



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 08:28 PM UTC

PDB ID : 2KXP / pdb_00002kxp
Title : Solution NMR structure of V-1 bound to capping protein (CP)
Authors : Zwolak, A.; Fujiwara, I.; Hammer III, J.A.; Tjandra, N.
Deposited on : 2010-05-11

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

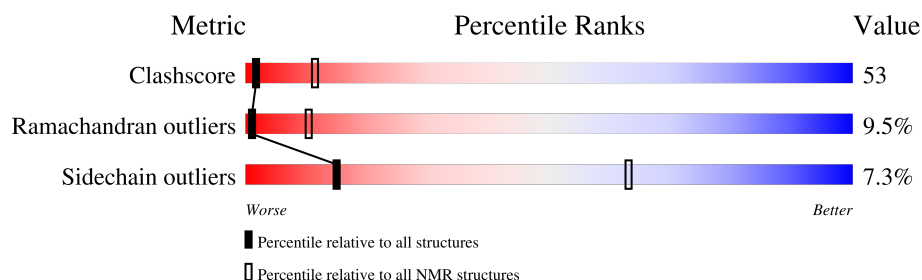
1 Overall quality at a glance

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	275	40% 48% 11% .
2	B	270	59% 36% 5%
3	C	118	28% 54% 17% .

2 Ensemble composition and analysis

This entry contains 10 models. Model 7 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:7-A:281, B:302-B:571 (545)	0.00	7
2	C:601-C:718 (118)	0.00	8

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 and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10511 atoms, of which 5229 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called F-actin-capping protein subunit alpha-1.

Mol	Chain	Residues	Atoms						Trace
1	A	275	Total	C	H	N	O	S	0
			4416	1413	2177	392	429	5	

- Molecule 2 is a protein called F-actin-capping protein subunit beta isoforms 1 and 2.

Mol	Chain	Residues	Atoms						Trace
2	B	270	Total	C	H	N	O	S	0
			4276	1334	2135	374	423	10	

- Molecule 3 is a protein called Myotrophin.

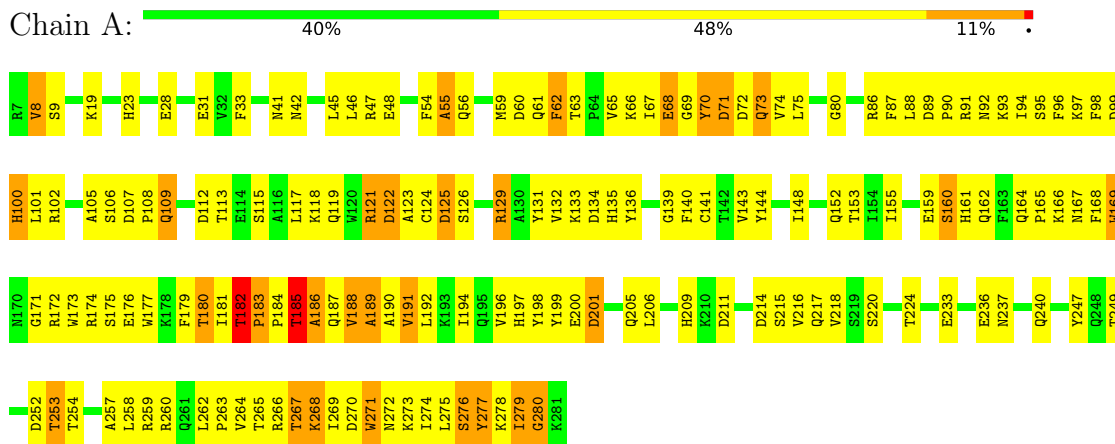
Mol	Chain	Residues	Atoms						Trace
3	C	118	Total	C	H	N	O	S	0
			1819	570	917	152	175	5	

4 Residue-property plots

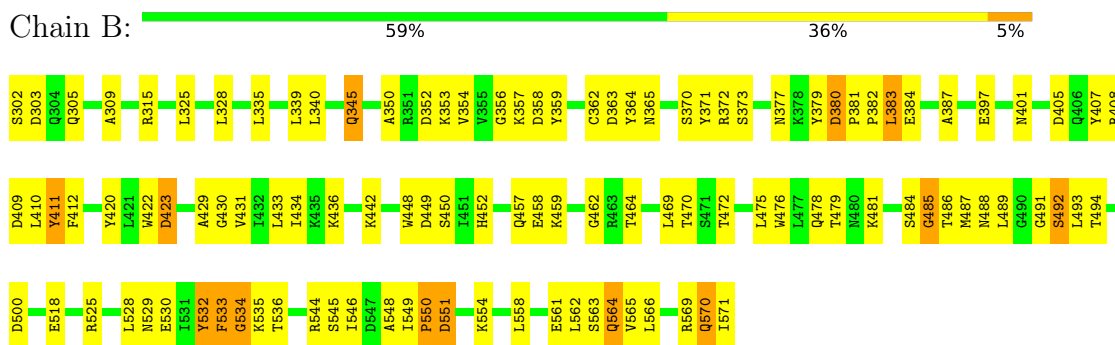
4.1 Average score per residue in the NMR ensemble

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.

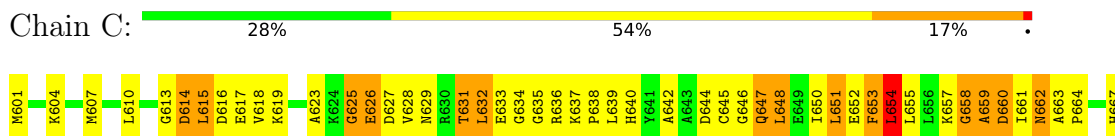
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 3: Myotrophin



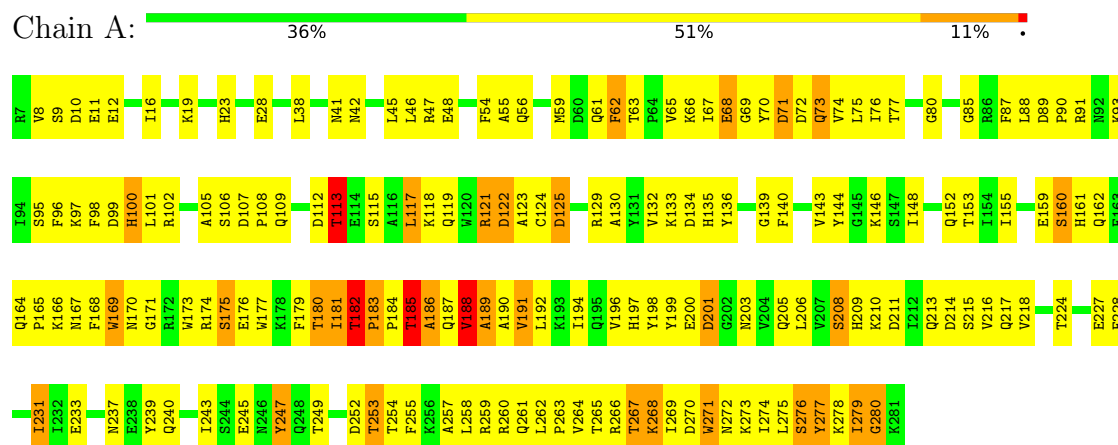


4.2 Scores per residue for each member of the ensemble

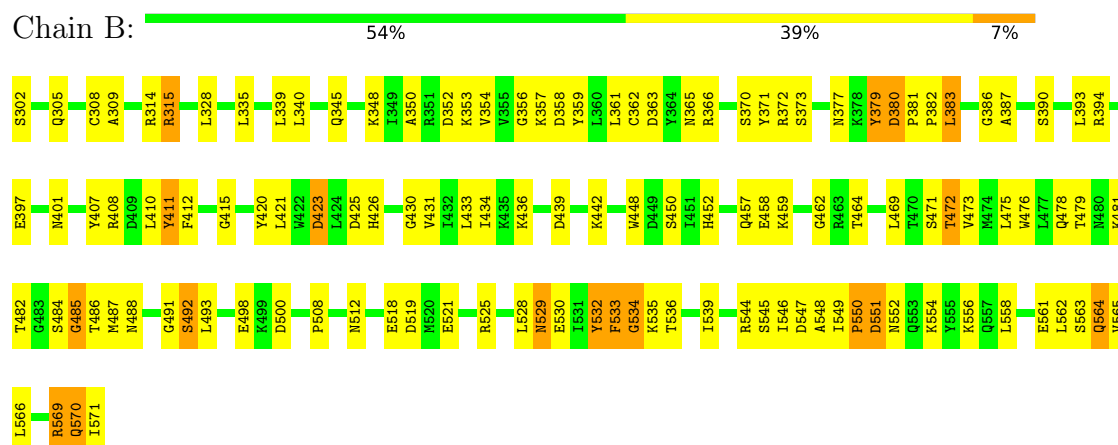
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

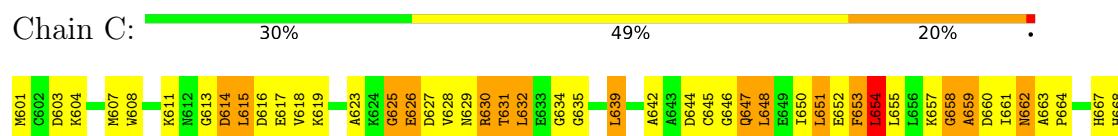
- Molecule 1: F-actin-capping protein subunit alpha-1

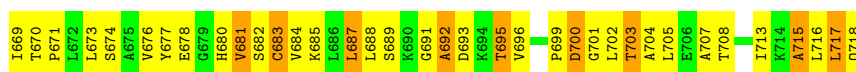


- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



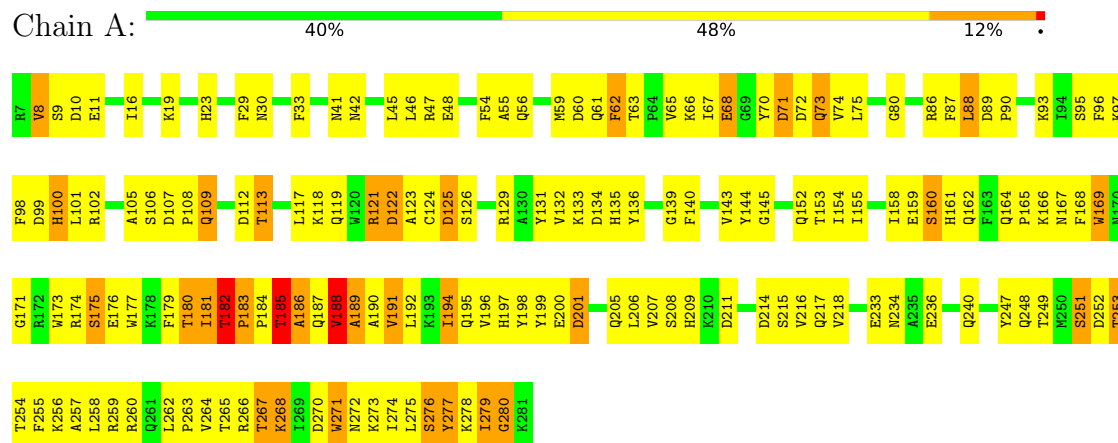
- Molecule 3: Myotrophin



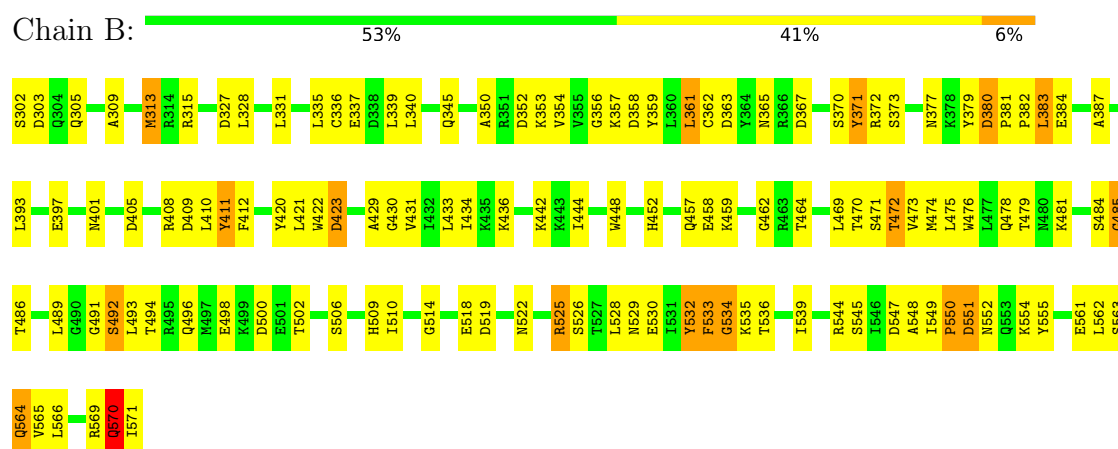


4.2.2 Score per residue for model 2

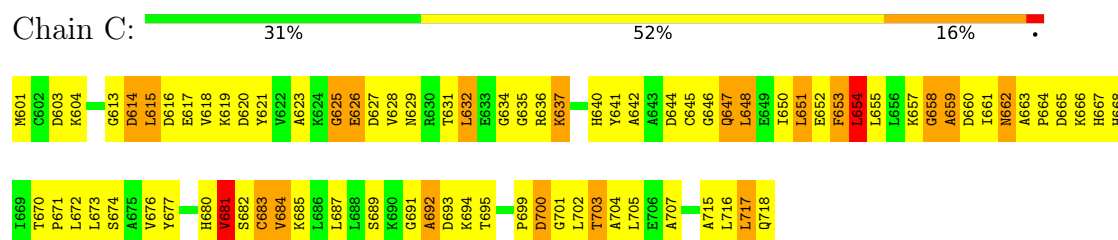
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

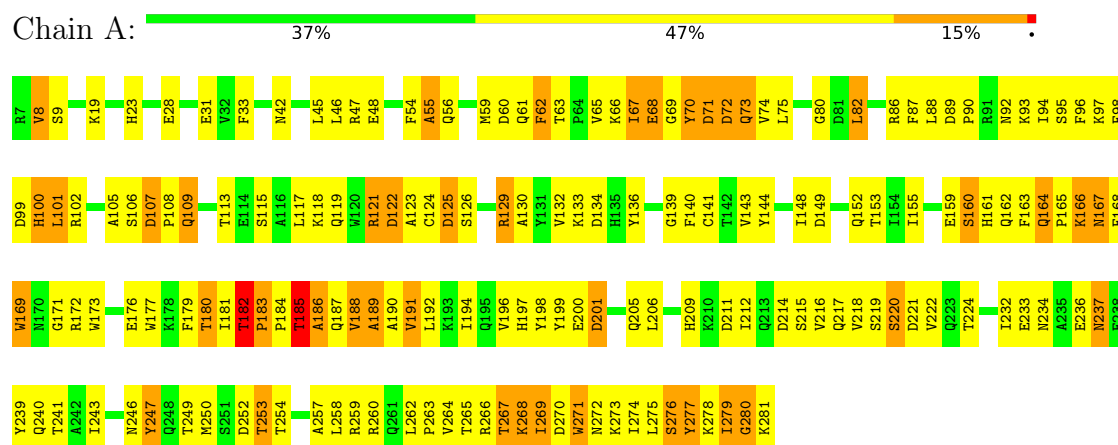


- Molecule 3: Myotrophin

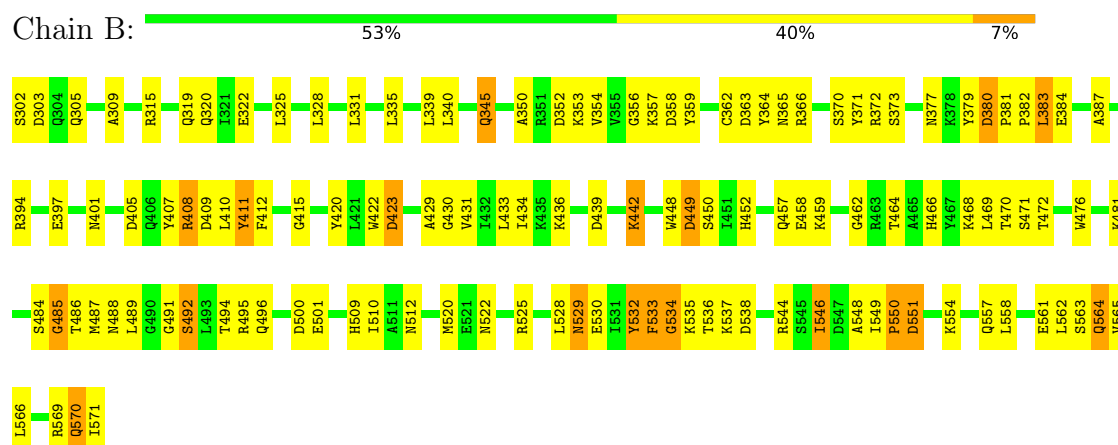


4.2.3 Score per residue for model 3

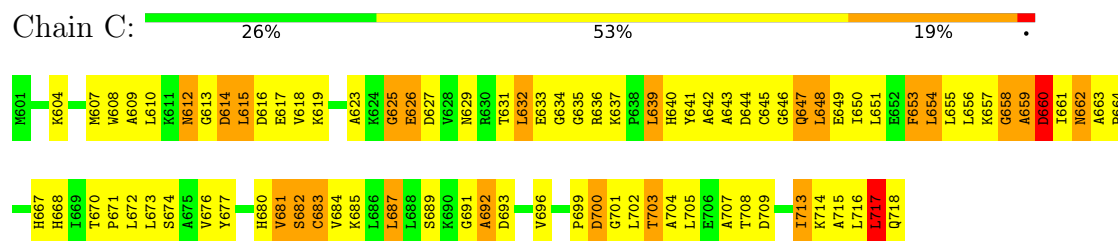
- Molecule 1: F-actin-capping protein subunit alpha-1



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



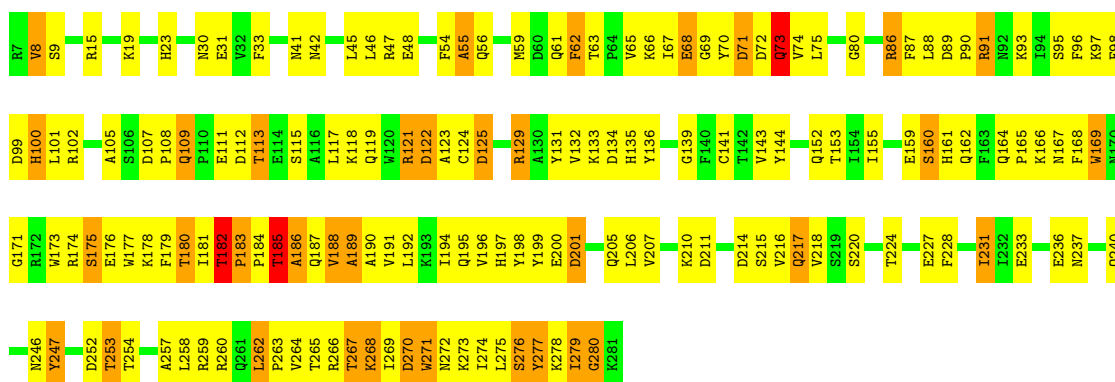
- Molecule 3: Myotrophin



4.2.4 Score per residue for model 4

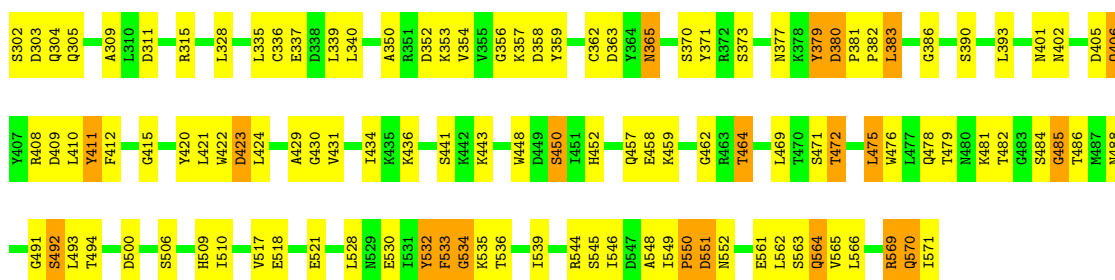
- Molecule 1: F-actin-capping protein subunit alpha-1





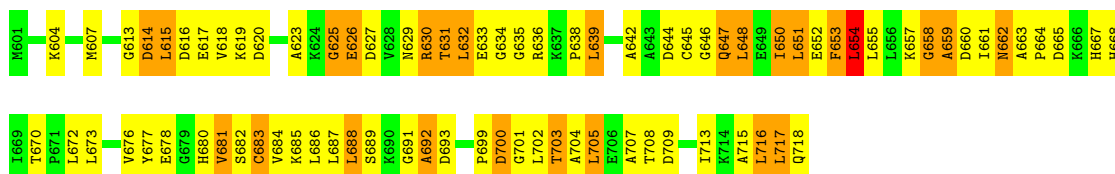
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B: 57% 35% 8%



- Molecule 3: Myotrophin

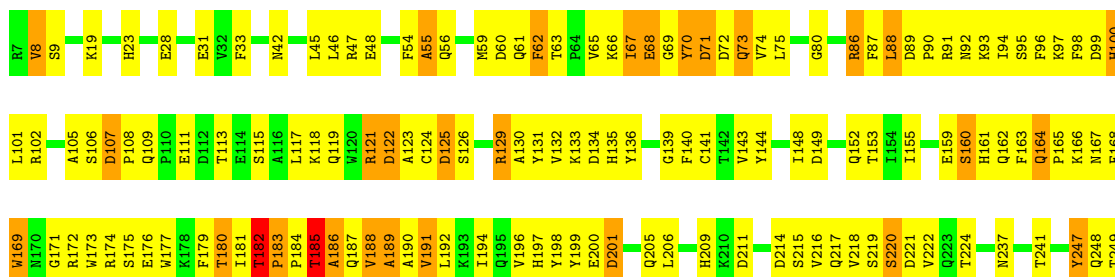
Chain C: 31% 47% 21%

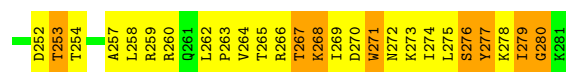


4.2.5 Score per residue for model 5

- Molecule 1: F-actin-capping protein subunit alpha-1

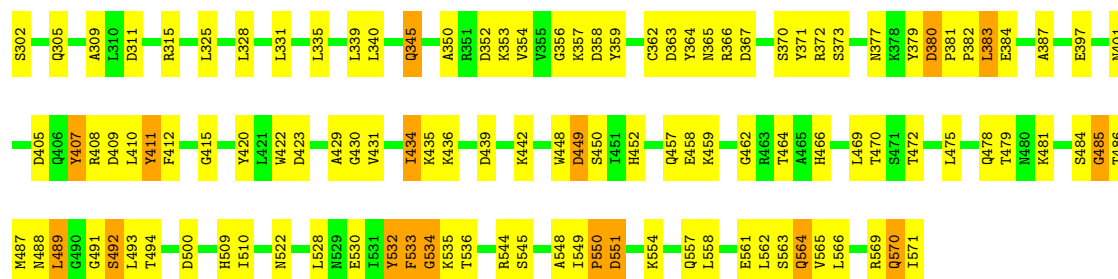
Chain A: 39% 47% 13%





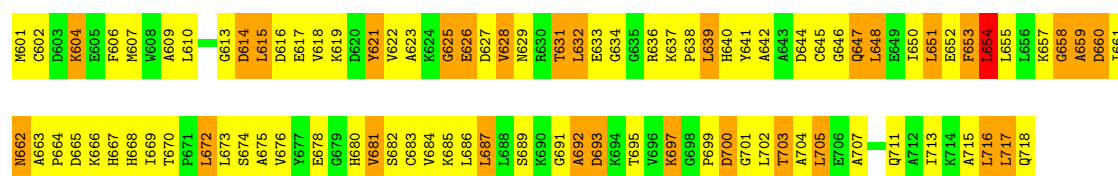
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B: 57% 36% 6%



- Molecule 3: Myotrophin

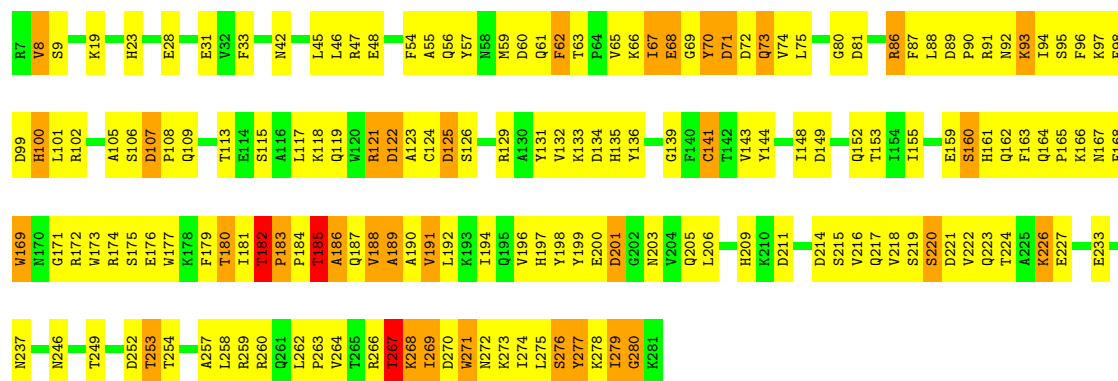
Chain C: 22% 53% 25%



4.2.6 Score per residue for model 6

- Molecule 1: F-actin-capping protein subunit alpha-1

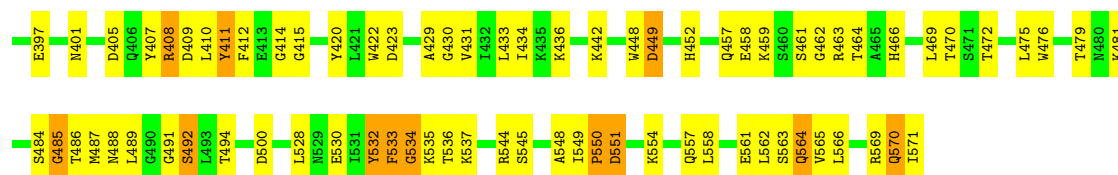
Chain A: 39% 48% 12%



- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

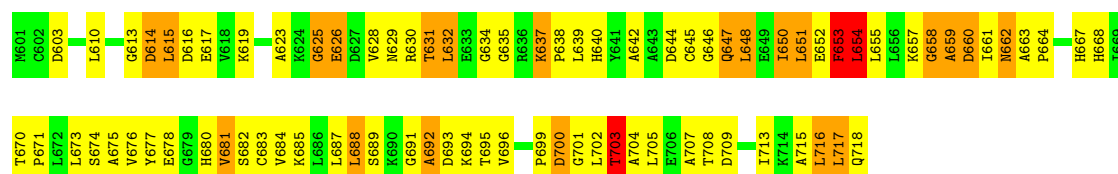
Chain B: 57% 37% 6%





• Molecule 3: Myotrophin

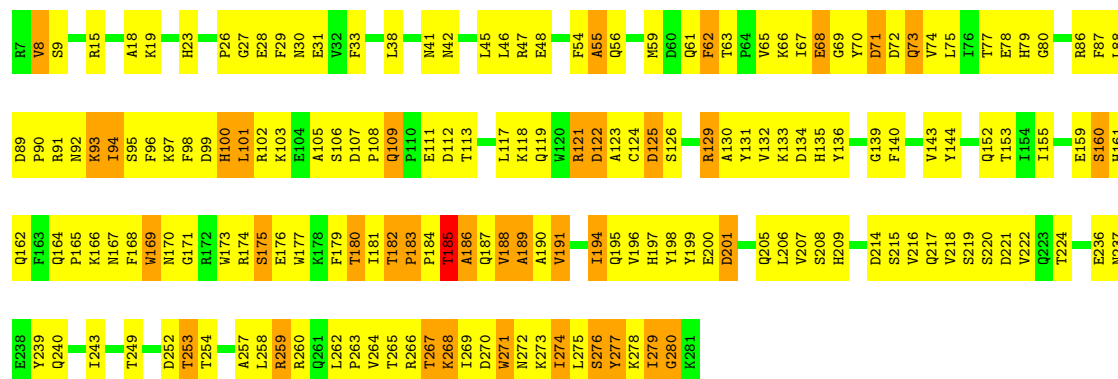
Chain C: 31% 49% 18%



4.2.7 Score per residue for model 7 (medoid)

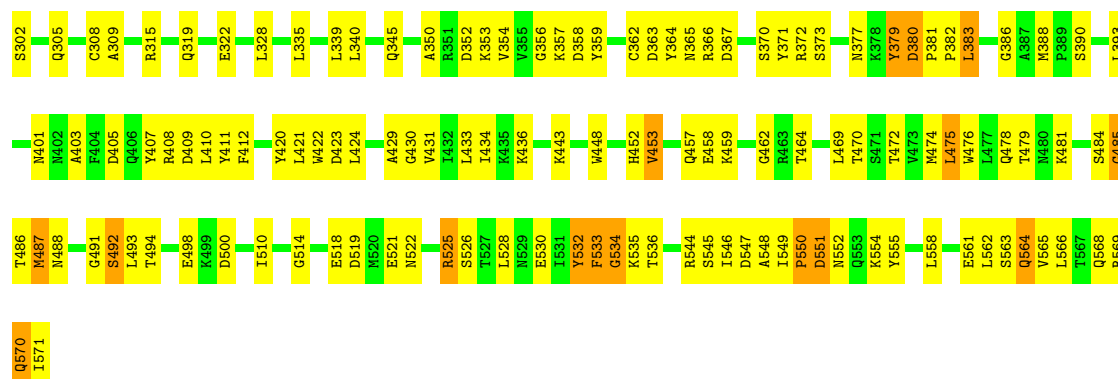
• Molecule 1: F-actin-capping protein subunit alpha-1

Chain A: 36% 51% 13%

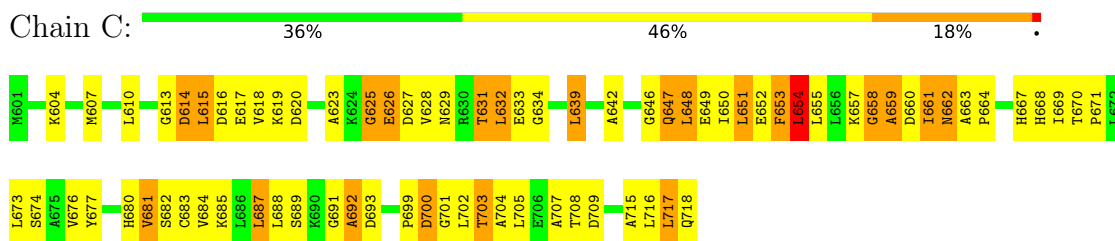


• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B: 53% 41% 6%

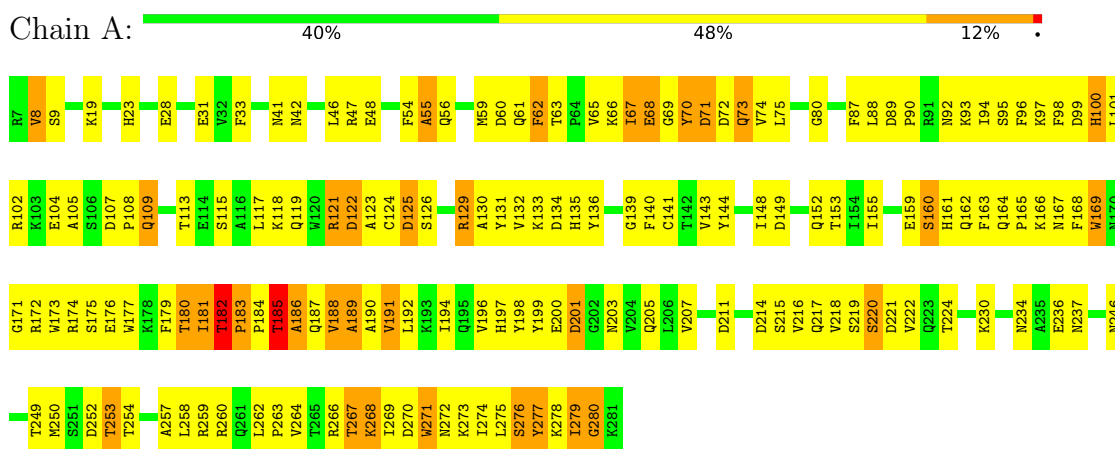


- Molecule 3: Myotrophin

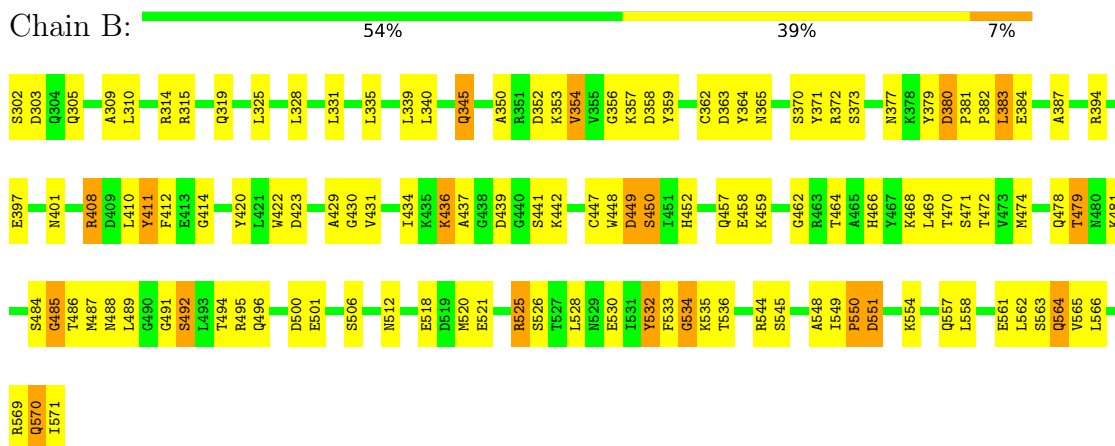


4.2.8 Score per residue for model 8

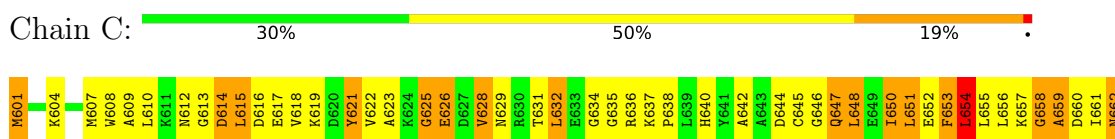
- Molecule 1: F-actin-capping protein subunit alpha-1

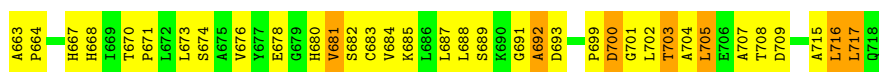


- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



- Molecule 3: Myotrophin

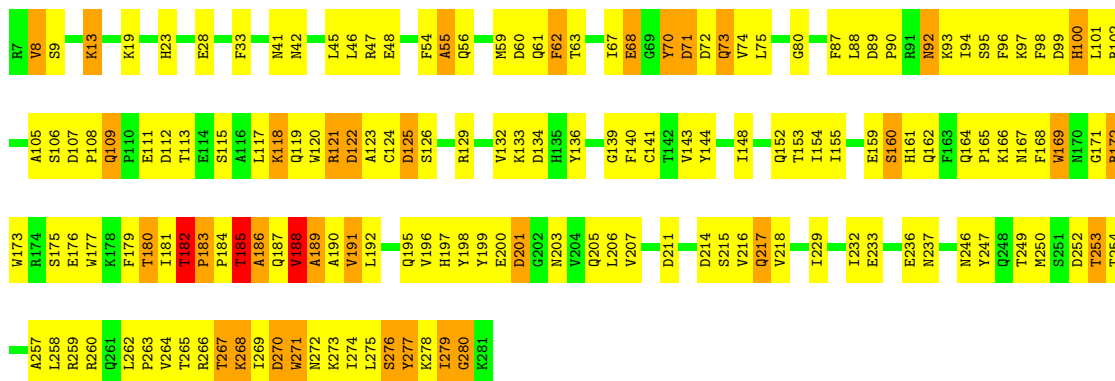




4.2.9 Score per residue for model 9

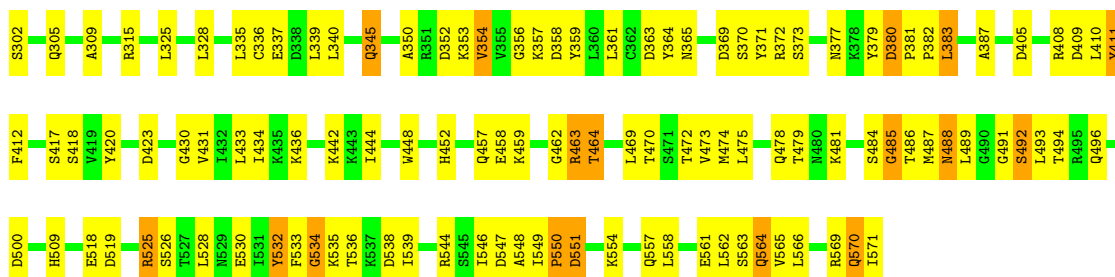
- Molecule 1: F-actin-capping protein subunit alpha-1

Chain A: 41% 45% 12%



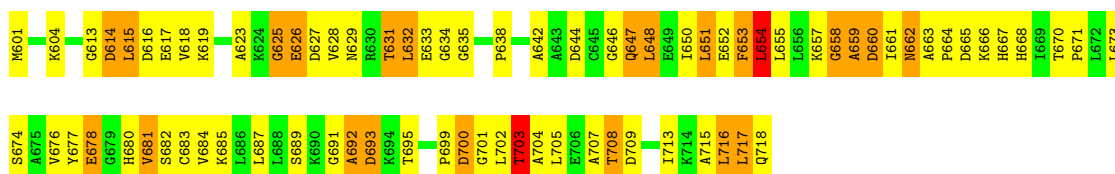
- Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2

Chain B: 57% 36% 6%



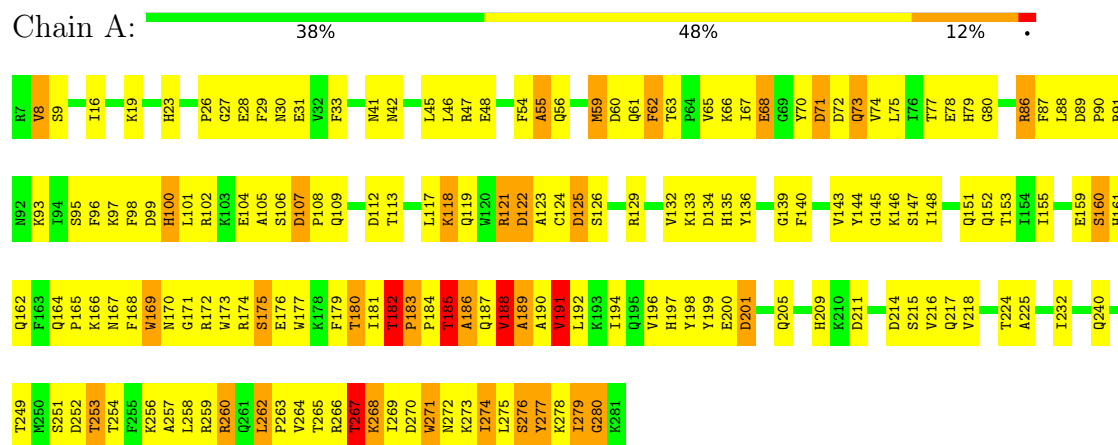
- Molecule 3: Myotrophin

Chain C: 34% 46% 19%

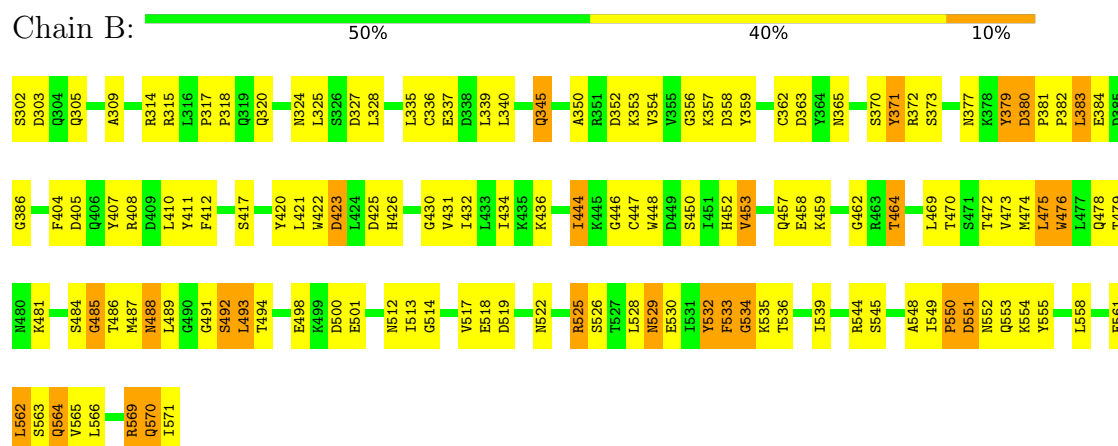


4.2.10 Score per residue for model 10

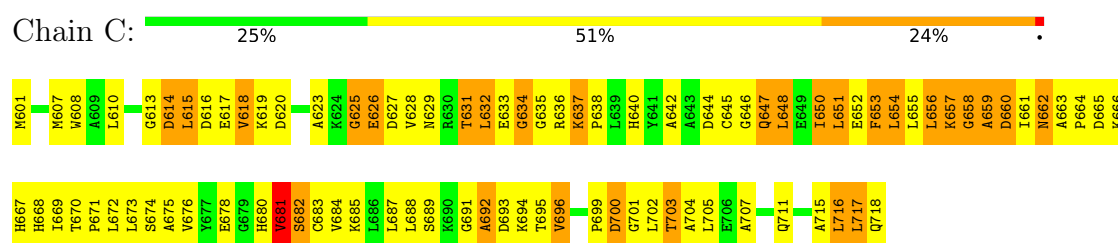
- Molecule 1: F-actin-capping protein subunit alpha-1



• Molecule 2: F-actin-capping protein subunit beta isoforms 1 and 2



• Molecule 3: Myotrophin



5 Refinement protocol and experimental data overview ⓘ

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

Of the 200 calculated structures, 10 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	refinement	2.23

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	2239	2177	2166	291±13
2	B	2141	2135	2128	160±9
3	C	902	917	909	129±8
All	All	52820	52290	52030	5557

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 53.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:SER:O	1:A:278:LYS:N	1.32	1.62	4	10
1:A:182:THR:OG1	1:A:184:PRO:HG3	1.25	1.30	7	1
3:C:688:LEU:HD13	3:C:689:SER:N	1.23	1.49	4	2
1:A:273:LYS:O	1:A:277:TYR:HB3	1.22	1.35	8	10
3:C:673:LEU:O	3:C:676:VAL:HG22	1.18	0.99	3	1
3:C:673:LEU:O	3:C:676:VAL:CG2	1.14	1.95	3	1
1:A:186:ALA:HB3	1:A:216:VAL:C	1.13	1.69	3	10
1:A:200:GLU:O	1:A:201:ASP:CG	1.11	1.92	10	7
1:A:186:ALA:O	1:A:216:VAL:O	1.11	1.68	7	10
1:A:187:GLN:O	1:A:188:VAL:HG23	1.09	1.44	4	10
3:C:691:GLY:O	3:C:693:ASP:N	1.09	1.85	4	10
1:A:186:ALA:HB3	1:A:216:VAL:O	1.08	1.47	3	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:279:ILE:O	1:A:280:GLY:O	1.08	1.72	4	10
3:C:662:ASN:C	3:C:664:PRO:HD2	1.08	1.74	3	10
1:A:273:LYS:O	1:A:277:TYR:CB	1.08	2.02	8	10
1:A:72:ASP:O	1:A:74:VAL:N	1.07	1.87	2	10
1:A:182:THR:OG1	1:A:184:PRO:CG	1.07	2.01	7	1
1:A:183:PRO:HA	1:A:218:VAL:HB	1.06	1.28	1	10
1:A:187:GLN:HA	1:A:215:SER:HA	1.05	1.28	5	10
3:C:651:LEU:N	3:C:651:LEU:HD13	1.05	1.66	9	3
3:C:716:LEU:O	3:C:717:LEU:HB2	1.04	1.52	10	9
2:B:371:TYR:O	2:B:379:TYR:HA	1.04	1.52	9	10
3:C:651:LEU:HD13	3:C:651:LEU:H	1.04	0.99	8	8
3:C:651:LEU:HD13	3:C:651:LEU:N	1.04	1.66	8	5
1:A:186:ALA:CB	1:A:216:VAL:O	1.03	2.07	3	10
1:A:185:THR:O	1:A:217:GLN:HA	1.03	1.54	6	10
3:C:688:LEU:HD22	3:C:688:LEU:C	1.02	1.79	4	2
1:A:152:GLN:O	1:A:181:ILE:HG13	1.01	1.55	10	1
1:A:186:ALA:HB1	1:A:216:VAL:HG13	1.01	1.32	3	4
1:A:260:ARG:O	2:B:411:TYR:CZ	1.00	2.14	7	1
3:C:651:LEU:H	3:C:651:LEU:CD1	1.00	1.67	9	8
1:A:186:ALA:CA	1:A:216:VAL:O	0.99	2.11	3	10
3:C:653:PHE:O	3:C:655:LEU:N	0.99	1.96	8	10
1:A:186:ALA:HB2	1:A:218:VAL:HG23	0.98	1.35	1	10
3:C:716:LEU:O	3:C:717:LEU:HB3	0.98	1.54	3	1
2:B:352:ASP:O	2:B:356:GLY:N	0.97	1.97	8	10
2:B:444:ILE:HD13	2:B:444:ILE:H	0.97	1.20	10	1
2:B:370:SER:HB3	2:B:381:PRO:HD2	0.96	1.37	3	4
1:A:186:ALA:C	1:A:216:VAL:O	0.96	2.08	8	10
3:C:688:LEU:HD22	3:C:688:LEU:O	0.95	1.60	6	2
1:A:187:GLN:O	1:A:188:VAL:CG2	0.95	2.15	4	10
2:B:370:SER:HB2	2:B:381:PRO:HD2	0.94	1.38	5	6
1:A:153:THR:HG23	1:A:179:PHE:C	0.92	1.89	4	3
3:C:688:LEU:HD13	3:C:689:SER:H	0.92	1.25	6	2
3:C:615:LEU:HD13	3:C:615:LEU:O	0.91	1.65	8	7
3:C:648:LEU:C	3:C:651:LEU:HD21	0.91	1.91	6	8
3:C:680:HIS:O	3:C:682:SER:N	0.91	2.04	3	10
1:A:107:ASP:CG	1:A:107:ASP:O	0.91	2.14	5	3
3:C:654:LEU:HD22	3:C:654:LEU:O	0.90	1.65	6	1
2:B:530:GLU:O	2:B:534:GLY:HA3	0.90	1.67	7	10
3:C:648:LEU:HD13	3:C:682:SER:OG	0.90	1.67	3	1
1:A:252:ASP:O	1:A:253:THR:OG1	0.89	1.91	4	10
3:C:621:TYR:CD1	3:C:622:VAL:N	0.89	2.40	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:481:LYS:O	2:B:485:GLY:N	0.89	2.06	4	10
3:C:653:PHE:C	3:C:655:LEU:H	0.88	1.77	5	10
3:C:717:LEU:HD12	3:C:718:GLN:N	0.88	1.83	3	1
1:A:152:GLN:O	1:A:181:ILE:CG1	0.87	2.23	10	1
3:C:621:TYR:OH	3:C:628:VAL:HG22	0.87	1.68	8	2
2:B:422:TRP:NE1	2:B:429:ALA:HB3	0.87	1.85	8	5
1:A:185:THR:O	1:A:217:GLN:CA	0.87	2.21	5	10
1:A:106:SER:O	1:A:107:ASP:OD1	0.86	1.92	3	3
3:C:621:TYR:CG	3:C:622:VAL:N	0.86	2.43	8	2
1:A:274:ILE:HD12	1:A:274:ILE:O	0.86	1.69	7	1
1:A:185:THR:C	1:A:217:GLN:HA	0.86	1.96	10	10
1:A:152:GLN:N	1:A:181:ILE:HG12	0.85	1.86	10	1
2:B:569:ARG:O	2:B:570:GLN:HB3	0.85	1.67	2	2
3:C:662:ASN:C	3:C:664:PRO:CD	0.85	2.50	5	10
2:B:493:LEU:HD13	2:B:494:THR:H	0.85	1.29	10	1
1:A:192:LEU:N	1:A:192:LEU:HD22	0.85	1.87	1	1
2:B:570:GLN:O	2:B:571:ILE:HB	0.85	1.72	9	10
3:C:648:LEU:HD13	3:C:648:LEU:N	0.84	1.88	5	8
2:B:561:GLU:O	2:B:565:VAL:HG23	0.84	1.72	7	10
1:A:74:VAL:C	1:A:75:LEU:HD22	0.84	1.97	9	1
1:A:186:ALA:O	1:A:216:VAL:N	0.84	2.11	6	10
1:A:182:THR:HB	1:A:184:PRO:CG	0.84	2.03	1	9
3:C:680:HIS:C	3:C:682:SER:H	0.84	1.81	4	10
2:B:422:TRP:CE2	2:B:429:ALA:HB3	0.84	2.08	4	7
1:A:153:THR:OG1	1:A:180:THR:HA	0.84	1.71	3	3
3:C:654:LEU:H	3:C:654:LEU:HD22	0.83	1.32	1	3
1:A:152:GLN:H	1:A:181:ILE:HG12	0.83	1.32	10	1
1:A:95:SER:O	1:A:109:GLN:N	0.83	2.12	6	10
2:B:361:LEU:HD23	2:B:362:CYS:H	0.82	1.34	2	1
1:A:95:SER:O	1:A:108:PRO:CA	0.82	2.28	4	10
1:A:186:ALA:CB	1:A:216:VAL:HG13	0.82	2.05	6	4
3:C:716:LEU:O	3:C:717:LEU:CB	0.82	2.28	3	10
3:C:676:VAL:HG23	3:C:677:TYR:H	0.81	1.32	3	1
1:A:219:SER:H	1:A:224:THR:CG2	0.81	1.88	5	5
2:B:570:GLN:O	2:B:571:ILE:CB	0.81	2.29	5	10
1:A:200:GLU:O	1:A:201:ASP:CB	0.81	2.29	5	10
2:B:408:ARG:HE	2:B:415:GLY:C	0.81	1.83	6	2
1:A:95:SER:O	1:A:108:PRO:HA	0.80	1.77	4	10
1:A:252:ASP:OD1	1:A:252:ASP:O	0.80	2.00	5	3
1:A:70:TYR:O	1:A:72:ASP:N	0.80	2.15	1	10
2:B:563:SER:O	2:B:565:VAL:N	0.80	2.15	2	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:688:LEU:C	3:C:688:LEU:CD2	0.80	2.52	4	2
3:C:703:THR:O	3:C:707:ALA:HB2	0.79	1.78	9	10
3:C:676:VAL:HG23	3:C:677:TYR:N	0.79	1.88	3	1
3:C:651:LEU:N	3:C:651:LEU:HD22	0.79	1.93	6	8
2:B:570:GLN:O	2:B:571:ILE:HG22	0.79	1.77	7	5
3:C:621:TYR:CD1	3:C:621:TYR:C	0.79	2.61	5	2
2:B:570:GLN:O	2:B:571:ILE:CG2	0.79	2.31	7	5
3:C:685:LYS:O	3:C:688:LEU:HD12	0.79	1.78	6	2
2:B:493:LEU:HD13	2:B:494:THR:N	0.79	1.91	10	1
1:A:270:ASP:O	1:A:273:LYS:N	0.79	2.14	6	10
2:B:562:LEU:O	2:B:565:VAL:HB	0.78	1.78	4	10
1:A:181:ILE:O	1:A:182:THR:HG23	0.78	1.78	1	9
1:A:181:ILE:HD12	1:A:181:ILE:O	0.78	1.77	10	1
3:C:691:GLY:C	3:C:693:ASP:N	0.78	2.41	9	10
3:C:650:ILE:O	3:C:654:LEU:HD12	0.78	1.78	6	2
3:C:663:ALA:N	3:C:664:PRO:CD	0.78	2.47	5	10
3:C:648:LEU:O	3:C:648:LEU:HD12	0.78	1.79	8	1
1:A:59:MET:HE3	1:A:87:PHE:CZ	0.78	2.14	1	1
1:A:188:VAL:CG1	1:A:189:ALA:N	0.78	2.47	10	10
1:A:201:ASP:CG	2:B:493:LEU:HD11	0.77	2.03	10	1
3:C:688:LEU:CD1	3:C:689:SER:N	0.77	2.42	4	2
1:A:168:PHE:O	1:A:169:TRP:HB3	0.77	1.80	8	10
1:A:208:SER:OG	2:B:487:MET:HA	0.77	1.79	1	1
1:A:173:TRP:CE3	1:A:194:ILE:HD11	0.77	2.15	7	1
1:A:177:TRP:CZ2	1:A:232:ILE:HG23	0.77	2.15	10	1
1:A:98:PHE:HA	1:A:105:ALA:HB1	0.77	1.57	5	10
1:A:77:THR:O	1:A:87:PHE:CE2	0.76	2.38	1	1
2:B:372:ARG:NH1	2:B:387:ALA:O	0.76	2.18	1	1
1:A:67:ILE:HD12	1:A:68:GLU:N	0.76	1.95	5	4
3:C:688:LEU:HD13	3:C:688:LEU:C	0.76	2.05	4	2
1:A:72:ASP:O	1:A:73:GLN:C	0.76	2.29	5	10
3:C:699:PRO:O	3:C:700:ASP:CG	0.76	2.29	4	3
1:A:98:PHE:HA	1:A:105:ALA:CB	0.76	2.11	10	10
3:C:691:GLY:C	3:C:693:ASP:H	0.76	1.89	8	10
2:B:444:ILE:HD13	2:B:444:ILE:N	0.75	1.95	10	1
2:B:569:ARG:C	2:B:570:GLN:CD	0.75	2.54	2	1
1:A:117:LEU:O	1:A:117:LEU:HG	0.75	1.80	9	9
2:B:370:SER:HB2	2:B:381:PRO:CD	0.75	2.12	9	6
1:A:249:THR:HA	1:A:252:ASP:OD1	0.75	1.81	6	1
1:A:173:TRP:CZ3	1:A:194:ILE:HD11	0.75	2.17	10	5
3:C:654:LEU:HD22	3:C:654:LEU:C	0.75	2.06	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:569:ARG:O	2:B:570:GLN:CB	0.75	2.35	1	10
1:A:160:SER:O	1:A:173:TRP:N	0.74	2.20	3	10
3:C:655:LEU:C	3:C:655:LEU:HD23	0.74	2.07	8	2
3:C:648:LEU:N	3:C:648:LEU:CD1	0.74	2.50	5	8
2:B:379:TYR:CE2	2:B:386:GLY:HA3	0.74	2.17	7	3
2:B:370:SER:HB3	2:B:381:PRO:CD	0.74	2.12	2	4
3:C:615:LEU:HD13	3:C:615:LEU:C	0.74	2.07	9	7
1:A:201:ASP:OD1	2:B:493:LEU:HD21	0.74	1.82	10	1
1:A:274:ILE:HD11	2:B:403:ALA:HB1	0.74	1.59	7	1
1:A:169:TRP:O	1:A:169:TRP:CD2	0.74	2.41	9	10
3:C:651:LEU:N	3:C:651:LEU:CD1	0.73	2.40	1	8
3:C:601:MET:O	3:C:602:CYS:SG	0.73	2.47	5	1
1:A:148:ILE:O	1:A:151:GLN:CG	0.73	2.36	10	1
1:A:276:SER:C	1:A:278:LYS:N	0.73	2.47	1	10
3:C:651:LEU:CD2	3:C:652:GLU:H	0.73	1.97	9	8
2:B:379:TYR:CZ	2:B:386:GLY:HA3	0.73	2.19	1	3
1:A:275:LEU:O	1:A:276:SER:CB	0.73	2.37	1	10
2:B:371:TYR:O	2:B:379:TYR:CA	0.73	2.36	5	10
1:A:259:ARG:CZ	2:B:448:TRP:CZ2	0.73	2.71	7	1
1:A:181:ILE:O	1:A:182:THR:HB	0.73	1.83	7	1
1:A:187:GLN:CA	1:A:215:SER:HA	0.72	2.13	9	10
1:A:67:ILE:HD12	1:A:68:GLU:H	0.72	1.44	3	4
2:B:569:ARG:O	2:B:570:GLN:HB2	0.72	1.83	3	8
1:A:256:LYS:NZ	3:C:636:ARG:NE	0.72	2.37	2	1
2:B:380:ASP:HB3	2:B:381:PRO:HD3	0.72	1.58	7	6
1:A:181:ILE:O	1:A:182:THR:OG1	0.72	2.07	2	9
3:C:680:HIS:C	3:C:682:SER:N	0.72	2.46	2	10
1:A:67:ILE:O	1:A:68:GLU:C	0.72	2.33	5	10
2:B:362:CYS:HG	2:B:365:ASN:CG	0.71	1.92	2	6
3:C:672:LEU:HD23	3:C:672:LEU:C	0.71	2.09	2	2
1:A:186:ALA:CB	1:A:216:VAL:C	0.71	2.58	9	10
3:C:654:LEU:HD13	3:C:655:LEU:N	0.71	2.00	6	1
1:A:183:PRO:HA	1:A:218:VAL:CB	0.71	2.14	2	10
3:C:653:PHE:C	3:C:655:LEU:N	0.71	2.43	6	10
1:A:8:VAL:HG13	1:A:8:VAL:O	0.71	1.86	7	9
1:A:192:LEU:N	1:A:192:LEU:CD1	0.71	2.54	3	7
2:B:470:THR:HG23	2:B:470:THR:O	0.71	1.85	7	2
1:A:95:SER:HB3	1:A:109:GLN:O	0.71	1.86	8	2
3:C:628:VAL:HG23	3:C:628:VAL:O	0.70	1.85	1	2
2:B:571:ILE:HG23	2:B:571:ILE:O	0.70	1.86	6	5
3:C:615:LEU:HD11	3:C:653:PHE:CE2	0.70	2.20	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:379:TYR:CE1	2:B:383:LEU:HB3	0.70	2.20	4	1
3:C:693:ASP:CG	3:C:696:VAL:HG13	0.70	2.10	10	1
1:A:169:TRP:HA	1:A:197:HIS:O	0.70	1.87	8	10
2:B:350:ALA:CB	2:B:359:TYR:CZ	0.70	2.74	9	10
1:A:200:GLU:O	1:A:201:ASP:HB2	0.70	1.87	1	9
3:C:702:LEU:O	3:C:703:THR:C	0.70	2.35	5	10
1:A:219:SER:H	1:A:224:THR:HG22	0.70	1.46	7	5
3:C:683:CYS:SG	3:C:684:VAL:N	0.70	2.65	5	3
1:A:263:PRO:O	1:A:266:ARG:N	0.70	2.24	8	10
2:B:439:ASP:CG	3:C:611:LYS:HZ1	0.70	1.93	1	1
1:A:121:ARG:HE	1:A:122:ASP:N	0.70	1.85	4	1
1:A:111:GLU:CG	1:A:111:GLU:O	0.70	2.40	7	1
1:A:187:GLN:O	1:A:216:VAL:HG12	0.70	1.86	8	4
1:A:187:GLN:O	1:A:188:VAL:CB	0.70	2.40	6	10
1:A:182:THR:HG1	1:A:184:PRO:HG3	0.69	1.42	7	1
1:A:59:MET:C	1:A:59:MET:SD	0.69	2.75	10	1
3:C:618:VAL:O	3:C:621:TYR:CD2	0.69	2.45	8	2
3:C:676:VAL:CG2	3:C:677:TYR:H	0.69	2.01	3	1
1:A:165:PRO:O	1:A:167:ASN:N	0.69	2.26	3	10
1:A:267:THR:O	1:A:268:LYS:C	0.69	2.36	3	10
2:B:532:TYR:O	2:B:536:THR:OG1	0.69	2.10	5	8
1:A:275:LEU:O	1:A:276:SER:OG	0.69	2.11	10	9
1:A:259:ARG:HG3	2:B:412:PHE:CE1	0.69	2.22	5	1
3:C:642:ALA:O	3:C:646:GLY:N	0.69	2.26	7	10
1:A:180:THR:O	1:A:181:ILE:HG23	0.69	1.88	10	1
1:A:179:PHE:O	1:A:180:THR:O	0.68	2.12	9	10
1:A:181:ILE:O	1:A:182:THR:CG2	0.68	2.41	1	9
1:A:107:ASP:O	1:A:107:ASP:OD1	0.68	2.12	5	3
1:A:259:ARG:HG2	1:A:260:ARG:H	0.68	1.47	5	5
1:A:194:ILE:HD13	1:A:195:GLN:N	0.68	2.03	2	1
1:A:169:TRP:CD1	2:B:535:LYS:HZ3	0.68	2.07	3	2
1:A:90:PRO:O	1:A:121:ARG:NH1	0.68	2.27	4	1
2:B:380:ASP:CB	2:B:381:PRO:HD3	0.68	2.19	8	10
2:B:361:LEU:HD11	2:B:371:TYR:CD1	0.68	2.24	2	1
1:A:161:HIS:CG	1:A:163:PHE:CZ	0.68	2.82	5	4
1:A:184:PRO:O	1:A:185:THR:HG23	0.68	1.88	7	1
1:A:168:PHE:HB3	1:A:199:TYR:O	0.68	1.89	5	10
3:C:651:LEU:HD22	3:C:652:GLU:H	0.68	1.47	9	8
2:B:412:PHE:CD1	2:B:436:LYS:HG3	0.68	2.23	5	1
1:A:188:VAL:HG12	1:A:189:ALA:N	0.68	2.03	4	10
1:A:129:ARG:NH2	1:A:133:LYS:HZ2	0.68	1.86	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:70:TYR:CZ	1:A:92:ASN:OD1	0.68	2.47	3	4
1:A:278:LYS:O	1:A:279:ILE:CG1	0.67	2.42	8	3
1:A:74:VAL:C	1:A:75:LEU:HD12	0.67	2.14	1	2
1:A:182:THR:HB	1:A:184:PRO:HG3	0.67	1.66	1	9
1:A:279:ILE:N	1:A:279:ILE:HD12	0.67	2.03	1	1
3:C:654:LEU:C	3:C:654:LEU:HD13	0.67	2.13	6	1
3:C:663:ALA:N	3:C:664:PRO:HD2	0.67	2.04	9	10
3:C:681:VAL:O	3:C:684:VAL:HG22	0.67	1.89	1	6
3:C:676:VAL:CG2	3:C:677:TYR:N	0.67	2.58	3	1
1:A:129:ARG:NH2	1:A:133:LYS:NZ	0.67	2.42	6	1
2:B:422:TRP:CZ3	2:B:424:LEU:HD21	0.67	2.24	7	1
1:A:70:TYR:O	1:A:71:ASP:C	0.67	2.38	2	10
1:A:70:TYR:CE1	1:A:92:ASN:CG	0.67	2.73	5	4
2:B:488:ASN:N	2:B:488:ASN:ND2	0.67	2.43	9	1
1:A:186:ALA:HB2	1:A:218:VAL:CG2	0.67	2.18	9	10
3:C:648:LEU:HA	3:C:651:LEU:HD21	0.67	1.66	5	1
1:A:172:ARG:NH1	1:A:174:ARG:NE	0.67	2.43	10	1
2:B:571:ILE:CG2	2:B:571:ILE:O	0.66	2.43	6	5
2:B:563:SER:C	2:B:565:VAL:N	0.66	2.53	8	10
1:A:74:VAL:HG22	1:A:75:LEU:N	0.66	2.05	7	10
3:C:615:LEU:O	3:C:615:LEU:HD22	0.66	1.90	9	6
2:B:350:ALA:O	2:B:358:ASP:HA	0.66	1.91	7	10
3:C:659:ALA:C	3:C:661:ILE:H	0.66	1.99	3	10
2:B:371:TYR:CD1	2:B:371:TYR:N	0.66	2.64	2	3
1:A:118:LYS:HZ3	1:A:121:ARG:NE	0.66	1.89	5	2
3:C:602:CYS:SG	3:C:606:PHE:CD2	0.66	2.89	5	1
2:B:492:SER:C	2:B:493:LEU:HD22	0.66	2.15	2	5
1:A:192:LEU:HD12	1:A:192:LEU:N	0.66	2.05	10	5
3:C:654:LEU:HD12	3:C:654:LEU:H	0.66	1.51	10	1
2:B:420:TYR:C	2:B:421:LEU:HD12	0.66	2.15	1	2
1:A:121:ARG:HH21	1:A:145:GLY:H	0.66	1.31	2	2
2:B:415:GLY:HA3	2:B:436:LYS:HD3	0.66	1.67	5	1
3:C:602:CYS:SG	3:C:606:PHE:CE2	0.66	2.89	5	1
1:A:89:ASP:O	1:A:93:LYS:HA	0.65	1.92	5	10
1:A:270:ASP:O	1:A:271:TRP:C	0.65	2.39	5	10
1:A:135:HIS:O	2:B:544:ARG:HG2	0.65	1.90	7	7
1:A:88:LEU:HD23	1:A:89:ASP:H	0.65	1.49	5	1
2:B:340:LEU:O	2:B:363:ASP:CB	0.65	2.45	3	10
1:A:75:LEU:HD22	1:A:75:LEU:N	0.65	2.06	9	1
1:A:75:LEU:CD2	1:A:75:LEU:N	0.65	2.59	9	1
2:B:350:ALA:HB1	2:B:359:TYR:CZ	0.65	2.27	5	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:654:LEU:CD1	3:C:654:LEU:N	0.65	2.59	6	1
2:B:528:LEU:O	2:B:532:TYR:HB2	0.65	1.92	2	10
2:B:361:LEU:HD11	2:B:371:TYR:CG	0.65	2.27	2	1
2:B:379:TYR:CD1	2:B:383:LEU:HB2	0.65	2.27	4	2
2:B:361:LEU:HD12	2:B:361:LEU:N	0.64	2.08	9	2
1:A:192:LEU:N	1:A:192:LEU:HD12	0.64	2.08	9	2
1:A:187:GLN:HA	1:A:215:SER:CA	0.64	2.17	8	10
1:A:100:HIS:N	1:A:100:HIS:CD2	0.64	2.63	7	1
1:A:161:HIS:CD2	1:A:163:PHE:CZ	0.64	2.86	3	4
1:A:61:GLN:O	1:A:62:PHE:C	0.64	2.41	9	10
2:B:544:ARG:HG2	2:B:545:SER:H	0.64	1.50	1	8
2:B:475:LEU:HD23	2:B:476:TRP:N	0.64	2.07	4	3
3:C:654:LEU:HD23	3:C:654:LEU:H	0.64	1.51	4	2
1:A:129:ARG:O	1:A:129:ARG:NE	0.64	2.30	7	1
1:A:59:MET:HG3	1:A:60:ASP:N	0.64	2.07	10	1
1:A:153:THR:HA	1:A:179:PHE:O	0.64	1.93	2	10
2:B:377:ASN:ND2	2:B:394:ARG:NE	0.64	2.46	3	3
1:A:198:TYR:O	1:A:198:TYR:CD1	0.64	2.51	3	7
2:B:361:LEU:HD23	2:B:362:CYS:N	0.64	2.07	2	1
3:C:685:LYS:O	3:C:688:LEU:CD1	0.64	2.46	6	2
1:A:181:ILE:O	1:A:182:THR:CB	0.64	2.46	3	10
2:B:563:SER:C	2:B:565:VAL:H	0.63	2.01	6	10
3:C:691:GLY:O	3:C:692:ALA:C	0.63	2.41	5	10
1:A:117:LEU:HD12	1:A:120:TRP:CD1	0.63	2.29	9	1
1:A:260:ARG:O	2:B:411:TYR:CE2	0.63	2.50	7	1
3:C:650:ILE:N	3:C:650:ILE:CD1	0.63	2.60	5	1
1:A:165:PRO:O	1:A:168:PHE:N	0.63	2.31	5	10
1:A:152:GLN:CB	1:A:181:ILE:HG21	0.63	2.24	10	1
1:A:165:PRO:C	1:A:167:ASN:H	0.63	2.02	6	10
1:A:59:MET:SD	1:A:59:MET:N	0.63	2.71	1	1
1:A:172:ARG:HH11	1:A:174:ARG:NE	0.63	1.91	10	1
1:A:100:HIS:CD2	1:A:100:HIS:H	0.63	2.11	1	3
1:A:165:PRO:C	1:A:167:ASN:N	0.63	2.56	2	10
1:A:195:GLN:NE2	1:A:205:GLN:NE2	0.63	2.46	9	1
1:A:148:ILE:O	1:A:151:GLN:HG2	0.63	1.93	10	1
1:A:152:GLN:HB2	1:A:181:ILE:HG21	0.63	1.69	10	1
2:B:530:GLU:O	2:B:534:GLY:CA	0.63	2.46	1	10
3:C:688:LEU:HD12	3:C:691:GLY:O	0.63	1.93	7	1
1:A:200:GLU:C	1:A:201:ASP:CG	0.62	2.66	10	7
1:A:118:LYS:HZ3	1:A:121:ARG:HE	0.62	1.37	5	2
1:A:121:ARG:O	1:A:122:ASP:C	0.62	2.42	5	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:570:GLN:O	2:B:570:GLN:OE1	0.62	2.16	2	1
2:B:364:TYR:CD1	2:B:422:TRP:CH2	0.62	2.87	8	4
1:A:263:PRO:HG3	2:B:411:TYR:CZ	0.62	2.29	10	1
1:A:196:VAL:O	1:A:205:GLN:HA	0.62	1.95	9	10
1:A:273:LYS:O	1:A:277:TYR:HB2	0.62	1.94	10	10
1:A:277:TYR:O	1:A:277:TYR:CD2	0.62	2.53	7	10
3:C:636:ARG:NH1	3:C:641:TYR:CE2	0.62	2.68	2	1
3:C:678:GLU:CD	3:C:678:GLU:O	0.62	2.43	9	1
1:A:259:ARG:NE	2:B:411:TYR:CD1	0.62	2.67	5	4
1:A:279:ILE:O	1:A:279:ILE:HG22	0.62	1.93	1	5
2:B:362:CYS:H	2:B:365:ASN:HD21	0.62	1.35	4	1
2:B:550:PRO:O	2:B:551:ASP:C	0.62	2.43	8	10
2:B:381:PRO:O	2:B:383:LEU:N	0.62	2.33	5	10
1:A:29:PHE:CD2	1:A:30:ASN:N	0.62	2.68	2	3
3:C:651:LEU:HD12	3:C:652:GLU:N	0.62	2.10	5	1
1:A:61:GLN:NE2	1:A:172:ARG:NH2	0.62	2.47	8	2
1:A:192:LEU:N	1:A:192:LEU:CD2	0.62	2.59	1	1
2:B:412:PHE:CD1	2:B:412:PHE:N	0.62	2.68	6	5
3:C:716:LEU:O	3:C:717:LEU:CG	0.62	2.48	7	3
3:C:636:ARG:NH1	3:C:641:TYR:CZ	0.62	2.67	2	1
2:B:372:ARG:NH2	2:B:397:GLU:OE2	0.62	2.32	5	2
1:A:92:ASN:N	1:A:92:ASN:HD22	0.62	1.92	9	1
2:B:448:TRP:CD1	2:B:448:TRP:C	0.61	2.79	8	10
1:A:92:ASN:OD1	1:A:94:ILE:HD13	0.61	1.95	6	4
3:C:673:LEU:HA	3:C:676:VAL:CG1	0.61	2.26	3	1
1:A:279:ILE:O	1:A:280:GLY:C	0.61	2.44	6	10
3:C:610:LEU:CD2	3:C:618:VAL:HG11	0.61	2.25	8	2
1:A:59:MET:SD	1:A:78:GLU:N	0.61	2.72	10	1
1:A:100:HIS:CD2	1:A:100:HIS:N	0.61	2.69	1	2
1:A:186:ALA:CB	1:A:218:VAL:HG23	0.61	2.21	2	10
1:A:263:PRO:HD3	2:B:411:TYR:CZ	0.61	2.31	4	8
1:A:277:TYR:CG	1:A:277:TYR:O	0.61	2.54	6	8
1:A:59:MET:SD	1:A:60:ASP:N	0.61	2.74	9	1
1:A:181:ILE:C	1:A:182:THR:OG1	0.61	2.43	2	9
1:A:184:PRO:C	1:A:185:THR:HG22	0.61	2.19	2	1
1:A:152:GLN:O	1:A:181:ILE:HB	0.61	1.95	1	9
1:A:187:GLN:O	1:A:188:VAL:HB	0.61	1.95	1	8
2:B:496:GLN:NE2	2:B:496:GLN:N	0.61	2.48	2	1
2:B:340:LEU:O	2:B:363:ASP:CG	0.61	2.44	8	4
1:A:46:LEU:HD23	1:A:46:LEU:O	0.61	1.95	1	1
2:B:350:ALA:HB2	2:B:361:LEU:HD11	0.61	1.72	9	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:453:VAL:O	2:B:470:THR:HG22	0.61	1.96	10	2
1:A:206:LEU:HD12	1:A:247:TYR:OH	0.61	1.94	9	3
3:C:651:LEU:H	3:C:651:LEU:CD2	0.61	2.07	6	7
3:C:680:HIS:O	3:C:681:VAL:HG22	0.61	1.96	6	5
3:C:699:PRO:O	3:C:700:ASP:HB2	0.61	1.96	8	7
1:A:149:ASP:OD1	1:A:149:ASP:O	0.61	2.19	6	3
1:A:91:ARG:NH2	1:A:141:CYS:SG	0.61	2.73	6	1
2:B:564:GLN:NE2	2:B:568:GLN:NE2	0.61	2.49	7	1
1:A:278:LYS:O	1:A:279:ILE:HG12	0.61	1.96	8	3
1:A:199:TYR:CG	1:A:199:TYR:O	0.61	2.54	10	1
3:C:673:LEU:HA	3:C:676:VAL:HG13	0.61	1.72	3	1
1:A:277:TYR:O	1:A:277:TYR:CG	0.60	2.54	7	2
1:A:152:GLN:O	1:A:181:ILE:HG23	0.60	1.96	10	1
1:A:271:TRP:O	1:A:274:ILE:N	0.60	2.33	1	10
1:A:274:ILE:N	1:A:274:ILE:HD12	0.60	2.11	1	1
1:A:198:TYR:O	1:A:198:TYR:CD2	0.60	2.54	2	1
1:A:256:LYS:NZ	3:C:636:ARG:HE	0.60	1.92	2	1
2:B:452:HIS:ND1	2:B:471:SER:OG	0.60	2.34	8	1
1:A:184:PRO:O	1:A:185:THR:OG1	0.60	2.19	5	9
3:C:700:ASP:CG	3:C:701:GLY:N	0.60	2.59	6	7
1:A:177:TRP:CE3	1:A:190:ALA:CB	0.60	2.85	10	1
1:A:206:LEU:C	1:A:206:LEU:HD23	0.60	2.21	9	2
3:C:651:LEU:N	3:C:651:LEU:CD2	0.60	2.61	7	7
1:A:97:LYS:O	1:A:105:ALA:HB1	0.60	1.97	9	10
1:A:121:ARG:HH21	1:A:145:GLY:N	0.60	1.93	2	2
2:B:469:LEU:HD12	2:B:470:THR:H	0.60	1.57	2	6
3:C:651:LEU:H	3:C:651:LEU:HD22	0.60	1.57	6	4
3:C:695:THR:HG23	3:C:695:THR:O	0.60	1.95	9	2
2:B:450:SER:OG	2:B:452:HIS:CE1	0.60	2.54	3	1
1:A:188:VAL:HG13	1:A:189:ALA:N	0.60	2.10	1	4
1:A:86:ARG:NH2	1:A:107:ASP:O	0.60	2.35	2	1
1:A:168:PHE:CD1	1:A:199:TYR:O	0.60	2.54	9	6
1:A:179:PHE:C	1:A:179:PHE:CD1	0.60	2.78	1	2
1:A:262:LEU:O	1:A:262:LEU:HD12	0.60	1.96	10	2
2:B:379:TYR:CE1	2:B:383:LEU:CB	0.60	2.85	4	1
3:C:613:GLY:O	3:C:615:LEU:N	0.60	2.33	7	10
1:A:61:GLN:O	1:A:63:THR:N	0.60	2.35	1	10
1:A:216:VAL:HG12	1:A:217:GLN:N	0.60	2.12	1	6
2:B:336:CYS:SG	2:B:337:GLU:N	0.60	2.75	9	4
1:A:177:TRP:HB3	1:A:179:PHE:CZ	0.60	2.32	8	7
1:A:216:VAL:HG22	1:A:217:GLN:N	0.60	2.12	5	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:TYR:OH	1:A:173:TRP:CE2	0.59	2.55	9	3
2:B:553:GLN:CD	2:B:553:GLN:H	0.59	2.05	10	1
1:A:274:ILE:O	1:A:274:ILE:HG22	0.59	1.97	3	5
2:B:313:MET:SD	2:B:313:MET:N	0.59	2.75	2	1
1:A:148:ILE:O	1:A:149:ASP:CG	0.59	2.45	5	4
2:B:459:LYS:CG	2:B:464:THR:O	0.59	2.50	9	6
3:C:644:ASP:OD1	3:C:644:ASP:O	0.59	2.21	6	2
2:B:478:GLN:CD	2:B:479:THR:H	0.59	2.05	9	1
2:B:491:GLY:O	2:B:492:SER:HB3	0.59	1.98	8	7
1:A:136:TYR:HH	1:A:173:TRP:CD1	0.59	2.15	2	5
1:A:239:TYR:CE2	1:A:243:ILE:HD11	0.59	2.33	7	3
2:B:476:TRP:CD1	2:B:476:TRP:C	0.59	2.80	4	2
1:A:159:GLU:CD	1:A:160:SER:N	0.59	2.61	10	9
2:B:422:TRP:N	2:B:422:TRP:CD1	0.59	2.69	7	3
3:C:650:ILE:N	3:C:650:ILE:HD12	0.59	2.10	5	1
1:A:182:THR:OG1	1:A:184:PRO:CD	0.59	2.50	7	1
1:A:65:VAL:HG22	1:A:66:LYS:N	0.59	2.12	1	9
1:A:72:ASP:C	1:A:74:VAL:N	0.59	2.61	8	10
1:A:159:GLU:OE2	1:A:173:TRP:O	0.59	2.19	1	1
2:B:370:SER:OG	2:B:381:PRO:HB2	0.59	1.96	10	4
2:B:487:MET:SD	2:B:487:MET:O	0.59	2.61	3	1
1:A:148:ILE:O	1:A:151:GLN:HG3	0.59	1.97	10	1
1:A:169:TRP:O	1:A:169:TRP:CE3	0.59	2.56	9	10
2:B:310:LEU:O	2:B:310:LEU:HD23	0.59	1.98	8	1
1:A:95:SER:N	1:A:109:GLN:O	0.59	2.35	1	10
2:B:383:LEU:HD23	2:B:384:GLU:H	0.59	1.58	10	6
3:C:688:LEU:C	3:C:688:LEU:CD1	0.59	2.72	4	2
2:B:463:ARG:CG	2:B:463:ARG:HH11	0.59	2.11	9	1
2:B:488:ASN:N	2:B:488:ASN:HD22	0.59	1.95	9	1
1:A:199:TYR:OH	2:B:314:ARG:NH2	0.59	2.35	10	1
1:A:237:ASN:ND2	1:A:237:ASN:C	0.59	2.61	3	2
2:B:544:ARG:HG2	2:B:545:SER:N	0.59	2.13	1	7
2:B:370:SER:OG	2:B:383:LEU:HD12	0.59	1.98	5	3
3:C:699:PRO:HG2	3:C:702:LEU:HD22	0.59	1.74	8	1
2:B:408:ARG:NH1	2:B:415:GLY:O	0.59	2.36	1	2
1:A:61:GLN:OE1	1:A:172:ARG:NH2	0.59	2.35	5	2
1:A:274:ILE:CG2	1:A:274:ILE:O	0.59	2.51	4	1
3:C:636:ARG:HH21	3:C:640:HIS:CD2	0.59	2.15	10	2
3:C:672:LEU:HD12	3:C:684:VAL:HG13	0.59	1.73	5	1
3:C:648:LEU:O	3:C:651:LEU:HD21	0.58	1.98	10	8
3:C:717:LEU:HD12	3:C:718:GLN:H	0.58	1.53	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:717:LEU:CD1	3:C:718:GLN:N	0.58	2.63	3	1
2:B:564:GLN:NE2	2:B:568:GLN:HE22	0.58	1.95	7	1
2:B:370:SER:HA	2:B:381:PRO:HG2	0.58	1.75	4	10
2:B:442:LYS:NZ	3:C:644:ASP:OD2	0.58	2.35	9	2
3:C:642:ALA:O	3:C:646:GLY:CA	0.58	2.52	3	10
3:C:642:ALA:O	3:C:646:GLY:HA3	0.58	1.99	10	10
3:C:630:ARG:HH11	3:C:630:ARG:CG	0.58	2.11	4	2
3:C:677:TYR:CD1	3:C:677:TYR:O	0.58	2.56	2	1
1:A:205:GLN:NE2	1:A:207:VAL:CG2	0.58	2.66	7	2
1:A:72:ASP:OD1	1:A:91:ARG:NE	0.58	2.36	5	2
1:A:177:TRP:CD2	1:A:190:ALA:CB	0.58	2.87	7	8
3:C:647:GLN:C	3:C:648:LEU:HG	0.58	2.22	3	1
1:A:176:GLU:O	1:A:190:ALA:HB1	0.58	1.99	5	10
2:B:570:GLN:O	2:B:571:ILE:CG1	0.58	2.51	1	5
1:A:131:TYR:OH	2:B:544:ARG:NH2	0.58	2.37	4	6
1:A:248:GLN:O	1:A:252:ASP:OD2	0.58	2.21	5	2
2:B:566:LEU:N	2:B:566:LEU:HD22	0.58	2.13	7	1
2:B:377:ASN:ND2	2:B:394:ARG:CZ	0.58	2.66	3	3
3:C:630:ARG:CD	3:C:630:ARG:H	0.58	2.12	1	1
2:B:422:TRP:CZ2	2:B:429:ALA:HB3	0.58	2.33	4	3
1:A:161:HIS:CD2	1:A:163:PHE:CE2	0.58	2.92	3	4
3:C:648:LEU:O	3:C:648:LEU:CD1	0.58	2.51	8	1
1:A:236:GLU:OE2	1:A:237:ASN:ND2	0.58	2.37	9	1
2:B:478:GLN:NE2	2:B:479:THR:H	0.58	1.97	9	1
1:A:91:ARG:HH22	1:A:129:ARG:NH2	0.58	1.95	10	1
1:A:274:ILE:O	1:A:274:ILE:CG2	0.58	2.51	9	4
2:B:525:ARG:HH11	2:B:525:ARG:CG	0.58	2.12	8	5
1:A:164:GLN:HB3	1:A:169:TRP:CE2	0.58	2.33	1	7
1:A:180:THR:OG1	1:A:181:ILE:N	0.58	2.37	2	7
1:A:251:SER:OG	2:B:533:PHE:HB3	0.58	1.98	2	1
2:B:322:GLU:H	2:B:322:GLU:CD	0.58	2.06	3	1
1:A:253:THR:OG1	3:C:636:ARG:NH2	0.58	2.36	8	1
1:A:173:TRP:CH2	1:A:194:ILE:HD11	0.57	2.34	4	2
1:A:243:ILE:HG12	2:B:487:MET:SD	0.57	2.39	7	1
2:B:442:LYS:NZ	3:C:640:HIS:NE2	0.57	2.52	8	1
1:A:146:LYS:CG	1:A:147:SER:N	0.57	2.67	10	1
1:A:19:LYS:O	1:A:23:HIS:CG	0.57	2.57	4	10
1:A:74:VAL:HG22	1:A:75:LEU:H	0.57	1.60	9	10
1:A:237:ASN:O	1:A:237:ASN:ND2	0.57	2.37	1	1
2:B:550:PRO:O	2:B:551:ASP:O	0.57	2.23	5	10
3:C:717:LEU:HG	3:C:718:GLN:H	0.57	1.58	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:216:VAL:CG2	1:A:217:GLN:N	0.57	2.67	3	4
2:B:432:ILE:O	2:B:452:HIS:ND1	0.57	2.36	10	1
1:A:89:ASP:O	1:A:93:LYS:CA	0.57	2.53	1	10
1:A:224:THR:OG1	1:A:228:PHE:CZ	0.57	2.56	1	1
3:C:701:GLY:O	3:C:705:LEU:CB	0.57	2.53	10	10
3:C:693:ASP:CG	3:C:694:LYS:N	0.57	2.62	10	2
1:A:246:ASN:HD21	2:B:481:LYS:NZ	0.57	1.97	4	1
1:A:121:ARG:HG2	1:A:122:ASP:N	0.57	2.14	2	1
1:A:206:LEU:HD23	1:A:206:LEU:O	0.57	1.99	5	3
2:B:408:ARG:C	2:B:408:ARG:CD	0.57	2.78	8	1
2:B:439:ASP:OD1	2:B:441:SER:N	0.57	2.37	8	1
3:C:651:LEU:HD12	3:C:652:GLU:H	0.57	1.60	5	1
2:B:439:ASP:OD1	2:B:442:LYS:N	0.57	2.37	8	1
1:A:259:ARG:HG2	1:A:260:ARG:N	0.57	2.15	5	3
1:A:261:GLN:O	1:A:262:LEU:HG	0.57	1.99	1	1
3:C:659:ALA:C	3:C:661:ILE:N	0.57	2.63	1	10
1:A:252:ASP:OD1	1:A:252:ASP:C	0.57	2.47	6	3
1:A:55:ALA:O	1:A:59:MET:SD	0.57	2.62	1	1
1:A:263:PRO:HA	2:B:410:LEU:O	0.57	2.00	8	10
2:B:412:PHE:O	2:B:436:LYS:NZ	0.57	2.38	10	8
2:B:569:ARG:HH11	2:B:569:ARG:CG	0.57	2.11	1	3
1:A:206:LEU:HD23	1:A:206:LEU:C	0.57	2.23	5	2
1:A:247:TYR:OH	2:B:536:THR:OG1	0.57	2.21	5	1
1:A:155:ILE:N	1:A:155:ILE:HD12	0.57	2.14	9	1
1:A:61:GLN:OE1	1:A:174:ARG:NH2	0.57	2.37	1	2
1:A:129:ARG:CG	1:A:129:ARG:HH11	0.57	2.13	3	4
2:B:496:GLN:H	2:B:496:GLN:CD	0.57	2.07	9	1
2:B:458:GLU:CD	2:B:459:LYS:N	0.57	2.63	10	1
1:A:188:VAL:HG13	1:A:189:ALA:H	0.57	1.59	2	10
2:B:544:ARG:CG	2:B:545:SER:N	0.57	2.68	1	4
1:A:125:ASP:CG	1:A:143:VAL:HB	0.57	2.24	2	1
3:C:674:SER:O	3:C:678:GLU:HG2	0.57	2.00	6	2
1:A:260:ARG:NH1	3:C:633:GLU:OE1	0.57	2.38	9	1
2:B:493:LEU:CD1	2:B:494:THR:N	0.57	2.66	10	1
1:A:188:VAL:O	1:A:189:ALA:HB2	0.56	2.01	6	10
1:A:236:GLU:CG	2:B:544:ARG:NH1	0.56	2.68	2	1
1:A:184:PRO:C	1:A:185:THR:OG1	0.56	2.47	7	1
3:C:651:LEU:O	3:C:655:LEU:HB2	0.56	2.00	4	8
3:C:662:ASN:CA	3:C:664:PRO:HD2	0.56	2.30	9	10
2:B:493:LEU:HD22	2:B:493:LEU:N	0.56	2.14	2	1
1:A:249:THR:OG1	3:C:677:TYR:CZ	0.56	2.59	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:394:ARG:NH1	2:B:397:GLU:OE1	0.56	2.38	8	1
1:A:260:ARG:NH1	3:C:633:GLU:CD	0.56	2.64	9	1
1:A:70:TYR:C	1:A:72:ASP:N	0.56	2.64	3	10
1:A:216:VAL:CG1	1:A:217:GLN:N	0.56	2.67	4	6
1:A:158:ILE:HD13	1:A:175:SER:OG	0.56	2.00	2	1
3:C:651:LEU:O	3:C:655:LEU:HB3	0.56	2.00	7	2
1:A:86:ARG:HH11	1:A:86:ARG:CG	0.56	2.14	10	5
2:B:362:CYS:O	2:B:365:ASN:ND2	0.56	2.39	4	1
2:B:379:TYR:CD1	2:B:383:LEU:CB	0.56	2.88	4	2
1:A:89:ASP:O	1:A:93:LYS:N	0.56	2.39	9	10
1:A:255:PHE:CE2	2:B:525:ARG:CZ	0.56	2.89	1	1
2:B:379:TYR:OH	2:B:387:ALA:O	0.56	2.21	6	6
1:A:199:TYR:CD1	1:A:199:TYR:N	0.56	2.73	8	2
1:A:89:ASP:HB3	1:A:94:ILE:HD13	0.56	1.77	7	1
1:A:129:ARG:NE	1:A:129:ARG:C	0.56	2.64	7	1
2:B:562:LEU:O	2:B:562:LEU:HD23	0.56	2.00	10	1
1:A:199:TYR:O	1:A:199:TYR:CG	0.56	2.59	9	5
2:B:549:ILE:O	2:B:551:ASP:N	0.56	2.39	6	10
1:A:266:ARG:O	1:A:267:THR:OG1	0.56	2.22	8	4
1:A:89:ASP:OD1	1:A:92:ASN:N	0.56	2.38	9	3
1:A:186:ALA:O	1:A:216:VAL:C	0.56	2.48	3	10
2:B:525:ARG:O	2:B:529:ASN:ND2	0.56	2.39	2	1
2:B:372:ARG:NH1	2:B:377:ASN:OD1	0.56	2.39	5	2
1:A:28:GLU:OE2	1:A:170:ASN:ND2	0.56	2.38	7	1
2:B:570:GLN:OE1	2:B:570:GLN:N	0.56	2.38	2	1
1:A:148:ILE:O	1:A:149:ASP:OD1	0.56	2.24	6	4
1:A:199:TYR:N	1:A:199:TYR:CD1	0.56	2.73	5	2
1:A:271:TRP:CZ2	2:B:514:GLY:C	0.56	2.84	7	2
3:C:649:GLU:O	3:C:653:PHE:CD1	0.56	2.59	3	1
1:A:91:ARG:CG	1:A:91:ARG:HH11	0.56	2.12	4	1
2:B:552:ASN:ND2	2:B:555:TYR:CD1	0.56	2.74	10	2
3:C:646:GLY:C	3:C:648:LEU:H	0.56	2.09	4	10
1:A:29:PHE:CG	1:A:30:ASN:N	0.56	2.73	10	3
1:A:153:THR:HG23	1:A:180:THR:N	0.56	2.15	4	3
2:B:411:TYR:N	2:B:411:TYR:CD1	0.56	2.73	10	1
3:C:631:THR:O	3:C:632:LEU:C	0.56	2.49	3	10
3:C:651:LEU:O	3:C:655:LEU:CB	0.56	2.54	9	10
3:C:667:HIS:ND1	3:C:667:HIS:N	0.56	2.53	7	2
2:B:325:LEU:CD2	2:B:345:GLN:NE2	0.56	2.69	6	5
1:A:113:THR:OG1	1:A:118:LYS:NZ	0.56	2.38	4	1
2:B:452:HIS:CE1	2:B:471:SER:OG	0.56	2.59	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:GLU:OE2	1:A:160:SER:N	0.55	2.35	1	1
1:A:267:THR:O	1:A:268:LYS:O	0.55	2.24	7	10
2:B:444:ILE:HG22	2:B:479:THR:OG1	0.55	2.01	2	1
1:A:118:LYS:HZ2	1:A:121:ARG:HH21	0.55	1.44	3	2
3:C:661:ILE:HD11	3:C:672:LEU:CD2	0.55	2.32	5	1
2:B:409:ASP:CG	3:C:604:LYS:HZ3	0.55	2.09	7	1
1:A:210:LYS:NZ	2:B:482:THR:O	0.55	2.39	4	2
3:C:699:PRO:O	3:C:700:ASP:CB	0.55	2.54	4	10
1:A:184:PRO:O	1:A:185:THR:CG2	0.55	2.54	7	1
2:B:380:ASP:OD1	2:B:381:PRO:N	0.55	2.40	7	1
1:A:169:TRP:CZ3	2:B:539:ILE:HD12	0.55	2.37	1	5
1:A:188:VAL:HB	1:A:214:ASP:O	0.55	2.01	3	10
1:A:129:ARG:HG3	1:A:130:ALA:N	0.55	2.16	8	4
1:A:26:PRO:O	1:A:170:ASN:ND2	0.55	2.40	10	1
3:C:642:ALA:O	3:C:651:LEU:HD12	0.55	2.02	2	8
3:C:646:GLY:C	3:C:648:LEU:N	0.55	2.64	3	10
3:C:644:ASP:OD1	3:C:644:ASP:C	0.55	2.45	6	3
1:A:179:PHE:O	1:A:179:PHE:CD2	0.55	2.60	9	1
2:B:418:SER:OG	2:B:420:TYR:OH	0.55	2.19	9	1
3:C:630:ARG:CG	3:C:630:ARG:NH1	0.55	2.68	4	2
3:C:717:LEU:CG	3:C:718:GLN:H	0.55	2.14	1	2
1:A:129:ARG:CG	1:A:129:ARG:NH1	0.55	2.69	3	4
1:A:261:GLN:CG	2:B:525:ARG:NH1	0.55	2.69	1	1
3:C:640:HIS:CE1	3:C:644:ASP:OD2	0.55	2.59	2	2
3:C:639:LEU:HD22	3:C:660:ASP:OD1	0.55	2.02	3	1
1:A:136:TYR:HH	1:A:173:TRP:NE1	0.55	1.99	8	4
1:A:229:ILE:O	1:A:232:ILE:HG12	0.55	2.02	9	1
1:A:169:TRP:CE3	1:A:169:TRP:C	0.55	2.85	9	9
3:C:673:LEU:O	3:C:676:VAL:HB	0.55	2.02	9	9
1:A:42:ASN:ND2	1:A:45:LEU:CD1	0.55	2.70	5	3
2:B:487:MET:HE1	2:B:489:LEU:HB2	0.55	1.77	5	1
2:B:420:TYR:N	2:B:420:TYR:CD1	0.55	2.74	9	1
3:C:656:LEU:HD23	3:C:656:LEU:O	0.55	2.00	10	1
3:C:659:ALA:O	3:C:661:ILE:N	0.55	2.40	2	10
3:C:705:LEU:C	3:C:705:LEU:HD23	0.55	2.26	2	4
2:B:383:LEU:CD2	2:B:384:GLU:H	0.55	2.15	10	6
2:B:340:LEU:O	2:B:363:ASP:HB2	0.55	2.02	6	4
2:B:449:ASP:N	2:B:449:ASP:OD1	0.55	2.37	3	3
3:C:716:LEU:O	3:C:717:LEU:HD13	0.55	2.02	8	2
2:B:350:ALA:CB	2:B:359:TYR:CE1	0.55	2.90	9	9
1:A:126:SER:O	1:A:129:ARG:CG	0.55	2.55	7	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:247:TYR:CE2	2:B:537:LYS:NZ	0.55	2.71	3	1
1:A:31:GLU:OE1	2:B:315:ARG:NE	0.55	2.39	10	2
3:C:675:ALA:O	3:C:678:GLU:HB2	0.55	2.02	10	3
2:B:443:LYS:NZ	3:C:677:TYR:CD2	0.55	2.75	7	1
3:C:628:VAL:HG11	3:C:654:LEU:O	0.55	2.02	7	4
1:A:173:TRP:CZ3	2:B:544:ARG:NH1	0.55	2.75	9	1
1:A:152:GLN:N	1:A:181:ILE:CG1	0.55	2.69	10	1
1:A:19:LYS:O	1:A:23:HIS:ND1	0.54	2.40	2	9
1:A:61:GLN:NE2	1:A:174:ARG:NH2	0.54	2.55	1	2
1:A:136:TYR:N	1:A:136:TYR:CD1	0.54	2.75	1	2
3:C:701:GLY:O	3:C:705:LEU:HB3	0.54	2.01	1	10
2:B:533:PHE:N	2:B:533:PHE:CD1	0.54	2.74	5	5
2:B:407:TYR:CD1	2:B:407:TYR:C	0.54	2.85	6	6
3:C:635:GLY:O	3:C:667:HIS:NE2	0.54	2.40	3	8
1:A:67:ILE:CD1	1:A:68:GLU:N	0.54	2.69	5	4
2:B:422:TRP:O	2:B:422:TRP:CD1	0.54	2.61	8	4
2:B:415:GLY:HA3	2:B:436:LYS:CD	0.54	2.33	5	1
1:A:201:ASP:OD1	2:B:493:LEU:CD2	0.54	2.55	10	1
3:C:654:LEU:H	3:C:654:LEU:CD2	0.54	2.13	4	5
1:A:159:GLU:OE2	1:A:161:HIS:ND1	0.54	2.41	9	6
2:B:459:LYS:HB2	2:B:464:THR:O	0.54	2.03	4	6
2:B:409:ASP:OD2	3:C:604:LYS:NZ	0.54	2.39	4	1
1:A:134:ASP:C	1:A:135:HIS:CD2	0.54	2.85	7	1
3:C:699:PRO:HB2	3:C:702:LEU:HD13	0.54	1.79	8	1
1:A:186:ALA:O	1:A:215:SER:C	0.54	2.51	9	10
1:A:260:ARG:O	2:B:411:TYR:CE1	0.54	2.61	8	9
1:A:70:TYR:CE1	1:A:92:ASN:ND2	0.54	2.76	5	4
3:C:678:GLU:OE1	3:C:680:HIS:ND1	0.54	2.40	9	1
1:A:55:ALA:HB1	1:A:59:MET:HE2	0.54	1.79	1	1
1:A:278:LYS:C	1:A:280:GLY:H	0.54	2.11	5	10
2:B:498:GLU:N	2:B:498:GLU:CD	0.54	2.65	2	4
1:A:255:PHE:CE1	2:B:529:ASN:OD1	0.54	2.61	2	1
1:A:271:TRP:CE2	2:B:514:GLY:HA3	0.54	2.37	2	1
1:A:266:ARG:C	1:A:267:THR:OG1	0.54	2.50	6	2
3:C:642:ALA:C	3:C:651:LEU:HD12	0.54	2.28	2	8
1:A:232:ILE:O	1:A:236:GLU:HG2	0.54	2.03	3	1
1:A:217:GLN:N	1:A:217:GLN:CD	0.54	2.66	4	2
2:B:566:LEU:N	2:B:566:LEU:CD2	0.54	2.71	7	1
1:A:246:ASN:O	1:A:250:MET:SD	0.54	2.65	8	2
1:A:68:GLU:OE1	1:A:69:GLY:N	0.54	2.40	4	7
1:A:75:LEU:HD12	1:A:75:LEU:N	0.54	2.18	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ARG:O	1:A:123:ALA:N	0.54	2.41	6	10
1:A:169:TRP:CB	1:A:198:TYR:CD2	0.54	2.91	1	2
1:A:179:PHE:CE2	1:A:228:PHE:CZ	0.54	2.95	1	1
1:A:259:ARG:NH2	2:B:407:TYR:OH	0.54	2.41	1	1
3:C:627:ASP:O	3:C:630:ARG:NE	0.54	2.41	1	1
3:C:662:ASN:OD1	3:C:663:ALA:N	0.54	2.41	2	6
1:A:28:GLU:OE1	2:B:315:ARG:NH1	0.54	2.41	3	3
3:C:639:LEU:HD23	3:C:671:PRO:HG3	0.54	1.80	6	1
1:A:111:GLU:O	1:A:111:GLU:HG3	0.54	2.01	7	1
1:A:240:GLN:HA	1:A:243:ILE:HD12	0.54	1.79	7	1
2:B:444:ILE:HG23	2:B:479:THR:OG1	0.54	2.03	9	1
1:A:76:ILE:HG23	1:A:87:PHE:CE2	0.54	2.37	1	1
3:C:612:ASN:HD22	3:C:612:ASN:N	0.54	2.00	3	1
2:B:443:LYS:CD	2:B:443:LYS:H	0.54	2.16	4	1
3:C:664:PRO:O	3:C:697:LYS:NZ	0.54	2.40	5	1
1:A:73:GLN:OE1	1:A:140:PHE:CZ	0.54	2.61	9	1
1:A:187:GLN:C	1:A:214:ASP:O	0.54	2.51	8	10
2:B:547:ASP:OD1	2:B:548:ALA:N	0.54	2.41	1	2
3:C:658:GLY:O	3:C:659:ALA:HB2	0.54	2.03	7	10
3:C:692:ALA:O	3:C:693:ASP:C	0.54	2.51	5	10
1:A:61:GLN:CD	1:A:172:ARG:NH2	0.54	2.66	6	3
1:A:73:GLN:OE1	1:A:73:GLN:N	0.54	2.41	4	1
1:A:86:ARG:CG	1:A:86:ARG:NH1	0.54	2.70	7	5
1:A:28:GLU:OE2	2:B:315:ARG:NE	0.54	2.40	9	1
1:A:99:ASP:O	1:A:102:ARG:O	0.53	2.26	3	10
1:A:177:TRP:CD2	1:A:190:ALA:HB2	0.53	2.38	7	8
3:C:615:LEU:O	3:C:615:LEU:CD1	0.53	2.51	8	7
1:A:251:SER:OG	2:B:533:PHE:CG	0.53	2.60	2	1
2:B:452:HIS:NE2	2:B:521:GLU:OE2	0.53	2.41	4	1
1:A:148:ILE:HG22	1:A:149:ASP:OD2	0.53	2.04	8	3
2:B:435:LYS:O	2:B:436:LYS:HD3	0.53	2.03	5	1
2:B:466:HIS:ND1	2:B:500:ASP:OD1	0.53	2.41	6	3
2:B:478:GLN:HG3	2:B:479:THR:N	0.53	2.18	5	1
1:A:99:ASP:OD2	1:A:102:ARG:NE	0.53	2.41	6	1
1:A:167:ASN:OD1	1:A:169:TRP:NE1	0.53	2.41	7	1
2:B:372:ARG:NH2	2:B:420:TYR:OH	0.53	2.40	7	1
2:B:472:THR:HG23	2:B:494:THR:HG22	0.53	1.79	7	1
2:B:418:SER:OG	2:B:420:TYR:CZ	0.53	2.59	9	1
1:A:152:GLN:O	1:A:181:ILE:CG2	0.53	2.57	10	1
1:A:246:ASN:OD1	2:B:481:LYS:NZ	0.53	2.40	6	1
3:C:633:GLU:OE1	3:C:634:GLY:N	0.53	2.42	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:TYR:N	1:A:155:ILE:O	0.53	2.41	6	10
1:A:237:ASN:HD21	2:B:546:ILE:CD1	0.53	2.17	1	1
1:A:278:LYS:C	1:A:280:GLY:N	0.53	2.67	10	10
2:B:425:ASP:OD1	2:B:426:HIS:N	0.53	2.42	10	2
3:C:715:ALA:C	3:C:716:LEU:HD12	0.53	2.29	1	1
1:A:33:PHE:CZ	1:A:46:LEU:HD21	0.53	2.39	2	9
2:B:466:HIS:CG	2:B:500:ASP:OD1	0.53	2.61	6	4
1:A:252:ASP:C	1:A:253:THR:HG1	0.53	2.04	4	1
1:A:55:ALA:O	1:A:56:GLN:C	0.53	2.52	9	10
1:A:152:GLN:HB2	1:A:181:ILE:HG13	0.53	1.80	1	1
1:A:184:PRO:O	1:A:185:THR:CB	0.53	2.57	6	10
2:B:373:SER:O	2:B:377:ASN:HA	0.53	2.04	3	10
3:C:672:LEU:C	3:C:672:LEU:CD2	0.53	2.82	4	2
1:A:70:TYR:CE2	1:A:92:ASN:OD1	0.53	2.62	8	4
1:A:91:ARG:CG	1:A:91:ARG:NH1	0.53	2.69	4	1
3:C:604:LYS:NZ	3:C:607:MET:CE	0.53	2.72	5	1
1:A:274:ILE:CD1	2:B:403:ALA:HB1	0.53	2.31	7	1
1:A:73:GLN:OE1	1:A:140:PHE:CE1	0.53	2.61	9	1
2:B:442:LYS:NZ	3:C:644:ASP:CG	0.53	2.67	9	1
1:A:237:ASN:HD21	2:B:546:ILE:HD12	0.53	1.64	1	1
2:B:340:LEU:O	2:B:363:ASP:HB3	0.53	2.03	10	6
2:B:350:ALA:HB3	2:B:359:TYR:CZ	0.53	2.38	9	10
3:C:695:THR:CG2	3:C:703:THR:OG1	0.53	2.57	1	1
3:C:700:ASP:CG	3:C:701:GLY:H	0.53	2.10	3	7
1:A:273:LYS:O	1:A:273:LYS:HG3	0.53	2.04	7	3
3:C:610:LEU:HD12	3:C:610:LEU:H	0.53	1.63	5	3
1:A:152:GLN:H	1:A:181:ILE:HG21	0.53	1.63	2	7
1:A:70:TYR:CE2	1:A:94:ILE:HD13	0.53	2.39	8	4
1:A:188:VAL:CG1	1:A:189:ALA:H	0.53	2.16	7	6
3:C:646:GLY:O	3:C:650:ILE:HD13	0.53	2.03	5	1
1:A:27:GLY:C	1:A:28:GLU:OE1	0.53	2.52	10	2
1:A:41:ASN:O	1:A:42:ASN:CG	0.53	2.51	7	7
1:A:209:HIS:CE1	2:B:486:THR:OG1	0.53	2.62	2	6
2:B:372:ARG:HG3	2:B:372:ARG:HH11	0.53	1.63	1	1
1:A:126:SER:O	1:A:129:ARG:HB3	0.53	2.04	10	4
2:B:473:VAL:O	2:B:492:SER:OG	0.53	2.23	10	3
1:A:169:TRP:CD1	2:B:535:LYS:NZ	0.53	2.76	3	2
2:B:319:GLN:NE2	2:B:488:ASN:CG	0.53	2.67	3	2
3:C:716:LEU:O	3:C:717:LEU:HD23	0.53	2.03	9	3
3:C:667:HIS:O	3:C:668:HIS:CG	0.53	2.62	6	1
1:A:259:ARG:NH2	2:B:521:GLU:OE2	0.53	2.42	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:GLY:CA	1:A:159:GLU:O	0.53	2.57	5	10
2:B:569:ARG:CG	2:B:569:ARG:NH1	0.53	2.68	1	3
1:A:194:ILE:HD13	1:A:195:GLN:H	0.53	1.60	2	1
1:A:86:ARG:NH2	1:A:107:ASP:OD2	0.53	2.40	3	1
1:A:220:SER:O	1:A:224:THR:HG23	0.53	2.04	7	5
3:C:655:LEU:C	3:C:655:LEU:CD2	0.53	2.78	3	2
1:A:253:THR:CG2	3:C:636:ARG:HH21	0.53	2.17	4	1
1:A:260:ARG:NH1	3:C:633:GLU:OE2	0.53	2.42	4	1
1:A:10:ASP:OD1	1:A:11:GLU:N	0.53	2.41	1	2
1:A:121:ARG:NH1	1:A:122:ASP:OD1	0.53	2.42	6	4
1:A:54:PHE:CD1	1:A:54:PHE:N	0.53	2.74	4	1
1:A:67:ILE:HD12	1:A:67:ILE:N	0.53	2.19	9	1
1:A:169:TRP:CD2	1:A:169:TRP:C	0.53	2.87	9	10
1:A:203:ASN:ND2	2:B:314:ARG:O	0.53	2.41	1	1
1:A:213:GLN:CD	1:A:213:GLN:N	0.53	2.67	1	1
3:C:603:ASP:OD1	3:C:604:LYS:N	0.53	2.42	2	1
1:A:92:ASN:OD1	1:A:94:ILE:CD1	0.53	2.57	6	4
3:C:693:ASP:OD2	3:C:695:THR:N	0.53	2.42	10	1
1:A:70:TYR:CZ	1:A:92:ASN:CG	0.52	2.87	8	4
1:A:164:GLN:OE1	1:A:167:ASN:ND2	0.52	2.42	3	1
3:C:668:HIS:O	3:C:668:HIS:ND1	0.52	2.43	3	1
1:A:72:ASP:O	1:A:91:ARG:NH2	0.52	2.41	5	1
2:B:434:ILE:HG23	2:B:436:LYS:HZ3	0.52	1.63	5	1
3:C:654:LEU:C	3:C:654:LEU:CD2	0.52	2.77	6	1
2:B:439:ASP:OD1	2:B:441:SER:OG	0.52	2.26	8	1
2:B:450:SER:OG	2:B:452:HIS:NE2	0.52	2.43	1	2
2:B:475:LEU:HD23	2:B:532:TYR:CD2	0.52	2.40	2	5
2:B:478:GLN:NE2	2:B:488:ASN:CG	0.52	2.67	5	1
1:A:182:THR:HG23	1:A:182:THR:O	0.52	2.03	7	1
1:A:173:TRP:CZ3	2:B:544:ARG:CZ	0.52	2.92	9	1
1:A:203:ASN:C	1:A:203:ASN:ND2	0.52	2.67	9	1
2:B:458:GLU:OE2	2:B:509:HIS:NE2	0.52	2.42	9	1
1:A:73:GLN:N	1:A:73:GLN:CD	0.52	2.67	1	1
1:A:237:ASN:ND2	2:B:546:ILE:CD1	0.52	2.73	1	1
2:B:350:ALA:CB	2:B:359:TYR:CE2	0.52	2.92	1	2
3:C:625:GLY:O	3:C:626:GLU:C	0.52	2.53	6	10
1:A:168:PHE:O	1:A:169:TRP:CB	0.52	2.55	8	8
3:C:680:HIS:O	3:C:681:VAL:CG2	0.52	2.57	7	5
2:B:525:ARG:CG	2:B:525:ARG:NH1	0.52	2.72	9	5
3:C:621:TYR:CE2	3:C:627:ASP:CG	0.52	2.88	2	1
3:C:686:LEU:N	3:C:686:LEU:CD2	0.52	2.72	5	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:478:GLN:OE1	2:B:488:ASN:CG	0.52	2.52	9	1
1:A:71:ASP:O	1:A:73:GLN:NE2	0.52	2.43	1	1
1:A:199:TYR:CD1	1:A:199:TYR:C	0.52	2.88	10	6
1:A:92:ASN:O	1:A:92:ASN:ND2	0.52	2.43	3	1
1:A:91:ARG:CZ	1:A:141:CYS:O	0.52	2.58	6	1
1:A:187:GLN:N	1:A:187:GLN:OE1	0.52	2.42	5	1
1:A:271:TRP:CZ2	2:B:514:GLY:CA	0.52	2.93	7	2
1:A:172:ARG:NH1	1:A:174:ARG:CZ	0.52	2.72	10	1
1:A:61:GLN:CD	1:A:174:ARG:NH2	0.52	2.67	1	2
2:B:442:LYS:NZ	3:C:677:TYR:O	0.52	2.42	1	1
2:B:478:GLN:CD	2:B:479:THR:N	0.52	2.68	1	2
3:C:615:LEU:C	3:C:615:LEU:CD1	0.52	2.82	2	7
1:A:93:LYS:CE	1:A:121:ARG:HH12	0.52	2.17	4	1
1:A:93:LYS:CE	1:A:121:ARG:HH22	0.52	2.17	4	1
1:A:86:ARG:HH11	1:A:86:ARG:HG2	0.52	1.63	7	3
3:C:674:SER:O	3:C:678:GLU:CG	0.52	2.58	6	2
1:A:99:ASP:OD2	1:A:102:ARG:NH2	0.52	2.42	6	1
1:A:195:GLN:HE21	1:A:205:GLN:NE2	0.52	2.03	9	1
1:A:232:ILE:CG1	1:A:233:GLU:N	0.52	2.72	9	1
1:A:95:SER:O	1:A:108:PRO:C	0.52	2.53	5	10
1:A:167:ASN:O	1:A:168:PHE:HB2	0.52	2.05	1	6
1:A:186:ALA:HB3	1:A:217:GLN:N	0.52	2.18	8	10
1:A:273:LYS:C	1:A:274:ILE:HD12	0.52	2.29	1	1
3:C:647:GLN:O	3:C:648:LEU:HB2	0.52	2.05	6	8
1:A:248:GLN:O	1:A:252:ASP:CG	0.52	2.53	2	2
2:B:491:GLY:O	2:B:492:SER:HB2	0.52	2.05	2	3
2:B:449:ASP:OD2	2:B:476:TRP:NE1	0.52	2.42	3	2
2:B:362:CYS:H	2:B:365:ASN:ND2	0.52	2.02	4	1
2:B:478:GLN:NE2	2:B:488:ASN:OD1	0.52	2.43	4	1
1:A:221:ASP:N	1:A:221:ASP:OD1	0.52	2.43	7	2
3:C:640:HIS:CE1	3:C:674:SER:OG	0.52	2.63	6	1
3:C:718:GLN:OXT	3:C:718:GLN:NE2	0.52	2.43	10	1
1:A:161:HIS:O	1:A:162:GLN:NE2	0.52	2.43	8	10
2:B:309:ALA:HB1	2:B:328:LEU:HD21	0.52	1.82	3	10
3:C:614:ASP:C	3:C:616:ASP:N	0.52	2.68	6	10
3:C:693:ASP:N	3:C:693:ASP:OD1	0.52	2.42	5	2
2:B:366:ARG:NH1	2:B:371:TYR:OH	0.52	2.43	7	1
1:A:259:ARG:HH22	2:B:521:GLU:CA	0.52	2.18	8	1
2:B:439:ASP:OD2	2:B:441:SER:OG	0.52	2.27	8	1
1:A:70:TYR:CD2	1:A:94:ILE:CD1	0.52	2.93	9	1
1:A:74:VAL:CG2	1:A:75:LEU:N	0.51	2.73	7	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:ARG:NH2	1:A:145:GLY:H	0.51	2.03	2	1
1:A:254:THR:OG1	2:B:444:ILE:CD1	0.51	2.59	2	1
2:B:487:MET:C	2:B:488:ASN:HD22	0.51	2.13	7	2
1:A:28:GLU:OE2	2:B:315:ARG:NH2	0.51	2.43	1	1
2:B:535:LYS:O	2:B:536:THR:C	0.51	2.53	8	10
3:C:601:MET:N	3:C:601:MET:SD	0.51	2.84	1	5
3:C:715:ALA:O	3:C:716:LEU:HG	0.51	2.05	1	1
3:C:607:MET:CE	3:C:633:GLU:OE2	0.51	2.58	5	2
3:C:671:PRO:O	3:C:674:SER:OG	0.51	2.27	7	5
3:C:677:TYR:O	3:C:677:TYR:HD1	0.51	1.89	2	1
1:A:82:LEU:HD13	1:A:82:LEU:O	0.51	2.05	3	1
1:A:259:ARG:HH22	2:B:521:GLU:C	0.51	2.13	8	1
2:B:463:ARG:CG	2:B:463:ARG:NH1	0.51	2.68	9	1
1:A:279:ILE:O	1:A:279:ILE:CG2	0.51	2.58	1	5
3:C:686:LEU:N	3:C:686:LEU:HD22	0.51	2.20	5	2
3:C:604:LYS:HZ1	3:C:607:MET:HE2	0.51	1.65	5	1
1:A:260:ARG:CG	2:B:411:TYR:O	0.51	2.59	9	2
2:B:407:TYR:O	2:B:411:TYR:CD1	0.51	2.64	10	1
1:A:173:TRP:CD1	1:A:174:ARG:N	0.51	2.79	5	8
2:B:478:GLN:NE2	2:B:479:THR:C	0.51	2.69	1	1
3:C:651:LEU:CD2	3:C:652:GLU:N	0.51	2.71	9	8
2:B:570:GLN:CD	2:B:570:GLN:N	0.51	2.66	2	1
1:A:149:ASP:O	1:A:149:ASP:OD2	0.51	2.28	3	1
2:B:365:ASN:ND2	2:B:365:ASN:C	0.51	2.68	4	1
2:B:408:ARG:NE	2:B:414:GLY:O	0.51	2.43	6	2
3:C:688:LEU:CD1	3:C:691:GLY:O	0.51	2.58	7	1
1:A:173:TRP:CH2	2:B:544:ARG:NH1	0.51	2.79	9	1
1:A:253:THR:HG22	1:A:254:THR:N	0.51	2.21	5	8
2:B:372:ARG:HH11	2:B:372:ARG:CG	0.51	2.18	1	1
1:A:62:PHE:CD1	1:A:62:PHE:N	0.51	2.78	8	6
1:A:237:ASN:O	1:A:241:THR:HG23	0.51	2.04	5	2
1:A:61:GLN:NE2	1:A:174:ARG:HH21	0.51	2.03	1	2
2:B:362:CYS:SG	2:B:365:ASN:CG	0.51	2.93	10	8
3:C:625:GLY:O	3:C:626:GLU:O	0.51	2.29	2	10
3:C:717:LEU:CG	3:C:718:GLN:N	0.51	2.73	1	2
1:A:275:LEU:O	1:A:276:SER:HB2	0.51	2.05	2	2
2:B:496:GLN:NE2	2:B:496:GLN:H	0.51	2.03	2	1
3:C:621:TYR:CE2	3:C:627:ASP:OD2	0.51	2.63	2	1
1:A:94:ILE:C	1:A:111:GLU:OE1	0.51	2.53	7	1
3:C:618:VAL:CG1	3:C:654:LEU:HD21	0.51	2.36	10	1
1:A:96:PHE:HA	1:A:108:PRO:HA	0.51	1.83	7	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:674:SER:HA	3:C:677:TYR:CE2	0.51	2.40	2	1
1:A:129:ARG:CD	1:A:129:ARG:C	0.51	2.83	3	3
1:A:226:LYS:HG3	1:A:227:GLU:N	0.51	2.20	6	1
1:A:279:ILE:N	1:A:279:ILE:CD1	0.51	2.73	1	1
2:B:493:LEU:N	2:B:493:LEU:CD2	0.51	2.73	2	1
3:C:633:GLU:OE1	3:C:636:ARG:NH2	0.51	2.44	3	1
2:B:498:GLU:N	2:B:498:GLU:OE1	0.51	2.44	10	1
1:A:90:PRO:CG	1:A:143:VAL:O	0.51	2.59	5	8
2:B:372:ARG:HB2	2:B:379:TYR:CZ	0.51	2.41	9	6
1:A:220:SER:O	1:A:224:THR:CG2	0.51	2.59	7	5
2:B:439:ASP:O	2:B:442:LYS:CG	0.51	2.59	3	1
1:A:167:ASN:OD1	1:A:169:TRP:CD1	0.51	2.64	7	1
2:B:372:ARG:NH1	2:B:372:ARG:CG	0.50	2.73	1	1
2:B:533:PHE:CD1	2:B:533:PHE:N	0.50	2.77	10	3
1:A:196:VAL:O	1:A:205:GLN:CG	0.50	2.60	4	4
3:C:655:LEU:HD23	3:C:656:LEU:N	0.50	2.20	3	2
3:C:703:THR:OG1	3:C:704:ALA:N	0.50	2.42	9	4
1:A:240:GLN:NE2	2:B:546:ILE:HD11	0.50	2.21	4	1
1:A:136:TYR:OH	1:A:173:TRP:NE1	0.50	2.44	10	4
2:B:364:TYR:O	2:B:420:TYR:CE2	0.50	2.64	7	1
1:A:59:MET:SD	1:A:59:MET:C	0.50	2.93	9	1
1:A:236:GLU:OE1	1:A:236:GLU:C	0.50	2.53	9	1
2:B:470:THR:O	2:B:470:THR:CG2	0.50	2.59	10	1
2:B:439:ASP:OD1	3:C:611:LYS:NZ	0.50	2.41	1	1
3:C:630:ARG:HH11	3:C:630:ARG:CB	0.50	2.19	1	1
1:A:173:TRP:CD1	1:A:173:TRP:C	0.50	2.90	6	8
1:A:181:ILE:HD12	1:A:181:ILE:C	0.50	2.32	10	1
1:A:237:ASN:ND2	2:B:546:ILE:HD12	0.50	2.22	1	1
2:B:550:PRO:O	2:B:552:ASN:ND2	0.50	2.44	1	1
3:C:645:CYS:SG	3:C:645:CYS:O	0.50	2.70	1	4
1:A:134:ASP:O	1:A:135:HIS:CD2	0.50	2.64	7	2
3:C:693:ASP:CG	3:C:694:LYS:H	0.50	2.14	10	2
3:C:644:ASP:O	3:C:645:CYS:SG	0.50	2.69	10	2
1:A:121:ARG:HD2	1:A:122:ASP:N	0.50	2.21	9	4
2:B:496:GLN:CD	2:B:496:GLN:N	0.50	2.70	9	1
1:A:274:ILE:N	1:A:274:ILE:CD1	0.50	2.74	1	1
2:B:380:ASP:CB	2:B:381:PRO:CD	0.50	2.90	2	10
2:B:439:ASP:CG	3:C:611:LYS:NZ	0.50	2.67	1	1
1:A:246:ASN:HD21	2:B:484:SER:CB	0.50	2.19	8	2
1:A:195:GLN:NE2	1:A:205:GLN:OE1	0.50	2.45	7	1
3:C:645:CYS:O	3:C:645:CYS:SG	0.50	2.69	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:GLN:O	1:A:61:GLN:NE2	0.50	2.44	10	1
2:B:352:ASP:N	2:B:357:LYS:O	0.50	2.45	2	10
1:A:70:TYR:O	1:A:72:ASP:OD1	0.50	2.29	3	1
2:B:372:ARG:NH2	2:B:397:GLU:OE1	0.50	2.41	8	2
2:B:363:ASP:OD1	2:B:364:TYR:CE1	0.50	2.65	7	1
2:B:388:MET:SD	2:B:388:MET:C	0.50	2.95	7	1
2:B:472:THR:HG22	2:B:472:THR:O	0.50	2.06	7	1
1:A:169:TRP:O	1:A:169:TRP:CG	0.50	2.65	2	10
2:B:462:GLY:C	2:B:464:THR:H	0.50	2.15	8	10
1:A:121:ARG:C	1:A:125:ASP:OD1	0.50	2.54	2	1
1:A:251:SER:OG	2:B:533:PHE:CB	0.50	2.60	2	1
1:A:31:GLU:CD	1:A:31:GLU:H	0.50	2.15	8	4
3:C:607:MET:SD	3:C:607:MET:C	0.50	2.95	4	1
3:C:668:HIS:CG	3:C:668:HIS:O	0.50	2.61	8	1
2:B:484:SER:O	2:B:485:GLY:C	0.50	2.55	8	10
3:C:644:ASP:OD2	3:C:678:GLU:OE2	0.50	2.29	5	2
3:C:614:ASP:O	3:C:617:GLU:N	0.50	2.41	3	10
1:A:200:GLU:O	1:A:201:ASP:HB3	0.50	2.04	2	3
1:A:272:ASN:H	1:A:272:ASN:HD22	0.50	1.50	2	1
3:C:637:LYS:CD	3:C:637:LYS:H	0.50	2.19	6	3
1:A:99:ASP:O	1:A:100:HIS:C	0.50	2.55	3	10
3:C:646:GLY:O	3:C:648:LEU:N	0.50	2.45	6	10
2:B:525:ARG:HH11	2:B:525:ARG:HG2	0.50	1.67	7	4
1:A:173:TRP:CH2	1:A:236:GLU:OE1	0.50	2.65	3	1
3:C:702:LEU:HG	3:C:703:THR:N	0.50	2.21	7	2
1:A:67:ILE:N	1:A:67:ILE:CD1	0.50	2.75	9	1
1:A:59:MET:SD	1:A:77:THR:HA	0.50	2.47	10	1
1:A:54:PHE:CG	1:A:100:HIS:CB	0.49	2.95	8	6
3:C:636:ARG:NH1	3:C:641:TYR:OH	0.49	2.45	5	1
1:A:65:VAL:CG2	1:A:66:LYS:N	0.49	2.75	1	9
2:B:379:TYR:CE1	2:B:386:GLY:HA3	0.49	2.41	1	1
1:A:90:PRO:HG2	1:A:143:VAL:O	0.49	2.08	9	2
2:B:464:THR:O	2:B:464:THR:HG23	0.49	2.06	3	3
1:A:201:ASP:OD2	2:B:493:LEU:HD11	0.49	2.07	10	1
3:C:692:ALA:C	3:C:693:ASP:OD1	0.49	2.55	10	1
2:B:315:ARG:HG2	2:B:315:ARG:HH11	0.49	1.67	1	8
2:B:393:LEU:N	2:B:393:LEU:CD2	0.49	2.76	7	4
3:C:716:LEU:O	3:C:717:LEU:CD1	0.49	2.61	8	3
1:A:259:ARG:CZ	2:B:448:TRP:CH2	0.49	2.95	7	1
1:A:104:GLU:OE1	1:A:104:GLU:N	0.49	2.45	8	1
2:B:407:TYR:CE2	2:B:411:TYR:CZ	0.49	3.00	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:654:LEU:O	3:C:654:LEU:CD2	0.49	2.50	6	1
3:C:610:LEU:HD21	3:C:618:VAL:HG11	0.49	1.84	8	1
1:A:237:ASN:C	1:A:237:ASN:HD22	0.49	2.13	3	1
3:C:708:THR:HG22	3:C:709:ASP:H	0.49	1.67	8	4
2:B:406:GLN:O	2:B:410:LEU:HD13	0.49	2.08	4	1
1:A:259:ARG:NH1	2:B:448:TRP:CH2	0.49	2.81	7	1
1:A:31:GLU:OE1	2:B:315:ARG:NH2	0.49	2.44	10	2
2:B:372:ARG:CZ	2:B:372:ARG:CB	0.49	2.88	1	1
2:B:478:GLN:CG	2:B:488:ASN:ND2	0.49	2.76	1	1
1:A:8:VAL:O	1:A:8:VAL:CG1	0.49	2.59	4	8
3:C:614:ASP:OD1	3:C:616:ASP:CG	0.49	2.56	3	1
3:C:704:ALA:HB3	3:C:717:LEU:HD23	0.49	1.82	3	1
3:C:673:LEU:HD21	3:C:703:THR:HA	0.49	1.83	9	1
2:B:469:LEU:HG	2:B:470:THR:N	0.49	2.22	5	6
2:B:442:LYS:NZ	2:B:442:LYS:CB	0.49	2.76	3	1
3:C:668:HIS:O	3:C:668:HIS:CG	0.49	2.65	3	1
2:B:311:ASP:OD1	2:B:315:ARG:NH1	0.49	2.46	4	1
2:B:406:GLN:N	2:B:406:GLN:OE1	0.49	2.45	4	1
3:C:636:ARG:NH2	3:C:640:HIS:CD2	0.49	2.80	10	2
1:A:195:GLN:HE21	1:A:205:GLN:HE21	0.49	1.51	9	1
2:B:442:LYS:NZ	3:C:644:ASP:OD1	0.49	2.46	9	1
2:B:569:ARG:O	2:B:570:GLN:CG	0.49	2.61	9	1
3:C:653:PHE:CD2	3:C:654:LEU:N	0.49	2.80	9	1
1:A:177:TRP:HA	1:A:190:ALA:HB2	0.49	1.85	3	10
2:B:309:ALA:O	2:B:313:MET:SD	0.49	2.71	2	1
2:B:313:MET:SD	2:B:328:LEU:HD22	0.49	2.47	2	1
1:A:230:LYS:O	1:A:234:ASN:ND2	0.49	2.45	8	1
1:A:201:ASP:OD1	1:A:201:ASP:O	0.49	2.31	4	3
1:A:205:GLN:OE1	1:A:207:VAL:CG2	0.49	2.61	9	2
2:B:525:ARG:C	2:B:525:ARG:CD	0.49	2.85	8	1
3:C:615:LEU:HD22	3:C:618:VAL:CG1	0.48	2.38	4	5
1:A:119:GLN:CD	1:A:119:GLN:H	0.48	2.15	2	1
1:A:217:GLN:CD	1:A:217:GLN:H	0.48	2.16	4	2
1:A:252:ASP:C	1:A:253:THR:OG1	0.48	2.56	4	1
3:C:644:ASP:CG	3:C:678:GLU:OE1	0.48	2.56	5	1
1:A:67:ILE:CD1	1:A:94:ILE:HD11	0.48	2.38	7	1
3:C:688:LEU:HD13	3:C:693:ASP:O	0.48	2.08	7	1
1:A:74:VAL:C	1:A:75:LEU:CD2	0.48	2.81	9	1
1:A:92:ASN:N	1:A:92:ASN:ND2	0.48	2.57	9	1
1:A:80:GLY:O	1:A:87:PHE:HA	0.48	2.08	4	10
1:A:118:LYS:HZ2	1:A:121:ARG:NH2	0.48	2.05	3	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:561:GLU:O	2:B:564:GLN:HG2	0.48	2.08	3	5
1:A:208:SER:HB2	2:B:487:MET:HE2	0.48	1.85	7	1
1:A:88:LEU:CD1	1:A:144:TYR:OH	0.48	2.62	10	1
1:A:70:TYR:O	1:A:71:ASP:OD1	0.48	2.31	1	1
1:A:80:GLY:O	1:A:88:LEU:N	0.48	2.47	1	10
1:A:255:PHE:CZ	2:B:529:ASN:ND2	0.48	2.81	2	1
2:B:469:LEU:CG	2:B:470:THR:N	0.48	2.77	5	6
1:A:269:ILE:CG2	1:A:270:ASP:N	0.48	2.75	6	3
2:B:405:ASP:O	2:B:408:ARG:NH1	0.48	2.46	5	1
2:B:439:ASP:OD2	2:B:442:LYS:NZ	0.48	2.44	5	1
2:B:478:GLN:OE1	2:B:487:MET:O	0.48	2.31	5	2
3:C:664:PRO:O	3:C:697:LYS:CE	0.48	2.62	5	1
2:B:365:ASN:HB3	2:B:420:TYR:CD2	0.48	2.43	9	1
3:C:618:VAL:HG11	3:C:654:LEU:HD11	0.48	1.85	10	1
1:A:91:ARG:NE	1:A:129:ARG:NH2	0.48	2.60	1	1
1:A:245:GLU:OE2	3:C:677:TYR:CE1	0.48	2.66	1	1
2:B:546:ILE:HG23	2:B:547:ASP:N	0.48	2.21	7	3
3:C:628:VAL:O	3:C:628:VAL:CG2	0.48	2.58	1	2
3:C:651:LEU:HD22	3:C:652:GLU:N	0.48	2.21	9	4
3:C:717:LEU:O	3:C:718:GLN:HB2	0.48	2.09	2	7
1:A:191:VAL:HG23	1:A:211:ASP:OD1	0.48	2.08	10	6
2:B:434:ILE:HG23	2:B:436:LYS:NZ	0.48	2.23	5	1
2:B:335:LEU:O	2:B:339:LEU:CG	0.48	2.62	1	10
2:B:462:GLY:C	2:B:464:THR:N	0.48	2.72	1	10
1:A:72:ASP:OD2	1:A:89:ASP:OD2	0.48	2.32	7	4
3:C:661:ILE:CD1	3:C:687:LEU:HD11	0.48	2.39	2	1
1:A:246:ASN:ND2	2:B:484:SER:OG	0.48	2.46	8	2
2:B:478:GLN:OE1	2:B:487:MET:C	0.48	2.57	5	1
2:B:442:LYS:NZ	3:C:645:CYS:SG	0.48	2.86	2	1
3:C:661:ILE:O	3:C:661:ILE:HG23	0.48	2.07	9	2
2:B:431:VAL:O	2:B:431:VAL:HG13	0.48	2.09	10	3
3:C:673:LEU:N	3:C:673:LEU:HD12	0.48	2.23	7	3
1:A:233:GLU:O	1:A:236:GLU:HG3	0.48	2.08	9	1
2:B:442:LYS:HZ3	3:C:678:GLU:HG2	0.48	1.69	9	1
1:A:262:LEU:O	1:A:262:LEU:CD1	0.48	2.62	10	1
2:B:407:TYR:CD2	2:B:411:TYR:CE1	0.48	3.01	10	1
1:A:54:PHE:CG	1:A:100:HIS:HB2	0.48	2.44	8	6
2:B:481:LYS:O	2:B:485:GLY:CA	0.48	2.62	3	10
2:B:563:SER:O	2:B:564:GLN:C	0.48	2.56	9	10
2:B:408:ARG:O	2:B:412:PHE:HB2	0.48	2.09	8	5
2:B:554:LYS:HG3	2:B:555:TYR:H	0.48	1.69	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ARG:NH2	1:A:130:ALA:HB2	0.48	2.23	3	3
1:A:237:ASN:OD1	2:B:546:ILE:CD1	0.48	2.62	3	1
2:B:304:GLN:CD	2:B:304:GLN:H	0.48	2.17	4	1
2:B:443:LYS:CD	2:B:443:LYS:N	0.48	2.77	4	1
1:A:92:ASN:ND2	1:A:92:ASN:O	0.48	2.46	8	3
2:B:418:SER:CB	2:B:420:TYR:OH	0.48	2.62	9	1
2:B:352:ASP:O	2:B:353:LYS:C	0.48	2.57	3	10
3:C:614:ASP:O	3:C:616:ASP:N	0.48	2.47	1	10
1:A:125:ASP:OD1	1:A:143:VAL:HG11	0.48	2.09	2	1
2:B:401:ASN:O	2:B:405:ASP:CG	0.48	2.56	6	5
2:B:409:ASP:OD1	2:B:409:ASP:O	0.48	2.32	6	2
2:B:434:ILE:HB	2:B:450:SER:OG	0.48	2.09	8	2
3:C:610:LEU:CD2	3:C:638:PRO:O	0.48	2.61	10	3
1:A:161:HIS:C	1:A:161:HIS:ND1	0.48	2.71	7	1
3:C:716:LEU:O	3:C:717:LEU:HD12	0.48	2.09	7	1
3:C:705:LEU:HD13	3:C:705:LEU:C	0.48	2.34	8	1
1:A:59:MET:HE3	1:A:87:PHE:CE1	0.48	2.44	1	1
2:B:366:ARG:CZ	2:B:371:TYR:OH	0.48	2.62	7	2
2:B:370:SER:CA	2:B:381:PRO:HG2	0.48	2.39	4	10
2:B:448:TRP:CZ2	2:B:473:VAL:HG11	0.48	2.44	9	2
1:A:101:LEU:N	1:A:101:LEU:CD2	0.48	2.76	7	1
2:B:478:GLN:CD	2:B:488:ASN:HD21	0.48	2.17	8	1
1:A:236:GLU:CD	1:A:237:ASN:N	0.48	2.71	9	1
2:B:364:TYR:CG	2:B:431:VAL:HG21	0.48	2.43	9	1
1:A:177:TRP:CE2	1:A:232:ILE:HG23	0.48	2.44	10	1
2:B:315:ARG:HH11	2:B:315:ARG:CG	0.48	2.22	1	2
2:B:420:TYR:O	2:B:430:GLY:HA2	0.48	2.09	6	10
2:B:491:GLY:O	2:B:492:SER:CB	0.48	2.62	3	10
2:B:448:TRP:CZ2	2:B:473:VAL:HG21	0.48	2.44	2	1
1:A:136:TYR:CE1	1:A:173:TRP:CD1	0.48	3.02	9	2
1:A:192:LEU:CD2	1:A:236:GLU:OE1	0.48	2.62	3	1
1:A:236:GLU:CG	1:A:237:ASN:N	0.48	2.77	9	1
2:B:518:GLU:CD	2:B:518:GLU:C	0.47	2.81	7	7
2:B:569:ARG:HH11	2:B:569:ARG:HG2	0.47	1.69	2	2
1:A:101:LEU:N	1:A:101:LEU:HD12	0.47	2.24	3	1
3:C:672:LEU:CD1	3:C:692:ALA:HB1	0.47	2.39	3	1
2:B:439:ASP:CG	2:B:441:SER:OG	0.47	2.57	8	1
1:A:164:GLN:CB	1:A:169:TRP:CZ2	0.47	2.97	1	2
1:A:263:PRO:O	1:A:264:VAL:C	0.47	2.57	3	10
3:C:625:GLY:C	3:C:626:GLU:CG	0.47	2.87	4	6
1:A:198:TYR:OH	1:A:200:GLU:OE1	0.47	2.32	10	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:672:LEU:CD1	3:C:684:VAL:HG13	0.47	2.40	5	1
2:B:442:LYS:CE	3:C:644:ASP:OD2	0.47	2.62	6	1
3:C:644:ASP:OD1	3:C:678:GLU:OE1	0.47	2.31	6	1
3:C:661:ILE:HG23	3:C:661:ILE:O	0.47	2.09	6	1
1:A:129:ARG:C	1:A:129:ARG:CD	0.47	2.86	7	1
2:B:388:MET:SD	2:B:388:MET:O	0.47	2.73	7	1
2:B:442:LYS:HZ2	3:C:644:ASP:HB3	0.47	1.67	2	1
1:A:117:LEU:CD1	1:A:146:LYS:C	0.47	2.87	1	1
3:C:639:LEU:HD23	3:C:639:LEU:O	0.47	2.09	5	4
1:A:89:ASP:OD1	1:A:89:ASP:C	0.47	2.56	7	5
3:C:661:ILE:O	3:C:662:ASN:CG	0.47	2.57	5	2
2:B:459:LYS:NZ	2:B:461:SER:O	0.47	2.41	6	1
1:A:59:MET:C	1:A:61:GLN:H	0.47	2.18	3	10
1:A:275:LEU:O	1:A:276:SER:HB3	0.47	2.10	5	6
1:A:121:ARG:O	1:A:125:ASP:OD1	0.47	2.31	2	1
3:C:627:ASP:OD1	3:C:627:ASP:O	0.47	2.32	2	3
1:A:197:HIS:CE1	1:A:199:TYR:CD1	0.47	3.03	8	4
2:B:372:ARG:HH22	2:B:397:GLU:CD	0.47	2.17	3	2
1:A:192:LEU:HD22	1:A:236:GLU:OE1	0.47	2.09	4	1
1:A:273:LYS:O	1:A:273:LYS:CG	0.47	2.61	5	2
3:C:713:ILE:O	3:C:716:LEU:CD2	0.47	2.63	5	1
1:A:77:THR:OG1	1:A:78:GLU:N	0.47	2.48	7	1
1:A:129:ARG:C	1:A:129:ARG:HE	0.47	2.16	7	1
3:C:654:LEU:C	3:C:654:LEU:HD12	0.47	2.35	9	1
3:C:680:HIS:C	3:C:681:VAL:HG22	0.47	2.34	7	5
1:A:70:TYR:CZ	1:A:92:ASN:ND2	0.47	2.83	8	4
3:C:615:LEU:HD22	3:C:618:VAL:HG23	0.47	1.85	8	1
1:A:121:ARG:CG	1:A:125:ASP:OD2	0.47	2.62	2	1
1:A:247:TYR:O	1:A:251:SER:OG	0.47	2.19	2	1
3:C:665:ASP:OD1	3:C:665:ASP:N	0.47	2.47	9	3
3:C:674:SER:HA	3:C:677:TYR:CZ	0.47	2.44	2	1
1:A:31:GLU:H	1:A:31:GLU:CD	0.47	2.17	4	1
1:A:273:LYS:NZ	1:A:277:TYR:CD2	0.47	2.83	5	1
3:C:713:ILE:O	3:C:716:LEU:HD21	0.47	2.10	5	1
1:A:89:ASP:CB	1:A:94:ILE:HD13	0.47	2.40	7	1
1:A:101:LEU:N	1:A:101:LEU:HD22	0.47	2.22	7	1
3:C:705:LEU:C	3:C:705:LEU:CD1	0.47	2.88	8	1
1:A:79:HIS:O	1:A:144:TYR:CZ	0.47	2.67	10	1
3:C:648:LEU:CD2	3:C:682:SER:OG	0.47	2.63	10	1
1:A:161:HIS:HB2	1:A:171:GLY:O	0.47	2.09	4	10
2:B:315:ARG:CG	2:B:315:ARG:NH1	0.47	2.76	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:705:LEU:C	3:C:705:LEU:CD2	0.47	2.87	1	4
3:C:717:LEU:HD23	3:C:718:GLN:N	0.47	2.24	1	2
1:A:201:ASP:CG	2:B:494:THR:O	0.47	2.58	7	3
1:A:265:THR:O	1:A:265:THR:HG22	0.47	2.10	10	2
1:A:272:ASN:ND2	2:B:506:SER:O	0.47	2.48	4	1
2:B:489:LEU:C	2:B:489:LEU:CD2	0.47	2.87	5	1
3:C:705:LEU:CD1	3:C:705:LEU:C	0.47	2.87	5	1
3:C:705:LEU:C	3:C:705:LEU:HD13	0.47	2.34	5	1
1:A:252:ASP:O	1:A:252:ASP:CG	0.47	2.57	6	1
3:C:644:ASP:CG	3:C:678:GLU:OE2	0.47	2.58	6	2
2:B:449:ASP:OD1	2:B:474:MET:O	0.47	2.33	8	1
1:A:75:LEU:N	1:A:75:LEU:CD1	0.47	2.78	2	2
2:B:362:CYS:O	2:B:365:ASN:OD1	0.47	2.32	2	8
2:B:422:TRP:CZ2	2:B:429:ALA:CB	0.47	2.97	4	3
1:A:221:ASP:OD1	1:A:221:ASP:N	0.47	2.45	3	3
3:C:713:ILE:CG2	3:C:714:LYS:N	0.47	2.78	3	1
2:B:489:LEU:C	2:B:489:LEU:HD23	0.47	2.34	5	1
1:A:172:ARG:C	1:A:172:ARG:HE	0.47	2.18	9	1
1:A:260:ARG:O	2:B:411:TYR:CD1	0.47	2.68	8	8
3:C:638:PRO:O	3:C:654:LEU:CD1	0.47	2.62	4	2
1:A:91:ARG:CD	1:A:91:ARG:C	0.47	2.88	7	1
2:B:563:SER:O	2:B:566:LEU:N	0.46	2.48	5	10
3:C:685:LYS:C	3:C:687:LEU:H	0.46	2.19	1	10
3:C:687:LEU:C	3:C:689:SER:N	0.46	2.73	2	10
3:C:654:LEU:HD13	3:C:654:LEU:N	0.46	2.23	6	2
2:B:358:ASP:OD1	2:B:358:ASP:O	0.46	2.33	4	2
1:A:256:LYS:HZ1	3:C:636:ARG:HE	0.46	1.53	2	1
1:A:187:GLN:N	1:A:187:GLN:CD	0.46	2.73	10	3
3:C:607:MET:SD	3:C:633:GLU:OE2	0.46	2.74	7	2
2:B:408:ARG:CD	2:B:414:GLY:O	0.46	2.63	8	1
1:A:120:TRP:HB2	1:A:154:ILE:HD11	0.46	1.86	9	1
1:A:133:LYS:O	1:A:133:LYS:CG	0.46	2.63	1	1
1:A:275:LEU:C	1:A:276:SER:OG	0.46	2.58	8	6
2:B:508:PRO:O	2:B:512:ASN:ND2	0.46	2.48	1	1
3:C:711:GLN:C	3:C:711:GLN:CD	0.46	2.84	5	1
1:A:31:GLU:CD	2:B:315:ARG:HH21	0.46	2.19	10	2
1:A:70:TYR:CE2	1:A:94:ILE:CD1	0.46	2.98	9	1
3:C:627:ASP:O	3:C:627:ASP:CG	0.46	2.58	10	1
2:B:434:ILE:HB	2:B:450:SER:CB	0.46	2.41	8	3
3:C:644:ASP:CG	3:C:678:GLU:CD	0.46	2.82	6	2
1:A:136:TYR:OH	1:A:173:TRP:CD1	0.46	2.68	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:TRP:CD2	1:A:232:ILE:HG12	0.46	2.46	10	1
1:A:200:GLU:O	1:A:201:ASP:OD1	0.46	2.29	10	1
1:A:87:PHE:HB2	1:A:96:PHE:CZ	0.46	2.46	5	9
2:B:304:GLN:CD	2:B:304:GLN:N	0.46	2.74	4	1
1:A:274:ILE:HD12	1:A:274:ILE:C	0.46	2.35	7	1
1:A:95:SER:CB	1:A:109:GLN:O	0.46	2.63	5	10
1:A:169:TRP:CA	1:A:197:HIS:O	0.46	2.62	5	10
1:A:194:ILE:CG2	1:A:208:SER:HB3	0.46	2.41	1	1
2:B:478:GLN:CG	2:B:479:THR:N	0.46	2.79	9	4
2:B:557:GLN:O	2:B:557:GLN:CD	0.46	2.59	6	5
1:A:107:ASP:OD1	1:A:107:ASP:C	0.46	2.59	6	2
2:B:463:ARG:HH11	2:B:463:ARG:HG2	0.46	1.70	9	1
1:A:85:GLY:O	1:A:98:PHE:CE1	0.46	2.68	1	1
1:A:118:LYS:O	1:A:119:GLN:C	0.46	2.59	4	10
2:B:471:SER:C	2:B:472:THR:HG22	0.46	2.35	4	3
2:B:569:ARG:O	2:B:570:GLN:CD	0.46	2.58	2	1
3:C:609:ALA:HB3	3:C:618:VAL:HG13	0.46	1.87	5	3
2:B:479:THR:HG23	2:B:479:THR:O	0.46	2.11	4	2
1:A:117:LEU:O	1:A:117:LEU:CG	0.46	2.60	9	1
1:A:28:GLU:OE2	1:A:170:ASN:OD1	0.46	2.34	10	1
3:C:693:ASP:OD1	3:C:696:VAL:HG22	0.46	2.10	10	1
2:B:425:ASP:OD1	2:B:425:ASP:N	0.46	2.47	1	1
3:C:661:ILE:O	3:C:661:ILE:HG13	0.46	2.11	1	3
1:A:121:ARG:CG	1:A:125:ASP:OD1	0.46	2.63	2	1
2:B:525:ARG:HG3	2:B:526:SER:N	0.46	2.25	2	5
2:B:487:MET:O	2:B:487:MET:CG	0.46	2.63	3	1
1:A:252:ASP:O	1:A:252:ASP:OD1	0.46	2.34	4	2
1:A:266:ARG:CG	1:A:266:ARG:O	0.46	2.62	5	1
1:A:259:ARG:NH2	2:B:521:GLU:HB3	0.46	2.25	7	1
2:B:458:GLU:OE1	2:B:459:LYS:N	0.46	2.48	10	1
1:A:233:GLU:C	1:A:233:GLU:CD	0.46	2.83	2	2
1:A:133:LYS:O	1:A:134:ASP:OD1	0.46	2.34	4	9
1:A:153:THR:HG23	1:A:179:PHE:O	0.46	2.10	4	3
2:B:402:ASN:O	2:B:406:GLN:NE2	0.46	2.49	4	1
1:A:247:TYR:OH	2:B:489:LEU:HD11	0.46	2.10	5	1
1:A:26:PRO:O	1:A:28:GLU:OE1	0.46	2.34	7	1
1:A:259:ARG:HH22	2:B:521:GLU:CB	0.46	2.23	8	1
2:B:365:ASN:CB	2:B:420:TYR:CD2	0.46	2.99	9	1
1:A:68:GLU:C	1:A:68:GLU:CD	0.46	2.84	7	7
2:B:484:SER:O	2:B:486:THR:N	0.46	2.49	6	10
1:A:159:GLU:CD	1:A:159:GLU:C	0.46	2.84	7	8

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:PRO:O	1:A:185:THR:HB	0.46	2.11	2	1
2:B:380:ASP:OD1	2:B:380:ASP:C	0.46	2.57	3	5
2:B:529:ASN:C	2:B:529:ASN:ND2	0.46	2.74	3	1
3:C:609:ALA:CB	3:C:618:VAL:HG13	0.46	2.40	5	3
1:A:179:PHE:CD1	1:A:228:PHE:CE1	0.46	3.04	4	1
1:A:206:LEU:C	1:A:206:LEU:CD2	0.46	2.87	9	2
2:B:434:ILE:HG23	2:B:436:LYS:CE	0.46	2.41	5	1
3:C:621:TYR:CZ	3:C:622:VAL:HB	0.46	2.46	8	2
3:C:700:ASP:OD2	3:C:701:GLY:N	0.46	2.49	5	1
1:A:57:TYR:O	1:A:60:ASP:OD1	0.46	2.32	6	1
3:C:687:LEU:HD23	3:C:687:LEU:C	0.46	2.35	8	1
2:B:431:VAL:O	2:B:431:VAL:CG1	0.46	2.64	10	1
1:A:91:ARG:HE	1:A:129:ARG:NH2	0.45	2.08	1	1
2:B:353:LYS:O	2:B:354:VAL:C	0.45	2.59	6	10
2:B:379:TYR:CZ	2:B:386:GLY:CA	0.45	2.96	1	1
1:A:56:GLN:O	1:A:60:ASP:OD2	0.45	2.34	3	3
1:A:206:LEU:HD12	2:B:488:ASN:O	0.45	2.11	3	2
3:C:661:ILE:CD1	3:C:692:ALA:HB2	0.45	2.41	6	3
1:A:59:MET:SD	1:A:60:ASP:OD1	0.45	2.74	9	1
1:A:203:ASN:C	1:A:203:ASN:HD22	0.45	2.19	9	1
1:A:45:LEU:CD1	1:A:45:LEU:N	0.45	2.79	9	3
2:B:350:ALA:HB3	2:B:359:TYR:CE2	0.45	2.46	2	6
1:A:198:TYR:CZ	1:A:200:GLU:HB3	0.45	2.45	2	2
3:C:640:HIS:ND1	3:C:674:SER:OG	0.45	2.46	6	1
1:A:207:VAL:HG21	2:B:319:GLN:NE2	0.45	2.26	7	2
2:B:546:ILE:CG2	2:B:547:ASP:N	0.45	2.79	7	1
1:A:13:LYS:NZ	1:A:13:LYS:CB	0.45	2.80	9	1
2:B:513:ILE:O	2:B:517:VAL:HG23	0.45	2.12	10	1
1:A:267:THR:O	1:A:267:THR:HG23	0.45	2.11	3	6
3:C:699:PRO:O	3:C:700:ASP:OD2	0.45	2.34	2	2
1:A:256:LYS:HZ1	3:C:636:ARG:NE	0.45	2.07	2	1
2:B:397:GLU:C	2:B:397:GLU:CD	0.45	2.84	2	1
1:A:269:ILE:HG22	1:A:270:ASP:N	0.45	2.26	5	3
2:B:564:GLN:OE1	2:B:564:GLN:O	0.45	2.35	9	1
1:A:144:TYR:CE2	1:A:146:LYS:HB2	0.45	2.46	10	1
2:B:405:ASP:OD2	2:B:408:ARG:NH2	0.45	2.47	10	1
1:A:80:GLY:O	1:A:87:PHE:CA	0.45	2.65	8	10
2:B:350:ALA:O	2:B:358:ASP:CA	0.45	2.64	2	10
3:C:662:ASN:O	3:C:663:ALA:C	0.45	2.59	2	10
1:A:221:ASP:CG	1:A:222:VAL:H	0.45	2.19	6	5
1:A:136:TYR:CE1	2:B:544:ARG:HB2	0.45	2.46	7	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:654:LEU:N	3:C:654:LEU:HD23	0.45	2.27	5	1
2:B:408:ARG:NE	2:B:415:GLY:O	0.45	2.48	6	1
2:B:442:LYS:HZ3	3:C:644:ASP:CG	0.45	2.20	9	1
2:B:404:PHE:CZ	2:B:432:ILE:HD13	0.45	2.47	10	1
1:A:45:LEU:N	1:A:45:LEU:HD12	0.45	2.27	9	6
1:A:112:ASP:OD1	1:A:112:ASP:O	0.45	2.35	10	6
1:A:113:THR:OG1	1:A:118:LYS:CE	0.45	2.64	1	1
3:C:715:ALA:O	3:C:716:LEU:CG	0.45	2.65	1	1
1:A:71:ASP:OD1	1:A:71:ASP:N	0.45	2.50	2	1
2:B:552:ASN:O	2:B:552:ASN:OD1	0.45	2.35	10	4
3:C:643:ALA:HB2	3:C:651:LEU:CD1	0.45	2.41	3	1
2:B:393:LEU:N	2:B:393:LEU:HD22	0.45	2.26	7	1
2:B:441:SER:OG	3:C:678:GLU:OE2	0.45	2.33	8	1
1:A:167:ASN:O	1:A:167:ASN:OD1	0.45	2.35	10	2
2:B:409:ASP:OD1	3:C:604:LYS:NZ	0.45	2.49	9	1
1:A:107:ASP:N	1:A:108:PRO:CD	0.45	2.79	4	10
1:A:194:ILE:CD1	1:A:195:GLN:N	0.45	2.79	2	1
2:B:319:GLN:NE2	2:B:488:ASN:OD1	0.45	2.49	3	2
1:A:88:LEU:HD23	1:A:89:ASP:N	0.45	2.23	5	1
1:A:260:ARG:HB2	2:B:411:TYR:O	0.45	2.12	2	1
2:B:489:LEU:O	2:B:489:LEU:HG	0.45	2.11	9	5
3:C:616:ASP:N	3:C:616:ASP:OD1	0.45	2.45	3	1
2:B:315:ARG:NH1	2:B:315:ARG:CG	0.45	2.79	9	2
2:B:337:GLU:C	2:B:337:GLU:CD	0.45	2.85	4	1
3:C:628:VAL:O	3:C:660:ASP:OD2	0.45	2.35	5	1
1:A:30:ASN:CG	1:A:31:GLU:N	0.45	2.75	7	1
1:A:152:GLN:O	1:A:180:THR:C	0.45	2.60	4	10
1:A:249:THR:O	1:A:253:THR:HB	0.45	2.12	8	9
1:A:269:ILE:CG1	1:A:270:ASP:N	0.45	2.79	10	4
2:B:348:LYS:O	2:B:361:LEU:HD12	0.45	2.11	1	1
1:A:75:LEU:HD21	1:A:140:PHE:HB2	0.45	1.88	10	5
1:A:82:LEU:C	1:A:82:LEU:CD1	0.45	2.90	3	1
1:A:129:ARG:HH11	1:A:129:ARG:HG2	0.45	1.72	8	3
2:B:472:THR:HG23	2:B:494:THR:OG1	0.45	2.12	5	6
3:C:630:ARG:HH11	3:C:630:ARG:HG2	0.45	1.71	4	1
2:B:412:PHE:CG	2:B:436:LYS:CE	0.45	3.00	5	1
3:C:662:ASN:O	3:C:697:LYS:NZ	0.45	2.47	5	1
1:A:274:ILE:O	1:A:274:ILE:CD1	0.45	2.56	7	1
3:C:638:PRO:O	3:C:654:LEU:HD22	0.45	2.12	9	1
1:A:240:GLN:CB	2:B:544:ARG:NH2	0.45	2.80	10	1
3:C:644:ASP:OD2	3:C:678:GLU:OE1	0.45	2.35	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASP:O	1:A:174:ARG:NH1	0.45	2.49	2	1
2:B:547:ASP:OD1	2:B:547:ASP:O	0.45	2.35	2	1
1:A:153:THR:HG1	1:A:180:THR:HA	0.45	1.70	3	1
3:C:644:ASP:OD1	3:C:678:GLU:OE2	0.45	2.35	4	2
1:A:237:ASN:OD1	2:B:544:ARG:NH2	0.45	2.50	8	4
1:A:41:ASN:O	1:A:42:ASN:ND2	0.45	2.50	7	1
1:A:72:ASP:CG	1:A:92:ASN:OD1	0.45	2.60	7	1
2:B:370:SER:CB	2:B:381:PRO:HD2	0.45	2.31	7	1
2:B:478:GLN:C	2:B:479:THR:HG22	0.45	2.36	8	1
1:A:232:ILE:HG13	1:A:233:GLU:N	0.45	2.26	9	1
1:A:259:ARG:CD	2:B:448:TRP:CH2	0.45	3.00	9	1
1:A:180:THR:O	1:A:181:ILE:CG2	0.45	2.65	10	1
1:A:75:LEU:HD11	1:A:140:PHE:CB	0.45	2.42	1	2
1:A:130:ALA:HA	1:A:133:LYS:HG2	0.45	1.88	1	1
1:A:270:ASP:O	1:A:272:ASN:N	0.45	2.50	5	10
1:A:278:LYS:O	1:A:280:GLY:N	0.45	2.50	6	10
1:A:54:PHE:HB3	1:A:100:HIS:CB	0.45	2.42	7	3
3:C:654:LEU:N	3:C:654:LEU:HD12	0.45	2.27	3	1
2:B:535:LYS:CD	2:B:535:LYS:N	0.45	2.80	4	1
1:A:92:ASN:HD22	1:A:92:ASN:H	0.45	1.52	9	1
3:C:678:GLU:CD	3:C:678:GLU:C	0.45	2.84	9	1
3:C:633:GLU:C	3:C:633:GLU:CD	0.45	2.85	10	1
2:B:556:LYS:CD	2:B:556:LYS:N	0.44	2.80	1	1
1:A:119:GLN:OE1	1:A:119:GLN:N	0.44	2.47	2	1
2:B:561:GLU:C	2:B:561:GLU:CD	0.44	2.85	2	1
1:A:221:ASP:CG	1:A:222:VAL:N	0.44	2.75	3	5
3:C:610:LEU:HG	3:C:618:VAL:HG11	0.44	1.88	5	1
2:B:564:GLN:HE21	2:B:568:GLN:NE2	0.44	2.09	7	1
1:A:74:VAL:CG2	1:A:75:LEU:H	0.44	2.25	4	9
1:A:169:TRP:HB3	1:A:198:TYR:CD2	0.44	2.47	1	2
2:B:370:SER:CB	2:B:381:PRO:HG2	0.44	2.42	4	6
2:B:500:ASP:OD1	2:B:500:ASP:O	0.44	2.35	4	6
1:A:164:GLN:OE1	1:A:164:GLN:C	0.44	2.60	3	1
3:C:626:GLU:O	3:C:627:ASP:OD1	0.44	2.34	3	3
1:A:41:ASN:O	1:A:42:ASN:OD1	0.44	2.35	9	3
1:A:117:LEU:HD13	1:A:152:GLN:HB3	0.44	1.90	8	2
2:B:372:ARG:CZ	2:B:377:ASN:OD1	0.44	2.65	5	2
3:C:626:GLU:O	3:C:626:GLU:OE1	0.44	2.34	6	1
3:C:716:LEU:O	3:C:717:LEU:CD2	0.44	2.65	9	2
1:A:251:SER:O	1:A:256:LYS:NZ	0.44	2.51	10	1
1:A:254:THR:O	1:A:257:ALA:HB3	0.44	2.13	1	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:478:GLN:CD	2:B:478:GLN:C	0.44	2.85	1	1
1:A:121:ARG:CG	1:A:125:ASP:CG	0.44	2.90	2	1
1:A:192:LEU:HD21	1:A:236:GLU:OE1	0.44	2.11	2	1
2:B:367:ASP:OD1	2:B:367:ASP:C	0.44	2.60	5	3
2:B:469:LEU:CD1	2:B:470:THR:H	0.44	2.25	6	4
1:A:86:ARG:N	1:A:86:ARG:CD	0.44	2.77	4	2
3:C:620:ASP:C	3:C:620:ASP:OD1	0.44	2.60	7	2
1:A:71:ASP:O	1:A:71:ASP:OD1	0.44	2.36	8	2
1:A:259:ARG:HH22	2:B:521:GLU:CG	0.44	2.25	7	1
2:B:322:GLU:OE2	2:B:345:GLN:CD	0.44	2.61	7	1
3:C:647:GLN:O	3:C:649:GLU:CD	0.44	2.60	7	1
1:A:161:HIS:ND1	1:A:161:HIS:N	0.44	2.66	9	1
1:A:107:ASP:N	1:A:107:ASP:OD1	0.44	2.48	10	1
1:A:76:ILE:CG2	1:A:87:PHE:CE2	0.44	3.01	1	1
1:A:273:LYS:CA	1:A:277:TYR:HB2	0.44	2.43	5	10
3:C:630:ARG:CD	3:C:630:ARG:N	0.44	2.81	1	1
3:C:685:LYS:C	3:C:687:LEU:N	0.44	2.76	10	10
1:A:117:LEU:HD22	1:A:152:GLN:HB3	0.44	1.89	7	5
1:A:164:GLN:C	1:A:164:GLN:OE1	0.44	2.61	6	5
3:C:718:GLN:OE1	3:C:718:GLN:OXT	0.44	2.35	2	2
2:B:452:HIS:CD2	2:B:452:HIS:N	0.44	2.84	4	2
1:A:209:HIS:O	1:A:209:HIS:ND1	0.44	2.50	5	1
3:C:621:TYR:OH	3:C:628:VAL:CG2	0.44	2.56	8	2
3:C:708:THR:O	3:C:709:ASP:OD1	0.44	2.35	8	2
1:A:28:GLU:OE2	2:B:315:ARG:NH1	0.44	2.50	8	1
1:A:61:GLN:C	1:A:63:THR:N	0.44	2.76	5	10
1:A:247:TYR:HH	2:B:536:THR:CB	0.44	2.25	1	1
2:B:522:ASN:O	2:B:525:ARG:HG3	0.44	2.12	7	3
1:A:106:SER:O	1:A:107:ASP:CG	0.44	2.59	3	2
1:A:191:VAL:CG2	1:A:211:ASP:OD1	0.44	2.66	3	5
2:B:434:ILE:HB	2:B:450:SER:HB3	0.44	1.90	4	1
2:B:412:PHE:CG	2:B:436:LYS:HE2	0.44	2.48	5	1
3:C:621:TYR:CD1	3:C:622:VAL:CA	0.44	3.01	5	2
3:C:694:LYS:O	3:C:695:THR:HG23	0.44	2.13	6	1
1:A:27:GLY:C	1:A:28:GLU:CD	0.44	2.85	7	2
3:C:711:GLN:CD	3:C:711:GLN:N	0.44	2.75	10	1
1:A:95:SER:O	1:A:108:PRO:CB	0.44	2.66	5	10
1:A:177:TRP:HA	1:A:190:ALA:CB	0.44	2.43	9	10
1:A:240:GLN:CD	1:A:240:GLN:C	0.44	2.86	4	4
2:B:457:GLN:O	2:B:458:GLU:C	0.44	2.61	3	10
1:A:131:TYR:O	1:A:135:HIS:ND1	0.44	2.47	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:ASP:OD2	2:B:494:THR:O	0.44	2.35	7	3
1:A:129:ARG:CZ	1:A:130:ALA:HB2	0.44	2.42	3	3
1:A:273:LYS:NZ	1:A:277:TYR:CE2	0.44	2.83	5	1
2:B:370:SER:CB	2:B:381:PRO:CG	0.44	2.95	4	10
2:B:554:LYS:O	2:B:558:LEU:N	0.44	2.49	6	8
1:A:167:ASN:N	1:A:167:ASN:HD22	0.44	2.11	3	1
1:A:212:ILE:N	1:A:212:ILE:HD12	0.44	2.28	3	1
1:A:233:GLU:CD	1:A:233:GLU:C	0.44	2.86	3	1
2:B:319:GLN:C	2:B:320:GLN:OE1	0.44	2.61	3	2
3:C:647:GLN:C	3:C:648:LEU:CG	0.44	2.91	3	1
1:A:240:GLN:HE21	2:B:546:ILE:CD1	0.44	2.26	4	1
3:C:661:ILE:HD11	3:C:672:LEU:HD23	0.44	1.90	5	1
2:B:365:ASN:OD1	2:B:365:ASN:C	0.44	2.61	7	3
2:B:380:ASP:OD1	2:B:381:PRO:CD	0.44	2.65	7	1
1:A:211:ASP:OD1	1:A:211:ASP:O	0.44	2.35	1	3
2:B:519:ASP:OD1	2:B:519:ASP:O	0.44	2.35	10	5
3:C:688:LEU:HD12	3:C:693:ASP:O	0.44	2.13	8	2
1:A:45:LEU:N	1:A:45:LEU:CD1	0.44	2.81	7	3
1:A:111:GLU:C	1:A:111:GLU:CD	0.44	2.85	4	3
3:C:650:ILE:CG2	3:C:654:LEU:HD21	0.44	2.43	4	1
3:C:667:HIS:C	3:C:668:HIS:CG	0.44	2.96	6	1
1:A:117:LEU:CD1	1:A:120:TRP:CD1	0.44	3.00	9	1
1:A:133:LYS:O	1:A:133:LYS:HD2	0.44	2.13	1	1
1:A:169:TRP:C	1:A:170:ASN:OD1	0.44	2.61	1	1
1:A:188:VAL:O	1:A:189:ALA:CB	0.44	2.66	10	9
2:B:302:SER:O	2:B:305:GLN:N	0.44	2.51	5	10
2:B:478:GLN:NE2	2:B:479:THR:N	0.44	2.66	1	1
3:C:667:HIS:O	3:C:668:HIS:C	0.44	2.61	6	10
1:A:272:ASN:OD1	2:B:506:SER:O	0.44	2.36	2	2
2:B:528:LEU:CD1	2:B:532:TYR:CE1	0.44	3.00	2	1
2:B:554:LYS:O	2:B:558:LEU:HD13	0.44	2.12	3	2
3:C:717:LEU:O	3:C:718:GLN:HB3	0.44	2.12	3	1
1:A:56:GLN:O	1:A:60:ASP:OD1	0.44	2.36	6	1
2:B:303:ASP:C	2:B:303:ASP:OD1	0.44	2.61	6	1
2:B:408:ARG:NH2	2:B:415:GLY:O	0.44	2.49	6	1
1:A:124:CYS:O	1:A:125:ASP:C	0.43	2.61	4	10
1:A:176:GLU:O	1:A:190:ALA:CB	0.43	2.66	8	10
1:A:246:ASN:CB	2:B:487:MET:HE3	0.43	2.43	3	1
1:A:233:GLU:O	1:A:237:ASN:CG	0.43	2.61	4	2
1:A:153:THR:OG1	1:A:179:PHE:C	0.43	2.61	10	5
3:C:668:HIS:O	3:C:668:HIS:CD2	0.43	2.71	8	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:ASP:OD1	1:A:60:ASP:O	0.43	2.36	10	1
1:A:91:ARG:NH2	1:A:129:ARG:NH2	0.43	2.66	10	1
3:C:654:LEU:N	3:C:654:LEU:HD13	0.43	2.27	1	2
1:A:121:ARG:HG2	1:A:125:ASP:CG	0.43	2.38	2	1
1:A:169:TRP:CZ3	2:B:539:ILE:HG23	0.43	2.48	10	3
1:A:233:GLU:OE1	1:A:234:ASN:OD1	0.43	2.36	3	1
2:B:501:GLU:OE2	2:B:512:ASN:OD1	0.43	2.36	8	3
3:C:648:LEU:CD1	3:C:682:SER:OG	0.43	2.56	3	1
1:A:131:TYR:OH	1:A:236:GLU:OE1	0.43	2.34	8	2
2:B:464:THR:HG23	2:B:464:THR:O	0.43	2.13	7	1
2:B:553:GLN:CD	2:B:553:GLN:N	0.43	2.75	10	1
1:A:47:ARG:O	1:A:48:GLU:C	0.43	2.62	3	10
1:A:90:PRO:HG3	1:A:143:VAL:O	0.43	2.14	1	7
2:B:397:GLU:O	2:B:401:ASN:ND2	0.43	2.52	8	2
1:A:86:ARG:HH12	1:A:109:GLN:NE2	0.43	2.10	2	1
1:A:121:ARG:HH21	1:A:145:GLY:CA	0.43	2.26	2	1
3:C:627:ASP:OD1	3:C:627:ASP:C	0.43	2.60	10	4
2:B:364:TYR:CE1	2:B:422:TRP:CZ2	0.43	3.06	8	2
2:B:441:SER:O	3:C:677:TYR:CD1	0.43	2.71	4	1
2:B:401:ASN:O	2:B:405:ASP:OD2	0.43	2.36	5	1
3:C:604:LYS:HG3	3:C:607:MET:HE2	0.43	1.90	8	1
1:A:59:MET:SD	1:A:60:ASP:CG	0.43	3.01	9	1
1:A:78:GLU:O	1:A:78:GLU:CD	0.43	2.61	10	1
2:B:458:GLU:OE1	2:B:459:LYS:O	0.43	2.37	10	1
3:C:654:LEU:H	3:C:654:LEU:CD1	0.43	2.19	10	1
2:B:372:ARG:CZ	2:B:387:ALA:O	0.43	2.65	1	1
1:A:82:LEU:HD13	1:A:82:LEU:C	0.43	2.38	3	1
1:A:259:ARG:NH2	2:B:411:TYR:CD2	0.43	2.86	3	1
2:B:366:ARG:CD	2:B:371:TYR:CZ	0.43	3.02	3	3
2:B:551:ASP:O	2:B:551:ASP:OD1	0.43	2.37	7	2
1:A:274:ILE:CD1	2:B:403:ALA:CB	0.43	2.96	7	1
1:A:104:GLU:N	1:A:104:GLU:CD	0.43	2.76	8	1
2:B:408:ARG:HH12	2:B:417:SER:N	0.43	2.11	9	2
1:A:200:GLU:C	1:A:201:ASP:OD1	0.43	2.61	10	1
2:B:408:ARG:HG2	2:B:409:ASP:N	0.43	2.28	2	2
3:C:671:PRO:O	3:C:674:SER:HB2	0.43	2.13	3	2
3:C:713:ILE:HD13	3:C:713:ILE:O	0.43	2.12	3	1
1:A:237:ASN:ND2	2:B:544:ARG:NH2	0.43	2.65	4	1
2:B:434:ILE:O	2:B:434:ILE:HG22	0.43	2.12	5	1
3:C:664:PRO:O	3:C:697:LYS:CD	0.43	2.67	5	1
1:A:172:ARG:HH11	1:A:174:ARG:CD	0.43	2.26	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:446:GLY:C	2:B:447:CYS:SG	0.43	3.01	10	1
1:A:73:GLN:N	1:A:73:GLN:OE1	0.43	2.52	1	1
3:C:607:MET:SD	3:C:641:TYR:CE2	0.43	3.11	3	1
2:B:517:VAL:O	2:B:521:GLU:OE1	0.43	2.36	4	1
3:C:647:GLN:O	3:C:649:GLU:OE1	0.43	2.36	7	1
2:B:350:ALA:HB1	2:B:359:TYR:CE1	0.43	2.48	9	1
1:A:12:GLU:O	1:A:16:ILE:HG12	0.43	2.13	1	1
1:A:174:ARG:C	1:A:175:SER:OG	0.43	2.62	1	3
2:B:335:LEU:O	2:B:339:LEU:HG	0.43	2.14	10	6
2:B:350:ALA:HB3	2:B:359:TYR:CE1	0.43	2.47	9	2
2:B:401:ASN:OD1	2:B:401:ASN:O	0.43	2.37	2	1
2:B:362:CYS:SG	2:B:365:ASN:ND2	0.43	2.92	4	1
1:A:111:GLU:O	1:A:111:GLU:OE1	0.43	2.37	9	2
3:C:687:LEU:C	3:C:687:LEU:CD2	0.43	2.91	8	1
1:A:197:HIS:ND1	1:A:205:GLN:CD	0.43	2.77	10	1
3:C:693:ASP:OD2	3:C:696:VAL:HG13	0.43	2.13	10	1
1:A:271:TRP:C	1:A:273:LYS:N	0.43	2.77	7	7
2:B:302:SER:O	2:B:305:GLN:HB2	0.43	2.14	1	10
1:A:106:SER:C	1:A:107:ASP:CG	0.43	2.86	2	2
3:C:648:LEU:HD22	3:C:682:SER:CB	0.43	2.44	3	1
3:C:704:ALA:HB3	3:C:717:LEU:CD2	0.43	2.43	3	1
2:B:407:TYR:O	2:B:407:TYR:CG	0.43	2.72	6	2
3:C:644:ASP:OD2	3:C:678:GLU:CD	0.43	2.62	5	1
2:B:408:ARG:CG	2:B:408:ARG:NH1	0.43	2.81	6	1
1:A:243:ILE:HG12	2:B:487:MET:CE	0.43	2.44	7	1
3:C:692:ALA:O	3:C:693:ASP:OD1	0.43	2.37	10	1
1:A:134:ASP:O	2:B:548:ALA:HA	0.43	2.14	10	10
2:B:478:GLN:NE2	2:B:479:THR:CA	0.43	2.82	1	1
1:A:16:ILE:HD12	2:B:327:ASP:CG	0.43	2.39	2	2
2:B:475:LEU:HD23	2:B:476:TRP:H	0.43	1.72	4	3
3:C:667:HIS:O	3:C:669:ILE:HG22	0.43	2.13	7	3
1:A:136:TYR:CD1	1:A:160:SER:CB	0.43	3.02	10	2
2:B:522:ASN:OD1	2:B:522:ASN:C	0.43	2.61	7	1
3:C:648:LEU:O	3:C:648:LEU:CG	0.43	2.65	8	1
1:A:78:GLU:CD	1:A:78:GLU:C	0.43	2.86	10	1
1:A:168:PHE:CG	1:A:199:TYR:O	0.43	2.72	9	5
1:A:191:VAL:HG13	1:A:191:VAL:O	0.43	2.14	2	8
2:B:519:ASP:OD1	2:B:519:ASP:C	0.43	2.62	10	5
3:C:662:ASN:C	3:C:662:ASN:OD1	0.43	2.62	2	1
3:C:672:LEU:HD23	3:C:672:LEU:O	0.43	2.14	4	2
1:A:175:SER:O	1:A:175:SER:OG	0.43	2.37	4	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:628:VAL:O	3:C:660:ASP:OD1	0.43	2.36	5	1
1:A:223:GLN:O	1:A:226:LYS:HG3	0.43	2.14	6	1
1:A:79:HIS:CE1	1:A:155:ILE:HD13	0.43	2.48	7	1
1:A:274:ILE:HD11	2:B:403:ALA:CB	0.43	2.39	7	1
2:B:352:ASP:OD1	2:B:359:TYR:CE1	0.43	2.72	8	1
1:A:59:MET:CG	1:A:60:ASP:N	0.43	2.70	10	1
3:C:620:ASP:OD1	3:C:620:ASP:C	0.42	2.62	10	2
1:A:161:HIS:NE2	1:A:163:PHE:CE2	0.42	2.87	3	4
2:B:372:ARG:HB2	2:B:379:TYR:CE2	0.42	2.49	5	3
2:B:538:ASP:OD1	2:B:538:ASP:C	0.42	2.62	3	2
2:B:422:TRP:HE1	2:B:429:ALA:HB3	0.42	1.69	8	1
3:C:647:GLN:O	3:C:648:LEU:CG	0.42	2.66	8	1
1:A:61:GLN:OE1	1:A:63:THR:OG1	0.42	2.37	10	1
3:C:619:LYS:O	3:C:623:ALA:HB2	0.42	2.14	6	10
1:A:259:ARG:HD2	2:B:448:TRP:CH2	0.42	2.49	4	2
3:C:673:LEU:N	3:C:673:LEU:CD1	0.42	2.82	5	3
2:B:409:ASP:O	2:B:409:ASP:CG	0.42	2.62	6	1
1:A:28:GLU:OE1	1:A:28:GLU:N	0.42	2.52	7	1
2:B:436:LYS:HD2	2:B:437:ALA:N	0.42	2.29	8	1
2:B:475:LEU:HB3	2:B:532:TYR:CZ	0.42	2.49	9	1
1:A:146:LYS:HG2	1:A:147:SER:N	0.42	2.28	10	1
1:A:112:ASP:O	1:A:112:ASP:CG	0.42	2.63	9	5
3:C:630:ARG:HH11	3:C:630:ARG:HB2	0.42	1.74	1	1
1:A:206:LEU:HD22	1:A:247:TYR:OH	0.42	2.13	2	1
1:A:179:PHE:CD1	1:A:188:VAL:HG22	0.42	2.49	5	4
2:B:411:TYR:OH	2:B:522:ASN:ND2	0.42	2.51	3	2
3:C:701:GLY:O	3:C:705:LEU:HB2	0.42	2.14	3	4
1:A:91:ARG:HH11	1:A:91:ARG:HG2	0.42	1.73	4	2
1:A:227:GLU:O	1:A:231:ILE:CD1	0.42	2.67	4	1
1:A:169:TRP:O	1:A:170:ASN:OD1	0.42	2.37	7	1
3:C:705:LEU:HD23	3:C:717:LEU:HD23	0.42	1.92	8	1
3:C:700:ASP:OD1	3:C:700:ASP:C	0.42	2.62	9	1
3:C:683:CYS:O	3:C:684:VAL:C	0.42	2.63	7	10
2:B:401:ASN:OD1	2:B:401:ASN:C	0.42	2.61	2	2
3:C:665:ASP:OD1	3:C:666:LYS:N	0.42	2.51	9	3
2:B:495:ARG:O	2:B:520:MET:HE3	0.42	2.13	3	2
2:B:475:LEU:HD23	2:B:532:TYR:CE2	0.42	2.49	5	1
1:A:206:LEU:O	1:A:206:LEU:HG	0.42	2.13	6	1
1:A:15:ARG:NH2	1:A:18:ALA:CB	0.42	2.82	7	1
2:B:525:ARG:CD	2:B:525:ARG:C	0.42	2.92	9	2
1:A:259:ARG:NH2	2:B:521:GLU:O	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:A:260:ARG:HG2	2:B:411:TYR:O	0.42	2.14	9	1
2:B:404:PHE:CZ	2:B:432:ILE:CD1	0.42	3.03	10	1
1:A:227:GLU:O	1:A:231:ILE:HD13	0.42	2.14	4	2
2:B:433:LEU:C	2:B:434:ILE:CG1	0.42	2.93	6	6
3:C:702:LEU:O	3:C:704:ALA:N	0.42	2.53	9	10
1:A:70:TYR:C	1:A:71:ASP:OD1	0.42	2.62	2	2
1:A:86:ARG:HH22	1:A:108:PRO:C	0.42	2.23	2	1
1:A:117:LEU:HD21	1:A:154:ILE:HD13	0.42	1.92	2	1
1:A:117:LEU:HD21	1:A:154:ILE:CD1	0.42	2.44	2	1
1:A:177:TRP:CE3	1:A:190:ALA:HB2	0.42	2.49	7	5
3:C:615:LEU:HA	3:C:618:VAL:CG2	0.42	2.45	3	3
3:C:647:GLN:CD	3:C:647:GLN:O	0.42	2.62	3	1
3:C:665:ASP:OD1	3:C:665:ASP:C	0.42	2.62	5	2
1:A:95:SER:OG	1:A:109:GLN:O	0.42	2.31	9	1
3:C:700:ASP:OD1	3:C:701:GLY:N	0.42	2.53	9	1
1:A:38:LEU:CD1	2:B:308:CYS:SG	0.42	3.08	1	2
1:A:75:LEU:HD11	1:A:140:PHE:HB2	0.42	1.91	1	2
1:A:264:VAL:HG23	1:A:265:THR:N	0.42	2.30	5	6
2:B:423:ASP:OD1	2:B:423:ASP:C	0.42	2.63	1	1
2:B:431:VAL:HA	2:B:452:HIS:O	0.42	2.15	7	10
2:B:474:MET:HA	2:B:492:SER:HB2	0.42	1.92	2	3
1:A:269:ILE:HG23	1:A:270:ASP:N	0.42	2.29	6	2
3:C:672:LEU:HD11	3:C:692:ALA:HB1	0.42	1.90	3	1
1:A:253:THR:HG23	3:C:636:ARG:HH21	0.42	1.72	4	1
3:C:616:ASP:O	3:C:616:ASP:OD1	0.42	2.37	5	1
1:A:169:TRP:C	1:A:169:TRP:CE3	0.42	2.98	8	1
2:B:431:VAL:HG13	2:B:431:VAL:O	0.42	2.15	8	1
1:A:169:TRP:HB2	1:A:198:TYR:CD2	0.42	2.50	1	2
3:C:677:TYR:O	3:C:677:TYR:CD2	0.42	2.73	1	1
1:A:173:TRP:CZ2	1:A:236:GLU:OE1	0.42	2.73	3	1
2:B:557:GLN:CD	2:B:557:GLN:C	0.42	2.87	5	5
2:B:434:ILE:HG23	2:B:436:LYS:HE2	0.42	1.92	5	1
3:C:630:ARG:HG2	3:C:631:THR:N	0.42	2.29	6	1
1:A:198:TYR:OH	2:B:535:LYS:NZ	0.42	2.50	7	1
2:B:569:ARG:O	2:B:570:GLN:OE1	0.42	2.37	9	1
2:B:459:LYS:CB	2:B:464:THR:O	0.42	2.68	5	10
1:A:234:ASN:OD1	1:A:234:ASN:C	0.42	2.61	2	1
1:A:136:TYR:CE1	2:B:544:ARG:HB3	0.42	2.50	3	1
1:A:30:ASN:OD1	1:A:30:ASN:C	0.42	2.60	4	1
1:A:148:ILE:C	1:A:149:ASP:CG	0.42	2.87	6	3
2:B:466:HIS:CE1	2:B:500:ASP:OD2	0.42	2.73	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:TRP:CD1	1:A:177:TRP:N	0.42	2.88	9	1
1:A:99:ASP:OD2	1:A:104:GLU:O	0.42	2.37	10	1
2:B:325:LEU:CD2	2:B:345:GLN:OE1	0.42	2.68	10	1
1:A:95:SER:HB3	1:A:109:GLN:CB	0.42	2.45	7	4
1:A:132:VAL:C	1:A:134:ASP:H	0.42	2.23	9	10
2:B:442:LYS:NZ	3:C:644:ASP:C	0.42	2.78	2	1
1:A:264:VAL:HG13	1:A:265:THR:N	0.42	2.30	3	1
2:B:452:HIS:HD1	2:B:471:SER:CB	0.42	2.28	3	1
1:A:195:GLN:OE1	1:A:205:GLN:OE1	0.42	2.37	4	1
3:C:607:MET:CG	3:C:608:TRP:N	0.42	2.82	10	2
1:A:95:SER:HB2	1:A:109:GLN:CB	0.42	2.45	9	1
1:A:192:LEU:HD22	1:A:192:LEU:H	0.42	1.65	1	1
2:B:529:ASN:ND2	2:B:529:ASN:C	0.42	2.78	1	2
1:A:134:ASP:C	1:A:135:HIS:CG	0.42	2.98	2	1
2:B:405:ASP:OD1	2:B:405:ASP:O	0.42	2.37	9	2
3:C:647:GLN:O	3:C:647:GLN:OE1	0.42	2.37	3	1
1:A:121:ARG:HE	1:A:122:ASP:CA	0.42	2.28	4	1
2:B:487:MET:C	2:B:487:MET:SD	0.42	3.03	5	1
2:B:320:GLN:O	2:B:324:ASN:CG	0.42	2.63	10	1
3:C:718:GLN:OXT	3:C:718:GLN:CD	0.42	2.62	10	1
3:C:613:GLY:C	3:C:615:LEU:N	0.41	2.78	3	10
2:B:303:ASP:OD1	2:B:303:ASP:C	0.41	2.62	2	2
2:B:405:ASP:C	2:B:405:ASP:OD1	0.41	2.63	2	1
1:A:166:LYS:C	1:A:167:ASN:HD22	0.41	2.22	3	1
2:B:439:ASP:O	2:B:442:LYS:HG2	0.41	2.15	3	1
1:A:144:TYR:HB2	1:A:155:ILE:HB	0.41	1.91	4	1
1:A:248:GLN:C	1:A:252:ASP:OD2	0.41	2.64	5	1
1:A:203:ASN:OD1	2:B:314:ARG:O	0.41	2.37	8	2
3:C:626:GLU:C	3:C:626:GLU:CD	0.41	2.88	6	1
3:C:610:LEU:HD21	3:C:618:VAL:HG21	0.41	1.92	7	1
1:A:273:LYS:HA	1:A:277:TYR:HB2	0.41	1.92	1	7
3:C:642:ALA:O	3:C:651:LEU:CD1	0.41	2.69	6	2
1:A:70:TYR:CD2	1:A:94:ILE:HD13	0.41	2.50	6	4
1:A:253:THR:CG2	3:C:636:ARG:NH2	0.41	2.83	4	1
1:A:206:LEU:O	1:A:206:LEU:CD2	0.41	2.67	5	1
1:A:90:PRO:O	1:A:121:ARG:CZ	0.41	2.69	9	1
2:B:405:ASP:OD1	2:B:405:ASP:C	0.41	2.61	9	1
3:C:604:LYS:O	3:C:608:TRP:N	0.41	2.41	3	2
1:A:125:ASP:OD1	1:A:125:ASP:N	0.41	2.53	2	1
3:C:648:LEU:CA	3:C:651:LEU:HD21	0.41	2.44	6	2
1:A:70:TYR:CE1	1:A:92:ASN:OD1	0.41	2.73	3	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:198:TYR:CD1	1:A:198:TYR:C	0.41	2.98	5	3
1:A:273:LYS:C	1:A:277:TYR:HB2	0.41	2.40	5	3
2:B:364:TYR:CD1	2:B:422:TRP:CZ2	0.41	3.08	3	2
3:C:661:ILE:O	3:C:662:ASN:OD1	0.41	2.38	4	1
1:A:164:GLN:CD	1:A:167:ASN:OD1	0.41	2.63	8	2
1:A:72:ASP:C	1:A:72:ASP:OD1	0.41	2.62	9	1
1:A:233:GLU:O	1:A:237:ASN:OD1	0.41	2.37	9	1
1:A:71:ASP:C	1:A:71:ASP:OD1	0.41	2.61	1	1
2:B:350:ALA:HB1	2:B:359:TYR:CE2	0.41	2.49	1	1
2:B:470:THR:HG22	2:B:470:THR:O	0.41	2.15	2	1
3:C:615:LEU:O	3:C:615:LEU:CD2	0.41	2.65	9	2
1:A:192:LEU:CD2	1:A:192:LEU:H	0.41	2.24	1	1
1:A:264:VAL:CG2	1:A:265:THR:N	0.41	2.82	1	3
1:A:256:LYS:NZ	3:C:636:ARG:CZ	0.41	2.84	2	1
2:B:302:SER:O	2:B:303:ASP:C	0.41	2.64	2	6
3:C:603:ASP:OD1	3:C:603:ASP:N	0.41	2.53	2	1
3:C:650:ILE:HG22	3:C:654:LEU:HD21	0.41	1.93	4	1
3:C:709:ASP:C	3:C:709:ASP:OD1	0.41	2.62	6	1
1:A:161:HIS:CD2	1:A:161:HIS:N	0.41	2.89	10	1
2:B:444:ILE:HG22	2:B:479:THR:HB	0.41	1.91	10	1
1:A:262:LEU:HD23	1:A:263:PRO:HD2	0.41	1.91	1	1
1:A:125:ASP:OD1	1:A:143:VAL:CG1	0.41	2.69	2	1
1:A:270:ASP:OD1	1:A:270:ASP:N	0.41	2.53	2	1
2:B:377:ASN:ND2	2:B:394:ARG:NH2	0.41	2.69	6	1
2:B:380:ASP:HB2	2:B:381:PRO:HD3	0.41	1.92	6	1
1:A:164:GLN:OE1	1:A:164:GLN:O	0.41	2.39	10	1
1:A:59:MET:C	1:A:61:GLN:N	0.41	2.79	1	10
3:C:614:ASP:C	3:C:616:ASP:H	0.41	2.24	8	7
1:A:129:ARG:HE	1:A:129:ARG:CA	0.41	2.27	7	1
1:A:274:ILE:CD1	1:A:274:ILE:C	0.41	2.93	7	1
2:B:401:ASN:O	2:B:401:ASN:OD1	0.41	2.39	7	1
1:A:54:PHE:CD1	1:A:100:HIS:CB	0.41	3.04	8	1
3:C:610:LEU:HD23	3:C:650:ILE:HG21	0.41	1.91	8	1
2:B:458:GLU:OE2	2:B:509:HIS:CD2	0.41	2.73	9	1
3:C:693:ASP:OD1	3:C:696:VAL:CG2	0.41	2.68	10	1
3:C:648:LEU:HD13	3:C:682:SER:CB	0.41	2.44	3	1
3:C:603:ASP:OD1	3:C:603:ASP:O	0.41	2.39	6	1
3:C:626:GLU:OE2	3:C:628:VAL:HG22	0.41	2.16	6	1
2:B:421:LEU:HD12	2:B:421:LEU:N	0.41	2.30	1	1
1:A:121:ARG:C	1:A:123:ALA:N	0.41	2.79	3	7
1:A:121:ARG:CG	1:A:122:ASP:N	0.41	2.82	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:361:LEU:CD2	2:B:362:CYS:N	0.41	2.82	2	1
2:B:442:LYS:NZ	3:C:644:ASP:HB3	0.41	2.31	2	1
2:B:509:HIS:O	2:B:510:ILE:C	0.41	2.64	3	4
3:C:658:GLY:O	3:C:659:ALA:CB	0.41	2.69	3	2
3:C:662:ASN:HD22	3:C:696:VAL:HG11	0.41	1.76	3	1
1:A:88:LEU:CD2	1:A:89:ASP:H	0.41	2.26	5	1
1:A:186:ALA:C	1:A:187:GLN:OE1	0.41	2.63	5	1
1:A:197:HIS:CD2	1:A:198:TYR:N	0.41	2.89	5	1
3:C:604:LYS:NZ	3:C:607:MET:HE2	0.41	2.27	5	1
2:B:408:ARG:CG	2:B:408:ARG:HH11	0.41	2.27	6	1
3:C:604:LYS:HA	3:C:607:MET:HE2	0.41	1.92	8	1
3:C:628:VAL:HG11	3:C:654:LEU:HB2	0.41	1.93	8	1
2:B:564:GLN:O	2:B:564:GLN:CD	0.41	2.63	9	1
2:B:372:ARG:NH1	2:B:420:TYR:OH	0.41	2.49	10	1
2:B:444:ILE:N	2:B:444:ILE:CD1	0.41	2.68	10	1
3:C:680:HIS:C	3:C:681:VAL:HG13	0.41	2.40	10	1
3:C:681:VAL:O	3:C:681:VAL:HG23	0.41	2.15	10	1
1:A:194:ILE:O	1:A:194:ILE:CG2	0.41	2.67	2	1
2:B:359:TYR:OH	2:B:380:ASP:OD1	0.41	2.36	2	1
2:B:422:TRP:O	2:B:423:ASP:C	0.41	2.64	2	4
2:B:570:GLN:O	2:B:570:GLN:CG	0.41	2.69	2	1
1:A:91:ARG:NE	1:A:125:ASP:OD2	0.41	2.54	4	1
2:B:311:ASP:OD1	2:B:315:ARG:NE	0.41	2.54	5	1
2:B:478:GLN:HE22	2:B:488:ASN:CG	0.41	2.23	5	1
1:A:198:TYR:O	1:A:198:TYR:HD1	0.41	1.98	6	1
2:B:479:THR:HG22	2:B:487:MET:HB3	0.41	1.92	6	1
1:A:126:SER:O	1:A:129:ARG:HG3	0.41	2.16	7	1
3:C:608:TRP:NE1	3:C:612:ASN:OD1	0.41	2.53	8	1
1:A:61:GLN:O	1:A:61:GLN:CG	0.41	2.69	10	1
1:A:136:TYR:HH	1:A:173:TRP:CG	0.41	2.34	10	1
1:A:224:THR:CG2	1:A:225:ALA:N	0.41	2.83	10	1
1:A:91:ARG:C	1:A:91:ARG:CD	0.40	2.93	1	1
3:C:717:LEU:O	3:C:718:GLN:CB	0.40	2.70	4	3
2:B:452:HIS:ND1	2:B:471:SER:CB	0.40	2.84	3	1
3:C:660:ASP:C	3:C:662:ASN:H	0.40	2.24	9	4
1:A:173:TRP:NE1	1:A:236:GLU:OE2	0.40	2.54	4	1
1:A:209:HIS:ND1	1:A:209:HIS:C	0.40	2.78	5	1
1:A:188:VAL:HG23	1:A:216:VAL:HG12	0.40	1.94	6	1
3:C:673:LEU:HD23	3:C:676:VAL:HG21	0.40	1.91	9	1
1:A:172:ARG:HH12	1:A:174:ARG:CZ	0.40	2.28	10	1
1:A:106:SER:O	1:A:107:ASP:CB	0.40	2.70	1	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:C:603:ASP:O	3:C:607:MET:HG3	0.40	2.15	1	1
1:A:272:ASN:OD1	1:A:272:ASN:O	0.40	2.38	3	1
2:B:468:LYS:CE	2:B:496:GLN:NE2	0.40	2.85	8	2
1:A:240:GLN:OE1	1:A:240:GLN:O	0.40	2.40	4	1
2:B:409:ASP:CG	3:C:604:LYS:NZ	0.40	2.79	4	1
1:A:42:ASN:ND2	1:A:45:LEU:HD12	0.40	2.31	5	1
2:B:408:ARG:CZ	2:B:414:GLY:O	0.40	2.69	6	1
2:B:510:ILE:HD12	2:B:510:ILE:H	0.40	1.76	7	1
3:C:676:VAL:HG12	3:C:677:TYR:N	0.40	2.30	9	1
2:B:408:ARG:HH11	2:B:408:ARG:HG3	0.40	1.76	10	1
2:B:553:GLN:H	2:B:553:GLN:NE2	0.40	2.14	10	1
1:A:122:ASP:C	1:A:122:ASP:OD1	0.40	2.64	1	1
1:A:273:LYS:C	1:A:277:TYR:CB	0.40	2.89	7	3
2:B:473:VAL:CG2	2:B:521:GLU:OE1	0.40	2.69	1	1
2:B:479:THR:CG2	2:B:487:MET:HB3	0.40	2.46	1	1
3:C:677:TYR:CD1	3:C:677:TYR:C	0.40	2.99	2	1
3:C:695:THR:O	3:C:695:THR:CG2	0.40	2.67	2	1
1:A:250:MET:SD	2:B:489:LEU:CD2	0.40	3.09	3	1
1:A:266:ARG:O	1:A:267:THR:HB	0.40	2.17	3	1
2:B:401:ASN:O	2:B:405:ASP:OD1	0.40	2.39	3	1
3:C:666:LYS:CD	3:C:666:LYS:N	0.40	2.84	5	1
1:A:81:ASP:OD1	1:A:81:ASP:C	0.40	2.63	6	1
3:C:637:LYS:H	3:C:637:LYS:HD2	0.40	1.76	6	1
1:A:181:ILE:C	1:A:181:ILE:CD1	0.40	2.94	10	1
1:A:72:ASP:OD2	1:A:89:ASP:OD1	0.40	2.40	1	1
1:A:240:GLN:CD	1:A:240:GLN:O	0.40	2.64	3	2
2:B:464:THR:O	2:B:464:THR:CG2	0.40	2.69	3	3
3:C:667:HIS:C	3:C:668:HIS:ND1	0.40	2.78	6	1
1:A:250:MET:HE1	2:B:487:MET:HE2	0.40	1.93	8	1
2:B:369:ASP:OD1	2:B:369:ASP:O	0.40	2.39	9	1
1:A:274:ILE:O	1:A:274:ILE:HG23	0.40	2.15	10	1
1:A:69:GLY:C	1:A:70:TYR:CD1	0.40	2.99	4	1
1:A:135:HIS:HB3	2:B:544:ARG:HE	0.40	1.77	4	1
1:A:220:SER:O	1:A:224:THR:OG1	0.40	2.30	4	1
3:C:687:LEU:O	3:C:689:SER:N	0.40	2.55	6	2
1:A:89:ASP:OD2	1:A:94:ILE:CD1	0.40	2.69	7	1
2:B:434:ILE:CB	2:B:450:SER:OG	0.40	2.69	8	1
3:C:613:GLY:C	3:C:615:LEU:H	0.40	2.23	8	1
2:B:379:TYR:N	2:B:379:TYR:CD1	0.40	2.90	9	1
2:B:317:PRO:HA	2:B:318:PRO:HD3	0.40	1.79	10	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	273/275 (99%)	194±0 (71±0%)	48±0 (17±0%)	32±0 (12±0%)	1	7
2	B	268/270 (99%)	227±0 (85±0%)	31±0 (12±0%)	10±0 (4±0%)	4	32
3	C	116/118 (98%)	62±0 (53±0%)	33±0 (28±0%)	21±0 (18±0%)	0	3
All	All	6570/6630 (99%)	4827 (73%)	1116 (17%)	627 (10%)	1	10

All 63 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	8	VAL	10
1	A	9	SER	10
1	A	62	PHE	10
1	A	68	GLU	10
1	A	71	ASP	10
1	A	73	GLN	10
1	A	101	LEU	10
1	A	113	THR	10
1	A	121	ARG	10
1	A	122	ASP	10
1	A	125	ASP	10
1	A	166	LYS	10
1	A	169	TRP	10
1	A	180	THR	10
1	A	182	THR	10
1	A	183	PRO	10
1	A	185	THR	10
1	A	186	ALA	10
1	A	188	VAL	10
1	A	189	ALA	10
1	A	191	VAL	10
1	A	201	ASP	10
1	A	253	THR	10
1	A	258	LEU	10
1	A	267	THR	10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	268	LYS	10
1	A	271	TRP	10
1	A	276	SER	10
1	A	277	TYR	10
1	A	279	ILE	10
1	A	280	GLY	10
2	B	382	PRO	10
2	B	423	ASP	10
2	B	485	GLY	10
2	B	492	SER	10
2	B	532	TYR	10
2	B	534	GLY	10
2	B	550	PRO	10
2	B	551	ASP	10
2	B	564	GLN	10
2	B	570	GLN	10
3	C	614	ASP	10
3	C	615	LEU	10
3	C	625	GLY	10
3	C	626	GLU	10
3	C	629	ASN	10
3	C	632	LEU	10
3	C	634	GLY	10
3	C	647	GLN	10
3	C	653	PHE	10
3	C	654	LEU	10
3	C	657	LYS	10
3	C	658	GLY	10
3	C	659	ALA	10
3	C	660	ASP	10
3	C	662	ASN	10
3	C	681	VAL	10
3	C	692	ALA	10
3	C	700	ASP	10
3	C	703	THR	10
3	C	715	ALA	10
3	C	717	LEU	10
1	A	55	ALA	7

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	243/243 (100%)	227±3 (93±1%)	16±3 (7±1%)	17 65
2	B	241/241 (100%)	228±3 (95±1%)	13±3 (5±1%)	21 71
3	C	96/96 (100%)	83±3 (86±3%)	13±3 (14±3%)	6 45
All	All	5800/5800 (100%)	5374 (93%)	426 (7%)	15 63

All 140 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	100	HIS	10
1	A	160	SER	10
1	A	185	THR	10
2	B	380	ASP	10
2	B	383	LEU	10
2	B	533	PHE	10
3	C	648	LEU	10
3	C	670	THR	10
1	A	175	SER	9
1	A	182	THR	9
3	C	650	ILE	9
3	C	651	LEU	9
1	A	262	LEU	9
2	B	345	GLN	8
2	B	411	TYR	8
3	C	654	LEU	8
1	A	115	SER	7
3	C	631	THR	7
1	A	109	GLN	6
2	B	525	ARG	6
3	C	637	LYS	6
1	A	141	CYS	6
3	C	716	LEU	6
3	C	639	LEU	5
3	C	713	ILE	5
2	B	331	LEU	5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
3	C	681	VAL	5
1	A	70	TYR	5
1	A	129	ARG	5
1	A	188	VAL	4
1	A	247	TYR	4
2	B	379	TYR	4
2	B	469	LEU	4
3	C	683	CYS	4
3	C	687	LEU	4
1	A	67	ILE	4
1	A	107	ASP	4
1	A	220	SER	4
2	B	449	ASP	4
1	A	86	ARG	4
1	A	181	ILE	3
2	B	390	SER	3
2	B	472	THR	3
2	B	529	ASN	3
2	B	569	ARG	3
3	C	696	VAL	3
3	C	708	THR	3
1	A	194	ILE	3
2	B	408	ARG	3
2	B	421	LEU	3
2	B	450	SER	3
2	B	464	THR	3
2	B	475	LEU	3
3	C	688	LEU	3
3	C	705	LEU	3
1	A	113	THR	2
1	A	148	ILE	2
1	A	208	SER	2
1	A	231	ILE	2
3	C	630	ARG	2
3	C	695	THR	2
1	A	88	LEU	2
1	A	259	ARG	2
2	B	371	TYR	2
2	B	476	TRP	2
1	A	164	GLN	2
1	A	269	ILE	2
3	C	682	SER	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	217	GLN	2
1	A	270	ASP	2
2	B	493	LEU	2
3	C	621	TYR	2
3	C	628	VAL	2
3	C	672	LEU	2
3	C	693	ASP	2
1	A	93	LYS	2
1	A	267	THR	2
2	B	463	ARG	2
3	C	703	THR	2
1	A	274	ILE	2
2	B	453	VAL	2
2	B	354	VAL	2
1	A	118	LYS	2
2	B	488	ASN	2
1	A	117	LEU	1
2	B	315	ARG	1
3	C	669	ILE	1
1	A	251	SER	1
2	B	313	MET	1
2	B	361	LEU	1
2	B	478	GLN	1
2	B	502	THR	1
2	B	570	GLN	1
3	C	684	VAL	1
1	A	72	ASP	1
1	A	82	LEU	1
1	A	167	ASN	1
1	A	237	ASN	1
1	A	281	LYS	1
2	B	442	LYS	1
2	B	546	ILE	1
3	C	612	ASN	1
3	C	660	ASP	1
3	C	717	LEU	1
1	A	15	ARG	1
1	A	73	GLN	1
1	A	91	ARG	1
1	A	178	LYS	1
2	B	365	ASN	1
2	B	406	GLN	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	B	424	LEU	1
2	B	407	TYR	1
2	B	434	ILE	1
2	B	489	LEU	1
3	C	604	LYS	1
3	C	697	LYS	1
1	A	226	LYS	1
2	B	537	LYS	1
3	C	653	PHE	1
1	A	94	ILE	1
1	A	103	LYS	1
2	B	474	MET	1
2	B	487	MET	1
3	C	661	ILE	1
2	B	436	LYS	1
2	B	447	CYS	1
2	B	479	THR	1
3	C	601	MET	1
1	A	13	LYS	1
1	A	92	ASN	1
1	A	172	ARG	1
3	C	678	GLU	1
1	A	59	MET	1
1	A	191	VAL	1
1	A	260	ARG	1
2	B	444	ILE	1
2	B	562	LEU	1
3	C	618	VAL	1
3	C	656	LEU	1
3	C	657	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [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