20
1:A:43:SER:CB	1:A:44:PRO:HD2	0.58	2.29	6	20
1:A:34:ILE:CG2	1:A:34:ILE:O	0.57	2.52	9	20
1:A:43:SER:O	1:A:45:CYS:N	0.57	2.37	10	20
1:A:68:PRO:HG2	1:A:79:ILE:HD12	0.57	1.75	5	4
1:A:18:PHE:CE2	1:A:47:ILE:HD12	0.57	2.34	9	15
1:A:49:PHE:CE1	1:A:63:LEU:CD2	0.57	2.88	1	5
1:A:94:VAL:O	1:A:95:GLU:C	0.57	2.43	2	20
1:A:67:ASN:N	1:A:68:PRO:CD	0.57	2.66	4	5
1:A:68:PRO:CG	1:A:79:ILE:CD1	0.57	2.81	5	4
1:A:89:TYR:CE1	1:A:102:ASN:OD1	0.57	2.57	14	1
1:A:38:TYR:CE2	1:A:45:CYS:SG	0.57	2.98	12	4
1:A:94:VAL:O	1:A:98:GLN:N	0.57	2.38	9	5
1:A:14:CYS:N	1:A:46:LYS:O	0.57	2.38	2	6
1:A:95:GLU:N	1:A:96:PRO:HD2	0.57	2.15	6	20
1:A:47:ILE:CD1	1:A:70:VAL:CG2	0.56	2.78	12	20
1:A:49:PHE:CB	1:A:63:LEU:HD11	0.56	2.29	12	1
1:A:17:LYS:CG	1:A:97:GLY:CA	0.56	2.84	9	2
1:A:94:VAL:O	1:A:97:GLY:N	0.56	2.38	9	3
1:A:65:THR:O	1:A:66:VAL:C	0.56	2.44	17	20
1:A:36:VAL:O	1:A:76:PRO:HA	0.56	1.99	5	18
1:A:66:VAL:HG12	1:A:67:ASN:OD1	0.56	2.00	5	1
1:A:62:ARG:O	1:A:82:GLU:N	0.56	2.39	3	17
1:A:92:ILE:O	1:A:99:LEU:N	0.56	2.38	10	18
1:A:18:PHE:CZ	1:A:48:PRO:HD2	0.56	2.36	7	16
1:A:38:TYR:CE1	1:A:40:GLY:CA	0.56	2.89	4	6
1:A:34:ILE:HG21	1:A:92:ILE:CD1	0.55	2.21	1	1
1:A:70:VAL:CG2	1:A:77:VAL:HG21	0.55	2.30	6	4
1:A:95:GLU:CB	1:A:96:PRO:CD	0.55	2.85	2	20
1:A:34:ILE:HG22	1:A:79:ILE:CB	0.55	2.32	6	20
1:A:62:ARG:O	1:A:81:ALA:HB1	0.55	2.01	12	6
1:A:18:PHE:CE1	1:A:48:PRO:HD2	0.55	2.37	7	18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:VAL:O	1:A:67:ASN:ND2	0.55	2.40	7	1
1:A:47:ILE:N	1:A:68:PRO:O	0.55	2.40	18	18
1:A:32:ILE:HD11	1:A:83:PRO:HB3	0.55	1.77	12	1
1:A:38:TYR:CZ	1:A:40:GLY:CA	0.55	2.90	13	3
1:A:38:TYR:O	1:A:73:LYS:O	0.55	2.25	6	20
1:A:45:CYS:SG	1:A:46:LYS:N	0.55	2.80	15	10
1:A:101:LEU:HD12	1:A:101:LEU:N	0.55	2.17	15	7
1:A:17:LYS:CG	1:A:97:GLY:HA3	0.54	2.32	6	20
1:A:47:ILE:HG21	1:A:79:ILE:HD11	0.54	1.80	9	5
1:A:15:THR:O	1:A:94:VAL:CG2	0.54	2.56	3	14
1:A:70:VAL:CG1	1:A:72:GLU:O	0.54	2.56	6	2
1:A:72:GLU:O	1:A:73:LYS:CD	0.54	2.56	17	1
1:A:24:ILE:HG22	1:A:103:TRP:CD2	0.54	2.38	2	2
1:A:27:THR:CG2	1:A:33:VAL:HG23	0.54	2.32	18	16
1:A:15:THR:HA	1:A:94:VAL:HG21	0.54	1.80	6	3
1:A:46:LYS:HA	1:A:68:PRO:O	0.54	2.03	5	20
1:A:17:LYS:CE	1:A:18:PHE:N	0.54	2.71	18	3
1:A:47:ILE:O	1:A:67:ASN:ND2	0.54	2.41	9	1
1:A:38:TYR:CZ	1:A:40:GLY:C	0.54	2.81	13	4
1:A:33:VAL:HG22	1:A:80:GLU:HG3	0.53	1.79	16	3
1:A:43:SER:O	1:A:45:CYS:SG	0.53	2.66	16	10
1:A:45:CYS:O	1:A:69:ILE:CG2	0.53	2.53	13	7
1:A:25:ALA:O	1:A:32:ILE:CA	0.53	2.56	13	10
1:A:46:LYS:HG3	1:A:69:ILE:CD1	0.53	2.33	12	18
1:A:50:GLU:O	1:A:51:ILE:CG2	0.53	2.56	1	1
1:A:51:ILE:O	1:A:51:ILE:CG2	0.53	2.56	12	2
1:A:63:LEU:HD13	1:A:80:GLU:O	0.53	2.03	9	6
1:A:14:CYS:O	1:A:48:PRO:CG	0.53	2.57	3	7
1:A:18:PHE:CE2	1:A:48:PRO:HD2	0.53	2.38	2	2
1:A:40:GLY:O	1:A:73:LYS:CD	0.53	2.57	15	5
1:A:18:PHE:O	1:A:99:LEU:CD1	0.53	2.56	6	16
1:A:46:LYS:CD	1:A:67:ASN:OD1	0.53	2.56	6	2
1:A:101:LEU:N	1:A:101:LEU:CD1	0.53	2.66	1	2
1:A:17:LYS:CE	1:A:18:PHE:O	0.53	2.57	9	3
1:A:50:GLU:O	1:A:91:ILE:CD1	0.53	2.57	12	5
1:A:64:ILE:N	1:A:80:GLU:O	0.53	2.42	7	15
1:A:34:ILE:HG22	1:A:79:ILE:CG1	0.53	2.34	5	6
1:A:46:LYS:O	1:A:47:ILE:HD13	0.53	2.04	13	4
1:A:14:CYS:SG	1:A:38:TYR:CE1	0.53	3.02	17	2
1:A:24:ILE:CG2	1:A:32:ILE:CG2	0.53	2.87	14	3
1:A:24:ILE:CG2	1:A:32:ILE:HG22	0.53	2.33	14	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LYS:O	1:A:39:GLU:N	0.53	2.40	1	12
1:A:63:LEU:CD2	1:A:81:ALA:CB	0.53	2.87	3	3
1:A:50:GLU:HG3	1:A:91:ILE:CG2	0.53	2.34	10	1
1:A:14:CYS:HB3	1:A:38:TYR:CE1	0.52	2.39	17	11
1:A:27:THR:CG2	1:A:80:GLU:OE2	0.52	2.57	12	12
1:A:37:GLN:CG	1:A:74:ASP:O	0.52	2.57	13	1
1:A:49:PHE:HB3	1:A:63:LEU:HD11	0.52	1.81	12	3
1:A:40:GLY:O	1:A:73:LYS:CG	0.52	2.57	18	2
1:A:21:VAL:HG23	1:A:36:VAL:C	0.52	2.25	14	10
1:A:67:ASN:O	1:A:67:ASN:ND2	0.52	2.42	5	1
1:A:38:TYR:OH	1:A:41:ASP:N	0.52	2.43	13	4
1:A:31:THR:CG2	1:A:64:ILE:HD13	0.52	2.35	7	12
1:A:40:GLY:O	1:A:73:LYS:CE	0.52	2.57	1	5
1:A:62:ARG:N	1:A:82:GLU:O	0.52	2.43	9	10
1:A:14:CYS:SG	1:A:46:LYS:O	0.52	2.68	2	16
1:A:14:CYS:HB3	1:A:38:TYR:CZ	0.52	2.40	19	8
1:A:38:TYR:CD1	1:A:38:TYR:C	0.52	2.80	1	1
1:A:17:LYS:CD	1:A:97:GLY:O	0.52	2.58	2	2
1:A:25:ALA:O	1:A:32:ILE:CG2	0.52	2.56	1	8
1:A:63:LEU:O	1:A:66:VAL:CG2	0.52	2.56	7	4
1:A:35:ARG:NE	1:A:78:ASN:OD1	0.52	2.43	8	1
1:A:68:PRO:HG2	1:A:79:ILE:HD13	0.52	1.82	13	1
1:A:46:LYS:CE	1:A:67:ASN:OD1	0.52	2.57	6	1
1:A:24:ILE:CG2	1:A:103:TRP:CE3	0.52	2.93	18	4
1:A:25:ALA:N	1:A:33:VAL:O	0.52	2.41	2	20
1:A:38:TYR:CE1	1:A:40:GLY:HA3	0.52	2.39	4	5
1:A:91:ILE:CG2	1:A:98:GLN:CD	0.51	2.79	13	20
1:A:31:THR:CG2	1:A:64:ILE:HG12	0.51	2.35	8	1
1:A:37:GLN:NE2	1:A:74:ASP:OD2	0.51	2.43	10	1
1:A:102:ASN:OD1	1:A:102:ASN:N	0.51	2.44	10	1
1:A:78:ASN:N	1:A:78:ASN:OD1	0.51	2.43	4	6
1:A:27:THR:O	1:A:28:GLN:CB	0.51	2.59	1	1
1:A:32:ILE:O	1:A:80:GLU:HA	0.51	2.05	5	20
1:A:66:VAL:O	1:A:67:ASN:C	0.51	2.48	1	14
1:A:38:TYR:CZ	1:A:40:GLY:HA3	0.51	2.40	13	2
1:A:90:ILE:N	1:A:101:LEU:O	0.51	2.43	11	14
1:A:68:PRO:HB3	1:A:79:ILE:CD1	0.51	2.36	5	4
1:A:50:GLU:C	1:A:51:ILE:HG23	0.51	2.26	1	1
1:A:38:TYR:CE2	1:A:40:GLY:C	0.51	2.83	5	3
1:A:25:ALA:O	1:A:32:ILE:HA	0.51	2.06	9	20
1:A:35:ARG:C	1:A:36:VAL:CG1	0.51	2.79	1	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:GLU:OE1	1:A:51:ILE:N	0.51	2.43	3	1
1:A:18:PHE:CE2	1:A:47:ILE:CG2	0.51	2.86	13	10
1:A:49:PHE:HE2	1:A:51:ILE:HD11	0.50	1.66	20	2
1:A:48:PRO:HB2	1:A:93:GLY:O	0.50	2.06	12	20
1:A:51:ILE:HG22	1:A:90:ILE:HA	0.50	1.82	1	1
1:A:46:LYS:HG2	1:A:69:ILE:CD1	0.50	2.36	6	8
1:A:78:ASN:OD1	1:A:78:ASN:N	0.50	2.43	8	2
1:A:50:GLU:HG2	1:A:91:ILE:CG2	0.50	2.37	17	2
1:A:38:TYR:CE1	1:A:39:GLU:O	0.50	2.64	1	2
1:A:94:VAL:N	1:A:98:GLN:HB2	0.50	2.21	9	9
1:A:17:LYS:HE2	1:A:18:PHE:N	0.50	2.21	18	2
1:A:17:LYS:N	1:A:39:GLU:O	0.50	2.43	7	7
1:A:21:VAL:HB	1:A:35:ARG:CG	0.50	2.36	7	16
1:A:49:PHE:CE1	1:A:90:ILE:HG23	0.50	2.41	2	8
1:A:26:GLU:N	1:A:26:GLU:OE1	0.50	2.45	14	2
1:A:63:LEU:CD1	1:A:65:THR:C	0.50	2.80	7	2
1:A:67:ASN:O	1:A:67:ASN:OD1	0.50	2.30	7	4
1:A:24:ILE:HG23	1:A:32:ILE:HB	0.50	1.82	13	1
1:A:63:LEU:HD12	1:A:66:VAL:CA	0.50	2.37	7	1
1:A:66:VAL:O	1:A:67:ASN:OD1	0.49	2.30	1	6
1:A:21:VAL:CG2	1:A:36:VAL:C	0.49	2.80	18	10
1:A:14:CYS:HB3	1:A:38:TYR:CE2	0.49	2.42	16	1
1:A:24:ILE:CG2	1:A:103:TRP:CD2	0.49	2.95	2	2
1:A:15:THR:HA	1:A:94:VAL:CG2	0.49	2.36	6	1
1:A:64:ILE:N	1:A:64:ILE:HD13	0.49	2.22	19	7
1:A:17:LYS:HE3	1:A:18:PHE:N	0.49	2.22	10	2
1:A:34:ILE:HG12	1:A:101:LEU:HD22	0.49	1.84	9	1
1:A:24:ILE:HG23	1:A:32:ILE:CG2	0.49	2.36	14	2
1:A:81:ALA:C	1:A:83:PRO:CD	0.49	2.81	20	2
1:A:22:LYS:HB3	1:A:35:ARG:HB3	0.49	1.83	1	17
1:A:68:PRO:HG2	1:A:79:ILE:CD1	0.49	2.38	10	2
1:A:15:THR:O	1:A:16:GLY:O	0.49	2.30	8	16
1:A:24:ILE:HG12	1:A:34:ILE:HG12	0.49	1.85	20	20
1:A:43:SER:OG	1:A:44:PRO:HD2	0.49	2.08	2	17
1:A:45:CYS:C	1:A:69:ILE:HG23	0.49	2.28	2	5
1:A:67:ASN:N	1:A:68:PRO:HD3	0.49	2.23	6	4
1:A:20:VAL:HG23	1:A:99:LEU:CD1	0.49	2.38	13	10
1:A:32:ILE:CG1	1:A:83:PRO:HD3	0.49	2.37	1	15
1:A:89:TYR:HA	1:A:101:LEU:O	0.49	2.07	10	17
1:A:90:ILE:O	1:A:101:LEU:N	0.49	2.42	10	2
1:A:95:GLU:CB	1:A:96:PRO:HD3	0.49	2.38	9	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:PHE:CZ	1:A:63:LEU:HD21	0.49	2.43	12	1
1:A:89:TYR:CE1	1:A:102:ASN:ND2	0.49	2.81	8	1
1:A:67:ASN:O	1:A:68:PRO:O	0.48	2.31	10	7
1:A:15:THR:CA	1:A:94:VAL:HG21	0.48	2.38	6	1
1:A:65:THR:CG2	1:A:68:PRO:CG	0.48	2.91	14	6
1:A:32:ILE:CG2	1:A:103:TRP:NE1	0.48	2.76	14	1
1:A:89:TYR:CE1	1:A:102:ASN:HB2	0.48	2.43	14	1
1:A:67:ASN:OD1	1:A:67:ASN:O	0.48	2.31	6	5
1:A:22:LYS:HB3	1:A:35:ARG:CG	0.48	2.39	14	12
1:A:72:GLU:O	1:A:73:LYS:HB3	0.48	2.08	13	8
1:A:94:VAL:O	1:A:96:PRO:N	0.48	2.47	2	13
1:A:72:GLU:C	1:A:73:LYS:CG	0.48	2.81	8	3
1:A:17:LYS:CE	1:A:96:PRO:O	0.48	2.62	17	2
1:A:18:PHE:CE1	1:A:47:ILE:HD12	0.48	2.43	2	1
1:A:41:ASP:N	1:A:41:ASP:OD1	0.48	2.46	6	2
1:A:46:LYS:CE	1:A:67:ASN:CG	0.48	2.82	6	1
1:A:78:ASN:ND2	1:A:78:ASN:N	0.48	2.60	18	2
1:A:92:ILE:O	1:A:98:GLN:HA	0.48	2.08	9	4
1:A:19:LYS:CE	1:A:37:GLN:HB3	0.48	2.38	17	1
1:A:90:ILE:CG2	1:A:101:LEU:CD1	0.48	2.92	20	1
1:A:38:TYR:CD2	1:A:73:LYS:HA	0.48	2.44	19	4
1:A:18:PHE:CB	1:A:92:ILE:CG2	0.48	2.91	19	7
1:A:18:PHE:O	1:A:99:LEU:CD2	0.48	2.57	9	1
1:A:37:GLN:NE2	1:A:74:ASP:CG	0.48	2.67	10	1
1:A:72:GLU:O	1:A:73:LYS:HB2	0.48	2.09	10	6
1:A:49:PHE:HB3	1:A:63:LEU:CD1	0.48	2.39	12	1
1:A:48:PRO:HB2	1:A:93:GLY:CA	0.48	2.39	9	20
1:A:27:THR:OG1	1:A:31:THR:OG1	0.48	2.32	12	6
1:A:45:CYS:O	1:A:69:ILE:HA	0.48	2.08	3	16
1:A:14:CYS:SG	1:A:38:TYR:CZ	0.48	3.07	17	3
1:A:17:LYS:HG2	1:A:97:GLY:CA	0.48	2.39	6	2
1:A:46:LYS:HE3	1:A:67:ASN:CB	0.48	2.39	8	1
1:A:22:LYS:CB	1:A:35:ARG:HB3	0.47	2.39	8	3
1:A:91:ILE:HG23	1:A:98:GLN:HG3	0.47	1.86	15	1
1:A:43:SER:OG	1:A:44:PRO:HD3	0.47	2.09	16	3
1:A:94:VAL:C	1:A:98:GLN:HB3	0.47	2.29	11	19
1:A:24:ILE:HG22	1:A:103:TRP:CZ3	0.47	2.45	7	1
1:A:64:ILE:CG1	1:A:80:GLU:HG2	0.47	2.39	20	3
1:A:40:GLY:O	1:A:73:LYS:NZ	0.47	2.46	1	2
1:A:47:ILE:O	1:A:67:ASN:OD1	0.47	2.32	3	8
1:A:19:LYS:CE	1:A:37:GLN:CD	0.47	2.83	17	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:TYR:OH	1:A:41:ASP:O	0.47	2.33	17	7
1:A:34:ILE:CD1	1:A:36:VAL:HG12	0.47	2.39	14	10
1:A:64:ILE:CB	1:A:80:GLU:HG2	0.47	2.39	20	8
1:A:18:PHE:CB	1:A:99:LEU:HD11	0.47	2.40	9	1
1:A:94:VAL:C	1:A:98:GLN:CB	0.47	2.83	5	18
1:A:44:PRO:HA	1:A:70:VAL:O	0.47	2.09	16	19
1:A:37:GLN:OE1	1:A:74:ASP:O	0.47	2.33	10	2
1:A:32:ILE:HG21	1:A:103:TRP:CD1	0.47	2.45	2	1
1:A:68:PRO:HB3	1:A:79:ILE:HD13	0.47	1.87	4	1
1:A:17:LYS:HA	1:A:97:GLY:O	0.47	2.09	6	4
1:A:31:THR:HG23	1:A:82:GLU:HB2	0.47	1.86	13	3
1:A:21:VAL:CG1	1:A:35:ARG:HG2	0.47	2.40	11	3
1:A:46:LYS:HB3	1:A:67:ASN:ND2	0.47	2.25	9	1
1:A:65:THR:CG2	1:A:68:PRO:HG3	0.47	2.40	14	6
1:A:18:PHE:CB	1:A:92:ILE:HG22	0.47	2.39	19	4
1:A:16:GLY:HA3	1:A:40:GLY:HA3	0.47	1.86	19	10
1:A:33:VAL:HA	1:A:79:ILE:O	0.47	2.09	12	12
1:A:34:ILE:CG2	1:A:79:ILE:HB	0.47	2.39	6	1
1:A:51:ILE:O	1:A:89:TYR:O	0.47	2.33	8	2
1:A:49:PHE:CE1	1:A:90:ILE:CG2	0.47	2.98	9	1
1:A:63:LEU:HD11	1:A:79:ILE:CG2	0.47	2.39	17	4
1:A:18:PHE:CE1	1:A:47:ILE:CG2	0.46	2.91	2	2
1:A:68:PRO:O	1:A:69:ILE:HG12	0.46	2.10	6	17
1:A:18:PHE:CZ	1:A:38:TYR:CD1	0.46	3.03	13	1
1:A:95:GLU:HB2	1:A:96:PRO:CD	0.46	2.40	12	2
1:A:65:THR:O	1:A:66:VAL:O	0.46	2.32	7	1
1:A:17:LYS:HE3	1:A:18:PHE:O	0.46	2.10	6	3
1:A:17:LYS:NZ	1:A:39:GLU:OE1	0.46	2.49	6	1
1:A:42:GLY:O	1:A:43:SER:CB	0.46	2.62	5	4
1:A:17:LYS:CE	1:A:97:GLY:O	0.46	2.64	2	1
1:A:46:LYS:HD3	1:A:67:ASN:ND2	0.46	2.26	14	6
1:A:41:ASP:HA	1:A:73:LYS:CD	0.46	2.40	19	1
1:A:24:ILE:CD1	1:A:34:ILE:HB	0.46	2.41	1	13
1:A:21:VAL:HG23	1:A:36:VAL:CA	0.46	2.40	10	12
1:A:21:VAL:N	1:A:35:ARG:O	0.46	2.46	6	7
1:A:46:LYS:CE	1:A:67:ASN:HB2	0.46	2.40	8	1
1:A:50:GLU:HG3	1:A:91:ILE:HD12	0.46	1.87	9	1
1:A:50:GLU:HG3	1:A:91:ILE:HG21	0.46	1.87	10	1
1:A:63:LEU:HB3	1:A:66:VAL:CG2	0.45	2.41	9	5
1:A:16:GLY:HA3	1:A:40:GLY:CA	0.45	2.42	4	7
1:A:32:ILE:HD12	1:A:90:ILE:CD1	0.45	2.37	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:ILE:HA	1:A:33:VAL:O	0.45	2.11	1	19
1:A:65:THR:CG2	1:A:68:PRO:HB3	0.45	2.42	10	9
1:A:21:VAL:CG2	1:A:37:GLN:HB2	0.45	2.42	2	5
1:A:43:SER:O	1:A:44:PRO:C	0.45	2.55	11	9
1:A:18:PHE:HB2	1:A:99:LEU:CD1	0.45	2.41	9	1
1:A:32:ILE:CG2	1:A:103:TRP:CE2	0.45	2.99	14	1
1:A:32:ILE:CD1	1:A:83:PRO:HG3	0.45	2.42	5	11
1:A:38:TYR:CD1	1:A:39:GLU:N	0.45	2.85	16	3
1:A:37:GLN:HG3	1:A:74:ASP:O	0.45	2.12	7	5
1:A:95:GLU:N	1:A:96:PRO:CD	0.45	2.79	9	3
1:A:32:ILE:CD1	1:A:103:TRP:CD1	0.45	2.88	14	1
1:A:49:PHE:CD1	1:A:63:LEU:HD23	0.45	2.46	16	2
1:A:50:GLU:CG	1:A:91:ILE:HD12	0.45	2.40	13	1
1:A:41:ASP:HA	1:A:73:LYS:HD3	0.45	1.89	19	1
1:A:34:ILE:CG2	1:A:92:ILE:CD1	0.45	2.84	1	1
1:A:94:VAL:O	1:A:98:GLN:HB3	0.45	2.12	7	13
1:A:43:SER:HB3	1:A:44:PRO:HD2	0.45	1.89	10	13
1:A:83:PRO:O	1:A:84:PRO:O	0.45	2.34	7	2
1:A:32:ILE:HG13	1:A:81:ALA:O	0.45	2.11	13	7
1:A:24:ILE:HD13	1:A:33:VAL:C	0.45	2.31	9	1
1:A:24:ILE:CD1	1:A:34:ILE:CB	0.45	2.94	8	13
1:A:46:LYS:CE	1:A:67:ASN:ND2	0.45	2.80	3	1
1:A:68:PRO:CG	1:A:79:ILE:HG12	0.45	2.41	3	3
1:A:51:ILE:CG2	1:A:90:ILE:HA	0.45	2.41	1	1
1:A:17:LYS:HD2	1:A:97:GLY:CA	0.45	2.42	2	2
1:A:38:TYR:CE1	1:A:40:GLY:N	0.45	2.84	4	3
1:A:81:ALA:C	1:A:83:PRO:HD3	0.45	2.32	14	2
1:A:21:VAL:HB	1:A:35:ARG:HG2	0.44	1.88	8	5
1:A:91:ILE:HG23	1:A:98:GLN:CD	0.44	2.33	20	8
1:A:92:ILE:O	1:A:98:GLN:CA	0.44	2.65	10	3
1:A:67:ASN:O	1:A:67:ASN:CG	0.44	2.55	7	1
1:A:65:THR:O	1:A:65:THR:HG22	0.44	2.11	10	3
1:A:32:ILE:CD1	1:A:90:ILE:CD1	0.44	2.93	11	1
1:A:51:ILE:CD1	1:A:81:ALA:HB1	0.44	2.40	14	3
1:A:48:PRO:HB2	1:A:93:GLY:C	0.44	2.32	12	14
1:A:36:VAL:O	1:A:77:VAL:N	0.44	2.50	4	7
1:A:46:LYS:HE3	1:A:67:ASN:ND2	0.44	2.27	3	1
1:A:24:ILE:O	1:A:103:TRP:CH2	0.44	2.70	6	1
1:A:27:THR:HG22	1:A:33:VAL:HG23	0.44	1.89	16	3
1:A:46:LYS:HD2	1:A:67:ASN:ND2	0.44	2.26	11	1
1:A:14:CYS:HB2	1:A:46:LYS:O	0.44	2.13	11	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LYS:CE	1:A:67:ASN:HA	0.44	2.42	4	1
1:A:38:TYR:CE2	1:A:73:LYS:CG	0.44	3.01	9	1
1:A:17:LYS:CD	1:A:97:GLY:HA3	0.44	2.43	13	2
1:A:95:GLU:O	1:A:96:PRO:C	0.44	2.55	15	2
1:A:15:THR:O	1:A:94:VAL:HG21	0.44	2.13	19	7
1:A:35:ARG:HA	1:A:77:VAL:O	0.44	2.12	5	10
1:A:62:ARG:CB	1:A:82:GLU:HB3	0.44	2.43	12	5
1:A:46:LYS:HG2	1:A:69:ILE:HD11	0.44	1.87	9	3
1:A:38:TYR:C	1:A:38:TYR:CD1	0.44	2.89	12	2
1:A:37:GLN:OE1	1:A:74:ASP:OD1	0.44	2.36	9	1
1:A:41:ASP:OD1	1:A:41:ASP:N	0.44	2.50	10	1
1:A:37:GLN:HG2	1:A:74:ASP:O	0.44	2.12	13	1
1:A:46:LYS:HE3	1:A:67:ASN:OD1	0.44	2.13	13	1
1:A:49:PHE:CE2	1:A:90:ILE:HG23	0.44	2.47	4	1
1:A:24:ILE:CD1	1:A:34:ILE:CG1	0.44	2.95	8	5
1:A:17:LYS:HG3	1:A:97:GLY:O	0.44	2.13	13	2
1:A:63:LEU:HD11	1:A:79:ILE:HG22	0.44	1.89	17	1
1:A:20:VAL:CG2	1:A:99:LEU:CD1	0.44	2.96	11	1
1:A:62:ARG:NH1	1:A:62:ARG:HG3	0.44	2.28	14	1
1:A:82:GLU:N	1:A:83:PRO:CD	0.44	2.80	20	1
1:A:61:GLY:CA	1:A:84:PRO:HD3	0.44	2.43	10	9
1:A:68:PRO:HG3	1:A:79:ILE:HG12	0.44	1.89	10	5
1:A:17:LYS:CD	1:A:96:PRO:O	0.44	2.66	17	1
1:A:46:LYS:HG2	1:A:67:ASN:OD1	0.44	2.13	4	3
1:A:66:VAL:O	1:A:67:ASN:CG	0.44	2.56	12	3
1:A:14:CYS:SG	1:A:45:CYS:C	0.43	2.96	16	6
1:A:34:ILE:HD12	1:A:92:ILE:CD1	0.43	2.43	6	6
1:A:34:ILE:HG13	1:A:101:LEU:CD1	0.43	2.43	9	2
1:A:90:ILE:O	1:A:100:LYS:HA	0.43	2.13	9	3
1:A:50:GLU:O	1:A:91:ILE:HB	0.43	2.14	7	8
1:A:46:LYS:HE3	1:A:67:ASN:HB2	0.43	1.90	8	1
1:A:27:THR:HG21	1:A:80:GLU:OE1	0.43	2.13	12	1
1:A:38:TYR:OH	1:A:41:ASP:C	0.43	2.57	10	2
1:A:19:LYS:HB2	1:A:39:GLU:CG	0.43	2.43	5	1
1:A:50:GLU:HG2	1:A:91:ILE:HB	0.43	1.90	10	2
1:A:72:GLU:O	1:A:73:LYS:HD3	0.43	2.13	17	1
1:A:49:PHE:CD2	1:A:63:LEU:CD1	0.43	2.99	3	1
1:A:24:ILE:HG12	1:A:101:LEU:CD2	0.43	2.43	10	1
1:A:74:ASP:O	1:A:76:PRO:HD3	0.43	2.13	10	9
1:A:46:LYS:CD	1:A:67:ASN:HB2	0.43	2.43	8	3
1:A:47:ILE:HG12	1:A:68:PRO:O	0.43	2.13	17	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ALA:O	1:A:83:PRO:HD3	0.43	2.13	13	1
1:A:94:VAL:C	1:A:96:PRO:HD2	0.43	2.34	19	14
1:A:91:ILE:HG23	1:A:98:GLN:CG	0.43	2.44	10	5
1:A:14:CYS:CB	1:A:46:LYS:O	0.43	2.66	16	1
1:A:24:ILE:CD1	1:A:34:ILE:HG12	0.43	2.44	20	6
1:A:17:LYS:HG3	1:A:97:GLY:CA	0.43	2.44	9	1
1:A:65:THR:O	1:A:65:THR:HG23	0.43	2.14	19	3
1:A:33:VAL:CG1	1:A:78:ASN:HB3	0.43	2.43	7	2
1:A:38:TYR:HB3	1:A:73:LYS:O	0.43	2.14	10	1
1:A:27:THR:C	1:A:28:GLN:CG	0.43	2.84	1	1
1:A:89:TYR:CD1	1:A:102:ASN:HB2	0.43	2.49	1	2
1:A:21:VAL:N	1:A:36:VAL:HA	0.43	2.29	17	10
1:A:64:ILE:CG2	1:A:80:GLU:HG2	0.43	2.44	13	7
1:A:43:SER:O	1:A:45:CYS:HB3	0.43	2.14	3	7
1:A:47:ILE:N	1:A:67:ASN:OD1	0.43	2.52	3	1
1:A:100:LYS:O	1:A:101:LEU:HD12	0.43	2.14	10	1
1:A:91:ILE:HG21	1:A:98:GLN:NE2	0.43	2.29	11	1
1:A:94:VAL:O	1:A:98:GLN:CB	0.42	2.67	5	6
1:A:65:THR:CG2	1:A:68:PRO:CB	0.42	2.97	10	1
1:A:27:THR:O	1:A:28:GLN:HB2	0.42	2.14	1	1
1:A:100:LYS:C	1:A:101:LEU:CD1	0.42	2.84	1	1
1:A:21:VAL:HG23	1:A:37:GLN:N	0.42	2.30	12	7
1:A:61:GLY:N	1:A:84:PRO:HG3	0.42	2.29	4	1
1:A:49:PHE:O	1:A:50:GLU:HB2	0.42	2.15	15	4
1:A:81:ALA:O	1:A:83:PRO:HD2	0.42	2.14	20	1
1:A:18:PHE:HB2	1:A:92:ILE:HG22	0.42	1.92	16	7
1:A:70:VAL:HG12	1:A:71:THR:N	0.42	2.29	10	1
1:A:91:ILE:CG2	1:A:98:GLN:NE2	0.42	2.82	11	1
1:A:97:GLY:O	1:A:98:GLN:C	0.42	2.56	2	2
1:A:41:ASP:OD1	1:A:73:LYS:HE2	0.42	2.15	4	1
1:A:46:LYS:HD2	1:A:67:ASN:OD1	0.42	2.15	4	1
1:A:41:ASP:O	1:A:41:ASP:OD1	0.42	2.37	5	1
1:A:34:ILE:O	1:A:79:ILE:N	0.42	2.52	17	5
1:A:42:GLY:O	1:A:43:SER:C	0.42	2.57	10	7
1:A:17:LYS:O	1:A:39:GLU:HB2	0.42	2.14	6	1
1:A:51:ILE:HG23	1:A:90:ILE:HG13	0.42	1.91	11	1
1:A:19:LYS:HB2	1:A:39:GLU:OE2	0.42	2.15	12	1
1:A:19:LYS:HE3	1:A:37:GLN:CB	0.42	2.44	17	1
1:A:17:LYS:CE	1:A:18:PHE:C	0.42	2.87	18	1
1:A:31:THR:HA	1:A:81:ALA:O	0.42	2.15	20	1
1:A:64:ILE:HB	1:A:80:GLU:HG2	0.42	1.92	15	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:PRO:HG3	1:A:79:ILE:CG2	0.42	2.44	15	1
1:A:61:GLY:CA	1:A:83:PRO:HA	0.42	2.45	20	2
1:A:51:ILE:HA	1:A:89:TYR:O	0.42	2.15	11	1
1:A:39:GLU:O	1:A:40:GLY:C	0.42	2.56	12	2
1:A:49:PHE:CD1	1:A:79:ILE:HD12	0.42	2.50	13	1
1:A:98:GLN:OE1	1:A:100:LYS:NZ	0.42	2.49	14	1
1:A:19:LYS:HE3	1:A:37:GLN:CD	0.42	2.35	17	1
1:A:40:GLY:O	1:A:73:LYS:HD2	0.41	2.15	14	2
1:A:40:GLY:O	1:A:73:LYS:HE3	0.41	2.15	18	1
1:A:34:ILE:HG13	1:A:101:LEU:HD22	0.41	1.91	1	1
1:A:20:VAL:CG2	1:A:99:LEU:HD22	0.41	2.45	4	1
1:A:31:THR:OG1	1:A:80:GLU:OE2	0.41	2.36	12	1
1:A:49:PHE:HA	1:A:91:ILE:O	0.41	2.15	12	4
1:A:17:LYS:HD2	1:A:97:GLY:O	0.41	2.15	2	1
1:A:16:GLY:HA3	1:A:38:TYR:OH	0.41	2.16	9	1
1:A:50:GLU:O	1:A:91:ILE:CG1	0.41	2.69	13	1
1:A:95:GLU:C	1:A:97:GLY:N	0.41	2.73	13	2
1:A:27:THR:HG21	1:A:80:GLU:CG	0.41	2.46	16	1
1:A:102:ASN:O	1:A:102:ASN:ND2	0.41	2.53	18	2
1:A:50:GLU:CG	1:A:91:ILE:HG22	0.41	2.46	10	1
1:A:24:ILE:HD11	1:A:34:ILE:CB	0.41	2.46	14	3
1:A:38:TYR:CZ	1:A:41:ASP:N	0.41	2.89	13	1
1:A:16:GLY:O	1:A:17:LYS:HE2	0.41	2.15	17	1
1:A:14:CYS:O	1:A:48:PRO:HD3	0.41	2.15	18	1
1:A:19:LYS:HE2	1:A:37:GLN:NE2	0.41	2.31	18	2
1:A:46:LYS:HG3	1:A:69:ILE:HD13	0.41	1.91	2	1
1:A:34:ILE:HG22	1:A:79:ILE:HG13	0.41	1.93	3	3
1:A:17:LYS:HG2	1:A:97:GLY:O	0.41	2.15	10	1
1:A:37:GLN:HG2	1:A:74:ASP:OD1	0.41	2.16	10	1
1:A:63:LEU:HB3	1:A:66:VAL:HG22	0.41	1.93	15	1
1:A:37:GLN:NE2	1:A:76:PRO:HD3	0.41	2.31	16	1
1:A:20:VAL:HG23	1:A:99:LEU:CD2	0.41	2.45	11	1
1:A:65:THR:HG23	1:A:68:PRO:HB3	0.41	1.93	14	1
1:A:26:GLU:HG3	1:A:26:GLU:O	0.41	2.15	1	1
1:A:65:THR:O	1:A:68:PRO:HD3	0.41	2.16	2	1
1:A:66:VAL:C	1:A:67:ASN:OD1	0.41	2.59	5	1
1:A:50:GLU:HG2	1:A:91:ILE:CB	0.41	2.46	17	2
1:A:36:VAL:HG23	1:A:37:GLN:N	0.41	2.31	14	2
1:A:61:GLY:HA2	1:A:82:GLU:O	0.41	2.15	16	1
1:A:47:ILE:O	1:A:67:ASN:HA	0.41	2.16	19	1
1:A:17:LYS:HE3	1:A:97:GLY:O	0.40	2.16	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:GLU:C	1:A:73:LYS:HG3	0.40	2.36	8	1
1:A:63:LEU:HA	1:A:81:ALA:HA	0.40	1.93	12	1
1:A:33:VAL:CG2	1:A:80:GLU:HG3	0.40	2.46	16	1
1:A:97:GLY:O	1:A:98:GLN:O	0.40	2.39	2	2
1:A:36:VAL:HG11	1:A:92:ILE:CD1	0.40	2.46	6	1
1:A:64:ILE:HG21	1:A:80:GLU:HG2	0.40	1.94	15	1
1:A:35:ARG:C	1:A:36:VAL:HG13	0.40	2.36	1	1
1:A:64:ILE:HG21	1:A:80:GLU:OE1	0.40	2.16	9	1
1:A:14:CYS:SG	1:A:47:ILE:CD1	0.40	3.06	12	1
1:A:64:ILE:HB	1:A:80:GLU:CG	0.40	2.46	13	1
1:A:21:VAL:HB	1:A:35:ARG:HG3	0.40	1.93	5	1
1:A:40:GLY:O	1:A:73:LYS:HD3	0.40	2.14	7	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	77/117 (66%)	60±2 (78±3%)	8±2 (11±2%)	9±1 (11±2%)	1 8
All	All	1540/2340 (66%)	1196 (78%)	170 (11%)	174 (11%)	1 8

All 16 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	16	GLY	20
1	A	43	SER	20
1	A	44	PRO	20
1	A	66	VAL	20
1	A	84	PRO	17
1	A	96	PRO	16
1	A	95	GLU	15
1	A	68	PRO	12
1	A	42	GLY	11
1	A	14	CYS	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	50	GLU	4
1	A	61	GLY	3
1	A	98	GLN	2
1	A	97	GLY	2
1	A	51	ILE	1
1	A	73	LYS	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	68/105 (65%)	50±2 (74±3%)	18±2 (26±3%)	2 23
All	All	1360/2100 (65%)	1009 (74%)	351 (26%)	2 23

All 42 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	24	ILE	20
1	A	31	THR	20
1	A	32	ILE	20
1	A	34	ILE	20
1	A	43	SER	20
1	A	62	ARG	20
1	A	94	VAL	20
1	A	98	GLN	20
1	A	69	ILE	17
1	A	17	LYS	15
1	A	100	LYS	15
1	A	35	ARG	13
1	A	63	LEU	13
1	A	29	HIS	12
1	A	73	LYS	12
1	A	95	GLU	10
1	A	45	CYS	10
1	A	65	THR	8
1	A	92	ILE	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	41	ASP	6
1	A	15	THR	6
1	A	50	GLU	5
1	A	28	GLN	4
1	A	46	LYS	4
1	A	22	LYS	3
1	A	80	GLU	3
1	A	82	GLU	3
1	A	78	ASN	3
1	A	37	GLN	3
1	A	102	ASN	2
1	A	71	THR	2
1	A	75	SER	2
1	A	26	GLU	2
1	A	23	GLU	2
1	A	14	CYS	2
1	A	101	LEU	1
1	A	51	ILE	1
1	A	67	ASN	1
1	A	99	LEU	1
1	A	103	TRP	1
1	A	19	LYS	1
1	A	90	ILE	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 monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

No chemical shift data were provided