



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 03:10 PM UTC

PDB ID : 2KDC / pdb_00002kdc
Title : NMR Solution Structure of E. coli diacylglycerol kinase (DAGK) in DPC micelles
Authors : Van Horn, W.D.; Kim, H.; Ellis, C.D.; Hadziselimovic, A.; Sulistijo, E.S.; Karra, M.D.; Tian, C.; Sonnichsen, F.D.; Sanders, C.R.
Deposited on : 2009-01-06

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

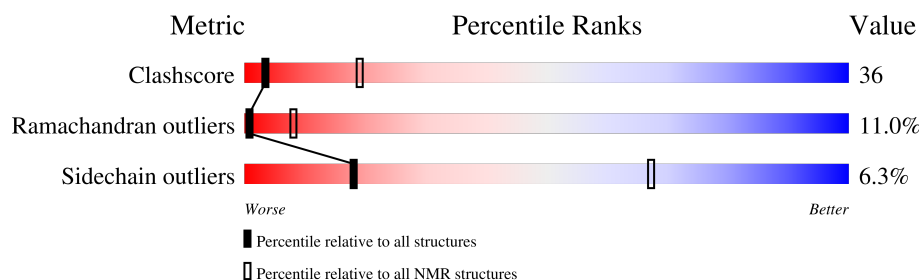
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	121	28% 45% 7% 21%
1	B	121	31% 42% 7% 21%
1	C	121	29% 45% 7% 20%

2 Ensemble composition and analysis

This entry contains 16 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:25-A:120, B:25-B:120, C:25-C:121 (289)	1.26	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 3 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 5, 8, 9, 15, 16
2	1, 6, 11, 12, 13, 14
3	2, 4, 7, 10

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 5658 atoms, of which 2889 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Diacylglycerol kinase.

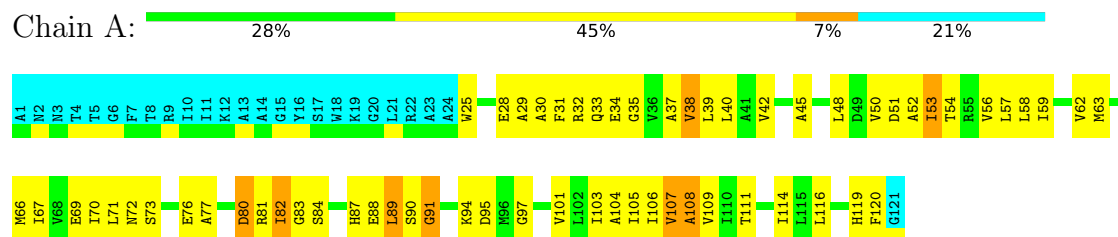
Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1886	600	963	156	162	5	
1	B	121	Total	C	H	N	O	S	0
			1886	600	963	156	162	5	
1	C	121	Total	C	H	N	O	S	0
			1886	600	963	156	162	5	

4 Residue-property plots

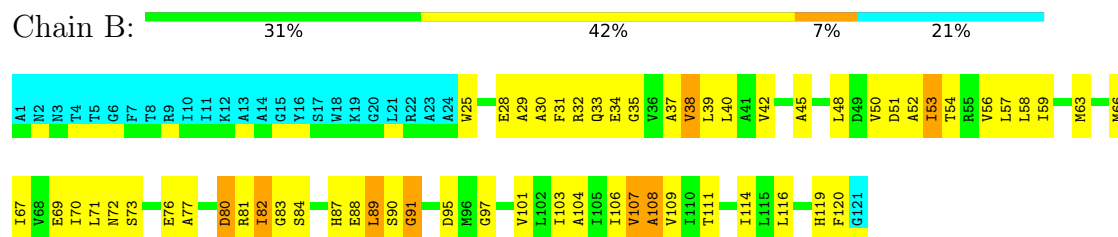
4.1 Average score per residue in the NMR ensemble

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.

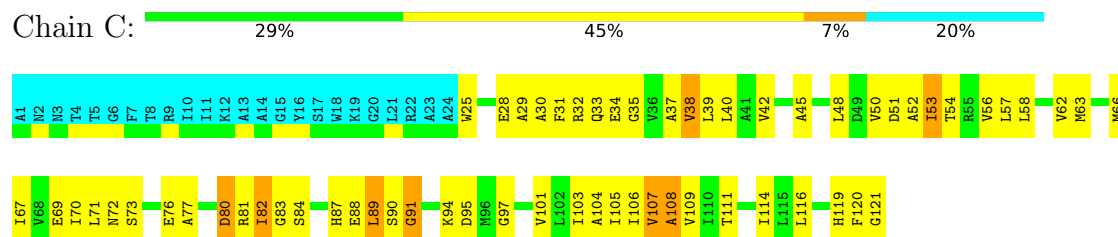
- Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase

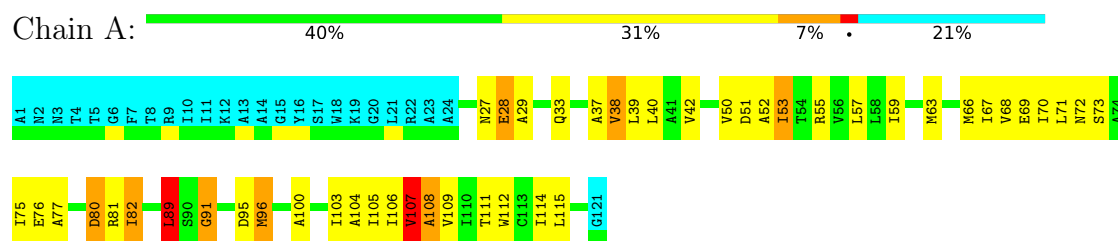


4.2 Scores per residue for each member of the ensemble

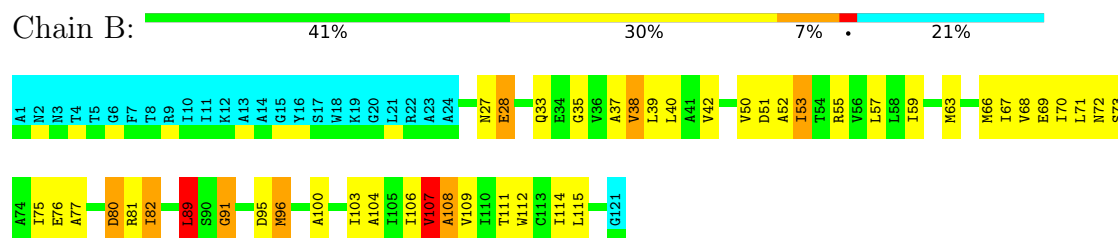
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

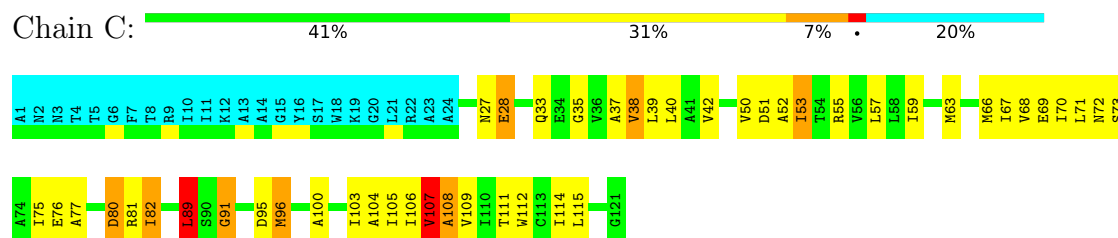
- Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase

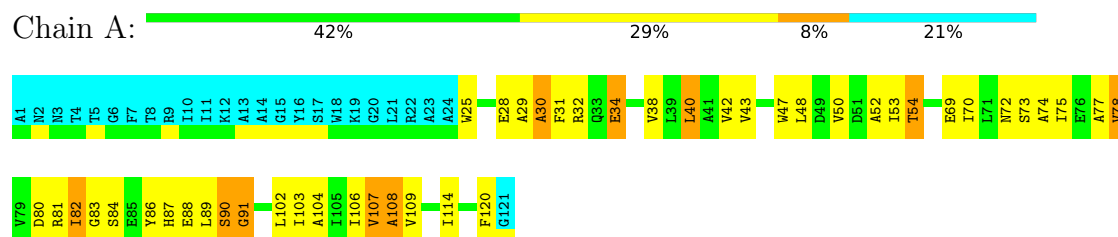


- Molecule 1: Diacylglycerol kinase

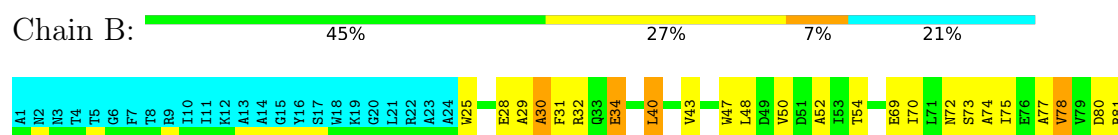


4.2.2 Score per residue for model 2

- Molecule 1: Diacylglycerol kinase



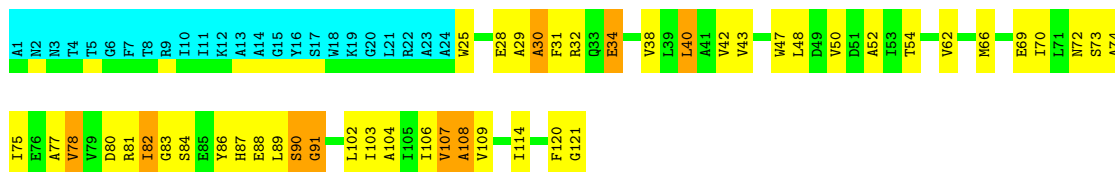
- Molecule 1: Diacylglycerol kinase





• Molecule 1: Diacylglycerol kinase

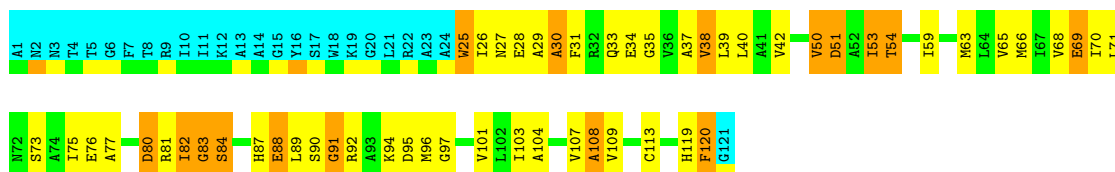
Chain C: 41% 31% 7% 20%



4.2.3 Score per residue for model 3 (medoid)

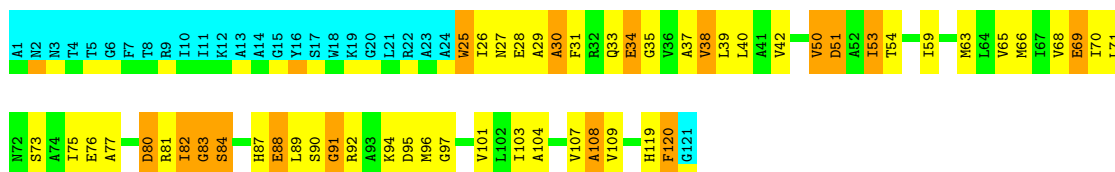
• Molecule 1: Diacylglycerol kinase

Chain A: 34% 32% 13% 21%



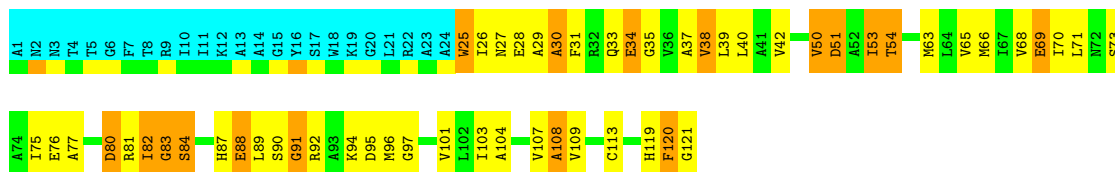
• Molecule 1: Diacylglycerol kinase

Chain B: 35% 31% 13% 21%



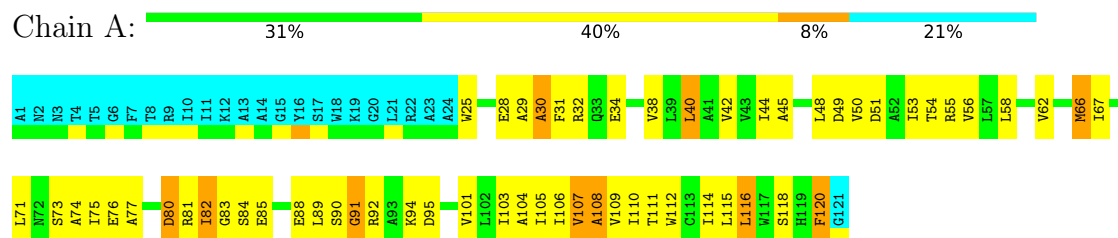
• Molecule 1: Diacylglycerol kinase

Chain C: 35% 31% 14% 20%

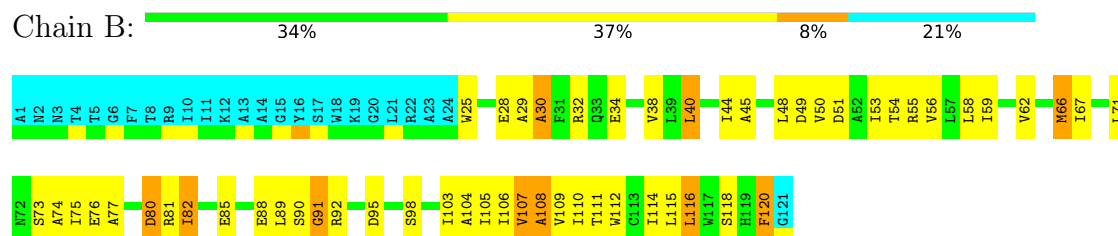


4.2.4 Score per residue for model 4

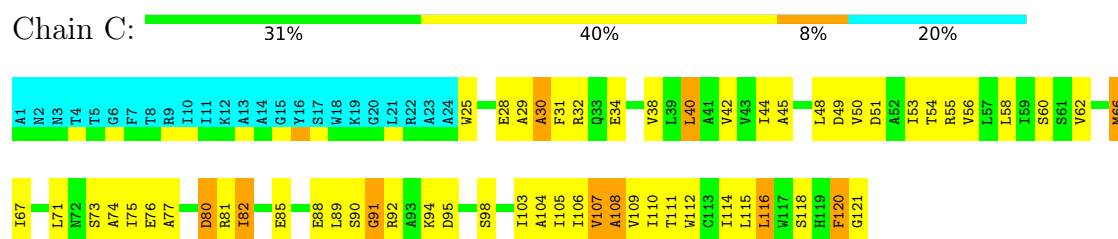
• Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase

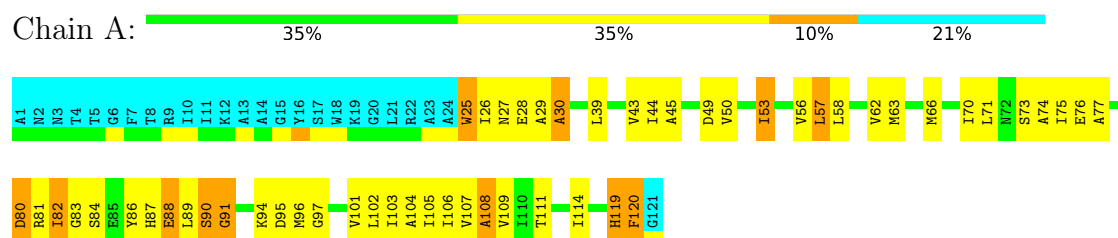


- Molecule 1: Diacylglycerol kinase

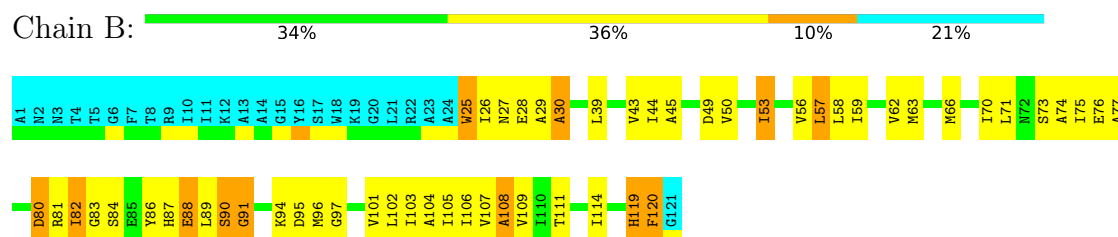


4.2.5 Score per residue for model 5

- Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase



Chain C:

A1 N2 N3 N4 T4 T5 G6 F7 F8 R9 R10 R11 R12 R13 R14 G15 G16 F17 F18 R19 R20 R21 R22 R23 A24 R25 R26 R27 R28 R29 R30 R31 R32 R33 R34 R35 R36 R37 R38 R39 R40 R41 R42 R43 R44 R45 R46 R47 R48 R49 R50 R51 R52 R53 R54 R55 R56 R57 R58 R59 R60 R61 R62 R63 R64 R65 R66 R67 R68 R69 R70 R71 R72 R73 R74 R75 R76 R77 R78 R79 R80 R81 R82 R83 R84 R85 R86 R87 R88 R89 R90 R91 R92 R93 R94 R95 R96 R97 R98 R99 R100 R101 R102 R103 R104 R105 R106 R107 R108 R109 R110 R111 R112 R113 R114 R115 R116 R117 R118 R119 R120 R121 R122 R123 R124 R125 R126 R127 R128 R129 R130 R131 R132 R133 R134 R135 R136 R137 R138 R139 R140 R141 R142 R143 R144 R145 R146 R147 R148 R149 R150 R151 R152 R153 R154 R155 R156 R157 R158 R159 R160 R161 R162 R163 R164 R165 R166 R167 R168 R169 R170 R171 R172 R173 R174 R175 R176 R177 R178 R179 R180 R181 R182 R183 R184 R185 R186 R187 R188 R189 R190 R191 R192 R193 R194 R195 R196 R197 R198 R199 R200

Chain A:

Top chart items: A1, N2, N3, T4, T5, G6, F7, T8, R9, I10, I11, K12, K13, A14, G15, Y16, S17, W18, K19, G20, L21, R22, A23, A24, W25, I26, N27, E28, A29, A30, F31, R32, G35, V36, A37, V38, L39, L40, A41, V42, V43, I44, A45, C46, W47, L48, D49, V50, D51, A52, T53, T54, R55, V56, L57, L58, I59, W62.

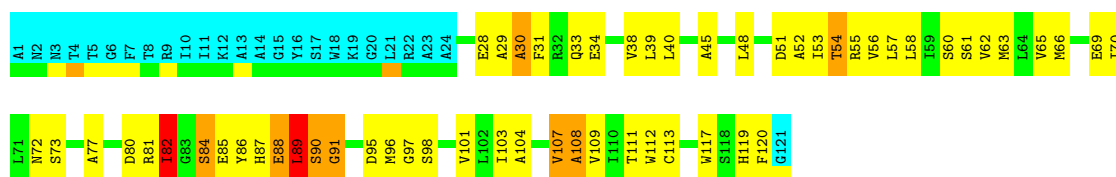
Bottom chart items: M66, I70, S73, A77, D80, R81, I82, G83, S84, E85, Y86, H87, E88, L89, S90, G91, R92, A93, K94, D95, M96, G97, S98, A99, A100, I101, L102, I103, A104, I105, I106, V107, A108, V109, I114, L115, W116, S117, S118, H119, F120, G121.

Chain B:

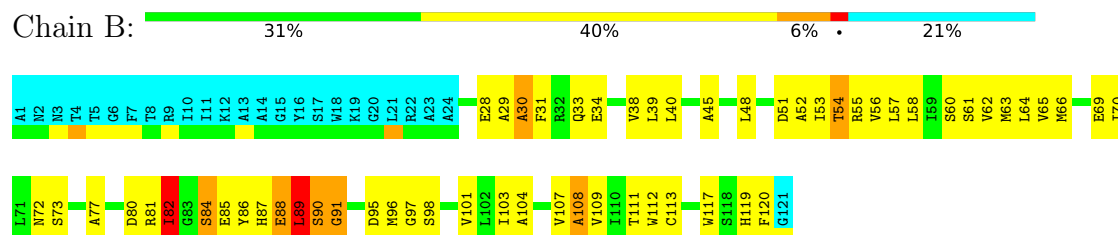
30% 40% 8% 21%

Chain C:

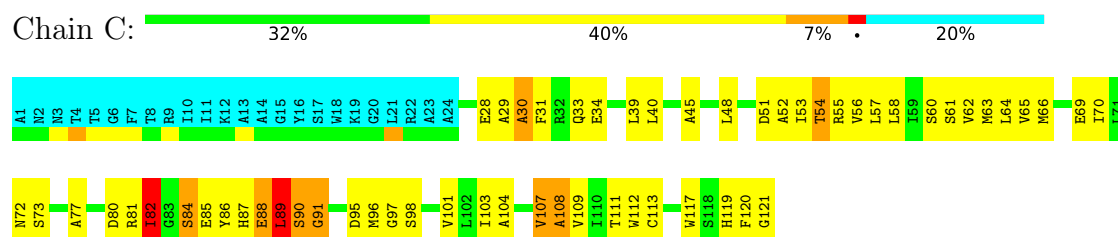
Chain A: 32% 39% 7% 21%



- Molecule 1: Diacylglycerol kinase

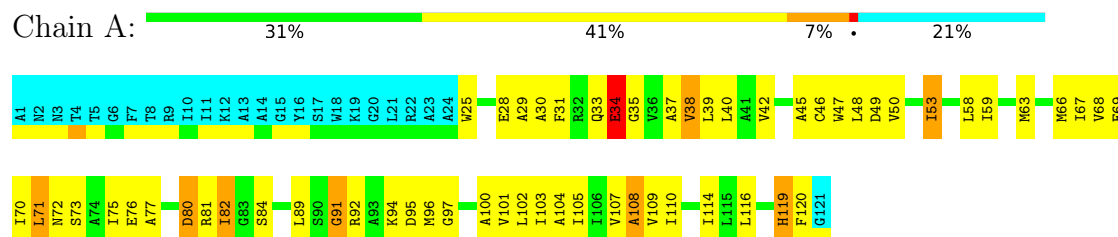


- Molecule 1: Diacylglycerol kinase

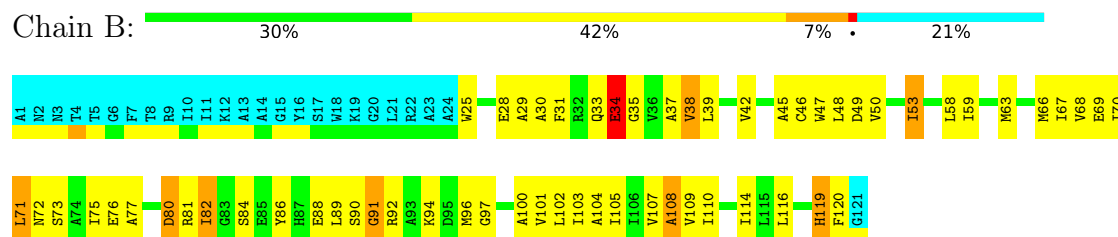


4.2.8 Score per residue for model 8

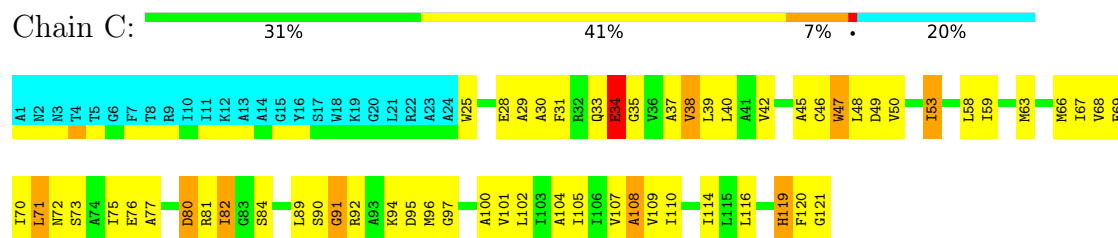
- Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase

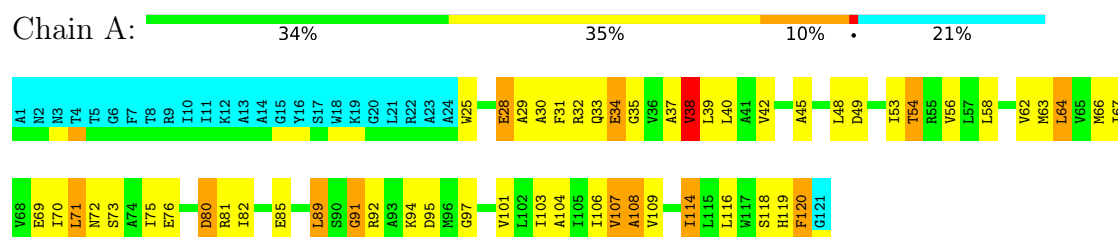


- Molecule 1: Diacylglycerol kinase

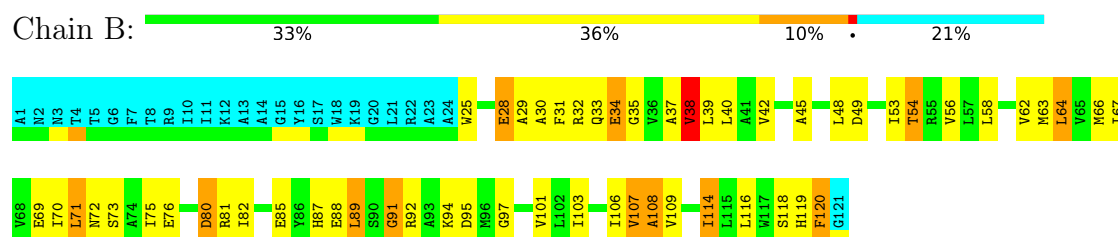


4.2.9 Score per residue for model 9

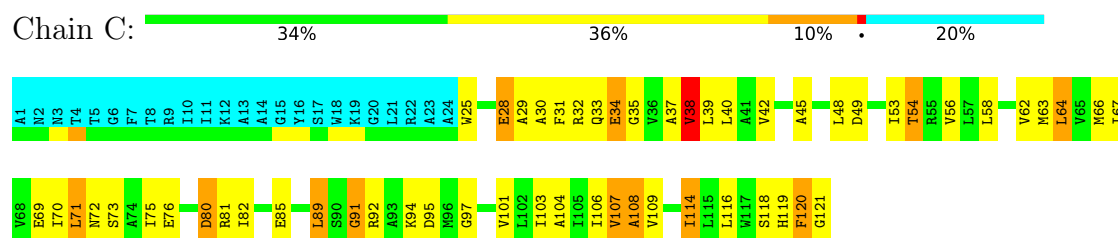
- Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase

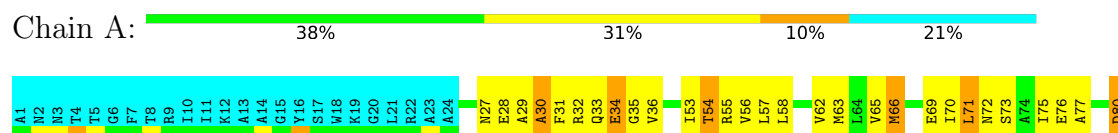


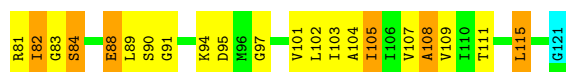
- Molecule 1: Diacylglycerol kinase



4.2.10 Score per residue for model 10

- Molecule 1: Diacylglycerol kinase

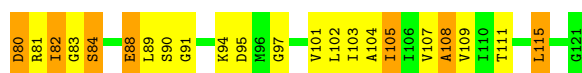




• Molecule 1: Diacylglycerol kinase

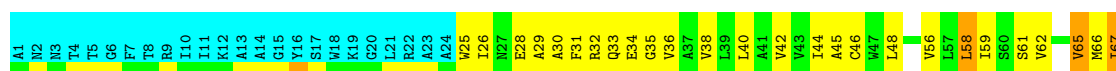


• Molecule 1: Diacylglycerol kinase

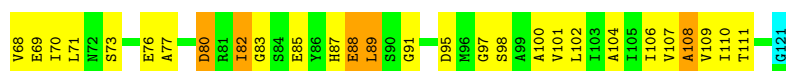
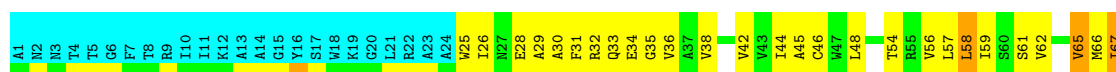


4.2.11 Score per residue for model 11

• Molecule 1: Diacylglycerol kinase

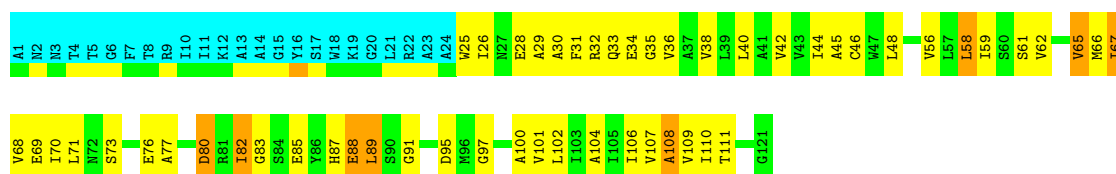


• Molecule 1: Diacylglycerol kinase



• Molecule 1: Diacylglycerol kinase



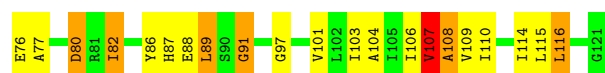




• Molecule 1: Diacylglycerol kinase

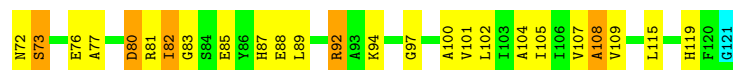
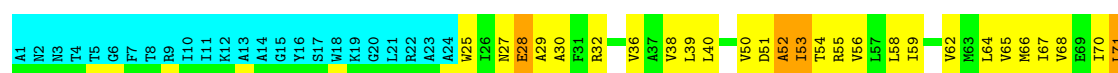


• Molecule 1: Diacylglycerol kinase

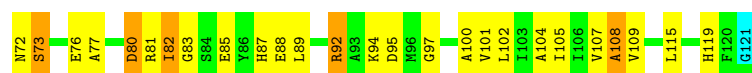
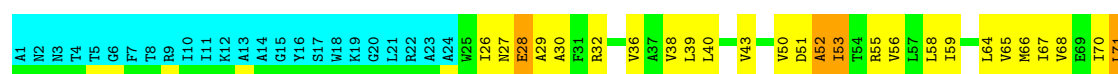


4.2.14 Score per residue for model 14

• Molecule 1: Diacylglycerol kinase

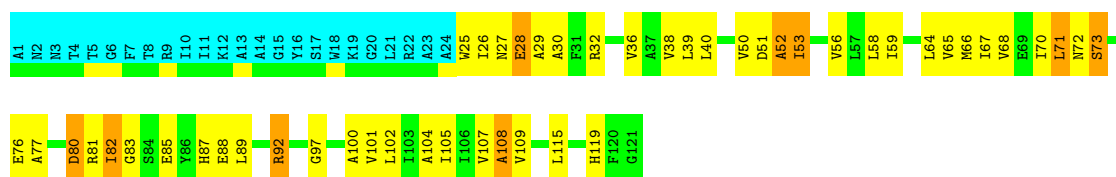


• Molecule 1: Diacylglycerol kinase



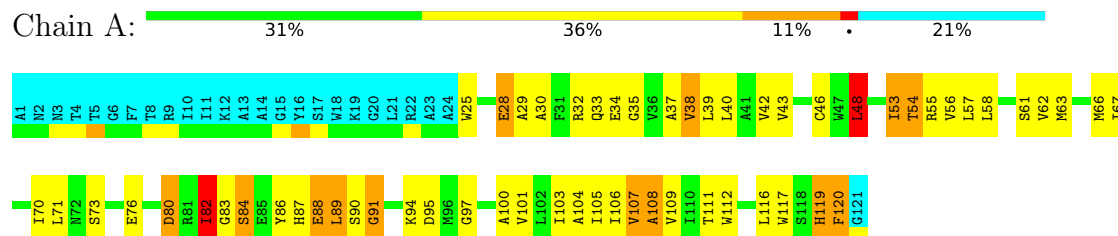
• Molecule 1: Diacylglycerol kinase



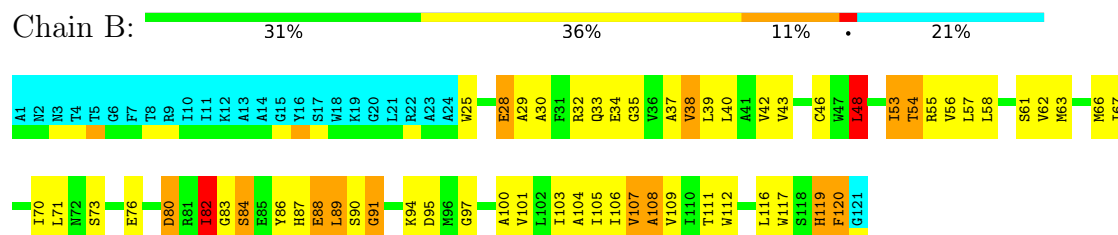


4.2.15 Score per residue for model 15

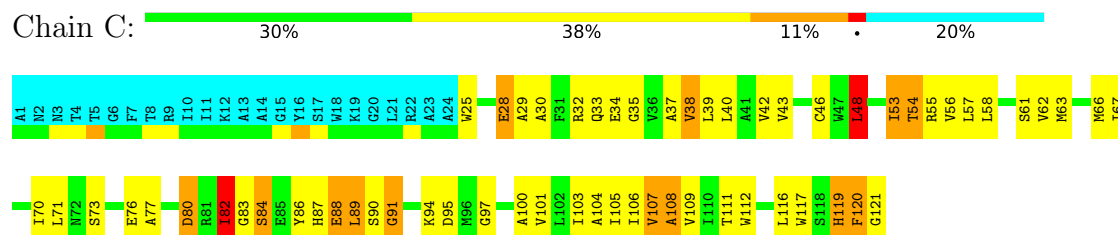
- Molecule 1: Diacylglycerol kinase



- Molecule 1: Diacylglycerol kinase

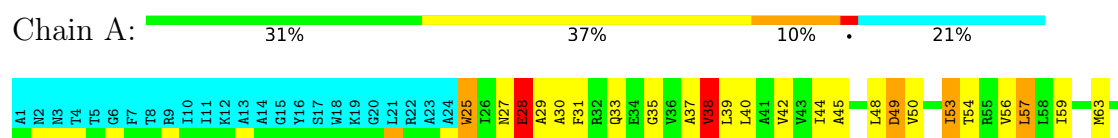


- Molecule 1: Diacylglycerol kinase



4.2.16 Score per residue for model 16

- Molecule 1: Diacylglycerol kinase

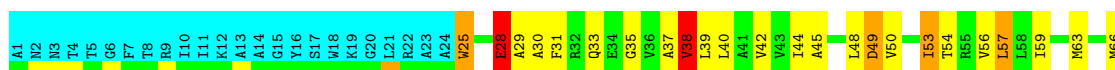




• Molecule 1: Diacylglycerol kinase



• Molecule 1: Diacylglycerol kinase



5 Refinement protocol and experimental data overview ⓘ

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

Of the 48 calculated structures, 16 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
X-PLOR NIH	structure solution	2.19
X-PLOR NIH	refinement	2.19

No chemical shift data was provided.

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	737	773	771	57±9
1	B	737	773	771	57±9
1	C	742	776	774	58±9
All	All	35456	37152	37056	2628

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 36.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:81:ARG:O	1:B:82:ILE:HG23	0.82	1.75	7	1
1:B:53:ILE:N	1:B:53:ILE:HD13	0.81	1.90	14	2
1:C:81:ARG:O	1:C:82:ILE:HG23	0.81	1.75	7	1
1:A:53:ILE:N	1:A:53:ILE:HD13	0.81	1.90	14	1
1:A:81:ARG:O	1:A:82:ILE:HG23	0.81	1.75	7	1
1:C:53:ILE:HD13	1:C:53:ILE:N	0.81	1.91	14	2
1:B:107:VAL:HG13	1:B:108:ALA:H	0.80	1.36	15	3
1:A:97:GLY:O	1:A:101:VAL:HG23	0.79	1.78	14	7
1:A:107:VAL:HG13	1:A:108:ALA:H	0.78	1.36	15	3
1:B:97:GLY:O	1:B:101:VAL:HG23	0.78	1.78	14	7
1:C:97:GLY:O	1:C:101:VAL:HG23	0.77	1.78	14	7
1:C:107:VAL:HG13	1:C:108:ALA:H	0.77	1.36	15	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:107:VAL:HG23	1:C:108:ALA:H	0.74	1.43	11	3
1:A:107:VAL:HG23	1:A:108:ALA:H	0.71	1.43	11	3
1:B:107:VAL:HG23	1:B:108:ALA:H	0.71	1.43	11	3
1:A:109:VAL:HG23	1:A:110:ILE:H	0.71	1.45	8	1
1:B:109:VAL:HG23	1:B:110:ILE:H	0.71	1.45	8	1
1:C:100:ALA:O	1:C:104:ALA:HB2	0.70	1.86	8	4
1:B:100:ALA:O	1:B:104:ALA:HB2	0.70	1.86	8	4
1:C:109:VAL:HG23	1:C:110:ILE:H	0.70	1.45	8	1
1:A:100:ALA:O	1:A:104:ALA:HB2	0.70	1.86	8	4
1:A:89:LEU:HD23	1:A:89:LEU:H	0.70	1.46	3	1
1:C:89:LEU:HD23	1:C:89:LEU:H	0.70	1.46	3	1
1:B:89:LEU:H	1:B:89:LEU:HD23	0.69	1.46	3	1
1:B:107:VAL:HG13	1:B:108:ALA:N	0.68	2.04	16	3
1:B:82:ILE:HD12	1:B:82:ILE:H	0.67	1.49	14	1
1:C:107:VAL:HG13	1:C:108:ALA:N	0.67	2.04	16	3
1:A:82:ILE:HD12	1:A:82:ILE:H	0.67	1.49	14	1
1:B:103:ILE:O	1:B:107:VAL:HG22	0.67	1.90	12	2
1:A:63:MET:SD	1:C:63:MET:HE1	0.67	2.30	5	1
1:A:82:ILE:HG23	1:A:83:GLY:H	0.67	1.50	15	1
1:B:63:MET:HE1	1:C:63:MET:SD	0.67	2.30	5	1
1:C:103:ILE:O	1:C:107:VAL:HG22	0.66	1.90	12	2
1:A:107:VAL:HG13	1:A:108:ALA:N	0.66	2.05	5	3
1:C:82:ILE:H	1:C:82:ILE:HD12	0.66	1.49	14	1
1:A:63:MET:HE1	1:B:63:MET:SD	0.66	2.30	5	1
1:C:82:ILE:HG23	1:C:83:GLY:H	0.66	1.50	15	1
1:A:103:ILE:O	1:A:107:VAL:HG22	0.65	1.90	12	2
1:B:82:ILE:HG23	1:B:83:GLY:H	0.65	1.50	15	1
1:B:26:ILE:N	1:B:26:ILE:HD12	0.65	2.06	6	1
1:A:26:ILE:HD12	1:A:26:ILE:N	0.65	2.06	6	1
1:B:56:VAL:HG21	1:C:53:ILE:HD11	0.64	1.69	5	1
1:C:26:ILE:HD12	1:C:26:ILE:N	0.64	2.06	6	1
1:B:101:VAL:HG13	1:B:102:LEU:N	0.64	2.08	6	4
1:A:101:VAL:HG13	1:A:102:LEU:N	0.64	2.08	5	4
1:C:101:VAL:HG13	1:C:102:LEU:N	0.63	2.08	8	4
1:C:109:VAL:HG23	1:C:110:ILE:N	0.63	2.08	8	1
1:B:107:VAL:HG23	1:B:108:ALA:N	0.63	2.09	11	1
1:A:56:VAL:HG21	1:B:53:ILE:HD11	0.63	1.69	5	1
1:C:53:ILE:N	1:C:53:ILE:CD1	0.63	2.62	14	2
1:A:31:PHE:CD1	1:A:32:ARG:N	0.63	2.67	2	3
1:A:53:ILE:N	1:A:53:ILE:CD1	0.62	2.62	14	2
1:A:101:VAL:HG23	1:A:102:LEU:H	0.62	1.55	12	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:59:ILE:HD12	1:B:59:ILE:N	0.62	2.10	14	1
1:A:37:ALA:O	1:A:39:LEU:N	0.62	2.33	12	9
1:A:107:VAL:HG23	1:A:108:ALA:N	0.62	2.09	11	1
1:C:37:ALA:O	1:C:39:LEU:N	0.62	2.33	12	9
1:B:37:ALA:O	1:B:39:LEU:N	0.62	2.33	12	9
1:C:107:VAL:HG23	1:C:108:ALA:N	0.62	2.09	11	1
1:B:53:ILE:N	1:B:53:ILE:CD1	0.62	2.62	14	2
1:A:59:ILE:HD12	1:A:59:ILE:N	0.62	2.10	14	1
1:A:109:VAL:HG23	1:A:110:ILE:N	0.62	2.08	8	1
1:B:109:VAL:HG23	1:B:110:ILE:N	0.62	2.09	8	1
1:B:101:VAL:HG23	1:B:102:LEU:N	0.62	2.09	12	2
1:B:31:PHE:CD1	1:B:32:ARG:N	0.62	2.67	2	3
1:C:31:PHE:CD1	1:C:32:ARG:N	0.62	2.67	2	3
1:A:101:VAL:HG23	1:A:102:LEU:N	0.62	2.09	12	2
1:C:59:ILE:N	1:C:59:ILE:HD12	0.62	2.09	14	1
1:A:53:ILE:HD11	1:C:56:VAL:HG21	0.62	1.68	5	1
1:C:101:VAL:HG23	1:C:102:LEU:N	0.62	2.09	12	2
1:A:53:ILE:HD13	1:A:53:ILE:N	0.61	2.08	3	1
1:B:25:TRP:NE1	1:B:33:GLN:NE2	0.61	2.48	9	1
1:B:101:VAL:HG23	1:B:102:LEU:H	0.61	1.55	12	2
1:C:31:PHE:CG	1:C:32:ARG:N	0.61	2.69	9	5
1:A:25:TRP:NE1	1:A:33:GLN:NE2	0.61	2.48	9	1
1:B:31:PHE:CG	1:B:32:ARG:N	0.61	2.69	9	5
1:C:25:TRP:NE1	1:C:33:GLN:NE2	0.61	2.48	9	1
1:A:31:PHE:CG	1:A:32:ARG:N	0.60	2.69	9	5
1:C:82:ILE:HD12	1:C:82:ILE:N	0.60	2.12	14	1
1:A:92:ARG:NH2	1:B:81:ARG:H	0.60	1.94	9	1
1:C:101:VAL:HG23	1:C:102:LEU:H	0.60	1.55	12	2
1:B:82:ILE:HD12	1:B:82:ILE:N	0.60	2.12	14	1
1:C:96:MET:SD	1:C:96:MET:N	0.60	2.75	3	4
1:A:96:MET:SD	1:A:96:MET:N	0.60	2.75	3	4
1:A:82:ILE:HD12	1:A:82:ILE:N	0.59	2.12	14	1
1:B:82:ILE:HG23	1:B:83:GLY:N	0.59	2.12	15	1
1:B:96:MET:SD	1:B:96:MET:N	0.59	2.75	3	2
1:B:25:TRP:HE1	1:B:33:GLN:NE2	0.59	1.95	9	1
1:B:114:ILE:HD13	1:B:114:ILE:O	0.59	1.97	9	1
1:C:25:TRP:HE1	1:C:33:GLN:NE2	0.59	1.95	9	1
1:A:25:TRP:HE1	1:A:33:GLN:NE2	0.59	1.95	9	1
1:B:96:MET:N	1:B:96:MET:SD	0.59	2.76	16	2
1:B:92:ARG:NH2	1:C:81:ARG:H	0.59	1.94	9	1
1:A:82:ILE:HG23	1:A:83:GLY:N	0.59	2.12	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:82:ILE:HG23	1:C:83:GLY:N	0.59	2.12	15	1
1:A:81:ARG:H	1:C:92:ARG:NH2	0.59	1.94	9	1
1:A:31:PHE:CD1	1:C:96:MET:SD	0.59	2.96	7	1
1:A:81:ARG:HE	1:C:92:ARG:NH1	0.58	1.96	4	1
1:B:92:ARG:NH1	1:C:81:ARG:HE	0.58	1.97	4	1
1:B:96:MET:SD	1:C:31:PHE:CD1	0.58	2.96	7	1
1:A:114:ILE:HD13	1:A:114:ILE:O	0.58	1.97	9	1
1:B:97:GLY:O	1:B:101:VAL:HG13	0.58	1.98	12	2
1:A:81:ARG:NE	1:C:92:ARG:HH12	0.58	1.97	4	1
1:A:92:ARG:NH1	1:B:81:ARG:HE	0.58	1.96	4	1
1:C:114:ILE:O	1:C:114:ILE:HD13	0.58	1.97	9	1
1:A:82:ILE:H	1:A:82:ILE:CD1	0.58	2.12	14	1
1:B:89:LEU:H	1:B:89:LEU:CD2	0.58	2.12	3	1
1:A:96:MET:SD	1:B:31:PHE:CD1	0.58	2.96	7	1
1:A:97:GLY:O	1:A:101:VAL:HG13	0.57	1.98	12	2
1:A:89:LEU:H	1:A:89:LEU:CD2	0.57	2.12	3	1
1:A:92:ARG:HH12	1:B:81:ARG:NE	0.57	1.97	4	1
1:C:97:GLY:O	1:C:101:VAL:HG13	0.57	1.98	12	2
1:C:82:ILE:H	1:C:82:ILE:CD1	0.57	2.12	14	1
1:B:92:ARG:HH12	1:C:81:ARG:NE	0.57	1.97	4	1
1:B:82:ILE:H	1:B:82:ILE:CD1	0.57	2.12	14	1
1:B:25:TRP:CD1	1:B:29:ALA:CB	0.57	2.88	4	1
1:C:53:ILE:HD13	1:C:53:ILE:H	0.57	1.58	14	1
1:C:25:TRP:CD1	1:C:29:ALA:CB	0.56	2.88	4	1
1:B:33:GLN:O	1:B:36:VAL:N	0.56	2.38	10	2
1:C:120:PHE:CD2	1:C:121:GLY:N	0.56	2.73	2	9
1:A:25:TRP:CD1	1:A:29:ALA:CB	0.56	2.88	4	1
1:C:119:HIS:ND1	1:C:120:PHE:N	0.56	2.53	15	3
1:A:63:MET:SD	1:B:63:MET:SD	0.56	3.04	5	3
1:B:63:MET:SD	1:C:63:MET:SD	0.56	3.04	5	3
1:C:33:GLN:O	1:C:36:VAL:N	0.56	2.38	10	2
1:A:53:ILE:O	1:A:56:VAL:N	0.56	2.39	15	9
1:B:53:ILE:O	1:B:56:VAL:N	0.56	2.39	15	9
1:A:119:HIS:ND1	1:A:120:PHE:N	0.56	2.53	15	3
1:B:53:ILE:HD13	1:B:53:ILE:H	0.56	1.58	14	1
1:B:119:HIS:ND1	1:B:120:PHE:N	0.56	2.53	15	3
1:C:89:LEU:H	1:C:89:LEU:CD2	0.56	2.12	3	1
1:C:107:VAL:CG1	1:C:108:ALA:H	0.56	2.14	16	3
1:A:33:GLN:O	1:A:36:VAL:N	0.56	2.38	10	2
1:B:31:PHE:CD2	1:B:32:ARG:N	0.56	2.74	13	2
1:C:53:ILE:O	1:C:56:VAL:N	0.55	2.39	15	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:107:VAL:CG1	1:B:108:ALA:H	0.55	2.14	16	3
1:C:31:PHE:CD2	1:C:32:ARG:N	0.55	2.74	13	2
1:A:53:ILE:HD13	1:A:53:ILE:H	0.55	1.57	14	1
1:A:63:MET:SD	1:C:63:MET:SD	0.55	3.04	5	3
1:B:66:MET:HE1	1:C:67:ILE:CD1	0.55	2.32	4	1
1:B:47:TRP:N	1:B:47:TRP:CD1	0.55	2.72	6	1
1:A:25:TRP:CD1	1:A:33:GLN:HE21	0.55	2.20	15	1
1:A:107:VAL:O	1:A:109:VAL:N	0.55	2.40	8	16
1:B:107:VAL:O	1:B:109:VAL:N	0.55	2.40	8	16
1:C:107:VAL:O	1:C:109:VAL:N	0.55	2.40	8	16
1:A:116:LEU:O	1:A:119:HIS:ND1	0.55	2.40	15	2
1:C:25:TRP:CD1	1:C:33:GLN:HE21	0.55	2.20	15	1
1:A:107:VAL:HG12	1:A:108:ALA:N	0.55	2.17	13	3
1:B:116:LEU:O	1:B:119:HIS:ND1	0.55	2.39	15	2
1:C:116:LEU:O	1:C:119:HIS:ND1	0.55	2.40	15	2
1:C:107:VAL:HG12	1:C:108:ALA:N	0.55	2.17	13	3
1:A:31:PHE:CD2	1:A:32:ARG:N	0.55	2.74	13	2
1:B:37:ALA:C	1:B:39:LEU:N	0.55	2.64	12	9
1:A:67:ILE:CD1	1:C:66:MET:HE1	0.55	2.32	4	1
1:C:53:ILE:O	1:C:55:ARG:N	0.55	2.40	15	4
1:A:37:ALA:C	1:A:39:LEU:N	0.54	2.65	16	9
1:A:66:MET:HE1	1:B:67:ILE:CD1	0.54	2.32	4	1
1:A:107:VAL:CG1	1:A:108:ALA:H	0.54	2.14	16	3
1:B:45:ALA:O	1:B:49:ASP:N	0.54	2.40	8	1
1:C:63:MET:CE	1:C:66:MET:SD	0.54	2.96	10	1
1:B:103:ILE:O	1:B:106:ILE:N	0.54	2.41	16	8
1:A:37:ALA:O	1:A:40:LEU:N	0.54	2.40	12	9
1:C:37:ALA:C	1:C:39:LEU:N	0.54	2.65	16	9
1:A:29:ALA:O	1:A:31:PHE:N	0.54	2.40	12	6
1:B:53:ILE:O	1:B:55:ARG:N	0.54	2.40	15	4
1:C:45:ALA:O	1:C:49:ASP:N	0.54	2.41	8	1
1:C:48:LEU:HD12	1:C:48:LEU:N	0.54	2.18	11	2
1:B:29:ALA:O	1:B:31:PHE:N	0.54	2.41	2	5
1:C:44:ILE:HG23	1:C:45:ALA:N	0.54	2.18	12	5
1:A:63:MET:CE	1:A:66:MET:SD	0.54	2.96	10	1
1:B:63:MET:CE	1:B:66:MET:SD	0.54	2.95	10	1
1:B:25:TRP:CD1	1:B:33:GLN:HE21	0.54	2.20	15	1
1:B:37:ALA:O	1:B:40:LEU:N	0.54	2.40	12	8
1:C:29:ALA:O	1:C:31:PHE:N	0.54	2.41	2	6
1:B:114:ILE:N	1:B:114:ILE:CD1	0.54	2.71	8	1
1:B:48:LEU:HD12	1:B:48:LEU:N	0.54	2.18	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:ILE:N	1:A:59:ILE:CD1	0.54	2.70	14	1
1:C:37:ALA:O	1:C:40:LEU:N	0.54	2.40	12	9
1:C:66:MET:O	1:C:69:GLU:N	0.54	2.41	11	4
1:C:119:HIS:O	1:C:121:GLY:N	0.54	2.41	6	4
1:B:35:GLY:O	1:B:38:VAL:HG22	0.54	2.03	6	1
1:C:47:TRP:N	1:C:47:TRP:CD1	0.54	2.72	6	1
1:C:38:VAL:O	1:C:42:VAL:HG22	0.54	2.03	15	1
1:B:70:ILE:O	1:B:73:SER:N	0.54	2.41	11	13
1:C:120:PHE:CG	1:C:121:GLY:N	0.54	2.76	2	5
1:A:44:ILE:HG23	1:A:45:ALA:N	0.54	2.17	6	5
1:A:45:ALA:O	1:A:49:ASP:N	0.54	2.41	8	1
1:C:114:ILE:N	1:C:114:ILE:CD1	0.54	2.71	8	1
1:B:25:TRP:CD1	1:B:33:GLN:NE2	0.54	2.76	9	1
1:A:38:VAL:O	1:A:42:VAL:HG22	0.54	2.03	15	1
1:B:38:VAL:O	1:B:42:VAL:HG23	0.54	2.03	6	8
1:C:103:ILE:O	1:C:106:ILE:N	0.54	2.41	16	9
1:A:53:ILE:O	1:A:55:ARG:N	0.54	2.40	15	4
1:C:116:LEU:O	1:C:119:HIS:CD2	0.54	2.61	16	2
1:C:25:TRP:CD1	1:C:33:GLN:NE2	0.54	2.76	9	1
1:B:107:VAL:HG12	1:B:108:ALA:N	0.53	2.17	13	3
1:B:44:ILE:HG23	1:B:45:ALA:N	0.53	2.17	6	5
1:A:114:ILE:CD1	1:A:114:ILE:N	0.53	2.71	8	1
1:C:59:ILE:N	1:C:59:ILE:CD1	0.53	2.70	14	1
1:A:114:ILE:N	1:A:114:ILE:CD1	0.53	2.71	16	1
1:B:114:ILE:CD1	1:B:114:ILE:N	0.53	2.71	16	1
1:A:38:VAL:O	1:A:42:VAL:HG23	0.53	2.03	6	10
1:A:103:ILE:O	1:A:106:ILE:N	0.53	2.41	1	8
1:A:35:GLY:O	1:A:38:VAL:HG22	0.53	2.03	6	1
1:A:116:LEU:O	1:A:119:HIS:CD2	0.53	2.61	16	2
1:B:59:ILE:N	1:B:59:ILE:CD1	0.53	2.70	14	1
1:C:38:VAL:O	1:C:42:VAL:HG23	0.53	2.03	6	10
1:A:66:MET:O	1:A:69:GLU:N	0.53	2.41	11	4
1:B:101:VAL:HG13	1:B:102:LEU:H	0.53	1.64	5	4
1:B:116:LEU:O	1:B:119:HIS:CD2	0.53	2.61	6	2
1:B:34:GLU:OE1	1:B:34:GLU:N	0.53	2.42	8	1
1:A:87:HIS:N	1:A:87:HIS:ND1	0.53	2.57	2	1
1:C:34:GLU:N	1:C:34:GLU:OE1	0.53	2.42	8	2
1:C:35:GLY:O	1:C:38:VAL:HG22	0.53	2.03	6	1
1:B:28:GLU:CD	1:B:29:ALA:N	0.53	2.67	9	1
1:C:28:GLU:CD	1:C:29:ALA:N	0.53	2.67	9	1
1:A:88:GLU:C	1:A:90:SER:H	0.53	2.12	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:88:GLU:C	1:C:90:SER:H	0.53	2.12	5	1
1:B:102:LEU:HD22	1:B:102:LEU:N	0.53	2.19	14	1
1:A:70:ILE:O	1:A:73:SER:N	0.53	2.39	14	12
1:A:101:VAL:HG13	1:A:102:LEU:H	0.53	1.64	6	4
1:B:84:SER:OG	1:B:87:HIS:CG	0.53	2.62	7	1
1:A:34:GLU:N	1:A:34:GLU:OE1	0.53	2.42	8	1
1:A:25:TRP:CD1	1:A:33:GLN:NE2	0.53	2.76	9	1
1:B:34:GLU:N	1:B:34:GLU:OE1	0.53	2.42	2	1
1:B:87:HIS:N	1:B:87:HIS:ND1	0.53	2.57	2	1
1:A:119:HIS:ND1	1:A:119:HIS:C	0.53	2.67	15	3
1:A:34:GLU:OE1	1:A:34:GLU:N	0.53	2.42	2	1
1:B:66:MET:O	1:B:69:GLU:N	0.53	2.41	11	4
1:C:107:VAL:CG1	1:C:108:ALA:N	0.53	2.72	16	3
1:A:84:SER:OG	1:A:87:HIS:CG	0.53	2.62	7	1
1:A:28:GLU:CD	1:A:29:ALA:N	0.53	2.67	9	1
1:B:97:GLY:O	1:B:101:VAL:HG22	0.53	2.04	11	2
1:A:28:GLU:O	1:A:32:ARG:NH2	0.53	2.42	15	1
1:B:38:VAL:O	1:B:42:VAL:HG22	0.53	2.03	15	1
1:C:114:ILE:CD1	1:C:114:ILE:N	0.53	2.71	16	1
1:B:39:LEU:HD12	1:B:39:LEU:N	0.53	2.19	7	3
1:B:88:GLU:C	1:B:90:SER:H	0.53	2.12	5	1
1:B:119:HIS:ND1	1:B:119:HIS:C	0.53	2.67	15	3
1:A:87:HIS:O	1:A:89:LEU:N	0.53	2.42	13	3
1:A:97:GLY:O	1:A:101:VAL:HG22	0.53	2.04	11	2
1:C:70:ILE:O	1:C:73:SER:N	0.53	2.39	14	14
1:C:87:HIS:N	1:C:87:HIS:ND1	0.53	2.56	2	1
1:A:71:LEU:O	1:A:75:ILE:HG23	0.53	2.04	10	3
1:C:71:LEU:O	1:C:75:ILE:HG23	0.53	2.04	10	3
1:A:87:HIS:CD2	1:A:88:GLU:N	0.53	2.77	14	1
1:A:107:VAL:CG1	1:A:108:ALA:N	0.52	2.72	16	3
1:C:119:HIS:ND1	1:C:119:HIS:C	0.52	2.67	15	4
1:C:81:ARG:O	1:C:82:ILE:CG2	0.52	2.55	7	1
1:B:71:LEU:O	1:B:75:ILE:HG23	0.52	2.03	10	3
1:C:87:HIS:CD2	1:C:88:GLU:N	0.52	2.77	14	1
1:B:38:VAL:O	1:B:42:VAL:HG13	0.52	2.05	15	1
1:A:39:LEU:N	1:A:39:LEU:HD12	0.52	2.19	5	1
1:C:39:LEU:N	1:C:39:LEU:HD12	0.52	2.19	7	3
1:B:87:HIS:O	1:B:89:LEU:N	0.52	2.42	13	3
1:B:28:GLU:O	1:B:32:ARG:NH2	0.52	2.42	15	1
1:C:28:GLU:O	1:C:32:ARG:NH2	0.52	2.42	15	1
1:B:69:GLU:O	1:B:72:ASN:N	0.52	2.42	7	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:69:GLU:O	1:C:72:ASN:N	0.52	2.42	7	4
1:A:39:LEU:HD12	1:A:39:LEU:N	0.52	2.19	7	2
1:C:84:SER:OG	1:C:87:HIS:CG	0.52	2.62	7	1
1:C:102:LEU:HD22	1:C:102:LEU:N	0.52	2.19	14	1
1:B:29:ALA:O	1:B:32:ARG:N	0.52	2.43	4	5
1:C:97:GLY:O	1:C:101:VAL:HG22	0.52	2.04	11	2
1:A:102:LEU:HD22	1:A:102:LEU:N	0.52	2.19	14	1
1:A:38:VAL:O	1:A:42:VAL:HG13	0.52	2.04	15	1
1:A:92:ARG:HH22	1:B:81:ARG:NH2	0.52	2.03	4	1
1:B:26:ILE:N	1:B:26:ILE:CD1	0.52	2.73	6	1
1:C:38:VAL:O	1:C:42:VAL:HG13	0.52	2.04	15	1
1:C:29:ALA:O	1:C:32:ARG:N	0.52	2.43	4	5
1:A:69:GLU:N	1:A:69:GLU:CD	0.52	2.68	10	2
1:C:26:ILE:N	1:C:26:ILE:CD1	0.52	2.73	6	1
1:A:115:LEU:O	1:A:119:HIS:CD2	0.52	2.63	14	1
1:A:119:HIS:CD2	1:A:119:HIS:N	0.52	2.77	14	1
1:B:115:LEU:O	1:B:119:HIS:CD2	0.52	2.63	14	1
1:A:29:ALA:O	1:A:32:ARG:N	0.52	2.43	4	5
1:A:81:ARG:NH2	1:C:92:ARG:HH22	0.52	2.03	4	1
1:A:48:LEU:HD12	1:A:48:LEU:N	0.52	2.18	11	2
1:B:70:ILE:CG2	1:B:71:LEU:N	0.52	2.73	16	1
1:B:87:HIS:CD2	1:B:88:GLU:N	0.52	2.77	14	1
1:C:120:PHE:CE2	1:C:121:GLY:O	0.52	2.63	2	1
1:A:114:ILE:N	1:A:114:ILE:HD12	0.52	2.20	8	2
1:C:85:GLU:N	1:C:85:GLU:CD	0.52	2.68	14	1
1:B:63:MET:CE	1:C:63:MET:SD	0.52	2.98	5	1
1:B:29:ALA:HB2	1:B:32:ARG:HH21	0.52	1.65	10	1
1:A:66:MET:O	1:A:70:ILE:N	0.51	2.43	6	10
1:A:75:ILE:HG23	1:C:78:VAL:HG22	0.51	1.82	2	1
1:A:89:LEU:HD23	1:A:89:LEU:N	0.51	2.19	3	1
1:A:26:ILE:N	1:A:26:ILE:CD1	0.51	2.73	6	1
1:C:87:HIS:O	1:C:89:LEU:N	0.51	2.42	13	3
1:C:115:LEU:O	1:C:119:HIS:CD2	0.51	2.63	14	1
1:C:66:MET:O	1:C:70:ILE:N	0.51	2.44	6	10
1:A:63:MET:CE	1:B:63:MET:SD	0.51	2.98	5	1
1:A:63:MET:HE1	1:A:66:MET:SD	0.51	2.46	10	1
1:B:85:GLU:N	1:B:85:GLU:CD	0.51	2.68	14	2
1:C:89:LEU:O	1:C:91:GLY:N	0.51	2.42	4	4
1:C:48:LEU:HD22	1:C:48:LEU:N	0.51	2.21	6	1
1:B:63:MET:HE1	1:B:66:MET:SD	0.51	2.45	10	1
1:B:69:GLU:CD	1:B:69:GLU:N	0.51	2.68	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:63:MET:HE1	1:C:66:MET:SD	0.51	2.45	10	1
1:A:25:TRP:N	1:A:25:TRP:CD1	0.51	2.77	12	1
1:A:70:ILE:CG2	1:A:71:LEU:N	0.51	2.73	16	1
1:C:101:VAL:HG13	1:C:102:LEU:H	0.51	1.63	6	4
1:C:114:ILE:N	1:C:114:ILE:HD12	0.51	2.21	8	2
1:C:70:ILE:CG2	1:C:71:LEU:N	0.51	2.73	16	1
1:A:69:GLU:O	1:A:72:ASN:N	0.51	2.42	7	4
1:B:29:ALA:C	1:B:31:PHE:N	0.51	2.69	12	5
1:B:78:VAL:HG22	1:C:75:ILE:HG23	0.51	1.82	2	1
1:A:85:GLU:CD	1:A:85:GLU:N	0.51	2.68	14	2
1:B:96:MET:SD	1:C:30:ALA:O	0.51	2.69	5	1
1:B:107:VAL:CG1	1:B:108:ALA:N	0.51	2.72	16	3
1:A:48:LEU:HD22	1:A:48:LEU:N	0.51	2.21	6	1
1:A:101:VAL:CG1	1:A:102:LEU:N	0.51	2.74	6	4
1:A:58:LEU:HD12	1:A:58:LEU:N	0.51	2.21	14	1
1:C:119:HIS:CD2	1:C:119:HIS:N	0.51	2.77	14	1
1:A:96:MET:HE1	1:B:73:SER:OG	0.51	2.05	3	1
1:A:119:HIS:C	1:A:119:HIS:ND1	0.51	2.68	9	1
1:C:69:GLU:CD	1:C:69:GLU:N	0.51	2.68	10	2
1:A:30:ALA:O	1:C:96:MET:SD	0.51	2.69	5	1
1:A:71:LEU:C	1:A:73:SER:N	0.51	2.69	12	2
1:C:33:GLN:C	1:C:35:GLY:N	0.51	2.69	3	9
1:A:78:VAL:HG22	1:B:75:ILE:HG23	0.51	1.82	2	1
1:A:63:MET:SD	1:A:63:MET:C	0.51	2.95	9	3
1:A:63:MET:SD	1:C:63:MET:CE	0.51	2.98	5	1
1:C:101:VAL:CG1	1:C:102:LEU:N	0.51	2.74	6	4
1:A:29:ALA:HB2	1:A:32:ARG:HH21	0.51	1.65	10	1
1:C:48:LEU:N	1:C:48:LEU:CD1	0.51	2.74	11	2
1:A:47:TRP:CD1	1:A:47:TRP:N	0.50	2.72	6	1
1:A:40:LEU:HD12	1:A:40:LEU:N	0.50	2.21	14	2
1:C:102:LEU:N	1:C:102:LEU:CD2	0.50	2.75	14	1
1:A:107:VAL:C	1:A:109:VAL:N	0.50	2.69	7	16
1:C:29:ALA:C	1:C:31:PHE:N	0.50	2.69	12	6
1:A:96:MET:SD	1:B:30:ALA:O	0.50	2.69	5	1
1:C:25:TRP:O	1:C:30:ALA:N	0.50	2.44	6	1
1:A:33:GLN:NE2	1:A:33:GLN:C	0.50	2.70	1	1
1:A:89:LEU:O	1:A:91:GLY:N	0.50	2.42	4	4
1:A:92:ARG:NH2	1:B:81:ARG:HH21	0.50	2.04	4	1
1:B:92:ARG:HH22	1:C:81:ARG:NH2	0.50	2.02	4	1
1:B:101:VAL:CG1	1:B:102:LEU:N	0.50	2.74	6	4
1:B:48:LEU:N	1:B:48:LEU:CD1	0.50	2.74	11	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:58:LEU:N	1:C:58:LEU:HD12	0.50	2.20	14	1
1:B:107:VAL:C	1:B:109:VAL:N	0.50	2.69	7	15
1:B:89:LEU:O	1:B:91:GLY:N	0.50	2.42	4	4
1:B:114:ILE:N	1:B:114:ILE:HD12	0.50	2.21	8	2
1:C:25:TRP:CD1	1:C:25:TRP:N	0.50	2.78	8	2
1:C:29:ALA:HB2	1:C:32:ARG:HH21	0.50	1.66	10	1
1:B:108:ALA:O	1:B:112:TRP:CD2	0.50	2.65	15	1
1:A:73:SER:O	1:A:77:ALA:N	0.50	2.45	4	14
1:B:96:MET:O	1:B:96:MET:SD	0.50	2.70	1	1
1:C:107:VAL:C	1:C:109:VAL:N	0.50	2.70	6	15
1:B:63:MET:SD	1:B:63:MET:C	0.50	2.95	3	3
1:B:69:GLU:N	1:B:69:GLU:CD	0.50	2.69	3	1
1:A:102:LEU:N	1:A:102:LEU:CD2	0.50	2.75	14	1
1:A:108:ALA:O	1:A:112:TRP:CD2	0.50	2.65	15	1
1:C:33:GLN:C	1:C:33:GLN:NE2	0.50	2.70	1	1
1:A:73:SER:OG	1:C:96:MET:HE1	0.50	2.06	3	1
1:B:104:ALA:O	1:B:108:ALA:HB3	0.50	2.07	4	1
1:A:48:LEU:N	1:A:48:LEU:CD1	0.50	2.74	11	2
1:B:58:LEU:HD12	1:B:58:LEU:N	0.50	2.20	14	1
1:A:96:MET:SD	1:A:96:MET:O	0.50	2.70	1	1
1:C:96:MET:SD	1:C:96:MET:O	0.50	2.70	1	1
1:A:29:ALA:C	1:A:31:PHE:N	0.50	2.69	12	5
1:A:73:SER:OG	1:A:74:ALA:N	0.50	2.45	2	3
1:C:73:SER:OG	1:C:74:ALA:N	0.50	2.45	2	3
1:A:33:GLN:C	1:A:35:GLY:N	0.50	2.69	8	8
1:B:31:PHE:CD1	1:B:31:PHE:C	0.50	2.90	8	3
1:B:96:MET:HE1	1:C:73:SER:OG	0.50	2.06	3	1
1:A:53:ILE:C	1:A:55:ARG:N	0.50	2.69	15	6
1:A:81:ARG:HH21	1:C:92:ARG:NH2	0.50	2.05	4	1
1:B:40:LEU:O	1:B:40:LEU:HD23	0.50	2.07	4	1
1:A:25:TRP:O	1:A:30:ALA:N	0.50	2.44	6	1
1:C:40:LEU:HD12	1:C:40:LEU:N	0.50	2.21	14	2
1:C:108:ALA:O	1:C:112:TRP:CD2	0.50	2.65	15	1
1:B:100:ALA:O	1:B:104:ALA:CB	0.50	2.60	11	3
1:C:63:MET:SD	1:C:63:MET:C	0.50	2.95	3	1
1:B:48:LEU:HD22	1:B:48:LEU:N	0.50	2.21	6	1
1:A:72:ASN:O	1:A:72:ASN:ND2	0.50	2.45	8	2
1:C:63:MET:SD	1:C:66:MET:SD	0.50	3.10	10	1
1:C:87:HIS:CD2	1:C:88:GLU:H	0.50	2.25	14	1
1:B:76:GLU:O	1:B:80:ASP:N	0.50	2.45	1	13
1:C:76:GLU:O	1:C:80:ASP:N	0.50	2.45	1	13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LEU:HD23	1:A:40:LEU:O	0.50	2.07	4	2
1:A:102:LEU:HD12	1:A:102:LEU:N	0.50	2.22	2	1
1:B:92:ARG:NH2	1:C:81:ARG:HH21	0.50	2.04	4	1
1:A:81:ARG:C	1:A:83:GLY:H	0.50	2.15	5	1
1:B:51:ASP:OD1	1:B:52:ALA:N	0.50	2.45	12	2
1:C:48:LEU:N	1:C:48:LEU:CD2	0.50	2.75	6	1
1:C:71:LEU:C	1:C:73:SER:N	0.50	2.69	13	2
1:B:73:SER:O	1:B:77:ALA:N	0.49	2.45	4	13
1:B:73:SER:OG	1:B:74:ALA:N	0.49	2.45	2	3
1:B:102:LEU:HD12	1:B:102:LEU:N	0.49	2.22	2	1
1:C:85:GLU:CD	1:C:85:GLU:N	0.49	2.70	4	1
1:B:48:LEU:N	1:B:48:LEU:CD2	0.49	2.75	6	1
1:B:40:LEU:N	1:B:40:LEU:HD12	0.49	2.21	14	2
1:B:109:VAL:CG2	1:B:110:ILE:H	0.49	2.20	8	1
1:A:87:HIS:CD2	1:A:88:GLU:H	0.49	2.25	14	1
1:C:100:ALA:O	1:C:104:ALA:CB	0.49	2.60	1	2
1:B:25:TRP:O	1:B:30:ALA:N	0.49	2.44	6	1
1:B:25:TRP:CD1	1:B:25:TRP:N	0.49	2.77	12	2
1:B:71:LEU:C	1:B:73:SER:N	0.49	2.69	12	2
1:B:102:LEU:N	1:B:102:LEU:CD2	0.49	2.75	14	1
1:A:116:LEU:O	1:A:116:LEU:HD23	0.49	2.08	16	1
1:C:31:PHE:CD1	1:C:31:PHE:C	0.49	2.90	8	3
1:B:53:ILE:C	1:B:55:ARG:N	0.49	2.70	7	6
1:C:53:ILE:C	1:C:55:ARG:N	0.49	2.69	15	5
1:A:51:ASP:OD1	1:A:52:ALA:N	0.49	2.45	12	2
1:B:87:HIS:CD2	1:B:88:GLU:H	0.49	2.25	14	1
1:A:103:ILE:O	1:A:107:VAL:N	0.49	2.45	4	8
1:B:81:ARG:C	1:B:83:GLY:H	0.49	2.16	5	1
1:A:48:LEU:N	1:A:48:LEU:CD2	0.49	2.75	6	1
1:C:51:ASP:OD1	1:C:52:ALA:N	0.49	2.45	12	2
1:C:63:MET:C	1:C:63:MET:SD	0.49	2.95	9	2
1:A:63:MET:SD	1:A:66:MET:SD	0.49	3.10	10	1
1:A:58:LEU:N	1:A:58:LEU:CD1	0.49	2.75	14	1
1:C:58:LEU:N	1:C:58:LEU:CD1	0.49	2.75	14	1
1:B:33:GLN:C	1:B:35:GLY:N	0.49	2.69	8	9
1:B:53:ILE:CD1	1:C:52:ALA:O	0.49	2.61	1	1
1:B:66:MET:O	1:B:70:ILE:N	0.49	2.44	6	10
1:B:103:ILE:O	1:B:107:VAL:N	0.49	2.45	4	9
1:C:102:LEU:N	1:C:102:LEU:HD12	0.49	2.22	2	1
1:C:40:LEU:HD23	1:C:40:LEU:O	0.49	2.07	4	1
1:C:104:ALA:O	1:C:108:ALA:HB3	0.49	2.07	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:81:ARG:C	1:C:83:GLY:H	0.49	2.15	5	1
1:B:116:LEU:O	1:B:116:LEU:HD23	0.49	2.08	16	2
1:B:33:GLN:C	1:B:33:GLN:NE2	0.49	2.70	1	1
1:A:100:ALA:O	1:A:104:ALA:CB	0.49	2.60	1	3
1:A:100:ALA:O	1:A:104:ALA:N	0.49	2.46	1	4
1:A:104:ALA:O	1:A:108:ALA:HB3	0.49	2.07	4	1
1:A:43:VAL:HG13	1:A:44:ILE:N	0.49	2.23	12	1
1:B:58:LEU:N	1:B:58:LEU:CD1	0.49	2.75	14	1
1:C:73:SER:O	1:C:77:ALA:N	0.49	2.46	11	14
1:B:63:MET:SD	1:B:66:MET:SD	0.49	3.10	10	1
1:A:82:ILE:CG2	1:A:83:GLY:N	0.49	2.75	14	2
1:A:59:ILE:O	1:A:63:MET:CG	0.49	2.61	16	1
1:B:89:LEU:C	1:B:91:GLY:H	0.49	2.16	5	12
1:A:57:LEU:O	1:A:57:LEU:HD13	0.49	2.08	6	2
1:B:28:GLU:O	1:B:31:PHE:CD2	0.49	2.66	2	1
1:C:28:GLU:O	1:C:31:PHE:CD2	0.49	2.66	2	1
1:A:31:PHE:CD1	1:A:31:PHE:C	0.49	2.90	8	3
1:A:33:GLN:O	1:A:35:GLY:N	0.49	2.46	8	6
1:A:81:ARG:HH21	1:C:92:ARG:HH22	0.49	1.51	4	1
1:A:89:LEU:C	1:A:91:GLY:N	0.49	2.71	5	1
1:A:57:LEU:HD13	1:A:57:LEU:C	0.49	2.33	6	1
1:C:71:LEU:C	1:C:73:SER:H	0.49	2.16	12	2
1:B:108:ALA:O	1:B:112:TRP:CE3	0.49	2.66	15	1
1:C:108:ALA:O	1:C:112:TRP:CE3	0.49	2.66	15	1
1:C:116:LEU:O	1:C:116:LEU:HD23	0.49	2.08	16	1
1:A:53:ILE:CD1	1:B:52:ALA:O	0.48	2.61	1	1
1:B:107:VAL:O	1:B:108:ALA:C	0.48	2.56	1	16
1:A:87:HIS:O	1:A:88:GLU:C	0.48	2.56	3	4
1:C:33:GLN:O	1:C:35:GLY:N	0.48	2.46	8	6
1:C:87:HIS:O	1:C:88:GLU:C	0.48	2.56	3	3
1:B:58:LEU:O	1:B:58:LEU:HD23	0.48	2.08	11	2
1:C:72:ASN:O	1:C:72:ASN:ND2	0.48	2.46	8	2
1:C:58:LEU:HD23	1:C:58:LEU:O	0.48	2.08	11	1
1:A:70:ILE:O	1:A:73:SER:CB	0.48	2.61	14	4
1:B:43:VAL:HG13	1:B:44:ILE:N	0.48	2.23	12	1
1:A:52:ALA:O	1:C:53:ILE:CD1	0.48	2.61	1	1
1:A:76:GLU:O	1:A:80:ASP:N	0.48	2.46	11	13
1:C:100:ALA:O	1:C:104:ALA:N	0.48	2.46	1	4
1:A:44:ILE:CG2	1:A:45:ALA:N	0.48	2.77	16	5
1:C:115:LEU:O	1:C:115:LEU:HD23	0.48	2.09	10	2
1:C:89:LEU:C	1:C:91:GLY:N	0.48	2.71	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:ASN:O	1:A:76:GLU:CG	0.48	2.62	12	1
1:A:53:ILE:O	1:A:54:THR:C	0.48	2.57	10	11
1:A:58:LEU:O	1:A:58:LEU:HD23	0.48	2.08	11	2
1:A:103:ILE:CD1	1:A:103:ILE:N	0.48	2.76	7	1
1:C:70:ILE:O	1:C:73:SER:CB	0.48	2.61	14	4
1:C:72:ASN:O	1:C:76:GLU:CG	0.48	2.62	12	1
1:B:82:ILE:CG2	1:B:83:GLY:N	0.48	2.75	14	2
1:C:59:ILE:O	1:C:63:MET:CG	0.48	2.61	16	1
1:A:107:VAL:O	1:A:108:ALA:C	0.48	2.57	12	16
1:B:33:GLN:O	1:B:35:GLY:N	0.48	2.46	8	6
1:C:57:LEU:C	1:C:57:LEU:HD13	0.48	2.33	6	1
1:A:40:LEU:N	1:A:40:LEU:CD1	0.48	2.75	14	2
1:B:72:ASN:ND2	1:B:72:ASN:O	0.48	2.45	8	1
1:C:82:ILE:CG2	1:C:83:GLY:N	0.48	2.75	14	1
1:B:100:ALA:O	1:B:104:ALA:N	0.48	2.46	1	4
1:C:75:ILE:CG2	1:C:76:GLU:N	0.48	2.77	1	3
1:C:107:VAL:O	1:C:108:ALA:C	0.48	2.57	12	16
1:B:44:ILE:CG2	1:B:45:ALA:N	0.48	2.77	16	5
1:A:27:ASN:CG	1:A:28:GLU:N	0.48	2.72	5	1
1:B:89:LEU:C	1:B:91:GLY:N	0.48	2.71	5	1
1:B:70:ILE:O	1:B:73:SER:CB	0.48	2.61	14	4
1:B:72:ASN:O	1:B:76:GLU:CG	0.48	2.61	12	1
1:A:108:ALA:O	1:A:112:TRP:CE3	0.48	2.66	15	1
1:C:81:ARG:O	1:C:82:ILE:O	0.48	2.32	4	9
1:A:28:GLU:O	1:A:31:PHE:CD2	0.48	2.66	2	1
1:B:87:HIS:O	1:B:88:GLU:C	0.48	2.56	3	4
1:C:40:LEU:N	1:C:40:LEU:CD1	0.48	2.75	14	2
1:A:25:TRP:CD1	1:A:25:TRP:N	0.48	2.78	8	1
1:A:71:LEU:C	1:A:73:SER:H	0.48	2.16	12	2
1:B:75:ILE:CG2	1:B:76:GLU:N	0.48	2.77	1	3
1:B:81:ARG:O	1:B:82:ILE:O	0.48	2.32	4	9
1:B:115:LEU:HD23	1:B:115:LEU:O	0.48	2.09	10	2
1:B:27:ASN:CG	1:B:28:GLU:N	0.48	2.72	5	1
1:C:57:LEU:HD13	1:C:57:LEU:O	0.48	2.08	6	2
1:B:40:LEU:N	1:B:40:LEU:CD1	0.48	2.75	14	2
1:B:119:HIS:CD2	1:B:119:HIS:N	0.48	2.77	14	1
1:A:81:ARG:O	1:A:82:ILE:O	0.48	2.32	4	9
1:B:59:ILE:O	1:B:63:MET:N	0.48	2.44	12	5
1:C:89:LEU:C	1:C:91:GLY:H	0.48	2.16	5	11
1:C:103:ILE:O	1:C:107:VAL:N	0.48	2.44	16	6
1:B:28:GLU:C	1:B:30:ALA:H	0.48	2.17	4	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:27:ASN:CG	1:C:28:GLU:N	0.48	2.72	5	1
1:C:103:ILE:CD1	1:C:103:ILE:N	0.48	2.76	7	1
1:B:110:ILE:HD12	1:B:110:ILE:N	0.48	2.23	13	1
1:A:89:LEU:C	1:A:91:GLY:H	0.48	2.16	5	12
1:B:103:ILE:O	1:B:104:ALA:C	0.48	2.57	16	9
1:A:92:ARG:NH2	1:B:81:ARG:HE	0.48	2.07	4	1
1:A:115:LEU:HD23	1:A:115:LEU:O	0.48	2.08	10	2
1:C:44:ILE:CG2	1:C:45:ALA:N	0.48	2.77	16	5
1:A:44:ILE:CG1	1:A:45:ALA:N	0.48	2.77	5	1
1:B:88:GLU:O	1:B:90:SER:N	0.48	2.47	5	1
1:C:77:ALA:O	1:C:82:ILE:N	0.48	2.44	12	2
1:B:57:LEU:C	1:B:57:LEU:HD13	0.48	2.33	6	1
1:B:28:GLU:C	1:B:30:ALA:N	0.48	2.72	4	8
1:C:53:ILE:O	1:C:54:THR:C	0.48	2.56	10	9
1:A:116:LEU:HD23	1:A:116:LEU:O	0.48	2.09	13	2
1:B:53:ILE:O	1:B:54:THR:C	0.48	2.56	10	8
1:A:77:ALA:O	1:A:82:ILE:N	0.48	2.44	12	2
1:A:116:LEU:C	1:A:118:SER:N	0.48	2.70	9	2
1:B:87:HIS:O	1:B:88:GLU:O	0.48	2.32	15	1
1:C:87:HIS:O	1:C:88:GLU:O	0.48	2.32	15	1
1:B:59:ILE:O	1:B:63:MET:CG	0.48	2.61	16	1
1:A:28:GLU:O	1:A:31:PHE:CE2	0.47	2.67	2	1
1:B:28:GLU:O	1:B:31:PHE:CE2	0.47	2.67	2	1
1:A:111:THR:HG23	1:A:112:TRP:N	0.47	2.24	4	1
1:B:105:ILE:O	1:B:109:VAL:CG2	0.47	2.62	14	4
1:A:39:LEU:N	1:A:39:LEU:CD1	0.47	2.77	5	2
1:A:66:MET:C	1:A:68:VAL:N	0.47	2.72	16	4
1:C:44:ILE:CG1	1:C:45:ALA:N	0.47	2.77	5	1
1:B:57:LEU:HD13	1:B:57:LEU:O	0.47	2.08	6	1
1:C:116:LEU:C	1:C:118:SER:N	0.47	2.70	9	2
1:A:58:LEU:O	1:A:62:VAL:HG12	0.47	2.09	9	1
1:A:119:HIS:CG	1:A:120:PHE:N	0.47	2.82	12	1
1:B:119:HIS:CG	1:B:120:PHE:N	0.47	2.82	12	1
1:A:86:TYR:CD1	1:A:86:TYR:O	0.47	2.68	13	3
1:B:40:LEU:HD23	1:B:40:LEU:O	0.47	2.10	2	1
1:C:28:GLU:O	1:C:31:PHE:CE2	0.47	2.66	2	1
1:C:29:ALA:O	1:C:30:ALA:C	0.47	2.57	4	13
1:A:70:ILE:CG1	1:A:71:LEU:N	0.47	2.78	3	1
1:B:92:ARG:O	1:B:96:MET:SD	0.47	2.73	6	3
1:A:105:ILE:O	1:A:109:VAL:CG2	0.47	2.63	5	5
1:B:111:THR:HG23	1:B:112:TRP:N	0.47	2.24	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:44:ILE:CG1	1:B:45:ALA:N	0.47	2.77	5	1
1:A:75:ILE:CG2	1:A:76:GLU:N	0.47	2.77	1	3
1:A:28:GLU:C	1:A:30:ALA:N	0.47	2.73	2	6
1:B:66:MET:C	1:B:68:VAL:N	0.47	2.72	16	4
1:B:92:ARG:NH2	1:C:81:ARG:HE	0.47	2.07	4	1
1:A:58:LEU:O	1:A:62:VAL:CG2	0.47	2.62	5	2
1:B:77:ALA:O	1:B:82:ILE:N	0.47	2.44	12	2
1:C:58:LEU:O	1:C:62:VAL:CG2	0.47	2.62	5	2
1:A:65:VAL:CG2	1:A:69:GLU:OE2	0.47	2.63	7	1
1:B:65:VAL:CG2	1:B:69:GLU:OE2	0.47	2.63	7	1
1:B:103:ILE:N	1:B:103:ILE:CD1	0.47	2.76	7	1
1:C:58:LEU:O	1:C:62:VAL:HG12	0.47	2.09	9	1
1:C:105:ILE:O	1:C:109:VAL:CG2	0.47	2.63	14	5
1:C:116:LEU:HD23	1:C:116:LEU:O	0.47	2.09	13	2
1:B:119:HIS:C	1:B:119:HIS:ND1	0.47	2.71	8	1
1:A:101:VAL:CG2	1:A:102:LEU:N	0.47	2.78	12	1
1:C:110:ILE:HD12	1:C:110:ILE:N	0.47	2.23	13	1
1:A:87:HIS:O	1:A:88:GLU:O	0.47	2.32	15	1
1:A:55:ARG:NH2	1:C:111:THR:OG1	0.47	2.48	1	1
1:A:28:GLU:C	1:A:30:ALA:H	0.47	2.18	2	8
1:C:40:LEU:O	1:C:40:LEU:HD23	0.47	2.10	2	1
1:C:86:TYR:CD1	1:C:86:TYR:O	0.47	2.68	13	3
1:B:92:ARG:HH12	1:C:81:ARG:HE	0.47	1.48	4	1
1:C:43:VAL:HG13	1:C:44:ILE:N	0.47	2.23	12	1
1:A:111:THR:OG1	1:B:55:ARG:NH2	0.47	2.48	1	1
1:B:111:THR:OG1	1:C:55:ARG:CZ	0.47	2.63	1	1
1:B:111:THR:CG2	1:B:112:TRP:N	0.47	2.77	4	2
1:A:29:ALA:O	1:A:30:ALA:C	0.47	2.57	4	14
1:C:28:GLU:C	1:C:30:ALA:H	0.47	2.18	7	8
1:B:89:LEU:HD23	1:B:89:LEU:N	0.47	2.19	3	1
1:B:39:LEU:N	1:B:39:LEU:CD1	0.47	2.77	5	2
1:B:58:LEU:O	1:B:62:VAL:CG2	0.47	2.62	5	2
1:C:109:VAL:CG2	1:C:110:ILE:H	0.47	2.20	8	1
1:B:58:LEU:O	1:B:62:VAL:HG12	0.47	2.09	9	1
1:A:62:VAL:O	1:A:65:VAL:HG12	0.47	2.09	11	1
1:B:62:VAL:O	1:B:65:VAL:HG12	0.47	2.09	11	1
1:A:82:ILE:HG22	1:A:83:GLY:N	0.47	2.24	14	1
1:A:111:THR:CG2	1:A:112:TRP:N	0.47	2.77	4	2
1:C:111:THR:CG2	1:C:112:TRP:N	0.47	2.77	4	2
1:C:66:MET:C	1:C:68:VAL:N	0.47	2.72	16	4
1:A:58:LEU:O	1:A:62:VAL:HG23	0.47	2.10	5	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:58:LEU:O	1:B:62:VAL:HG23	0.47	2.10	5	4
1:B:89:LEU:HD23	1:B:89:LEU:O	0.47	2.10	11	1
1:B:38:VAL:O	1:B:42:VAL:CG1	0.47	2.63	12	2
1:C:103:ILE:O	1:C:104:ALA:C	0.47	2.57	2	10
1:B:86:TYR:O	1:B:86:TYR:CD1	0.47	2.68	15	3
1:C:70:ILE:CG1	1:C:71:LEU:N	0.47	2.78	3	1
1:A:51:ASP:O	1:B:53:ILE:CD1	0.47	2.63	4	1
1:A:53:ILE:CD1	1:C:51:ASP:O	0.47	2.63	4	1
1:C:38:VAL:O	1:C:42:VAL:CG1	0.47	2.63	12	2
1:C:119:HIS:CG	1:C:120:PHE:N	0.47	2.82	12	1
1:B:70:ILE:HG23	1:B:71:LEU:N	0.47	2.25	16	1
1:B:68:VAL:O	1:B:72:ASN:CG	0.47	2.58	14	2
1:B:29:ALA:O	1:B:30:ALA:C	0.47	2.58	5	13
1:C:97:GLY:O	1:C:101:VAL:N	0.47	2.48	9	7
1:B:92:ARG:HH22	1:C:81:ARG:HH21	0.47	1.51	4	1
1:C:58:LEU:O	1:C:62:VAL:HG23	0.47	2.10	5	4
1:A:39:LEU:O	1:A:43:VAL:HG23	0.47	2.10	15	2
1:B:81:ARG:O	1:B:82:ILE:CG2	0.47	2.55	7	1
1:C:65:VAL:CG2	1:C:69:GLU:OE2	0.47	2.63	7	1
1:B:43:VAL:CG1	1:B:44:ILE:N	0.47	2.78	12	1
1:C:68:VAL:O	1:C:72:ASN:CG	0.46	2.58	14	2
1:C:28:GLU:C	1:C:30:ALA:N	0.46	2.73	2	7
1:B:70:ILE:CG1	1:B:71:LEU:N	0.46	2.78	3	1
1:A:92:ARG:HH12	1:B:81:ARG:HE	0.46	1.48	4	1
1:C:27:ASN:CG	1:C:28:GLU:H	0.46	2.18	5	1
1:A:81:ARG:O	1:A:82:ILE:CG2	0.46	2.56	7	1
1:A:111:THR:OG1	1:B:55:ARG:CZ	0.46	2.63	1	1
1:C:111:THR:HG23	1:C:112:TRP:N	0.46	2.24	4	1
1:C:39:LEU:N	1:C:39:LEU:CD1	0.46	2.77	7	2
1:B:116:LEU:C	1:B:118:SER:N	0.46	2.70	9	2
1:B:46:CYS:C	1:B:48:LEU:N	0.46	2.72	15	2
1:B:42:VAL:O	1:B:46:CYS:SG	0.46	2.70	11	1
1:C:89:LEU:HD23	1:C:89:LEU:O	0.46	2.10	11	1
1:A:59:ILE:O	1:A:63:MET:N	0.46	2.48	13	5
1:A:110:ILE:N	1:A:110:ILE:HD12	0.46	2.23	13	2
1:C:43:VAL:CG1	1:C:44:ILE:N	0.46	2.78	12	1
1:A:90:SER:O	1:A:91:GLY:O	0.46	2.33	5	6
1:C:90:SER:O	1:C:91:GLY:O	0.46	2.33	5	6
1:A:92:ARG:O	1:A:96:MET:SD	0.46	2.73	6	3
1:C:114:ILE:HG23	1:C:115:LEU:N	0.46	2.26	12	3
1:C:62:VAL:O	1:C:65:VAL:HG12	0.46	2.09	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:VAL:O	1:A:42:VAL:CG1	0.46	2.63	12	2
1:B:82:ILE:HG22	1:B:83:GLY:N	0.46	2.24	14	1
1:A:110:ILE:N	1:A:110:ILE:CD1	0.46	2.79	13	2
1:C:118:SER:C	1:C:120:PHE:H	0.46	2.19	4	1
1:A:89:LEU:O	1:A:89:LEU:HD23	0.46	2.10	11	1
1:B:71:LEU:C	1:B:73:SER:H	0.46	2.16	12	2
1:A:55:ARG:CZ	1:C:111:THR:OG1	0.46	2.63	1	1
1:A:68:VAL:O	1:A:72:ASN:CG	0.46	2.58	14	2
1:C:92:ARG:O	1:C:96:MET:SD	0.46	2.73	6	3
1:A:118:SER:C	1:A:120:PHE:H	0.46	2.19	4	1
1:B:118:SER:C	1:B:120:PHE:H	0.46	2.19	4	1
1:A:116:LEU:O	1:A:119:HIS:CG	0.46	2.69	8	1
1:A:35:GLY:O	1:A:38:VAL:N	0.46	2.46	11	1
1:A:103:ILE:O	1:A:104:ALA:C	0.46	2.57	16	10
1:C:69:GLU:O	1:C:70:ILE:C	0.46	2.59	2	4
1:C:114:ILE:H	1:C:114:ILE:HD12	0.46	1.71	5	1
1:C:101:VAL:O	1:C:104:ALA:HB3	0.46	2.11	12	3
1:A:81:ARG:HE	1:C:92:ARG:NH2	0.46	2.08	4	1
1:A:27:ASN:CG	1:A:28:GLU:H	0.46	2.19	5	1
1:A:88:GLU:O	1:A:90:SER:N	0.46	2.47	5	1
1:C:39:LEU:O	1:C:43:VAL:HG23	0.46	2.10	15	2
1:A:97:GLY:O	1:A:101:VAL:HG12	0.46	2.11	6	3
1:A:114:ILE:HG23	1:A:115:LEU:N	0.46	2.26	12	3
1:B:107:VAL:CG2	1:B:108:ALA:N	0.46	2.79	11	1
1:A:38:VAL:O	1:A:42:VAL:CG2	0.46	2.64	8	5
1:B:38:VAL:O	1:B:42:VAL:CG2	0.46	2.64	8	5
1:A:101:VAL:O	1:A:104:ALA:HB3	0.46	2.11	12	4
1:B:97:GLY:O	1:B:101:VAL:N	0.46	2.48	3	6
1:B:39:LEU:O	1:B:43:VAL:HG23	0.46	2.10	15	3
1:C:61:SER:OG	1:C:62:VAL:N	0.46	2.49	15	3
1:B:109:VAL:CG2	1:B:110:ILE:N	0.46	2.78	8	1
1:B:116:LEU:O	1:B:119:HIS:CG	0.46	2.69	8	1
1:C:109:VAL:CG2	1:C:110:ILE:N	0.46	2.78	8	1
1:A:43:VAL:CG1	1:A:44:ILE:N	0.46	2.78	12	1
1:B:101:VAL:CG2	1:B:102:LEU:N	0.46	2.78	12	1
1:C:82:ILE:HG22	1:C:83:GLY:N	0.46	2.24	14	1
1:C:81:ARG:O	1:C:82:ILE:C	0.46	2.59	12	9
1:C:97:GLY:O	1:C:101:VAL:HG12	0.46	2.11	6	3
1:B:111:THR:OG1	1:C:55:ARG:NH2	0.45	2.48	1	1
1:B:51:ASP:O	1:C:53:ILE:CD1	0.45	2.63	4	1
1:A:114:ILE:H	1:A:114:ILE:HD12	0.45	1.71	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:88:GLU:O	1:C:90:SER:N	0.45	2.47	5	1
1:C:103:ILE:N	1:C:103:ILE:HD12	0.45	2.26	7	1
1:C:58:LEU:O	1:C:62:VAL:HG13	0.45	2.11	10	1
1:A:42:VAL:O	1:A:46:CYS:SG	0.45	2.70	11	1
1:A:49:ASP:CG	1:A:50:VAL:N	0.45	2.74	16	1
1:A:37:ALA:C	1:A:39:LEU:H	0.45	2.20	16	7
1:A:69:GLU:O	1:A:70:ILE:C	0.45	2.59	2	4
1:B:89:LEU:CD2	1:B:89:LEU:N	0.45	2.80	3	1
1:A:106:ILE:O	1:A:110:ILE:N	0.45	2.49	13	2
1:B:106:ILE:O	1:B:110:ILE:N	0.45	2.49	13	2
1:C:110:ILE:N	1:C:110:ILE:CD1	0.45	2.79	13	2
1:B:60:SER:OG	1:B:61:SER:N	0.45	2.50	7	1
1:B:103:ILE:N	1:B:103:ILE:HD12	0.45	2.26	7	1
1:A:46:CYS:C	1:A:48:LEU:N	0.45	2.75	8	2
1:C:69:GLU:O	1:C:73:SER:N	0.45	2.50	9	1
1:C:35:GLY:O	1:C:38:VAL:N	0.45	2.46	11	2
1:B:49:ASP:CG	1:B:50:VAL:N	0.45	2.74	16	1
1:A:97:GLY:O	1:A:101:VAL:N	0.45	2.48	5	6
1:C:106:ILE:O	1:C:110:ILE:N	0.45	2.49	4	2
1:A:61:SER:OG	1:A:62:VAL:N	0.45	2.49	15	3
1:C:116:LEU:O	1:C:119:HIS:CG	0.45	2.69	8	1
1:A:58:LEU:N	1:A:58:LEU:CD2	0.45	2.80	9	1
1:A:69:GLU:O	1:A:73:SER:N	0.45	2.50	9	1
1:C:58:LEU:CD2	1:C:58:LEU:N	0.45	2.80	9	1
1:B:58:LEU:O	1:B:62:VAL:HG13	0.45	2.11	10	1
1:B:25:TRP:CD1	1:B:25:TRP:C	0.45	2.94	16	1
1:C:70:ILE:HG23	1:C:71:LEU:N	0.45	2.25	16	1
1:B:69:GLU:O	1:B:70:ILE:C	0.45	2.59	7	4
1:B:97:GLY:O	1:B:101:VAL:HG12	0.45	2.11	6	4
1:B:58:LEU:N	1:B:58:LEU:CD2	0.45	2.80	9	1
1:A:70:ILE:HG23	1:A:71:LEU:N	0.45	2.25	16	1
1:A:57:LEU:C	1:A:57:LEU:HD23	0.45	2.37	1	1
1:B:90:SER:O	1:B:91:GLY:O	0.45	2.33	5	6
1:B:110:ILE:N	1:B:110:ILE:CD1	0.45	2.80	4	2
1:A:103:ILE:N	1:A:103:ILE:HD12	0.45	2.26	7	1
1:B:37:ALA:C	1:B:39:LEU:H	0.45	2.20	16	7
1:C:25:TRP:C	1:C:27:ASN:N	0.45	2.75	5	1
1:A:33:GLN:O	1:A:34:GLU:C	0.45	2.60	10	7
1:C:26:ILE:O	1:C:30:ALA:HB2	0.45	2.12	11	1
1:A:81:ARG:O	1:A:82:ILE:C	0.45	2.60	1	9
1:B:81:ARG:O	1:B:82:ILE:C	0.45	2.60	16	9

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:38:VAL:O	1:C:42:VAL:CG2	0.45	2.64	8	5
1:C:75:ILE:HG23	1:C:76:GLU:N	0.45	2.27	1	2
1:C:89:LEU:HD23	1:C:89:LEU:N	0.45	2.19	3	1
1:A:81:ARG:HE	1:C:92:ARG:CZ	0.45	2.25	4	1
1:B:92:ARG:CZ	1:C:81:ARG:HE	0.45	2.25	4	1
1:B:87:HIS:ND1	1:B:87:HIS:N	0.45	2.64	5	1
1:C:37:ALA:C	1:C:39:LEU:H	0.45	2.20	16	6
1:B:61:SER:OG	1:B:62:VAL:N	0.45	2.49	15	3
1:C:57:LEU:C	1:C:57:LEU:HD23	0.45	2.37	1	1
1:C:59:ILE:O	1:C:63:MET:N	0.45	2.48	13	3
1:B:33:GLN:O	1:B:34:GLU:C	0.45	2.60	11	8
1:A:49:ASP:CG	1:A:50:VAL:H	0.45	2.20	4	2
1:B:27:ASN:CG	1:B:28:GLU:H	0.45	2.19	5	1
1:B:114:ILE:HD12	1:B:114:ILE:H	0.45	1.71	5	1
1:B:51:ASP:CG	1:B:52:ALA:H	0.45	2.20	7	3
1:B:69:GLU:O	1:B:73:SER:N	0.45	2.50	9	1
1:A:58:LEU:O	1:A:62:VAL:HG13	0.45	2.11	10	1
1:A:107:VAL:CG2	1:A:108:ALA:N	0.45	2.79	11	1
1:C:107:VAL:CG2	1:C:108:ALA:H	0.45	2.21	11	1
1:B:49:ASP:N	1:B:49:ASP:OD1	0.45	2.49	9	1
1:A:25:TRP:CD1	1:A:25:TRP:C	0.45	2.94	16	1
1:C:49:ASP:CG	1:C:50:VAL:N	0.45	2.74	16	1
1:B:57:LEU:C	1:B:57:LEU:HD23	0.45	2.37	1	1
1:C:43:VAL:O	1:C:47:TRP:CD1	0.45	2.70	2	1
1:B:101:VAL:O	1:B:104:ALA:HB3	0.45	2.11	12	4
1:A:75:ILE:HD11	1:C:74:ALA:HB1	0.45	1.89	4	1
1:B:110:ILE:N	1:B:110:ILE:HD12	0.45	2.27	4	1
1:C:110:ILE:N	1:C:110:ILE:HD12	0.45	2.27	4	1
1:C:51:ASP:CG	1:C:52:ALA:H	0.45	2.20	6	3
1:A:60:SER:OG	1:A:61:SER:N	0.45	2.50	7	1
1:C:46:CYS:C	1:C:48:LEU:N	0.45	2.72	15	2
1:A:36:VAL:C	1:A:38:VAL:N	0.45	2.75	14	1
1:C:60:SER:OG	1:C:61:SER:N	0.44	2.50	7	1
1:A:26:ILE:O	1:A:30:ALA:HB2	0.44	2.12	11	1
1:B:107:VAL:CG2	1:B:108:ALA:H	0.44	2.21	11	1
1:B:85:GLU:C	1:B:87:HIS:N	0.44	2.75	16	1
1:A:69:GLU:O	1:A:73:SER:OG	0.44	2.34	1	1
1:A:34:GLU:OE1	1:A:34:GLU:CA	0.44	2.65	8	2
1:B:34:GLU:OE1	1:B:34:GLU:CA	0.44	2.65	8	2
1:A:84:SER:OG	1:A:86:TYR:CE2	0.44	2.71	5	1
1:C:91:GLY:O	1:C:95:ASP:CG	0.44	2.60	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:113:CYS:HG	1:B:117:TRP:CD1	0.44	2.30	7	1
1:A:82:ILE:N	1:A:82:ILE:CD1	0.44	2.78	14	1
1:A:96:MET:SD	1:A:96:MET:C	0.44	3.00	1	1
1:A:92:ARG:CZ	1:B:81:ARG:HE	0.44	2.25	4	1
1:A:51:ASP:CG	1:A:52:ALA:H	0.44	2.20	7	3
1:B:64:LEU:O	1:B:67:ILE:HG22	0.44	2.13	9	1
1:B:116:LEU:HD23	1:B:116:LEU:O	0.44	2.11	4	1
1:A:25:TRP:C	1:A:27:ASN:N	0.44	2.75	5	1
1:C:64:LEU:O	1:C:67:ILE:HG22	0.44	2.13	9	1
1:B:53:ILE:CD1	1:B:53:ILE:H	0.44	2.26	3	1
1:C:33:GLN:O	1:C:34:GLU:C	0.44	2.60	11	8
1:C:87:HIS:ND1	1:C:87:HIS:N	0.44	2.64	5	1
1:B:66:MET:O	1:B:67:ILE:C	0.44	2.61	16	3
1:B:106:ILE:CG2	1:B:110:ILE:HD12	0.44	2.43	11	1
1:C:107:VAL:CG2	1:C:108:ALA:N	0.44	2.79	11	1
1:B:76:GLU:O	1:B:80:ASP:CB	0.44	2.66	12	1
1:A:43:VAL:O	1:A:47:TRP:CD1	0.44	2.70	2	1
1:C:76:GLU:O	1:C:80:ASP:CG	0.44	2.61	3	6
1:B:95:ASP:O	1:B:98:SER:OG	0.44	2.36	7	3
1:C:49:ASP:CG	1:C:50:VAL:H	0.44	2.20	4	2
1:B:114:ILE:HG23	1:B:115:LEU:N	0.44	2.26	12	3
1:A:113:CYS:HG	1:A:117:TRP:CD1	0.44	2.29	7	1
1:B:58:LEU:N	1:B:58:LEU:HD22	0.44	2.28	9	1
1:C:106:ILE:CG2	1:C:110:ILE:HD12	0.44	2.43	11	1
1:B:30:ALA:O	1:B:34:GLU:OE2	0.44	2.36	8	2
1:B:43:VAL:O	1:B:47:TRP:CD1	0.44	2.70	2	1
1:A:50:VAL:O	1:A:51:ASP:O	0.44	2.36	3	1
1:B:76:GLU:O	1:B:80:ASP:CG	0.44	2.61	3	6
1:C:101:VAL:CG2	1:C:102:LEU:N	0.44	2.78	12	1
1:B:75:ILE:HG23	1:B:76:GLU:N	0.44	2.27	1	2
1:A:30:ALA:O	1:A:34:GLU:OE2	0.44	2.36	8	2
1:A:88:GLU:C	1:A:89:LEU:HD12	0.44	2.38	2	1
1:B:50:VAL:O	1:B:51:ASP:O	0.44	2.36	3	1
1:C:49:ASP:OD1	1:C:49:ASP:N	0.44	2.50	9	1
1:A:85:GLU:N	1:A:85:GLU:OE1	0.44	2.51	14	1
1:C:86:TYR:O	1:C:89:LEU:HD21	0.44	2.13	16	1
1:A:103:ILE:C	1:A:107:VAL:HG22	0.44	2.38	1	1
1:C:30:ALA:O	1:C:34:GLU:OE2	0.44	2.36	2	2
1:C:89:LEU:CD2	1:C:89:LEU:N	0.44	2.80	3	1
1:A:101:VAL:CG1	1:A:102:LEU:H	0.44	2.26	5	4
1:B:85:GLU:CG	1:B:86:TYR:N	0.44	2.81	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:112:TRP:CD1	1:B:112:TRP:O	0.44	2.71	7	1
1:B:26:ILE:O	1:B:30:ALA:HB2	0.44	2.12	11	1
1:C:34:GLU:OE1	1:C:34:GLU:CA	0.43	2.65	8	2
1:A:76:GLU:O	1:A:80:ASP:CG	0.43	2.61	3	6
1:A:87:HIS:ND1	1:A:87:HIS:N	0.43	2.64	5	1
1:C:107:VAL:O	1:C:111:THR:OG1	0.43	2.36	5	7
1:A:58:LEU:N	1:A:58:LEU:HD22	0.43	2.28	9	1
1:A:106:ILE:CG2	1:A:110:ILE:HD12	0.43	2.43	11	1
1:C:86:TYR:O	1:C:89:LEU:CD2	0.43	2.66	16	1
1:B:33:GLN:C	1:B:33:GLN:CD	0.43	2.87	1	1
1:C:96:MET:SD	1:C:96:MET:C	0.43	3.00	1	1
1:C:50:VAL:O	1:C:51:ASP:O	0.43	2.36	3	1
1:B:107:VAL:O	1:B:111:THR:OG1	0.43	2.36	15	8
1:A:76:GLU:O	1:A:80:ASP:CB	0.43	2.66	12	1
1:C:76:GLU:O	1:C:80:ASP:CB	0.43	2.66	12	1
1:A:25:TRP:CD1	1:A:33:GLN:OE1	0.43	2.71	16	1
1:A:57:LEU:HD23	1:A:57:LEU:O	0.43	2.13	15	4
1:C:88:GLU:C	1:C:89:LEU:HD12	0.43	2.38	2	1
1:B:50:VAL:O	1:B:51:ASP:CG	0.43	2.61	14	2
1:A:91:GLY:O	1:A:95:ASP:CG	0.43	2.61	5	1
1:B:91:GLY:O	1:B:95:ASP:CG	0.43	2.61	5	1
1:A:95:ASP:O	1:A:98:SER:OG	0.43	2.36	7	1
1:B:62:VAL:O	1:B:66:MET:CG	0.43	2.67	9	1
1:A:59:ILE:O	1:A:62:VAL:N	0.43	2.51	13	1
1:C:59:ILE:O	1:C:62:VAL:N	0.43	2.51	13	1
1:C:76:GLU:O	1:C:76:GLU:CD	0.43	2.62	14	1
1:B:82:ILE:CG2	1:B:83:GLY:H	0.43	2.25	15	1
1:B:117:TRP:N	1:B:117:TRP:CD1	0.43	2.85	15	1
1:B:96:MET:SD	1:B:96:MET:C	0.43	3.00	1	1
1:B:103:ILE:C	1:B:107:VAL:HG22	0.43	2.38	1	1
1:B:88:GLU:C	1:B:89:LEU:HD12	0.43	2.38	2	1
1:A:50:VAL:O	1:A:51:ASP:CG	0.43	2.61	14	2
1:B:83:GLY:O	1:B:84:SER:O	0.43	2.37	10	4
1:B:94:LYS:O	1:B:97:GLY:N	0.43	2.52	3	4
1:C:94:LYS:O	1:C:97:GLY:N	0.43	2.52	3	3
1:A:74:ALA:HB1	1:B:75:ILE:HD11	0.43	1.89	4	1
1:A:107:VAL:O	1:A:111:THR:OG1	0.43	2.37	16	7
1:C:101:VAL:CG1	1:C:102:LEU:H	0.43	2.26	6	4
1:A:85:GLU:CG	1:A:86:TYR:N	0.43	2.81	7	1
1:C:112:TRP:CD1	1:C:112:TRP:O	0.43	2.71	7	1
1:C:113:CYS:HG	1:C:117:TRP:CD1	0.43	2.30	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:VAL:CG2	1:A:110:ILE:H	0.43	2.20	8	1
1:C:104:ALA:O	1:C:108:ALA:N	0.43	2.51	8	1
1:A:49:ASP:OD1	1:A:49:ASP:N	0.43	2.50	9	1
1:A:72:ASN:OD1	1:A:72:ASN:O	0.43	2.37	10	1
1:B:51:ASP:O	1:B:52:ALA:O	0.43	2.37	13	3
1:B:57:LEU:O	1:B:57:LEU:HD13	0.43	2.14	16	1
1:A:29:ALA:O	1:A:33:GLN:N	0.43	2.49	9	2
1:B:69:GLU:O	1:B:73:SER:OG	0.43	2.34	1	1
1:C:69:GLU:O	1:C:73:SER:OG	0.43	2.33	11	2
1:A:81:ARG:NE	1:C:92:ARG:HH22	0.43	2.12	4	1
1:B:49:ASP:CG	1:B:50:VAL:H	0.43	2.20	4	1
1:B:92:ARG:HH22	1:C:81:ARG:NE	0.43	2.11	4	1
1:B:90:SER:O	1:B:90:SER:OG	0.43	2.37	7	1
1:A:76:GLU:O	1:A:80:ASP:OD2	0.43	2.37	8	2
1:A:62:VAL:O	1:A:66:MET:CG	0.43	2.67	9	1
1:C:62:VAL:O	1:C:66:MET:CG	0.43	2.67	9	1
1:B:58:LEU:O	1:B:62:VAL:HG22	0.43	2.14	10	1
1:A:51:ASP:O	1:A:52:ALA:O	0.43	2.36	13	3
1:B:86:TYR:O	1:B:89:LEU:CD2	0.43	2.66	16	1
1:A:75:ILE:HG23	1:A:76:GLU:N	0.43	2.28	5	2
1:C:57:LEU:HD23	1:C:57:LEU:O	0.43	2.14	5	2
1:B:37:ALA:O	1:B:38:VAL:C	0.43	2.62	9	3
1:C:50:VAL:O	1:C:51:ASP:CG	0.43	2.62	14	2
1:C:53:ILE:CD1	1:C:53:ILE:H	0.43	2.26	3	1
1:B:74:ALA:HB1	1:C:75:ILE:HD11	0.43	1.89	4	1
1:A:45:ALA:O	1:A:49:ASP:O	0.43	2.37	5	1
1:A:104:ALA:O	1:A:108:ALA:N	0.43	2.51	8	1
1:A:64:LEU:O	1:A:67:ILE:HG22	0.43	2.13	9	1
1:C:65:VAL:O	1:C:69:GLU:OE1	0.43	2.37	10	1
1:A:103:ILE:HG22	1:A:107:VAL:HG23	0.43	1.90	13	1
1:A:64:LEU:N	1:A:64:LEU:CD2	0.43	2.81	14	1
1:C:64:LEU:N	1:C:64:LEU:CD2	0.43	2.81	14	1
1:A:114:ILE:O	1:B:51:ASP:CG	0.43	2.62	1	1
1:A:81:ARG:HE	1:C:92:ARG:HH12	0.43	1.48	4	1
1:A:92:ARG:HH22	1:B:81:ARG:NE	0.43	2.11	4	1
1:B:91:GLY:O	1:B:95:ASP:OD1	0.43	2.37	12	5
1:C:91:GLY:O	1:C:95:ASP:OD1	0.43	2.37	12	5
1:C:45:ALA:O	1:C:48:LEU:O	0.43	2.37	11	4
1:C:114:ILE:CG2	1:C:115:LEU:N	0.43	2.82	12	1
1:C:85:GLU:N	1:C:85:GLU:OE1	0.43	2.51	14	1
1:A:86:TYR:O	1:A:89:LEU:CD2	0.43	2.67	16	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:86:TYR:O	1:B:89:LEU:HD21	0.43	2.13	16	1
1:A:73:SER:OG	1:C:95:ASP:CG	0.43	2.62	1	2
1:B:94:LYS:O	1:B:95:ASP:C	0.43	2.62	5	5
1:C:37:ALA:O	1:C:38:VAL:C	0.43	2.62	9	3
1:C:94:LYS:O	1:C:95:ASP:C	0.43	2.62	5	9
1:C:34:GLU:O	1:C:38:VAL:HG23	0.43	2.14	11	2
1:C:88:GLU:C	1:C:90:SER:N	0.43	2.77	5	1
1:A:112:TRP:O	1:A:112:TRP:CD1	0.43	2.71	7	1
1:C:85:GLU:CG	1:C:86:TYR:N	0.43	2.81	7	1
1:B:76:GLU:O	1:B:80:ASP:OD2	0.43	2.37	8	2
1:C:25:TRP:HE1	1:C:33:GLN:CD	0.43	2.22	9	1
1:A:58:LEU:O	1:A:62:VAL:HG22	0.43	2.14	10	2
1:C:88:GLU:CD	1:C:88:GLU:C	0.43	2.87	12	1
1:B:76:GLU:O	1:B:76:GLU:CD	0.43	2.62	14	1
1:A:95:ASP:CG	1:B:73:SER:OG	0.43	2.62	11	2
1:A:53:ILE:CD1	1:A:53:ILE:H	0.43	2.26	3	1
1:A:83:GLY:O	1:A:84:SER:O	0.43	2.37	12	4
1:C:83:GLY:O	1:C:84:SER:O	0.43	2.37	12	4
1:C:95:ASP:O	1:C:98:SER:OG	0.43	2.36	7	2
1:A:46:CYS:O	1:A:48:LEU:N	0.43	2.52	8	1
1:A:66:MET:O	1:A:67:ILE:C	0.43	2.61	16	3
1:B:105:ILE:O	1:B:109:VAL:HG22	0.43	2.14	8	1
1:C:58:LEU:N	1:C:58:LEU:HD22	0.43	2.28	9	1
1:B:25:TRP:CD1	1:B:33:GLN:OE1	0.43	2.71	16	1
1:C:66:MET:O	1:C:68:VAL:N	0.43	2.52	16	1
1:B:84:SER:OG	1:B:86:TYR:CE2	0.43	2.71	5	1
1:C:86:TYR:C	1:C:88:GLU:N	0.43	2.77	6	1
1:C:46:CYS:O	1:C:48:LEU:N	0.43	2.52	8	1
1:C:29:ALA:HB2	1:C:32:ARG:NH2	0.43	2.29	10	1
1:C:58:LEU:O	1:C:62:VAL:HG22	0.43	2.14	10	1
1:A:107:VAL:O	1:A:111:THR:CB	0.43	2.67	12	2
1:A:38:VAL:O	1:A:42:VAL:HG12	0.43	2.14	12	1
1:B:64:LEU:CD2	1:B:64:LEU:N	0.43	2.81	14	1
1:A:86:TYR:O	1:A:89:LEU:HD21	0.43	2.13	16	1
1:C:25:TRP:CD1	1:C:25:TRP:C	0.43	2.94	16	1
1:B:114:ILE:O	1:C:51:ASP:CG	0.42	2.62	1	1
1:A:34:GLU:O	1:A:38:VAL:HG23	0.42	2.14	11	2
1:B:107:VAL:O	1:B:111:THR:CB	0.42	2.67	11	3
1:A:45:ALA:O	1:A:48:LEU:O	0.42	2.37	6	4
1:A:105:ILE:O	1:A:109:VAL:HG22	0.42	2.14	8	1
1:B:104:ALA:O	1:B:108:ALA:N	0.42	2.51	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:107:VAL:O	1:C:111:THR:CB	0.42	2.67	11	2
1:B:38:VAL:O	1:B:42:VAL:HG12	0.42	2.14	12	1
1:C:51:ASP:O	1:C:52:ALA:O	0.42	2.37	12	3
1:C:103:ILE:CG2	1:C:107:VAL:HG23	0.42	2.44	13	1
1:A:76:GLU:O	1:A:76:GLU:CD	0.42	2.61	14	1
1:B:82:ILE:N	1:B:82:ILE:CD1	0.42	2.78	14	1
1:C:85:GLU:C	1:C:87:HIS:N	0.42	2.75	16	1
1:A:33:GLN:C	1:A:33:GLN:CD	0.42	2.87	1	1
1:B:114:ILE:O	1:C:51:ASP:OD1	0.42	2.38	1	1
1:A:94:LYS:O	1:A:97:GLY:N	0.42	2.52	3	4
1:B:65:VAL:O	1:B:69:GLU:OE2	0.42	2.37	3	1
1:B:57:LEU:O	1:B:57:LEU:HD23	0.42	2.14	5	3
1:A:118:SER:OG	1:B:49:ASP:C	0.42	2.62	6	1
1:B:55:ARG:HH21	1:C:57:LEU:HD12	0.42	1.74	7	1
1:B:25:TRP:HE1	1:B:33:GLN:CD	0.42	2.22	9	1
1:B:85:GLU:OE2	1:C:76:GLU:CD	0.42	2.62	9	1
1:C:42:VAL:O	1:C:46:CYS:SG	0.42	2.70	11	1
1:B:88:GLU:CD	1:B:88:GLU:C	0.42	2.87	12	1
1:B:59:ILE:O	1:B:62:VAL:N	0.42	2.52	13	1
1:B:85:GLU:N	1:B:85:GLU:OE1	0.42	2.51	14	1
1:A:37:ALA:O	1:A:38:VAL:C	0.42	2.62	3	2
1:B:25:TRP:C	1:B:27:ASN:N	0.42	2.75	5	1
1:B:119:HIS:CD2	1:B:120:PHE:N	0.42	2.88	6	1
1:C:32:ARG:O	1:C:36:VAL:HG12	0.42	2.15	6	1
1:B:85:GLU:CD	1:C:76:GLU:OE2	0.42	2.63	9	1
1:C:29:ALA:O	1:C:33:GLN:N	0.42	2.49	9	1
1:B:72:ASN:O	1:B:72:ASN:OD1	0.42	2.37	10	1
1:C:38:VAL:O	1:C:42:VAL:HG12	0.42	2.14	12	1
1:B:64:LEU:N	1:B:64:LEU:HD22	0.42	2.29	14	1
1:B:101:VAL:HG22	1:C:26:ILE:HG21	0.42	1.92	14	1
1:B:95:ASP:CG	1:C:73:SER:OG	0.42	2.62	1	2
1:B:118:SER:OG	1:C:49:ASP:C	0.42	2.62	6	1
1:B:28:GLU:CD	1:B:28:GLU:C	0.42	2.87	9	1
1:C:72:ASN:O	1:C:72:ASN:OD1	0.42	2.37	10	1
1:B:114:ILE:CG2	1:B:115:LEU:N	0.42	2.82	12	1
1:A:82:ILE:CG2	1:A:83:GLY:H	0.42	2.25	15	1
1:A:117:TRP:N	1:A:117:TRP:CD1	0.42	2.85	15	1
1:A:49:ASP:OD1	1:C:118:SER:O	0.42	2.38	16	1
1:C:25:TRP:CD1	1:C:33:GLN:OE1	0.42	2.71	16	1
1:A:27:ASN:O	1:A:27:ASN:OD1	0.42	2.37	1	1
1:A:51:ASP:CG	1:C:114:ILE:O	0.42	2.62	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:ILE:O	1:B:51:ASP:OD1	0.42	2.37	1	1
1:C:103:ILE:C	1:C:107:VAL:HG22	0.42	2.38	1	1
1:A:87:HIS:C	1:A:89:LEU:H	0.42	2.22	2	1
1:B:87:HIS:C	1:B:89:LEU:H	0.42	2.22	2	1
1:A:109:VAL:O	1:A:113:CYS:SG	0.42	2.71	3	1
1:B:34:GLU:O	1:B:38:VAL:HG23	0.42	2.13	11	2
1:A:49:ASP:C	1:C:118:SER:OG	0.42	2.62	6	1
1:A:58:LEU:HD12	1:C:107:VAL:CG2	0.42	2.45	8	1
1:A:76:GLU:OE2	1:C:85:GLU:CD	0.42	2.63	9	1
1:A:85:GLU:OE2	1:B:76:GLU:CD	0.42	2.63	9	1
1:B:29:ALA:HB2	1:B:32:ARG:NH2	0.42	2.29	10	1
1:B:35:GLY:O	1:B:38:VAL:N	0.42	2.49	10	2
1:C:57:LEU:O	1:C:57:LEU:HD23	0.42	2.13	15	2
1:B:36:VAL:C	1:B:38:VAL:N	0.42	2.75	14	1
1:C:64:LEU:N	1:C:64:LEU:HD22	0.42	2.29	14	1
1:C:82:ILE:N	1:C:82:ILE:CD1	0.42	2.78	14	1
1:C:27:ASN:OD1	1:C:27:ASN:O	0.42	2.37	1	1
1:A:94:LYS:O	1:A:95:ASP:C	0.42	2.62	9	8
1:B:45:ALA:O	1:B:48:LEU:O	0.42	2.37	6	4
1:B:57:LEU:C	1:B:57:LEU:CD1	0.42	2.93	6	1
1:C:76:GLU:O	1:C:80:ASP:OD1	0.42	2.38	9	1
1:B:72:ASN:O	1:B:72:ASN:ND2	0.42	2.52	12	1
1:C:103:ILE:HG22	1:C:107:VAL:HG23	0.42	1.90	13	1
1:B:27:ASN:OD1	1:B:27:ASN:O	0.42	2.37	1	1
1:C:33:GLN:C	1:C:33:GLN:CD	0.42	2.86	1	1
1:B:50:VAL:O	1:B:51:ASP:C	0.42	2.63	3	1
1:A:91:GLY:O	1:A:95:ASP:OD1	0.42	2.37	12	5
1:B:45:ALA:O	1:B:49:ASP:O	0.42	2.37	5	1
1:B:101:VAL:CG1	1:B:102:LEU:H	0.42	2.26	6	3
1:C:84:SER:OG	1:C:86:TYR:CE2	0.42	2.71	5	1
1:A:66:MET:SD	1:C:99:ALA:CB	0.42	3.08	6	1
1:C:76:GLU:O	1:C:80:ASP:OD2	0.42	2.37	8	2
1:A:76:GLU:CD	1:C:85:GLU:OE2	0.42	2.63	9	1
1:C:28:GLU:CD	1:C:28:GLU:C	0.42	2.87	9	1
1:B:103:ILE:CG2	1:B:107:VAL:HG23	0.42	2.44	13	1
1:A:66:MET:O	1:A:68:VAL:N	0.42	2.52	16	1
1:A:51:ASP:OD1	1:C:114:ILE:O	0.42	2.38	1	1
1:C:87:HIS:C	1:C:89:LEU:H	0.42	2.22	2	1
1:B:99:ALA:CB	1:C:66:MET:SD	0.42	3.08	6	1
1:C:57:LEU:C	1:C:57:LEU:CD1	0.42	2.93	6	1
1:B:81:ARG:C	1:B:82:ILE:CG1	0.42	2.93	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:81:ARG:C	1:C:82:ILE:CG1	0.42	2.93	7	1
1:A:65:VAL:O	1:A:69:GLU:OE1	0.42	2.37	10	1
1:B:65:VAL:O	1:B:69:GLU:OE1	0.42	2.37	10	1
1:B:88:GLU:OE2	1:C:72:ASN:CG	0.42	2.63	10	2
1:C:119:HIS:CD2	1:C:119:HIS:C	0.42	2.97	16	2
1:A:65:VAL:O	1:A:69:GLU:OE2	0.42	2.37	3	1
1:B:58:LEU:HD23	1:B:58:LEU:C	0.42	2.40	4	1
1:C:118:SER:C	1:C:120:PHE:N	0.42	2.77	4	2
1:B:25:TRP:NE1	1:B:27:ASN:HD21	0.42	2.13	5	1
1:A:119:HIS:CD2	1:A:120:PHE:N	0.42	2.88	6	1
1:B:32:ARG:O	1:B:36:VAL:HG12	0.42	2.14	6	1
1:B:86:TYR:C	1:B:88:GLU:N	0.42	2.78	8	3
1:B:46:CYS:O	1:B:48:LEU:N	0.42	2.52	8	1
1:A:28:GLU:CD	1:A:28:GLU:C	0.42	2.87	9	1
1:B:88:GLU:OE1	1:B:95:ASP:OD2	0.42	2.38	11	1
1:A:54:THR:O	1:A:57:LEU:N	0.42	2.53	13	1
1:A:103:ILE:CG2	1:A:107:VAL:HG23	0.42	2.44	13	1
1:B:92:ARG:NH1	1:C:77:ALA:HB2	0.42	2.30	14	1
1:C:117:TRP:CD1	1:C:117:TRP:N	0.42	2.85	15	1
1:B:66:MET:O	1:B:68:VAL:N	0.42	2.52	16	1
1:A:105:ILE:O	1:A:109:VAL:HG23	0.42	2.15	12	3
1:C:105:ILE:O	1:C:109:VAL:HG23	0.42	2.15	12	2
1:C:68:VAL:C	1:C:69:GLU:OE1	0.42	2.63	3	1
1:C:109:VAL:O	1:C:113:CYS:SG	0.42	2.71	3	1
1:C:45:ALA:O	1:C:49:ASP:O	0.42	2.37	5	1
1:A:57:LEU:HD12	1:C:55:ARG:HH21	0.42	1.74	7	1
1:A:25:TRP:HE1	1:A:33:GLN:CD	0.42	2.22	9	1
1:A:76:GLU:O	1:A:80:ASP:OD1	0.42	2.38	9	1
1:A:72:ASN:CG	1:C:88:GLU:OE2	0.42	2.63	16	2
1:A:88:GLU:OE1	1:A:95:ASP:OD2	0.42	2.38	11	1
1:B:56:VAL:O	1:B:59:ILE:N	0.42	2.53	11	2
1:A:88:GLU:CD	1:A:88:GLU:C	0.42	2.87	12	1
1:B:103:ILE:HG22	1:B:107:VAL:HG23	0.42	1.90	13	1
1:A:64:LEU:N	1:A:64:LEU:HD22	0.42	2.29	14	1
1:B:57:LEU:HD13	1:B:57:LEU:C	0.42	2.40	16	1
1:A:27:ASN:O	1:A:28:GLU:CB	0.41	2.68	1	1
1:B:57:LEU:HD23	1:B:57:LEU:O	0.41	2.14	1	1
1:A:68:VAL:C	1:A:69:GLU:OE1	0.41	2.63	3	1
1:A:118:SER:C	1:A:120:PHE:N	0.41	2.77	4	2
1:A:25:TRP:NE1	1:A:27:ASN:HD21	0.41	2.13	5	1
1:A:88:GLU:C	1:A:90:SER:N	0.41	2.77	5	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ARG:O	1:A:36:VAL:HG12	0.41	2.14	6	1
1:C:105:ILE:O	1:C:109:VAL:HG22	0.41	2.14	8	1
1:A:85:GLU:CD	1:B:76:GLU:OE2	0.41	2.63	9	1
1:B:103:ILE:HD12	1:C:62:VAL:HG12	0.41	1.92	10	1
1:A:56:VAL:O	1:A:59:ILE:N	0.41	2.53	11	2
1:A:92:ARG:NH1	1:B:77:ALA:HB2	0.41	2.30	14	1
1:C:77:ALA:O	1:C:80:ASP:N	0.41	2.53	14	1
1:C:57:LEU:HD13	1:C:57:LEU:C	0.41	2.40	16	1
1:A:58:LEU:O	1:A:58:LEU:HD13	0.41	2.15	6	1
1:B:104:ALA:O	1:B:108:ALA:CB	0.41	2.69	8	1
1:A:29:ALA:HB2	1:A:32:ARG:NH2	0.41	2.28	10	1
1:A:114:ILE:CG2	1:A:115:LEU:N	0.41	2.82	12	1
1:A:77:ALA:HB2	1:C:92:ARG:NH1	0.41	2.30	14	1
1:C:27:ASN:O	1:C:28:GLU:CB	0.41	2.68	1	1
1:B:118:SER:C	1:B:120:PHE:N	0.41	2.77	4	1
1:C:85:GLU:CD	1:C:85:GLU:H	0.41	2.24	4	1
1:A:99:ALA:CB	1:B:66:MET:SD	0.41	3.08	6	1
1:C:119:HIS:CD2	1:C:120:PHE:N	0.41	2.88	6	1
1:A:69:GLU:OE1	1:C:98:SER:OG	0.41	2.37	7	1
1:A:107:VAL:CG2	1:B:58:LEU:HD12	0.41	2.45	8	1
1:C:59:ILE:O	1:C:63:MET:CB	0.41	2.68	8	1
1:A:62:VAL:HG12	1:C:103:ILE:HD12	0.41	1.92	10	1
1:A:88:GLU:OE2	1:B:72:ASN:CG	0.41	2.63	16	2
1:B:119:HIS:O	1:B:120:PHE:O	0.41	2.39	15	1
1:B:27:ASN:O	1:B:28:GLU:CB	0.41	2.68	1	1
1:A:50:VAL:O	1:A:51:ASP:C	0.41	2.62	3	1
1:B:59:ILE:O	1:B:63:MET:CB	0.41	2.68	8	2
1:A:57:LEU:C	1:A:57:LEU:CD1	0.41	2.93	6	2
1:B:38:VAL:HG22	1:C:64:LEU:HD22	0.41	1.92	7	1
1:C:56:VAL:O	1:C:59:ILE:N	0.41	2.53	13	2
1:A:77:ALA:O	1:A:80:ASP:N	0.41	2.53	14	1
1:A:119:HIS:O	1:A:120:PHE:O	0.41	2.39	15	1
1:B:88:GLU:OE1	1:C:72:ASN:O	0.41	2.38	16	1
1:C:114:ILE:HD12	1:C:115:LEU:N	0.41	2.30	1	1
1:B:50:VAL:C	1:B:51:ASP:CG	0.41	2.89	14	2
1:C:65:VAL:O	1:C:69:GLU:OE2	0.41	2.37	3	1
1:A:58:LEU:C	1:A:58:LEU:HD23	0.41	2.40	4	1
1:A:83:GLY:O	1:A:84:SER:OG	0.41	2.37	6	1
1:A:81:ARG:C	1:A:82:ILE:CG1	0.41	2.93	7	1
1:B:107:VAL:CG2	1:C:58:LEU:HD12	0.41	2.45	8	1
1:C:66:MET:O	1:C:67:ILE:C	0.41	2.63	11	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:101:VAL:CG2	1:B:102:LEU:H	0.41	2.26	12	1
1:A:67:ILE:O	1:A:71:LEU:CB	0.41	2.69	14	1
1:A:118:SER:O	1:B:49:ASP:OD1	0.41	2.38	16	1
1:B:85:GLU:CD	1:B:85:GLU:H	0.41	2.24	4	1
1:A:55:ARG:HH21	1:B:57:LEU:HD12	0.41	1.75	7	1
1:C:88:GLU:OE1	1:C:95:ASP:OD2	0.41	2.38	11	1
1:C:67:ILE:O	1:C:71:LEU:CB	0.41	2.69	14	2
1:A:101:VAL:HG22	1:B:26:ILE:HG21	0.41	1.93	14	1
1:A:88:GLU:OE1	1:B:72:ASN:O	0.41	2.38	16	1
1:A:59:ILE:O	1:A:63:MET:CB	0.41	2.69	3	2
1:C:90:SER:O	1:C:90:SER:OG	0.41	2.37	7	1
1:B:70:ILE:O	1:B:73:SER:OG	0.41	2.36	12	1
1:C:50:VAL:O	1:C:51:ASP:C	0.41	2.62	3	1
1:B:58:LEU:HD13	1:B:58:LEU:O	0.41	2.15	6	1
1:A:109:VAL:CG2	1:A:110:ILE:N	0.41	2.78	8	1
1:B:76:GLU:O	1:B:80:ASP:OD1	0.41	2.38	9	1
1:B:107:VAL:C	1:B:111:THR:OG1	0.41	2.64	11	1
1:B:68:VAL:C	1:B:69:GLU:OE1	0.41	2.63	3	1
1:C:58:LEU:C	1:C:58:LEU:HD23	0.41	2.41	4	1
1:A:86:TYR:C	1:A:88:GLU:N	0.41	2.77	6	1
1:B:105:ILE:O	1:B:109:VAL:HG23	0.41	2.15	12	3
1:C:27:ASN:O	1:C:27:ASN:ND2	0.41	2.54	6	1
1:C:58:LEU:O	1:C:58:LEU:HD13	0.41	2.15	6	1
1:C:104:ALA:O	1:C:108:ALA:CB	0.41	2.68	8	1
1:B:29:ALA:O	1:B:33:GLN:N	0.41	2.49	9	1
1:B:116:LEU:O	1:B:118:SER:N	0.41	2.54	9	1
1:A:103:ILE:HD12	1:B:62:VAL:HG12	0.41	1.92	10	1
1:A:58:LEU:O	1:A:61:SER:OG	0.41	2.36	11	1
1:B:58:LEU:O	1:B:61:SER:OG	0.41	2.37	11	1
1:C:107:VAL:C	1:C:111:THR:OG1	0.41	2.64	11	1
1:A:119:HIS:CD2	1:A:119:HIS:C	0.41	2.97	16	2
1:B:32:ARG:O	1:B:36:VAL:N	0.41	2.52	14	1
1:B:67:ILE:O	1:B:71:LEU:CB	0.41	2.69	14	1
1:C:36:VAL:C	1:C:38:VAL:N	0.41	2.76	14	1
1:C:119:HIS:O	1:C:120:PHE:O	0.41	2.39	15	1
1:A:85:GLU:C	1:A:87:HIS:N	0.41	2.75	16	1
1:B:114:ILE:HD12	1:B:115:LEU:N	0.41	2.31	1	1
1:A:83:GLY:O	1:A:84:SER:C	0.41	2.64	4	1
1:C:115:LEU:HD23	1:C:115:LEU:C	0.41	2.41	4	1
1:A:27:ASN:ND2	1:A:27:ASN:O	0.41	2.54	6	1
1:C:46:CYS:O	1:C:47:TRP:C	0.41	2.64	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:50:VAL:C	1:C:51:ASP:CG	0.41	2.89	14	1
1:A:89:LEU:CD2	1:A:89:LEU:N	0.40	2.80	3	1
1:A:101:VAL:O	1:A:104:ALA:CB	0.40	2.69	3	2
1:B:101:VAL:O	1:B:104:ALA:CB	0.40	2.69	3	2
1:A:85:GLU:CD	1:A:85:GLU:H	0.40	2.24	4	1
1:A:38:VAL:HG22	1:B:64:LEU:HD22	0.40	1.92	7	1
1:A:104:ALA:O	1:A:108:ALA:CB	0.40	2.68	8	1
1:B:54:THR:O	1:B:57:LEU:N	0.40	2.53	13	2
1:B:51:ASP:O	1:B:52:ALA:C	0.40	2.65	14	1
1:A:72:ASN:O	1:C:88:GLU:OE1	0.40	2.38	16	1
1:A:114:ILE:HD12	1:A:115:LEU:N	0.40	2.31	1	1
1:A:40:LEU:O	1:A:44:ILE:HG22	0.40	2.16	11	1
1:C:40:LEU:O	1:C:44:ILE:HG22	0.40	2.16	11	1
1:C:70:ILE:O	1:C:73:SER:OG	0.40	2.36	12	1
1:C:58:LEU:O	1:C:58:LEU:HD23	0.40	2.16	4	1
1:C:25:TRP:CG	1:C:27:ASN:OD1	0.40	2.75	5	1
1:C:94:LYS:O	1:C:98:SER:N	0.40	2.43	5	1
1:A:107:VAL:C	1:A:111:THR:OG1	0.40	2.64	11	1
1:B:118:SER:OG	1:C:51:ASP:OD2	0.40	2.39	13	1
1:A:50:VAL:HG22	1:A:51:ASP:N	0.40	2.31	14	1
1:C:89:LEU:N	1:C:89:LEU:CD1	0.40	2.85	2	1
1:B:59:ILE:CD1	1:C:60:SER:OG	0.40	2.70	4	1
1:A:101:VAL:CG2	1:A:102:LEU:H	0.40	2.26	12	1
1:C:62:VAL:O	1:C:66:MET:N	0.40	2.49	2	1
1:C:25:TRP:NE1	1:C:27:ASN:HD21	0.40	2.13	5	1
1:C:112:TRP:CD1	1:C:112:TRP:C	0.40	3.00	7	1
1:A:64:LEU:O	1:A:64:LEU:HD13	0.40	2.17	9	1
1:B:77:ALA:O	1:B:80:ASP:N	0.40	2.53	14	1
1:C:68:VAL:O	1:C:72:ASN:ND2	0.40	2.55	14	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	96/121 (79%)	68±2 (71±2%)	17±3 (18±3%)	10±2 (11±2%)	1 8

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	96/121 (79%)	68±2 (71±3%)	17±3 (18±3%)	10±2 (11±3%)	1	8
1	C	96/121 (79%)	68±2 (71±2%)	17±3 (18±3%)	11±2 (11±3%)	1	8
All	All	4608/5808 (79%)	3283 (71%)	820 (18%)	505 (11%)	1	8

All 75 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	80	ASP	16
1	A	82	ILE	16
1	A	108	ALA	16
1	B	80	ASP	16
1	B	82	ILE	16
1	B	108	ALA	16
1	C	80	ASP	16
1	C	82	ILE	16
1	C	108	ALA	16
1	A	91	GLY	13
1	B	91	GLY	13
1	C	91	GLY	13
1	A	107	VAL	10
1	C	107	VAL	10
1	A	28	GLU	9
1	A	38	VAL	9
1	B	28	GLU	9
1	B	38	VAL	9
1	B	107	VAL	9
1	C	28	GLU	9
1	C	38	VAL	9
1	A	89	LEU	8
1	B	89	LEU	8
1	C	89	LEU	8
1	B	90	SER	8
1	C	90	SER	8
1	A	88	GLU	8
1	B	88	GLU	8
1	C	88	GLU	8
1	A	53	ILE	7
1	B	53	ILE	7
1	C	53	ILE	7
1	A	30	ALA	7
1	A	90	SER	7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	30	ALA	7
1	C	30	ALA	7
1	A	120	PHE	7
1	B	120	PHE	7
1	C	120	PHE	7
1	A	84	SER	6
1	B	84	SER	6
1	C	84	SER	6
1	A	50	VAL	5
1	B	50	VAL	5
1	C	50	VAL	5
1	A	34	GLU	5
1	B	34	GLU	5
1	C	34	GLU	5
1	A	52	ALA	4
1	B	52	ALA	4
1	C	52	ALA	4
1	A	83	GLY	3
1	B	83	GLY	3
1	C	83	GLY	3
1	A	54	THR	3
1	B	54	THR	3
1	C	54	THR	3
1	A	25	TRP	2
1	A	51	ASP	2
1	B	25	TRP	2
1	B	51	ASP	2
1	C	25	TRP	2
1	C	51	ASP	2
1	A	48	LEU	2
1	B	48	LEU	2
1	C	48	LEU	2
1	A	47	TRP	1
1	B	47	TRP	1
1	C	47	TRP	1
1	A	85	GLU	1
1	B	85	GLU	1
1	C	85	GLU	1
1	A	49	ASP	1
1	B	49	ASP	1
1	C	49	ASP	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	79/95 (83%)	74±2 (94±2%)	5±2 (6±2%)	18	67
1	B	79/95 (83%)	74±2 (94±2%)	5±2 (6±2%)	18	67
1	C	79/95 (83%)	74±2 (94±2%)	5±2 (6±2%)	18	67
All	All	3792/4560 (83%)	3552 (94%)	240 (6%)	18	67

All 90 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	71	LEU	11
1	B	71	LEU	11
1	C	71	LEU	11
1	A	53	ILE	6
1	B	53	ILE	6
1	C	53	ILE	6
1	A	82	ILE	5
1	B	82	ILE	5
1	C	82	ILE	5
1	A	54	THR	4
1	B	54	THR	4
1	C	54	THR	4
1	A	38	VAL	4
1	B	38	VAL	4
1	C	38	VAL	4
1	A	67	ILE	3
1	A	89	LEU	3
1	A	107	VAL	3
1	B	67	ILE	3
1	B	89	LEU	3
1	B	107	VAL	3
1	C	67	ILE	3
1	C	89	LEU	3
1	C	107	VAL	3
1	A	114	ILE	3
1	B	114	ILE	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	114	ILE	3
1	A	66	MET	3
1	A	116	LEU	3
1	B	66	MET	3
1	B	116	LEU	3
1	C	66	MET	3
1	C	116	LEU	3
1	A	57	LEU	3
1	A	119	HIS	3
1	B	57	LEU	3
1	B	119	HIS	3
1	C	57	LEU	3
1	C	119	HIS	3
1	A	25	TRP	2
1	A	34	GLU	2
1	A	40	LEU	2
1	A	48	LEU	2
1	B	25	TRP	2
1	B	34	GLU	2
1	B	40	LEU	2
1	B	48	LEU	2
1	C	25	TRP	2
1	C	34	GLU	2
1	C	40	LEU	2
1	C	48	LEU	2
1	A	39	LEU	2
1	A	58	LEU	2
1	B	39	LEU	2
1	B	58	LEU	2
1	C	39	LEU	2
1	C	58	LEU	2
1	A	65	VAL	2
1	B	65	VAL	2
1	C	65	VAL	2
1	A	73	SER	2
1	A	92	ARG	2
1	B	73	SER	2
1	B	92	ARG	2
1	C	73	SER	2
1	C	92	ARG	2
1	A	96	MET	1
1	B	96	MET	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	C	96	MET	1
1	A	78	VAL	1
1	B	78	VAL	1
1	C	78	VAL	1
1	A	69	GLU	1
1	B	69	GLU	1
1	C	69	GLU	1
1	A	84	SER	1
1	B	84	SER	1
1	C	84	SER	1
1	A	64	LEU	1
1	B	64	LEU	1
1	C	64	LEU	1
1	A	105	ILE	1
1	A	115	LEU	1
1	B	105	ILE	1
1	B	115	LEU	1
1	C	105	ILE	1
1	C	115	LEU	1
1	A	28	GLU	1
1	B	28	GLU	1
1	C	28	GLU	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 oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided