



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 11:28 AM UTC

PDB ID : 2XDF / pdb_00002xdf
Title : Solution Structure of the Enzyme I Dimer Complexed with HPr Using Residual Dipolar Couplings and Small Angle X-Ray Scattering
Authors : Schwieters, C.D.; Suh, J.-Y.; Grishaev, A.; Guirlando, R.; Takayama, Y.; Clore, G.M.
Deposited on : 2010-04-30

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

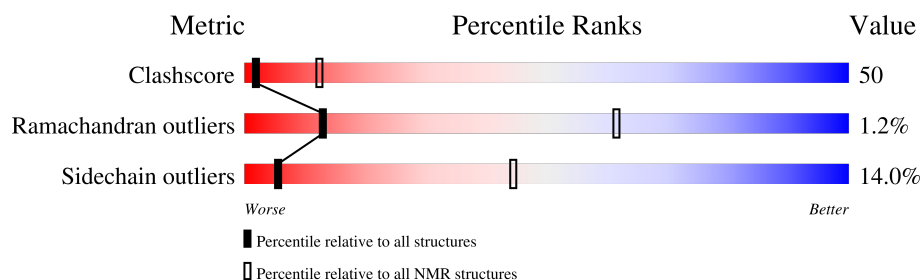
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

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	573	58% 27% 14%
1	B	573	58% 29% 13%
2	C	85	72% 26% ..
2	D	85	72% 26% ..

2 Ensemble composition and analysis ⓘ

This entry contains 2 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20502 atoms, of which 10338 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE.

Mol	Chain	Residues	Atoms						Trace
1	A	573	Total	C	H	N	O	S	0
			8956	2790	4514	757	874	21	
1	B	573	Total	C	H	N	O	S	0
			8956	2790	4514	757	874	21	

- Molecule 2 is a protein called PHOSPHOCARRIER PROTEIN HPR.

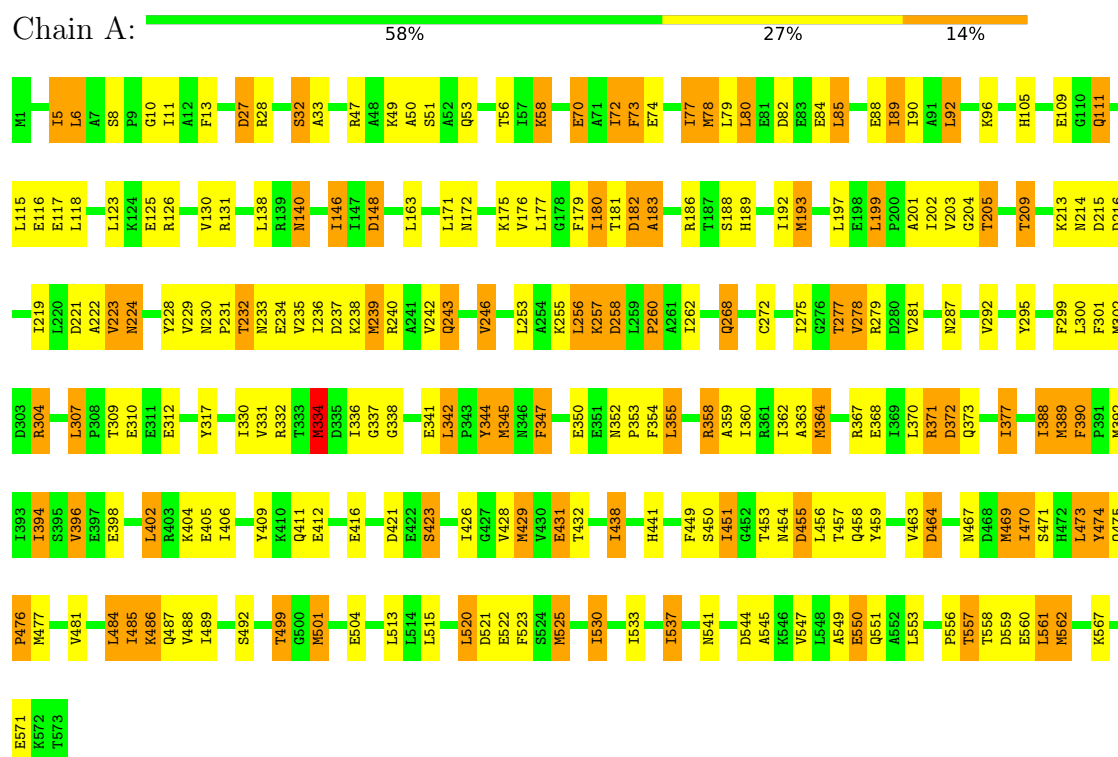
Mol	Chain	Residues	Atoms						Trace
2	C	85	Total	C	H	N	O	S	0
			1295	401	655	107	130	2	
2	D	85	Total	C	H	N	O	S	0
			1295	401	655	107	130	2	

4 Residue-property plots

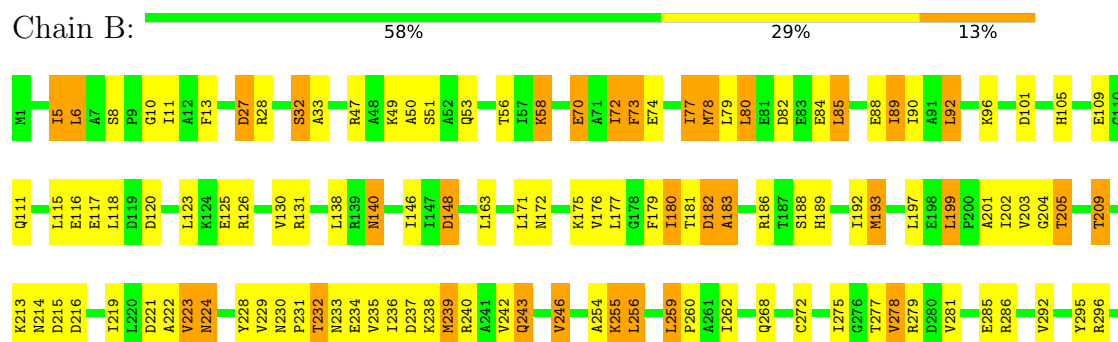
4.1 Average score per residue in the NMR ensemble

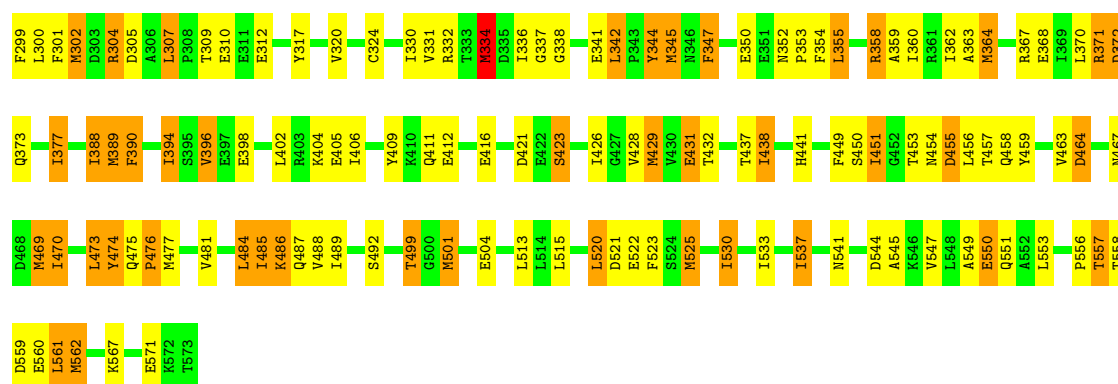
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE



• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE





• Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain C: 72% 26% ..



• Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain D: 72% 26% ..



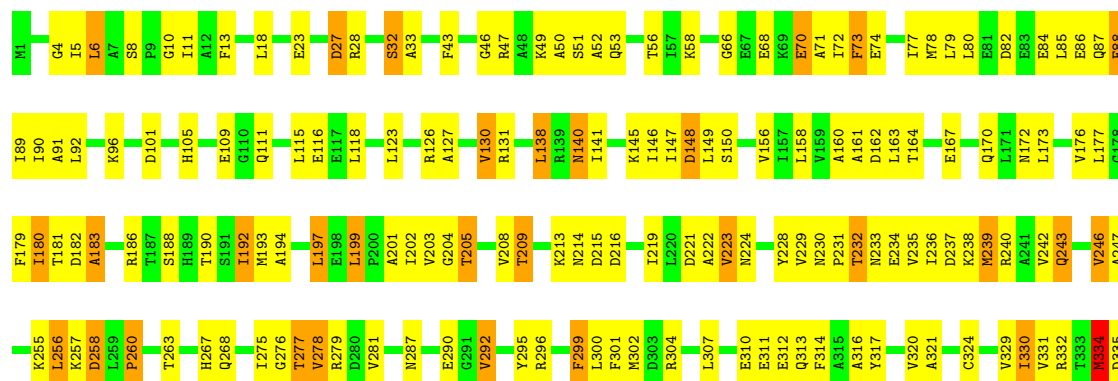
4.2 Scores per residue for each member of the ensemble

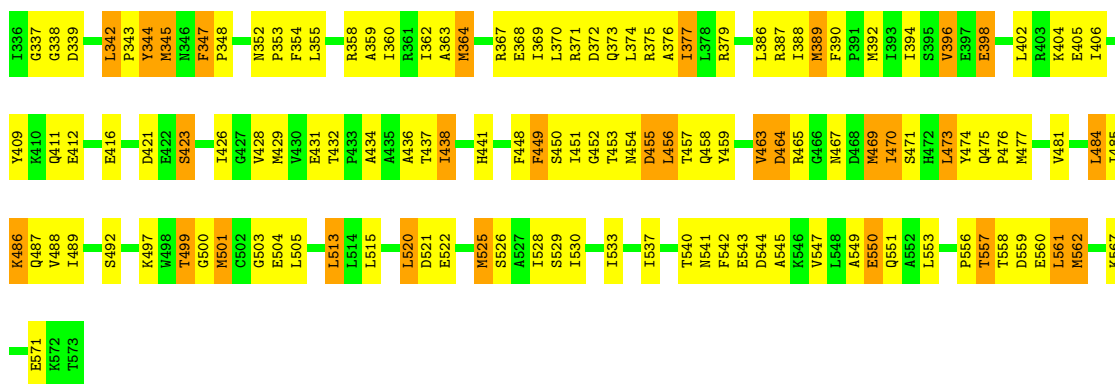
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE

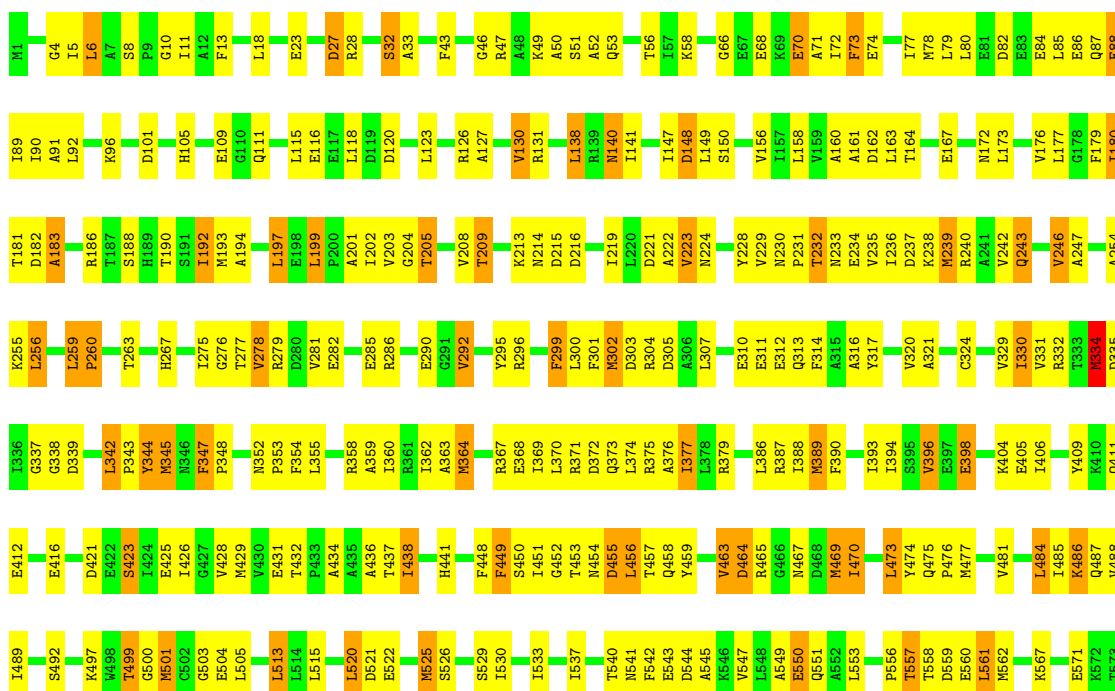
Chain A: 48% 41% 10%





• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE

Chain B: 48% 41% 10%



• Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain C: 66% 32% 2%



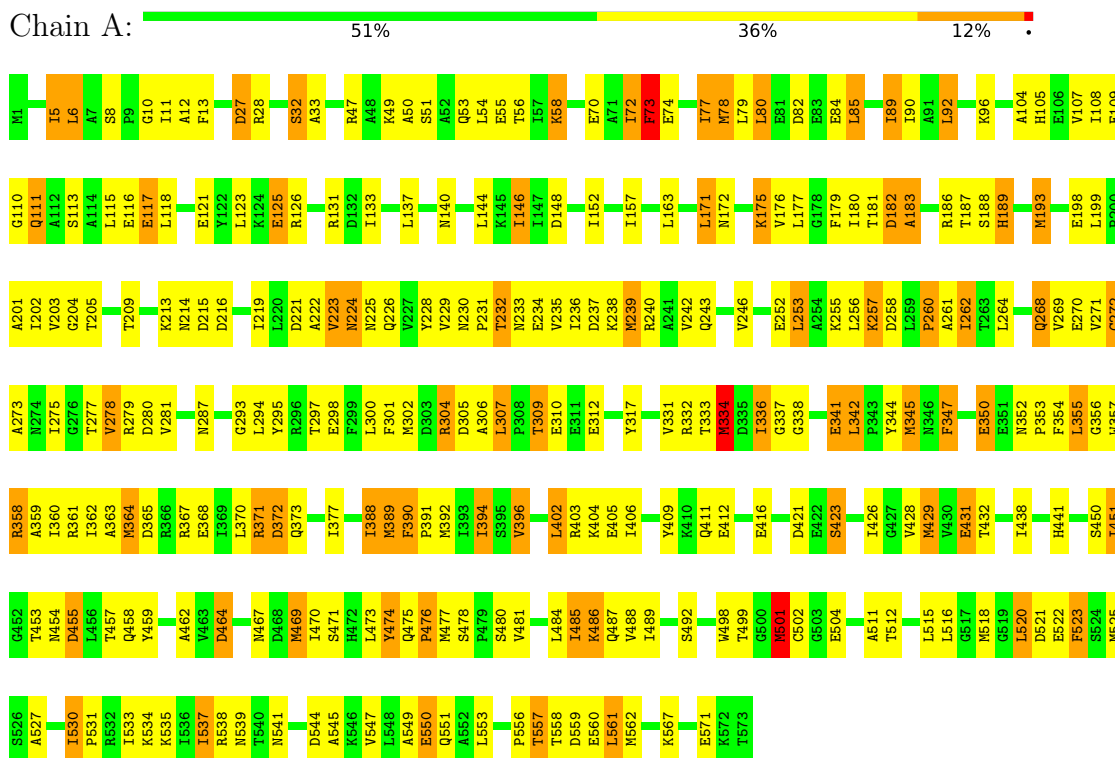
• Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain D: 68% 29% 3%

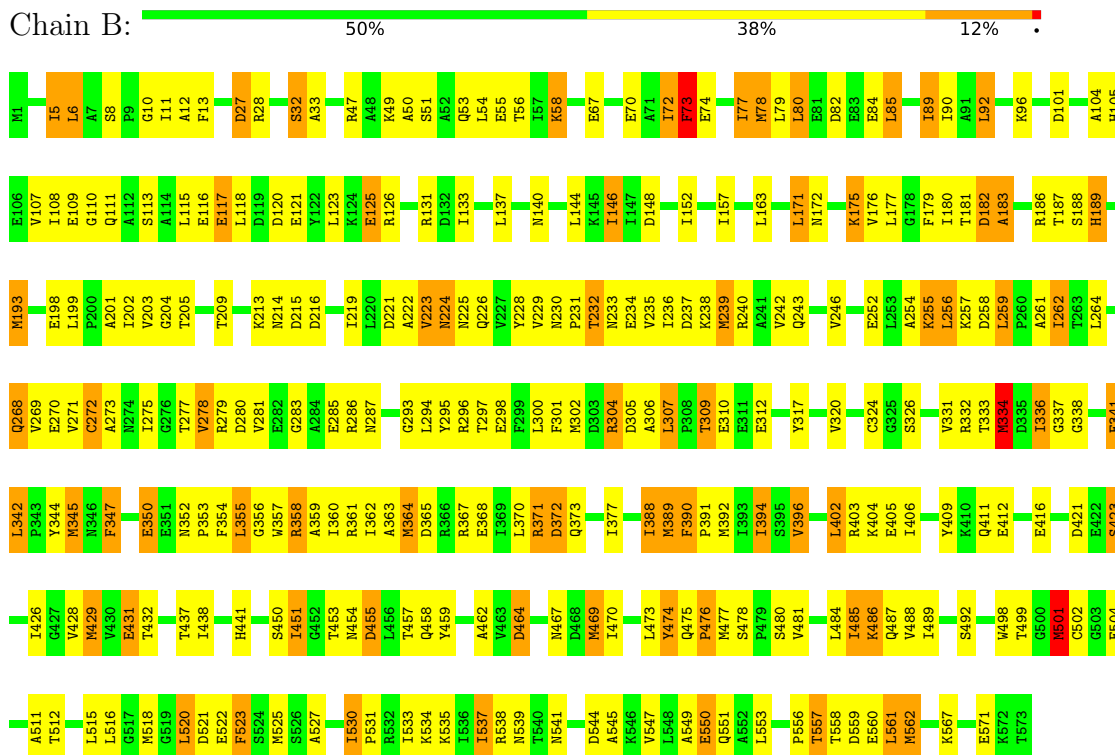


4.2.2 Score per residue for model 2

• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE



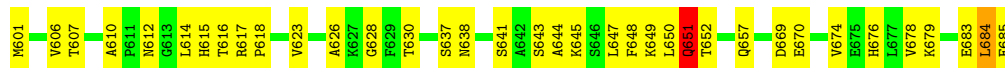
• Molecule 1: PHOSPHOENOLPYRUVATE-PROTEIN PHOSPHOTRANSFERASE



● Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain C:  60% 38% ..

● Molecule 2: PHOSPHOCARRIER PROTEIN HPR

Chain D:  58% 40% ..

5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 2 were deposited, based on the following criterion: *BEST EXPERIMENT FIT, AND THEN LOWEST ENERGY*.

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

Software name	Classification	Version
Xplor-NIH	refinement	2.25
Xplor-NIH	structure solution	

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.37±0.00	21±0/4495 (0.5± 0.0%)	1.16±0.00	8±0/6061 (0.1± 0.0%)
1	B	1.37±0.00	22±0/4495 (0.5± 0.0%)	1.17±0.00	8±0/6061 (0.1± 0.0%)
2	C	1.53±0.00	0±0/647 (0.0± 0.0%)	1.18±0.00	1±0/871 (0.1± 0.0%)
2	D	1.54±0.00	0±0/647 (0.0± 0.0%)	1.19±0.00	1±0/871 (0.1± 0.0%)
All	All	1.39	86/20568 (0.4%)	1.17	37/27728 (0.1%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	345	MET	SD-CE	14.01	2.14	1.79	2	2
1	B	345	MET	SD-CE	13.99	2.14	1.79	1	2
1	A	469	MET	SD-CE	13.78	2.13	1.79	2	2
1	B	469	MET	SD-CE	13.71	2.13	1.79	2	2
1	A	364	MET	SD-CE	10.62	2.06	1.79	2	2
1	B	364	MET	SD-CE	10.61	2.06	1.79	2	2
1	B	562	MET	SD-CE	8.81	2.01	1.79	2	2
1	A	562	MET	SD-CE	8.77	2.01	1.79	1	2
1	A	562	MET	CG-SD	7.54	1.99	1.80	2	2
1	B	562	MET	CG-SD	7.53	1.99	1.80	1	2
1	A	239	MET	SD-CE	7.23	1.97	1.79	1	2
1	B	239	MET	SD-CE	7.17	1.97	1.79	2	2
1	A	364	MET	CG-SD	6.82	1.97	1.80	1	2
1	B	364	MET	CG-SD	6.81	1.97	1.80	1	2
1	A	475	GLN	CA-C	-6.60	1.45	1.52	1	2
1	B	475	GLN	CA-C	-6.57	1.45	1.52	1	2
1	B	345	MET	CG-SD	6.46	1.96	1.80	1	2
1	A	525	MET	SD-CE	6.45	1.95	1.79	1	2
1	B	525	MET	SD-CE	6.44	1.95	1.79	2	2
1	A	345	MET	CG-SD	6.42	1.96	1.80	2	2
1	A	501	MET	CG-SD	6.22	1.96	1.80	1	2
1	A	334	MET	CG-SD	6.20	1.96	1.80	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	B	334	MET	CG-SD	6.15	1.96	1.80	2	2
1	B	501	MET	CG-SD	6.10	1.96	1.80	1	2
1	A	389	MET	SD-CE	5.99	1.94	1.79	2	2
1	B	389	MET	SD-CE	5.93	1.94	1.79	2	2
1	B	239	MET	CG-SD	5.79	1.95	1.80	2	2
1	A	239	MET	CG-SD	5.78	1.95	1.80	1	2
1	A	475	GLN	C-O	-5.75	1.19	1.24	1	2
1	B	475	GLN	C-O	-5.71	1.19	1.24	1	2
1	B	120	ASP	N-CA	5.52	1.52	1.46	2	2
1	A	477	MET	SD-CE	5.48	1.93	1.79	1	2
1	B	477	MET	SD-CE	5.44	1.93	1.79	1	2
1	A	429	MET	SD-CE	5.31	1.92	1.79	2	2
1	B	429	MET	SD-CE	5.26	1.92	1.79	1	2
1	A	334	MET	SD-CE	5.20	1.92	1.79	2	2
1	B	334	MET	SD-CE	5.19	1.92	1.79	2	2
1	B	525	MET	CG-SD	5.13	1.93	1.80	1	2
1	A	525	MET	CG-SD	5.10	1.93	1.80	1	2
1	B	469	MET	CG-SD	5.09	1.93	1.80	2	2
1	A	469	MET	CG-SD	5.05	1.93	1.80	2	2
1	A	550	GLU	N-CA	-5.01	1.40	1.46	1	2
1	B	550	GLU	N-CA	-5.01	1.40	1.46	1	2

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	561	LEU	CA-CB-CG	6.63	139.50	116.30	1	2
1	B	561	LEU	CA-CB-CG	6.63	139.49	116.30	1	2
1	B	487	GLN	N-CA-C	-5.76	105.14	111.82	1	2
1	A	487	GLN	N-CA-C	-5.75	105.15	111.82	1	2
2	C	645	LYS	N-CA-C	-5.70	106.55	112.93	1	2
2	D	645	LYS	N-CA-C	-5.70	106.55	112.93	2	2
1	A	224	ASN	N-CA-C	-5.45	106.31	113.17	2	2
1	B	338	GLY	N-CA-C	-5.35	100.49	113.18	1	2
1	A	338	GLY	N-CA-C	-5.34	100.52	113.18	1	2
1	B	224	ASN	N-CA-C	-5.25	106.56	113.17	2	2
1	A	342	LEU	CA-C-N	5.23	126.38	119.84	1	2
1	A	342	LEU	C-N-CA	5.23	126.38	119.84	1	2
1	B	342	LEU	CA-C-N	5.23	126.38	119.84	1	2
1	B	342	LEU	C-N-CA	5.23	126.38	119.84	1	2
1	A	73	PHE	CA-CB-CG	-5.13	108.67	113.80	2	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	170	GLN	CB-CG-CD	-5.13	103.89	112.60	1	1
1	B	73	PHE	CA-CB-CG	-5.06	108.74	113.80	1	2
1	B	476	PRO	N-CA-C	-5.02	107.86	114.03	1	2
1	A	476	PRO	N-CA-C	-5.01	107.86	114.03	1	2

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	4442	4514	4506	510±8
1	B	4442	4514	4506	509±6
2	C	640	655	650	41±3
2	D	640	655	650	41±2
All	All	20328	20676	20624	2060

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ARG:HH22	2:C:619:ALA:CB	1.61	1.04	1	1
1:B:126:ARG:HH22	2:D:619:ALA:CB	1.55	1.04	1	1
1:B:78:MET:HE2	2:D:627:LYS:CD	1.50	1.36	1	1
1:B:314:PHE:CE2	1:B:376:ALA:HA	1.49	1.41	1	1
1:A:314:PHE:CE2	1:A:376:ALA:HA	1.48	1.40	1	1
1:B:562:MET:SD	1:B:562:MET:CE	1.48	2.01	2	1
1:A:562:MET:CE	1:A:562:MET:SD	1.46	2.01	1	1
1:A:78:MET:HE2	2:C:627:LYS:CD	1.46	1.38	1	1
1:B:364:MET:SD	1:B:364:MET:CE	1.44	2.06	2	2
1:A:364:MET:SD	1:A:364:MET:CE	1.44	2.06	1	2
1:B:126:ARG:NH2	2:D:619:ALA:CB	1.39	1.84	1	1
1:A:276:GLY:HA2	1:A:299:PHE:CD2	1.37	1.54	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:78:MET:CE	2:D:627:LYS:HD2	1.36	1.47	1	1
1:B:276:GLY:HA2	1:B:299:PHE:CD2	1.36	1.55	1	1
1:A:469:MET:SD	1:A:469:MET:CE	1.36	2.14	2	2
1:B:469:MET:CE	1:B:469:MET:SD	1.36	2.13	1	2
1:A:126:ARG:NH2	2:C:619:ALA:CB	1.35	1.84	1	1
1:B:345:MET:SD	1:B:345:MET:CE	1.35	2.14	1	2
1:A:345:MET:SD	1:A:345:MET:CE	1.34	2.14	1	2
1:A:78:MET:CE	2:C:627:LYS:HD2	1.33	1.51	1	1
1:A:276:GLY:HA2	1:A:299:PHE:CE2	1.33	1.58	1	1
1:B:276:GLY:HA2	1:B:299:PHE:CE2	1.32	1.58	1	1
1:A:470:ILE:O	1:A:473:LEU:CD2	1.31	1.79	1	1
1:A:515:LEU:C	1:A:520:LEU:HD11	1.29	1.51	2	1
1:B:470:ILE:O	1:B:473:LEU:CD2	1.29	1.78	1	1
1:B:470:ILE:O	1:B:473:LEU:HD22	1.29	1.07	1	1
1:B:515:LEU:C	1:B:520:LEU:HD11	1.29	1.52	2	1
1:A:515:LEU:CA	1:A:520:LEU:HD21	1.28	1.58	2	1
1:B:515:LEU:CA	1:B:520:LEU:HD21	1.28	1.57	2	1
1:A:470:ILE:O	1:A:473:LEU:HD22	1.26	1.07	1	1
1:A:126:ARG:NH2	2:C:619:ALA:HB3	1.24	1.41	1	1
1:B:464:ASP:OD1	1:B:467:ASN:ND2	1.24	1.70	1	2
1:B:515:LEU:O	1:B:520:LEU:HG	1.24	1.30	2	1
1:A:515:LEU:O	1:A:520:LEU:HG	1.22	1.30	2	1
1:B:126:ARG:NH2	2:D:619:ALA:HB3	1.22	1.41	1	1
1:B:367:ARG:O	1:B:371:ARG:HG3	1.22	1.34	2	1
1:A:276:GLY:O	1:A:299:PHE:CD1	1.22	1.91	1	1
1:B:111:GLN:OE1	2:D:648:PHE:HB3	1.22	1.33	1	1
1:B:276:GLY:O	1:B:299:PHE:CD1	1.22	1.92	1	1
1:A:464:ASP:OD1	1:A:467:ASN:ND2	1.21	1.71	1	2
1:A:314:PHE:CE2	1:A:376:ALA:CA	1.21	2.23	1	1
1:A:449:PHE:CE2	1:A:499:THR:OG1	1.21	1.87	1	1
1:B:449:PHE:CE2	1:B:500:GLY:O	1.20	1.95	1	1
1:B:449:PHE:CE2	1:B:499:THR:OG1	1.20	1.87	1	1
1:A:431:GLU:HG3	1:A:452:GLY:O	1.20	1.34	1	1
1:B:314:PHE:CE2	1:B:376:ALA:CA	1.20	2.23	1	1
1:A:515:LEU:O	1:A:520:LEU:CG	1.19	1.90	2	1
1:B:272:CYS:SG	1:B:293:GLY:N	1.19	2.16	2	1
1:A:449:PHE:CE2	1:A:500:GLY:O	1.18	1.94	1	1
1:B:515:LEU:O	1:B:520:LEU:CG	1.18	1.90	2	1
1:A:272:CYS:SG	1:A:293:GLY:N	1.18	2.15	2	1
1:B:527:ALA:O	1:B:530:ILE:CG2	1.18	1.92	2	1
1:A:527:ALA:O	1:A:530:ILE:CG2	1.17	1.93	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:GLN:OE1	2:C:648:PHE:HB3	1.17	1.34	1	1
1:B:431:GLU:HG3	1:B:452:GLY:O	1.17	1.34	1	1
1:A:367:ARG:O	1:A:371:ARG:HG3	1.17	1.34	2	1
1:B:456:LEU:HD13	1:B:457:THR:N	1.13	1.59	1	1
1:B:314:PHE:CZ	1:B:376:ALA:HA	1.12	1.78	1	1
1:A:314:PHE:CZ	1:A:376:ALA:HA	1.11	1.79	1	1
1:A:456:LEU:HD13	1:A:457:THR:N	1.11	1.59	1	1
1:B:243:GLN:O	1:B:246:VAL:HG22	1.10	1.47	1	1
1:B:463:VAL:HG11	1:B:473:LEU:HG	1.10	1.20	1	1
1:A:243:GLN:O	1:A:246:VAL:HG22	1.09	1.47	1	1
1:A:314:PHE:CD2	1:A:376:ALA:HA	1.09	1.81	1	1
1:B:314:PHE:CD2	1:B:376:ALA:HA	1.09	1.81	1	1
1:A:296:ARG:O	1:A:299:PHE:CE2	1.08	2.06	1	1
1:A:515:LEU:C	1:A:520:LEU:CD1	1.08	2.27	2	1
1:A:463:VAL:HG11	1:A:473:LEU:HG	1.07	1.20	1	1
1:B:296:ARG:O	1:B:299:PHE:CE2	1.07	2.07	1	1
1:A:464:ASP:OD1	1:B:355:LEU:O	1.06	1.72	1	2
1:B:515:LEU:C	1:B:520:LEU:CD1	1.06	2.28	2	1
1:A:360:ILE:HD12	1:A:391:PRO:O	1.05	1.52	2	1
1:B:360:ILE:HD12	1:B:391:PRO:O	1.04	1.53	2	1
1:A:296:ARG:O	1:A:299:PHE:CD2	1.03	2.12	1	1
1:A:527:ALA:O	1:A:530:ILE:HG22	1.02	1.48	2	1
1:B:269:VAL:HG11	1:B:523:PHE:CE2	1.02	1.88	2	1
1:A:276:GLY:CA	1:A:299:PHE:CD2	1.02	2.42	1	1
1:B:296:ARG:O	1:B:299:PHE:CD2	1.02	2.12	1	1
1:A:269:VAL:HG11	1:A:523:PHE:CE2	1.02	1.88	2	1
1:B:276:GLY:CA	1:B:299:PHE:CD2	1.02	2.42	1	1
1:B:527:ALA:O	1:B:530:ILE:HG22	1.02	1.50	2	1
1:B:296:ARG:O	1:B:299:PHE:CZ	1.02	2.13	1	1
1:B:275:ILE:O	1:B:299:PHE:CE2	1.01	2.12	1	1
1:B:367:ARG:O	1:B:371:ARG:CG	1.01	2.08	2	1
1:A:126:ARG:HH22	2:C:619:ALA:HB2	1.01	1.07	1	1
1:A:331:VAL:HG12	1:A:387:ARG:O	1.01	1.55	1	1
1:B:331:VAL:HG12	1:B:387:ARG:O	1.01	1.55	1	1
1:B:126:ARG:HH22	2:D:619:ALA:HB2	1.01	1.07	1	1
1:A:355:LEU:O	1:B:464:ASP:OD1	1.01	1.78	1	2
1:A:296:ARG:O	1:A:299:PHE:CZ	1.00	2.14	1	1
1:A:449:PHE:CD2	1:A:449:PHE:O	1.00	2.13	1	1
1:B:449:PHE:O	1:B:449:PHE:CD2	1.00	2.13	1	1
1:A:367:ARG:O	1:A:371:ARG:CG	1.00	2.08	2	1
1:A:221:ASP:HA	1:A:239:MET:CE	1.00	1.87	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:232:THR:HG22	1:B:233:ASN:N	1.00	1.70	2	2
1:B:232:THR:CG2	1:B:233:ASN:H	1.00	1.69	2	2
1:A:275:ILE:O	1:A:299:PHE:CE2	1.00	2.13	1	1
1:B:541:ASN:O	1:B:544:ASP:OD1	1.00	1.80	2	2
1:B:515:LEU:HA	1:B:520:LEU:HD21	0.99	1.02	2	1
1:A:232:THR:HG22	1:A:233:ASN:N	0.99	1.71	1	2
1:A:232:THR:CG2	1:A:233:ASN:H	0.99	1.69	1	2
1:B:221:ASP:HA	1:B:239:MET:CE	0.99	1.87	2	2
1:A:11:ILE:HD13	1:A:221:ASP:O	0.99	1.57	2	2
1:A:449:PHE:CZ	1:A:451:ILE:HB	0.99	1.93	1	1
1:A:541:ASN:O	1:A:544:ASP:OD1	0.99	1.79	1	2
1:A:232:THR:CG2	1:A:233:ASN:N	0.98	2.26	2	2
1:B:449:PHE:CZ	1:B:451:ILE:HB	0.98	1.93	1	1
1:A:515:LEU:HA	1:A:520:LEU:HD21	0.98	1.02	2	1
1:A:314:PHE:CE2	1:A:379:ARG:CB	0.98	2.46	1	1
1:B:11:ILE:HD13	1:B:221:ASP:O	0.98	1.57	2	2
1:B:314:PHE:CE2	1:B:379:ARG:CB	0.98	2.46	1	1
1:A:221:ASP:OD2	1:A:225:ASN:N	0.97	1.98	2	1
1:A:276:GLY:O	1:A:299:PHE:CE1	0.96	2.18	1	1
1:B:221:ASP:OD2	1:B:225:ASN:N	0.96	1.99	2	1
1:B:533:ILE:O	1:B:537:ILE:HG23	0.95	1.61	2	1
1:A:464:ASP:CG	1:B:355:LEU:O	0.95	2.08	1	2
1:B:232:THR:CG2	1:B:233:ASN:N	0.94	2.26	1	2
1:B:449:PHE:CD2	1:B:449:PHE:C	0.94	2.44	1	1
1:B:276:GLY:O	1:B:299:PHE:CE1	0.94	2.19	1	1
1:A:276:GLY:CA	1:A:299:PHE:CE2	0.94	2.51	1	1
1:B:515:LEU:CA	1:B:520:LEU:CD2	0.93	2.46	2	1
1:B:276:GLY:CA	1:B:299:PHE:CE2	0.93	2.51	1	1
1:A:104:ALA:O	1:A:107:VAL:HG22	0.93	1.63	2	1
1:B:292:VAL:CG1	1:B:329:VAL:HG22	0.93	1.94	1	1
1:B:314:PHE:CE2	1:B:379:ARG:HB2	0.93	1.99	1	1
1:A:221:ASP:HA	1:A:239:MET:HE2	0.93	1.41	2	2
1:A:292:VAL:CG1	1:A:329:VAL:HG22	0.93	1.93	1	1
1:A:533:ILE:O	1:A:537:ILE:HG23	0.92	1.61	2	1
1:A:314:PHE:CE2	1:A:379:ARG:HB2	0.92	1.99	1	1
1:A:449:PHE:CD2	1:A:449:PHE:C	0.92	2.44	1	1
1:A:515:LEU:CA	1:A:520:LEU:CD2	0.92	2.47	2	1
1:A:449:PHE:HE2	1:A:500:GLY:O	0.92	1.45	1	1
1:A:242:VAL:O	1:A:246:VAL:HG13	0.92	1.64	1	1
1:B:359:ALA:O	1:B:362:ILE:HG22	0.92	1.65	1	2
1:B:104:ALA:O	1:B:107:VAL:HG22	0.91	1.64	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:292:VAL:HG21	1:A:329:VAL:HG13	0.91	1.40	1	1
1:A:175:LYS:C	1:A:175:LYS:CD	0.91	2.42	2	1
1:B:292:VAL:HG21	1:B:329:VAL:HG13	0.91	1.40	1	1
1:B:449:PHE:O	1:B:449:PHE:HD2	0.91	1.48	1	1
1:B:54:LEU:HD12	1:B:55:GLU:N	0.91	1.81	2	1
1:B:175:LYS:CD	1:B:175:LYS:C	0.90	2.43	2	1
1:B:242:VAL:O	1:B:246:VAL:HG13	0.90	1.64	1	1
1:B:221:ASP:CG	1:B:226:GLN:H	0.90	1.74	2	1
1:B:299:PHE:HD1	1:B:300:LEU:N	0.90	1.64	1	1
1:A:360:ILE:CD1	1:A:391:PRO:O	0.90	2.20	2	1
1:B:516:LEU:N	1:B:520:LEU:HD11	0.90	1.82	2	1
1:A:299:PHE:HD1	1:A:300:LEU:N	0.90	1.63	1	1
1:A:516:LEU:N	1:A:520:LEU:HD11	0.89	1.81	2	1
1:A:489:ILE:HA	1:A:499:THR:HG21	0.89	1.44	1	1
1:A:359:ALA:O	1:A:362:ILE:HG22	0.89	1.65	1	2
1:B:301:PHE:CG	1:B:342:LEU:HD22	0.89	2.03	2	1
1:A:269:VAL:HG13	1:A:521:ASP:O	0.89	1.66	2	1
1:B:221:ASP:HA	1:B:239:MET:HE2	0.89	1.41	2	2
1:B:269:VAL:HG13	1:B:521:ASP:O	0.89	1.66	2	1
1:A:221:ASP:CG	1:A:226:GLN:H	0.88	1.74	2	1
1:A:54:LEU:HD12	1:A:55:GLU:N	0.88	1.81	2	1
1:A:449:PHE:O	1:A:449:PHE:HD2	0.88	1.48	1	1
1:B:449:PHE:HE2	1:B:500:GLY:O	0.88	1.45	1	1
1:A:292:VAL:CG2	1:A:329:VAL:HG13	0.88	1.98	1	1
1:A:296:ARG:O	1:A:299:PHE:CE1	0.88	2.27	1	1
1:A:301:PHE:CG	1:A:342:LEU:HD22	0.88	2.04	2	1
1:A:372:ASP:C	1:A:372:ASP:OD1	0.87	2.17	2	1
1:A:355:LEU:O	1:B:464:ASP:CG	0.87	2.17	1	2
1:B:292:VAL:CG2	1:B:329:VAL:HG13	0.87	1.98	1	1
1:A:275:ILE:O	1:A:299:PHE:HE2	0.87	1.47	1	1
1:B:296:ARG:O	1:B:299:PHE:CE1	0.87	2.26	1	1
1:B:489:ILE:HG12	1:B:499:THR:HG21	0.87	1.44	2	1
1:B:263:THR:HG22	1:B:267:HIS:H	0.87	1.30	1	1
1:B:360:ILE:CD1	1:B:391:PRO:O	0.87	2.22	2	1
1:B:431:GLU:HG2	1:B:455:ASP:CB	0.86	1.99	1	1
1:A:489:ILE:HG12	1:A:499:THR:HG21	0.86	1.44	2	1
1:A:296:ARG:O	1:A:299:PHE:CG	0.86	2.28	1	1
1:A:12:ALA:HB1	1:A:177:LEU:HD13	0.86	1.47	2	1
1:B:372:ASP:OD1	1:B:372:ASP:C	0.86	2.17	2	1
1:B:296:ARG:O	1:B:299:PHE:CG	0.86	2.28	1	1
1:B:12:ALA:HB1	1:B:177:LEU:HD13	0.86	1.47	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:489:ILE:HA	1:B:499:THR:HG21	0.86	1.44	1	1
1:A:269:VAL:HG11	1:A:523:PHE:CZ	0.86	2.06	2	1
1:B:515:LEU:HA	1:B:520:LEU:CD2	0.86	1.98	2	1
1:B:269:VAL:HG11	1:B:523:PHE:CZ	0.86	2.06	2	1
1:A:431:GLU:HG2	1:A:455:ASP:CB	0.85	2.00	1	1
1:B:275:ILE:O	1:B:299:PHE:HE2	0.85	1.47	1	1
1:A:228:TYR:HB3	1:A:231:PRO:HG3	0.85	1.45	2	2
1:A:515:LEU:HB3	1:A:520:LEU:CD1	0.85	2.01	2	1
1:B:228:TYR:HB3	1:B:231:PRO:HG3	0.85	1.46	2	2
1:A:263:THR:HG22	1:A:267:HIS:H	0.85	1.30	1	1
1:B:50:ALA:O	1:B:54:LEU:HG	0.85	1.70	2	1
1:B:544:ASP:OD1	1:B:545:ALA:N	0.85	2.10	2	2
1:A:50:ALA:O	1:A:54:LEU:HG	0.85	1.70	2	1
1:B:115:LEU:HD11	2:D:651:GLN:HB3	0.85	1.48	2	1
1:B:527:ALA:O	1:B:530:ILE:HG23	0.85	1.69	2	1
1:A:544:ASP:OD1	1:A:545:ALA:N	0.85	2.10	2	2
1:A:115:LEU:HD11	2:C:651:GLN:HB3	0.84	1.48	2	1
1:B:175:LYS:C	1:B:175:LYS:HD3	0.84	1.96	2	1
1:A:175:LYS:C	1:A:175:LYS:HD3	0.84	1.97	2	1
1:B:51:SER:HA	1:B:54:LEU:HD21	0.84	1.49	2	1
1:B:278:VAL:O	1:B:281:VAL:HG22	0.84	1.73	2	1
1:B:515:LEU:C	1:B:520:LEU:CG	0.84	2.50	2	1
1:B:515:LEU:HB3	1:B:520:LEU:CD1	0.84	2.01	2	1
1:A:515:LEU:C	1:A:520:LEU:CG	0.83	2.50	2	1
1:A:78:MET:CE	2:C:627:LYS:CD	0.83	2.32	1	1
1:A:302:MET:HB2	1:A:342:LEU:HD21	0.83	1.49	1	1
1:B:449:PHE:CD2	1:B:499:THR:CB	0.83	2.60	1	1
1:A:449:PHE:CD2	1:A:499:THR:CB	0.83	2.60	1	1
1:B:78:MET:CE	2:D:627:LYS:CD	0.83	2.28	1	1
1:A:337:GLY:O	1:A:358:ARG:CZ	0.83	2.27	2	1
1:B:337:GLY:O	1:B:358:ARG:CZ	0.83	2.27	2	1
1:B:314:PHE:CZ	1:B:376:ALA:CA	0.83	2.56	1	1
1:A:350:GLU:N	1:A:350:GLU:CD	0.83	2.37	2	1
1:A:314:PHE:CE2	1:A:379:ARG:HB3	0.83	2.09	1	1
1:A:336:ILE:H	1:A:336:ILE:HD12	0.83	1.34	2	1
1:A:304:ARG:O	1:A:344:TYR:CZ	0.83	2.32	1	1
1:B:314:PHE:CE2	1:B:379:ARG:HB3	0.83	2.08	1	1
1:B:304:ARG:O	1:B:344:TYR:CZ	0.82	2.32	1	1
1:B:394:ILE:HD13	1:B:394:ILE:H	0.82	1.33	2	1
1:B:177:LEU:HD12	1:B:177:LEU:H	0.82	1.35	1	1
1:A:51:SER:HA	1:A:54:LEU:HD21	0.82	1.49	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:394:ILE:HD13	1:A:394:ILE:H	0.82	1.34	2	1
1:B:463:VAL:CG1	1:B:473:LEU:HG	0.81	2.04	1	1
1:B:350:GLU:CD	1:B:350:GLU:N	0.81	2.37	2	1
1:A:177:LEU:H	1:A:177:LEU:HD12	0.81	1.34	1	1
1:B:296:ARG:O	1:B:299:PHE:CD1	0.81	2.32	1	1
1:A:474:TYR:CG	1:A:474:TYR:O	0.81	2.34	2	1
1:B:360:ILE:HD13	1:B:390:PHE:CD2	0.81	2.10	2	1
1:A:314:PHE:CZ	1:A:376:ALA:CA	0.81	2.56	1	1
1:A:556:PRO:HB3	1:B:441:HIS:ND1	0.81	1.89	1	2
1:B:449:PHE:CD2	1:B:499:THR:CA	0.81	2.63	1	1
1:A:356:GLY:O	1:A:358:ARG:HG2	0.81	1.75	2	1
1:A:527:ALA:O	1:A:530:ILE:HG23	0.81	1.72	2	1
1:A:449:PHE:CD2	1:A:499:THR:CA	0.81	2.63	1	1
1:B:534:LYS:O	1:B:537:ILE:HG13	0.81	1.76	2	1
1:A:463:VAL:CG1	1:A:473:LEU:HG	0.80	2.04	1	1
1:A:296:ARG:O	1:A:299:PHE:CD1	0.80	2.34	1	1
1:B:464:ASP:OD1	1:B:464:ASP:N	0.80	2.15	1	2
1:A:126:ARG:HD3	2:C:616:THR:OG1	0.80	1.76	2	1
1:A:111:GLN:CD	2:C:648:PHE:HB3	0.80	2.01	1	2
1:A:299:PHE:CD1	1:A:300:LEU:N	0.80	2.49	1	1
1:B:456:LEU:HD11	1:B:481:VAL:CG1	0.80	2.07	1	1
1:B:356:GLY:O	1:B:358:ARG:HG2	0.80	1.74	2	1
1:B:449:PHE:CD2	1:B:499:THR:HA	0.80	2.11	1	1
1:B:177:LEU:HD12	1:B:177:LEU:O	0.80	1.77	2	1
1:B:474:TYR:O	1:B:474:TYR:CG	0.80	2.34	2	2
1:A:177:LEU:O	1:A:177:LEU:HD12	0.80	1.77	2	1
1:B:388:ILE:HD12	1:B:389:MET:N	0.80	1.92	2	1
1:A:74:GLU:OE1	2:C:624:LYS:NZ	0.80	2.15	1	1
1:B:336:ILE:HD12	1:B:336:ILE:H	0.80	1.34	2	1
1:A:199:LEU:HD23	1:A:199:LEU:O	0.79	1.78	1	1
1:A:205:THR:OG1	1:A:208:VAL:HG22	0.79	1.76	1	1
1:A:449:PHE:CD2	1:A:499:THR:HA	0.79	2.11	1	1
1:B:111:GLN:CD	2:D:648:PHE:HB3	0.79	2.01	1	2
1:B:126:ARG:HD3	2:D:616:THR:OG1	0.79	1.77	2	1
1:A:360:ILE:HD13	1:A:390:PHE:CD2	0.79	2.11	2	1
1:A:534:LYS:O	1:A:537:ILE:HG13	0.79	1.76	2	1
1:A:431:GLU:HG2	1:A:455:ASP:HB3	0.79	1.54	1	1
1:B:199:LEU:HD23	1:B:199:LEU:O	0.79	1.78	1	1
1:B:299:PHE:CD1	1:B:300:LEU:N	0.79	2.50	1	1
1:B:74:GLU:OE1	2:D:624:LYS:NZ	0.78	2.16	1	1
1:A:456:LEU:HD11	1:A:481:VAL:CG1	0.78	2.07	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:431:GLU:HG2	1:B:455:ASP:HB3	0.78	1.53	1	1
1:B:449:PHE:CD1	1:B:488:VAL:HG11	0.78	2.14	1	1
1:A:302:MET:SD	1:A:342:LEU:HG	0.78	2.19	2	1
1:A:438:ILE:CG2	1:A:441:HIS:HB2	0.78	2.09	2	1
1:A:353:PRO:O	1:A:358:ARG:CD	0.78	2.32	2	1
1:A:449:PHE:CD1	1:A:488:VAL:HG11	0.78	2.14	1	1
1:B:205:THR:OG1	1:B:208:VAL:HG22	0.78	1.78	1	1
1:A:301:PHE:CD2	1:A:342:LEU:HD22	0.78	2.14	2	1
1:A:388:ILE:HD12	1:A:389:MET:N	0.78	1.94	2	1
1:B:438:ILE:CG2	1:B:441:HIS:HB2	0.78	2.08	2	1
1:A:11:ILE:CD1	1:A:221:ASP:O	0.78	2.32	2	2
1:A:160:ALA:O	1:A:181:THR:HG23	0.78	1.79	1	1
1:A:515:LEU:HA	1:A:520:LEU:CD2	0.77	1.98	2	1
1:B:353:PRO:O	1:B:358:ARG:CD	0.77	2.32	2	1
1:B:13:PHE:CZ	1:B:240:ARG:HD2	0.77	2.15	2	2
1:B:11:ILE:CD1	1:B:221:ASP:O	0.77	2.33	2	2
1:B:160:ALA:O	1:B:181:THR:HG23	0.77	1.79	1	1
1:B:50:ALA:O	1:B:54:LEU:CG	0.77	2.33	2	1
1:B:476:PRO:O	1:B:481:VAL:CG2	0.77	2.33	2	1
1:B:402:LEU:HD13	1:B:403:ARG:N	0.76	1.96	2	1
1:A:476:PRO:O	1:A:481:VAL:CG2	0.76	2.33	2	1
1:A:50:ALA:O	1:A:54:LEU:CG	0.76	2.33	2	1
1:B:175:LYS:HD3	1:B:176:VAL:N	0.76	1.96	2	1
1:A:13:PHE:CZ	1:A:240:ARG:HD2	0.76	2.15	1	2
1:A:317:TYR:OH	1:A:331:VAL:HB	0.76	1.80	1	1
1:B:79:LEU:HD13	2:D:647:LEU:HB3	0.76	1.56	1	2
1:B:301:PHE:CD2	1:B:342:LEU:HD22	0.76	2.14	2	1
1:B:337:GLY:O	1:B:358:ARG:NE	0.76	2.19	2	1
1:A:79:LEU:HD13	2:C:647:LEU:HB3	0.76	1.56	1	2
1:A:314:PHE:CE2	1:A:376:ALA:C	0.76	2.63	1	1
1:B:314:PHE:CE2	1:B:376:ALA:C	0.76	2.63	1	1
1:A:307:LEU:O	1:A:307:LEU:HD23	0.76	1.80	2	1
1:B:115:LEU:CD1	2:D:651:GLN:HB3	0.76	2.09	2	1
1:A:314:PHE:CD2	1:A:376:ALA:CA	0.76	2.61	1	1
1:B:314:PHE:CD2	1:B:376:ALA:CA	0.76	2.61	1	1
1:A:115:LEU:CD1	2:C:651:GLN:HB3	0.76	2.09	2	1
1:A:177:LEU:HD12	1:A:177:LEU:C	0.76	2.06	2	1
1:A:402:LEU:HD13	1:A:403:ARG:N	0.76	1.96	2	1
1:A:449:PHE:CE2	1:A:499:THR:CB	0.75	2.70	1	1
1:A:449:PHE:HD2	1:A:499:THR:HA	0.75	1.42	1	1
1:B:431:GLU:CG	1:B:452:GLY:O	0.75	2.28	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:278:VAL:O	1:A:281:VAL:HG22	0.75	1.80	2	1
1:A:292:VAL:HG11	1:A:329:VAL:HG22	0.75	1.58	1	1
1:A:431:GLU:HG3	1:A:452:GLY:C	0.75	2.06	1	1
1:B:296:ARG:N	1:B:299:PHE:CE2	0.75	2.55	1	1
1:B:449:PHE:CE2	1:B:499:THR:CB	0.75	2.69	1	1
1:B:307:LEU:HD23	1:B:307:LEU:O	0.75	1.81	2	1
1:B:454:ASN:O	1:B:457:THR:HG22	0.75	1.82	2	1
1:A:70:GLU:CD	1:A:70:GLU:C	0.75	2.55	1	2
1:A:449:PHE:CE1	1:A:451:ILE:HB	0.75	2.16	1	1
1:B:304:ARG:NH1	1:B:342:LEU:HD23	0.75	1.97	2	1
1:A:337:GLY:O	1:A:358:ARG:NE	0.75	2.19	2	1
1:B:162:ASP:HA	1:B:181:THR:HG21	0.75	1.57	1	1
1:A:515:LEU:O	1:A:520:LEU:CD1	0.75	2.30	2	1
1:A:431:GLU:CD	1:A:455:ASP:HB2	0.75	2.07	1	1
1:B:431:GLU:CD	1:B:455:ASP:HB2	0.75	2.07	1	1
1:B:449:PHE:CE1	1:B:451:ILE:HB	0.75	2.16	1	1
1:B:177:LEU:HD12	1:B:177:LEU:C	0.75	2.06	2	1
1:B:317:TYR:OH	1:B:331:VAL:HB	0.74	1.82	1	1
1:A:464:ASP:OD1	1:A:464:ASP:N	0.74	2.14	1	2
1:B:70:GLU:C	1:B:70:GLU:CD	0.74	2.55	1	2
1:A:454:ASN:O	1:A:457:THR:HG22	0.74	1.82	2	1
1:A:162:ASP:HA	1:A:181:THR:HG21	0.74	1.57	1	1
1:B:314:PHE:CZ	1:B:375:ARG:C	0.74	2.65	1	1
1:B:362:ILE:CG2	1:B:363:ALA:N	0.74	2.50	2	2
1:B:449:PHE:HD2	1:B:499:THR:HA	0.74	1.42	1	1
1:A:301:PHE:O	1:A:304:ARG:CD	0.74	2.36	2	1
1:B:372:ASP:CG	1:B:373:GLN:N	0.74	2.45	1	1
1:B:431:GLU:HG3	1:B:452:GLY:C	0.74	2.07	1	1
1:B:515:LEU:O	1:B:520:LEU:CD1	0.74	2.31	2	1
1:A:175:LYS:HD3	1:A:176:VAL:N	0.74	1.96	2	1
1:A:296:ARG:C	1:A:299:PHE:CE2	0.74	2.66	1	1
1:A:449:PHE:CD1	1:A:488:VAL:CG1	0.74	2.71	1	1
1:B:292:VAL:HG11	1:B:329:VAL:HG22	0.74	1.59	1	1
1:A:296:ARG:N	1:A:299:PHE:CE2	0.73	2.55	1	1
1:A:314:PHE:CZ	1:A:375:ARG:C	0.73	2.65	1	1
1:A:314:PHE:CD2	1:A:376:ALA:O	0.73	2.40	1	1
1:A:362:ILE:CG2	1:A:363:ALA:N	0.73	2.50	2	2
1:A:463:VAL:HG21	1:A:473:LEU:CD2	0.73	2.12	1	1
1:B:314:PHE:CD2	1:B:376:ALA:O	0.73	2.40	1	1
1:B:449:PHE:CD1	1:B:488:VAL:CG1	0.73	2.71	1	1
1:A:512:THR:O	1:A:516:LEU:HG	0.73	1.83	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:126:ARG:HH11	2:D:651:GLN:NE2	0.73	1.81	2	1
1:A:317:TYR:CZ	1:A:331:VAL:HB	0.73	2.18	1	1
1:A:456:LEU:C	1:A:456:LEU:HD22	0.73	2.09	1	1
1:B:272:CYS:SG	1:B:293:GLY:CA	0.73	2.76	2	1
1:B:263:THR:OG1	1:B:540:THR:HG23	0.73	1.84	1	1
1:B:296:ARG:C	1:B:299:PHE:CE2	0.73	2.66	1	1
1:A:272:CYS:SG	1:A:273:ALA:N	0.73	2.62	2	1
1:A:10:GLY:O	1:A:11:ILE:HD13	0.73	1.82	1	2
1:B:362:ILE:HG23	1:B:363:ALA:N	0.73	1.99	1	2
1:B:353:PRO:O	1:B:358:ARG:HD3	0.73	1.84	2	1
1:A:372:ASP:CG	1:A:373:GLN:N	0.73	2.45	1	1
1:A:464:ASP:CG	1:A:467:ASN:ND2	0.73	2.46	1	1
1:B:228:TYR:CD2	1:B:235:VAL:HG11	0.73	2.19	1	2
1:B:232:THR:O	1:B:236:ILE:HG13	0.73	1.84	2	2
1:A:228:TYR:CD2	1:A:235:VAL:HG11	0.73	2.19	2	2
1:B:317:TYR:CZ	1:B:331:VAL:HB	0.73	2.19	1	1
1:A:272:CYS:SG	1:A:293:GLY:CA	0.73	2.76	2	1
1:B:512:THR:O	1:B:516:LEU:HG	0.73	1.83	2	1
1:A:304:ARG:O	1:A:344:TYR:CE1	0.72	2.42	1	1
1:B:456:LEU:HD22	1:B:456:LEU:O	0.72	1.84	1	1
1:B:74:GLU:HA	1:B:77:ILE:CG2	0.72	2.14	2	1
1:B:485:ILE:HD11	1:B:501:MET:SD	0.72	2.24	2	1
1:A:232:THR:O	1:A:236:ILE:HG13	0.72	1.84	1	2
1:B:464:ASP:CG	1:B:467:ASN:ND2	0.72	2.46	1	1
1:B:530:ILE:HD12	1:B:530:ILE:O	0.72	1.84	2	1
1:A:126:ARG:HD3	2:C:651:GLN:CG	0.72	2.14	1	1
1:A:434:ALA:O	1:A:437:THR:OG1	0.72	2.07	1	1
1:B:179:PHE:CZ	1:B:181:THR:OG1	0.72	2.40	1	1
1:B:302:MET:HB2	1:B:342:LEU:HD21	0.72	1.60	1	1
1:A:485:ILE:HD11	1:A:501:MET:SD	0.72	2.24	2	1
1:A:456:LEU:HD22	1:A:456:LEU:O	0.72	1.84	1	1
1:A:441:HIS:ND1	1:B:556:PRO:HB3	0.72	1.99	1	2
1:B:456:LEU:HD22	1:B:456:LEU:C	0.72	2.09	1	1
1:B:463:VAL:HG21	1:B:473:LEU:CD2	0.72	2.14	1	1
1:B:10:GLY:O	1:B:11:ILE:HD13	0.72	1.85	1	2
1:A:263:THR:OG1	1:A:540:THR:HG23	0.72	1.84	1	1
1:B:219:ILE:HD11	1:B:236:ILE:HG12	0.72	1.62	2	2
1:B:228:TYR:CB	1:B:231:PRO:HG3	0.72	2.14	1	2
1:B:434:ALA:O	1:B:437:THR:OG1	0.72	2.07	1	1
1:A:74:GLU:HA	1:A:77:ILE:CG2	0.72	2.14	2	1
1:A:353:PRO:O	1:A:358:ARG:HD3	0.72	1.84	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:80:LEU:HD13	1:B:80:LEU:O	0.72	1.84	2	1
1:B:272:CYS:SG	1:B:273:ALA:N	0.72	2.62	2	1
1:A:80:LEU:HD13	1:A:80:LEU:O	0.72	1.84	2	1
1:A:228:TYR:CB	1:A:231:PRO:HG3	0.71	2.14	2	2
1:A:456:LEU:CD1	1:A:457:THR:N	0.71	2.50	1	1
1:B:126:ARG:HD3	2:D:651:GLN:CG	0.71	2.14	1	1
1:B:515:LEU:C	1:B:520:LEU:HD21	0.71	2.09	2	1
1:B:304:ARG:O	1:B:344:TYR:CE1	0.71	2.43	1	1
1:B:456:LEU:CD1	1:B:457:THR:N	0.71	2.50	1	1
1:A:428:VAL:HG12	1:A:429:MET:O	0.71	1.85	2	1
1:A:354:PHE:H	1:B:352:ASN:HD21	0.71	1.27	1	2
1:A:362:ILE:HG23	1:A:363:ALA:N	0.71	1.99	1	2
1:A:294:LEU:HD11	1:A:332:ARG:NH2	0.71	2.00	2	1
1:A:530:ILE:O	1:A:530:ILE:HD12	0.71	1.85	2	1
1:A:476:PRO:O	1:A:481:VAL:HG21	0.71	1.85	2	1
1:A:431:GLU:CG	1:A:452:GLY:O	0.71	2.28	1	1
1:B:428:VAL:HG12	1:B:429:MET:O	0.71	1.85	2	1
1:A:567:LYS:O	1:A:571:GLU:HG3	0.70	1.87	1	2
1:A:126:ARG:HD3	2:C:651:GLN:HG3	0.70	1.62	1	1
1:A:73:PHE:O	1:A:77:ILE:HG22	0.70	1.87	2	1
1:B:301:PHE:O	1:B:304:ARG:CD	0.70	2.39	2	1
1:A:179:PHE:CZ	1:A:181:THR:OG1	0.70	2.40	1	1
1:B:456:LEU:HD11	1:B:481:VAL:HG13	0.70	1.63	1	1
1:A:347:PHE:N	1:A:347:PHE:CD1	0.70	2.59	2	1
1:B:377:ILE:C	1:B:377:ILE:HD12	0.70	2.11	1	1
1:A:126:ARG:HH11	2:C:651:GLN:NE2	0.70	1.84	2	1
1:B:73:PHE:O	1:B:77:ILE:HG22	0.70	1.87	2	1
1:A:90:ILE:HD12	1:A:91:ALA:N	0.70	2.01	1	1
1:A:456:LEU:HD11	1:A:481:VAL:HG13	0.70	1.64	1	1
1:B:90:ILE:HD12	1:B:91:ALA:N	0.70	2.01	1	1
1:B:304:ARG:CG	1:B:306:ALA:O	0.70	2.40	2	1
1:A:377:ILE:C	1:A:377:ILE:HD12	0.69	2.11	1	1
1:B:567:LYS:O	1:B:571:GLU:HG3	0.69	1.87	1	2
1:A:476:PRO:C	1:A:481:VAL:HG21	0.69	2.12	2	1
1:A:515:LEU:C	1:A:520:LEU:HD21	0.69	2.11	2	1
1:B:476:PRO:O	1:B:481:VAL:HG21	0.69	1.85	2	1
1:A:464:ASP:OD1	1:A:467:ASN:CG	0.69	2.35	2	2
1:B:11:ILE:HD12	1:B:239:MET:CE	0.69	2.16	2	2
1:A:219:ILE:HD11	1:A:236:ILE:HG12	0.69	1.62	1	2
1:A:228:TYR:CG	1:A:235:VAL:HG11	0.69	2.22	2	2
1:B:228:TYR:CG	1:B:235:VAL:HG11	0.69	2.23	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HD12	1:A:239:MET:CE	0.69	2.17	2	2
1:A:377:ILE:HD12	1:A:377:ILE:O	0.69	1.87	1	1
1:B:13:PHE:CE2	1:B:240:ARG:HD2	0.69	2.23	1	2
1:B:377:ILE:HD12	1:B:377:ILE:O	0.69	1.87	1	1
1:A:304:ARG:NH1	1:A:342:LEU:HD23	0.69	2.03	2	1
1:B:476:PRO:C	1:B:481:VAL:HG21	0.69	2.12	2	1
1:B:6:LEU:N	1:B:6:LEU:HD22	0.69	2.03	2	1
1:A:232:THR:HG23	1:A:233:ASN:H	0.69	1.47	1	2
1:B:181:THR:O	1:B:205:THR:CG2	0.69	2.41	1	1
1:B:126:ARG:HD3	2:D:651:GLN:HG3	0.69	1.62	1	1
1:A:556:PRO:HB3	1:B:441:HIS:CG	0.69	2.23	1	2
1:B:464:ASP:OD1	1:B:467:ASN:CG	0.69	2.36	2	2
1:A:181:THR:O	1:A:205:THR:CG2	0.68	2.41	1	1
1:B:294:LEU:HD11	1:B:332:ARG:NH2	0.68	2.03	2	1
1:A:264:LEU:HD23	1:A:264:LEU:C	0.68	2.13	2	1
1:A:467:ASN:ND2	1:A:470:ILE:CG1	0.68	2.56	1	1
1:A:6:LEU:N	1:A:6:LEU:HD22	0.68	2.03	2	1
1:A:13:PHE:CE2	1:A:240:ARG:HD2	0.68	2.23	2	2
1:B:314:PHE:CE2	1:B:376:ALA:O	0.68	2.47	1	1
1:A:304:ARG:CG	1:A:306:ALA:O	0.68	2.41	2	1
1:B:317:TYR:CE2	1:B:386:LEU:HD22	0.68	2.24	1	1
1:B:301:PHE:O	1:B:304:ARG:NH1	0.68	2.26	2	1
1:B:467:ASN:ND2	1:B:470:ILE:CG1	0.68	2.56	1	1
1:A:314:PHE:CE2	1:A:376:ALA:O	0.68	2.47	1	1
1:A:177:LEU:HD12	1:A:177:LEU:N	0.68	2.03	1	1
1:A:317:TYR:CE1	1:A:331:VAL:HG21	0.68	2.24	1	1
1:B:177:LEU:HD12	1:B:177:LEU:N	0.68	2.03	1	1
1:A:515:LEU:CB	1:A:520:LEU:CD2	0.68	2.72	2	1
1:B:530:ILE:HD12	1:B:530:ILE:C	0.68	2.14	2	1
1:A:107:VAL:HG23	1:A:108:ILE:N	0.67	2.04	2	1
1:B:107:VAL:HG23	1:B:108:ILE:N	0.67	2.03	2	1
1:B:264:LEU:C	1:B:264:LEU:HD23	0.67	2.13	2	1
1:A:13:PHE:CG	1:A:240:ARG:NH1	0.67	2.63	2	2
1:B:13:PHE:CG	1:B:240:ARG:NH1	0.67	2.63	2	2
1:A:336:ILE:HD12	1:A:336:ILE:N	0.67	2.05	2	1
1:A:355:LEU:CD2	1:A:355:LEU:N	0.67	2.58	2	1
1:A:389:MET:HE2	1:A:428:VAL:C	0.67	2.15	1	1
1:A:515:LEU:CB	1:A:520:LEU:HD21	0.67	2.20	2	1
1:B:157:ILE:CG1	1:B:177:LEU:HD21	0.67	2.19	2	1
1:B:515:LEU:O	1:B:520:LEU:CD2	0.67	2.42	2	1
1:A:221:ASP:HA	1:A:239:MET:HE1	0.67	1.66	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:352:ASN:HD21	1:B:354:PHE:H	0.67	1.30	2	2
1:B:232:THR:HG23	1:B:233:ASN:H	0.67	1.48	1	2
1:B:263:THR:OG1	1:B:540:THR:O	0.67	2.11	1	1
1:B:296:ARG:CA	1:B:299:PHE:CE2	0.67	2.77	1	1
1:A:304:ARG:O	1:A:344:TYR:OH	0.67	2.12	1	1
1:B:296:ARG:C	1:B:299:PHE:CZ	0.67	2.72	1	1
1:B:296:ARG:CB	1:B:299:PHE:CD2	0.67	2.78	1	1
1:A:304:ARG:NE	1:A:306:ALA:O	0.67	2.28	2	1
1:B:515:LEU:CB	1:B:520:LEU:CD2	0.67	2.72	2	1
1:A:314:PHE:CZ	1:A:376:ALA:N	0.67	2.63	1	1
1:A:515:LEU:HB3	1:A:520:LEU:HD13	0.67	1.66	2	1
1:A:127:ALA:O	1:A:130:VAL:HG22	0.67	1.90	1	1
1:A:179:PHE:CE1	1:A:190:THR:HG21	0.67	2.25	1	1
1:A:276:GLY:HA2	1:A:299:PHE:CG	0.67	2.21	1	1
1:A:157:ILE:CG1	1:A:177:LEU:HD21	0.67	2.19	2	1
1:B:336:ILE:HD12	1:B:336:ILE:N	0.67	2.05	2	1
1:A:296:ARG:CB	1:A:299:PHE:CD2	0.66	2.79	1	1
1:B:221:ASP:HA	1:B:239:MET:HE1	0.66	1.66	1	2
1:B:304:ARG:O	1:B:344:TYR:OH	0.66	2.13	1	1
1:B:389:MET:HE2	1:B:428:VAL:C	0.66	2.16	1	1
1:A:230:ASN:N	1:A:231:PRO:CD	0.66	2.59	1	2
1:A:296:ARG:C	1:A:299:PHE:CZ	0.66	2.73	1	1
1:A:367:ARG:C	1:A:371:ARG:HG3	0.66	2.15	2	1
1:A:292:VAL:HG21	1:A:329:VAL:CG1	0.66	2.18	1	1
1:A:296:ARG:CA	1:A:299:PHE:CE2	0.66	2.78	1	1
1:B:179:PHE:CE1	1:B:190:THR:HG21	0.66	2.26	1	1
1:B:314:PHE:CZ	1:B:376:ALA:N	0.66	2.62	1	1
1:A:73:PHE:C	1:A:73:PHE:CD2	0.66	2.73	2	1
1:A:232:THR:HG22	1:A:234:GLU:H	0.66	1.50	1	2
1:B:230:ASN:N	1:B:231:PRO:CD	0.66	2.59	1	2
1:B:292:VAL:HG21	1:B:329:VAL:CG1	0.66	2.19	1	1
1:B:296:ARG:CB	1:B:299:PHE:CE2	0.66	2.79	1	1
1:B:126:ARG:NH1	2:D:651:GLN:NE2	0.66	2.43	2	1
1:A:314:PHE:CD2	1:A:379:ARG:HB3	0.66	2.25	1	1
1:A:263:THR:OG1	1:A:540:THR:O	0.65	2.12	1	1
1:A:530:ILE:HD12	1:A:530:ILE:C	0.65	2.16	2	1
1:B:515:LEU:HB3	1:B:520:LEU:HD13	0.65	1.67	2	1
1:B:515:LEU:CB	1:B:520:LEU:HD21	0.65	2.19	2	1
1:A:317:TYR:CE2	1:A:386:LEU:HD22	0.65	2.26	1	1
1:B:314:PHE:CD2	1:B:379:ARG:HB3	0.65	2.25	1	1
1:B:73:PHE:C	1:B:73:PHE:CD2	0.65	2.74	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:259:LEU:HB2	1:B:262:ILE:CG1	0.65	2.21	2	1
1:A:230:ASN:N	1:A:231:PRO:HD3	0.65	2.07	1	2
1:B:317:TYR:CE1	1:B:331:VAL:HG21	0.65	2.27	1	1
1:A:515:LEU:O	1:A:520:LEU:CD2	0.65	2.43	2	1
1:A:276:GLY:CA	1:A:299:PHE:CG	0.65	2.80	1	1
1:A:402:LEU:HD13	1:A:402:LEU:C	0.65	2.17	2	1
1:B:355:LEU:N	1:B:355:LEU:CD2	0.65	2.60	2	1
1:A:10:GLY:O	1:A:222:ALA:HB3	0.65	1.92	1	2
1:A:198:GLU:O	1:A:199:LEU:HD22	0.65	1.91	2	1
1:A:406:ILE:HD13	1:A:426:ILE:HD13	0.65	1.68	1	2
1:B:406:ILE:HD13	1:B:426:ILE:HD13	0.65	1.68	1	2
1:B:438:ILE:O	1:B:438:ILE:HG23	0.65	1.92	1	1
1:B:232:THR:HG22	1:B:234:GLU:H	0.65	1.51	2	2
1:A:175:LYS:CD	1:A:176:VAL:N	0.65	2.59	2	1
1:B:269:VAL:CG1	1:B:523:PHE:CZ	0.65	2.80	2	1
1:B:515:LEU:C	1:B:520:LEU:CD2	0.65	2.69	2	1
1:A:331:VAL:HG13	1:A:331:VAL:O	0.65	1.91	1	1
1:B:10:GLY:O	1:B:222:ALA:HB3	0.65	1.92	2	2
1:B:276:GLY:HA2	1:B:299:PHE:CG	0.65	2.21	1	1
1:A:269:VAL:HG13	1:A:521:ASP:C	0.65	2.17	2	1
1:B:11:ILE:HD12	1:B:239:MET:HE1	0.65	1.69	1	2
1:B:295:TYR:OH	1:B:300:LEU:HD22	0.65	1.92	1	1
1:A:314:PHE:CE2	1:A:375:ARG:O	0.65	2.50	1	1
1:B:374:LEU:HA	1:B:377:ILE:CG2	0.64	2.22	1	1
1:A:72:ILE:HD11	2:C:616:THR:HG21	0.64	1.69	2	1
1:A:438:ILE:HG22	1:A:441:HIS:HB2	0.64	1.67	2	1
1:B:198:GLU:O	1:B:199:LEU:HD22	0.64	1.91	2	1
1:B:269:VAL:HG13	1:B:521:ASP:C	0.64	2.16	2	1
1:B:230:ASN:N	1:B:231:PRO:HD3	0.64	2.07	1	2
1:A:11:ILE:HD12	1:A:239:MET:HE1	0.64	1.69	1	2
1:A:295:TYR:OH	1:A:300:LEU:HD22	0.64	1.92	1	1
1:A:126:ARG:NH1	2:C:651:GLN:NE2	0.64	2.46	2	1
1:B:301:PHE:C	1:B:342:LEU:HD21	0.64	2.18	2	1
1:A:449:PHE:CE1	1:A:488:VAL:HG11	0.64	2.27	1	1
1:B:314:PHE:CE2	1:B:375:ARG:O	0.64	2.50	1	1
1:A:357:TRP:CD1	1:A:358:ARG:NH2	0.64	2.66	2	1
1:A:515:LEU:C	1:A:520:LEU:CD2	0.64	2.70	2	1
1:B:367:ARG:C	1:B:371:ARG:HG3	0.64	2.15	2	1
1:B:402:LEU:HD13	1:B:402:LEU:C	0.64	2.16	2	1
1:B:317:TYR:OH	1:B:373:GLN:NE2	0.64	2.30	2	1
1:B:347:PHE:N	1:B:347:PHE:CD1	0.64	2.59	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:374:LEU:HA	1:A:377:ILE:CG2	0.64	2.22	1	1
1:A:449:PHE:HZ	1:A:451:ILE:HB	0.64	1.50	1	1
1:B:276:GLY:CA	1:B:299:PHE:CG	0.64	2.80	1	1
1:B:525:MET:HG3	1:B:526:SER:N	0.64	2.08	1	1
1:B:175:LYS:CD	1:B:176:VAL:N	0.64	2.59	2	1
1:B:70:GLU:CG	1:B:71:ALA:N	0.64	2.61	1	1
1:B:449:PHE:CE1	1:B:488:VAL:HG11	0.64	2.26	1	1
1:B:451:ILE:CG2	1:B:451:ILE:O	0.64	2.46	1	1
1:A:438:ILE:HG23	1:A:438:ILE:O	0.64	1.92	1	1
1:A:451:ILE:O	1:A:451:ILE:CG2	0.64	2.46	1	1
1:A:261:ALA:C	1:A:537:ILE:HD13	0.63	2.18	2	1
1:A:304:ARG:NH1	1:A:304:ARG:O	0.63	2.31	2	1
1:B:453:THR:HG22	1:B:503:GLY:HA3	0.63	1.70	1	1
1:B:72:ILE:HD11	2:D:616:THR:HG21	0.63	1.69	2	1
1:B:192:ILE:C	1:B:192:ILE:HD12	0.63	2.19	1	1
1:A:221:ASP:OD2	1:A:224:ASN:C	0.63	2.40	2	1
1:B:221:ASP:OD2	1:B:224:ASN:C	0.63	2.40	2	1
1:B:394:ILE:HD13	1:B:394:ILE:N	0.63	2.00	2	1
1:A:296:ARG:CB	1:A:299:PHE:CE2	0.63	2.80	1	1
1:A:463:VAL:CG2	1:A:473:LEU:HD21	0.63	2.23	1	1
1:B:127:ALA:O	1:B:130:VAL:HG22	0.63	1.93	1	1
1:A:126:ARG:CD	2:C:616:THR:OG1	0.63	2.46	2	1
1:A:301:PHE:O	1:A:304:ARG:NH1	0.63	2.32	2	1
1:B:304:ARG:NH1	1:B:304:ARG:O	0.63	2.32	2	1
1:B:357:TRP:CD1	1:B:358:ARG:NH2	0.63	2.66	2	1
1:B:11:ILE:HG23	1:B:239:MET:CE	0.63	2.24	1	2
1:A:126:ARG:HD3	2:C:651:GLN:CD	0.63	2.19	1	1
1:A:537:ILE:O	1:A:540:THR:HG22	0.63	1.94	1	1
1:B:342:LEU:HD12	1:B:344:TYR:CE1	0.63	2.29	1	1
1:A:301:PHE:C	1:A:342:LEU:HD21	0.63	2.18	2	1
1:B:252:GLU:OE1	1:B:255:LYS:NZ	0.63	2.32	2	1
1:B:537:ILE:O	1:B:540:THR:HG22	0.63	1.93	1	1
1:B:304:ARG:HE	1:B:306:ALA:C	0.63	2.01	2	1
1:A:525:MET:HG3	1:A:526:SER:N	0.62	2.08	1	1
1:B:276:GLY:HA2	1:B:299:PHE:CZ	0.62	2.24	1	1
1:A:11:ILE:HG23	1:A:239:MET:CE	0.62	2.24	1	2
1:A:441:HIS:CG	1:B:556:PRO:HB3	0.62	2.28	1	2
1:B:4:GLY:HA3	1:B:202:ILE:HD11	0.62	1.71	1	1
1:B:331:VAL:HG13	1:B:331:VAL:O	0.62	1.92	1	1
1:A:256:LEU:O	1:A:258:ASP:N	0.62	2.32	2	1
1:B:126:ARG:HD3	2:D:651:GLN:CD	0.62	2.19	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:304:ARG:HG2	1:A:306:ALA:H	0.62	1.55	2	1
1:A:192:ILE:HD12	1:A:192:ILE:C	0.62	2.20	1	1
1:B:525:MET:CG	1:B:526:SER:N	0.62	2.62	1	1
1:A:70:GLU:CG	1:A:71:ALA:N	0.62	2.62	1	1
1:B:50:ALA:O	1:B:54:LEU:CD2	0.62	2.47	2	1
1:A:394:ILE:HD13	1:A:394:ILE:N	0.62	2.00	2	1
1:B:115:LEU:HD11	2:D:651:GLN:CB	0.62	2.23	2	1
1:A:342:LEU:HD12	1:A:344:TYR:CE1	0.62	2.30	1	1
1:B:541:ASN:O	1:B:544:ASP:CG	0.62	2.43	1	2
1:B:126:ARG:CD	2:D:616:THR:OG1	0.62	2.47	2	1
1:A:317:TYR:OH	1:A:373:GLN:NE2	0.62	2.33	2	1
1:B:304:ARG:HG2	1:B:306:ALA:H	0.62	1.54	2	1
1:A:269:VAL:CG1	1:A:523:PHE:CZ	0.62	2.81	2	1
1:A:173:LEU:N	1:A:173:LEU:HD22	0.61	2.10	1	1
1:A:525:MET:CG	1:A:526:SER:N	0.61	2.62	1	1
1:B:261:ALA:C	1:B:537:ILE:HD13	0.61	2.19	2	1
1:B:304:ARG:NE	1:B:306:ALA:O	0.61	2.33	2	1
1:A:453:THR:HG22	1:A:503:GLY:HA3	0.61	1.70	1	1
1:A:513:LEU:H	1:A:513:LEU:HD22	0.61	1.53	1	1
1:A:115:LEU:HD11	2:C:651:GLN:CB	0.61	2.23	2	1
1:A:489:ILE:O	1:A:492:SER:HB2	0.61	1.95	1	2
1:A:58:LYS:HB2	1:A:73:PHE:CG	0.61	2.30	2	1
1:A:337:GLY:O	1:A:358:ARG:CD	0.61	2.49	2	1
1:B:72:ILE:HD13	1:B:72:ILE:O	0.61	1.95	2	1
1:A:50:ALA:O	1:A:54:LEU:CD2	0.61	2.48	2	1
1:B:350:GLU:HB3	1:B:357:TRP:CZ2	0.61	2.31	2	1
1:B:438:ILE:HG22	1:B:441:HIS:HB2	0.61	1.70	2	1
1:A:221:ASP:CG	1:A:239:MET:SD	0.61	2.83	1	1
1:A:228:TYR:HB3	1:A:231:PRO:CG	0.61	2.25	1	2
1:A:238:LYS:O	1:A:242:VAL:HG23	0.61	1.95	2	2
1:B:238:LYS:O	1:B:242:VAL:HG23	0.61	1.96	2	2
1:A:111:GLN:NE2	2:C:648:PHE:HB3	0.61	2.10	2	1
1:B:58:LYS:HB2	1:B:73:PHE:CG	0.61	2.30	2	1
1:B:463:VAL:CG2	1:B:473:LEU:HD21	0.61	2.25	1	1
2:D:679:LYS:NZ	2:D:683:GLU:OE1	0.61	2.30	2	1
1:A:276:GLY:HA2	1:A:299:PHE:CZ	0.61	2.25	1	1
1:A:541:ASN:O	1:A:544:ASP:CG	0.61	2.43	1	2
1:A:181:THR:O	1:A:205:THR:HG23	0.61	1.95	1	1
1:B:431:GLU:CG	1:B:455:ASP:CB	0.61	2.78	1	1
1:A:394:ILE:N	1:A:394:ILE:CD1	0.61	2.64	2	1
1:B:111:GLN:NE2	2:D:648:PHE:HB3	0.61	2.10	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:258:ASP:O	1:B:259:LEU:C	0.61	2.42	2	1
1:B:337:GLY:O	1:B:358:ARG:CD	0.61	2.49	2	1
1:B:221:ASP:CG	1:B:239:MET:SD	0.60	2.84	1	1
1:B:228:TYR:HB3	1:B:231:PRO:CG	0.60	2.25	2	2
1:B:360:ILE:CD1	1:B:390:PHE:CD2	0.60	2.84	2	1
1:A:453:THR:HA	1:A:456:LEU:HD12	0.60	1.73	1	1
1:A:456:LEU:HD13	1:A:457:THR:CA	0.60	2.26	1	1
1:A:342:LEU:O	1:A:347:PHE:CZ	0.60	2.54	2	1
1:A:515:LEU:CB	1:A:520:LEU:CD1	0.60	2.78	2	1
1:B:513:LEU:HD22	1:B:513:LEU:H	0.60	1.54	1	1
1:A:350:GLU:N	1:A:350:GLU:OE2	0.60	2.33	2	1
1:B:107:VAL:CG2	1:B:108:ILE:N	0.60	2.64	2	1
1:B:309:THR:OG1	1:B:310:GLU:N	0.60	2.32	2	1
1:A:304:ARG:NH2	1:A:312:GLU:OE2	0.60	2.33	1	1
1:B:179:PHE:CE1	1:B:181:THR:OG1	0.60	2.51	1	1
1:A:221:ASP:OD2	1:A:226:GLN:N	0.60	2.34	2	1
1:B:342:LEU:O	1:B:347:PHE:CZ	0.60	2.55	2	1
1:B:394:ILE:N	1:B:394:ILE:CD1	0.60	2.64	2	1
1:A:4:GLY:HA3	1:A:202:ILE:HD11	0.60	1.72	1	1
1:B:173:LEU:N	1:B:173:LEU:HD22	0.60	2.10	1	1
1:B:292:VAL:HG13	1:B:329:VAL:HG22	0.60	1.71	1	1
1:A:73:PHE:CD2	1:A:74:GLU:N	0.60	2.69	2	1
1:B:489:ILE:O	1:B:492:SER:HB2	0.60	1.95	1	2
1:A:292:VAL:HG13	1:A:329:VAL:HG22	0.60	1.71	1	1
1:A:350:GLU:HB3	1:A:357:TRP:CZ2	0.60	2.32	2	1
1:B:259:LEU:O	1:B:260:PRO:O	0.60	2.20	1	1
1:A:172:ASN:O	1:A:176:VAL:HG12	0.60	1.97	2	2
1:A:467:ASN:ND2	1:A:470:ILE:HG12	0.60	2.12	1	1
1:B:367:ARG:CZ	1:B:371:ARG:NH2	0.60	2.65	1	1
1:A:72:ILE:HD13	1:A:72:ILE:O	0.60	1.95	2	1
1:B:221:ASP:OD2	1:B:226:GLN:N	0.60	2.33	2	1
1:A:302:MET:N	1:A:342:LEU:HD21	0.60	2.12	2	1
1:B:350:GLU:N	1:B:350:GLU:OE2	0.60	2.32	2	1
1:B:515:LEU:CB	1:B:520:LEU:CD1	0.60	2.79	2	1
1:A:68:GLU:N	1:A:68:GLU:CD	0.59	2.60	1	1
1:B:470:ILE:C	1:B:473:LEU:HD22	0.59	2.09	1	1
1:A:79:LEU:O	1:A:82:ASP:CG	0.59	2.45	2	1
1:A:179:PHE:CE1	1:A:181:THR:OG1	0.59	2.51	1	1
1:A:262:ILE:N	1:A:537:ILE:CD1	0.59	2.65	2	1
1:B:73:PHE:CD2	1:B:74:GLU:N	0.59	2.70	2	1
1:B:152:ILE:HG21	1:B:175:LYS:CG	0.59	2.27	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:79:LEU:O	1:B:82:ASP:CG	0.59	2.46	2	1
1:B:68:GLU:N	1:B:68:GLU:CD	0.59	2.61	1	1
1:B:70:GLU:HG3	1:B:71:ALA:N	0.59	2.13	1	1
2:D:618:PRO:HB3	2:D:684:LEU:HD13	0.59	1.73	2	1
1:A:367:ARG:CZ	1:A:371:ARG:NH2	0.59	2.65	1	1
1:B:181:THR:O	1:B:205:THR:HG23	0.59	1.96	1	1
1:B:53:GLN:O	1:B:56:THR:OG1	0.59	2.20	2	2
1:A:309:THR:OG1	1:A:310:GLU:N	0.59	2.33	2	1
1:A:352:ASN:ND2	1:B:354:PHE:H	0.59	1.96	2	1
1:B:259:LEU:CB	1:B:262:ILE:HG12	0.59	2.26	2	1
1:B:262:ILE:N	1:B:537:ILE:CD1	0.59	2.65	2	1
1:A:152:ILE:HG21	1:A:175:LYS:CG	0.59	2.27	2	1
1:A:261:ALA:HA	1:A:537:ILE:HD11	0.59	1.74	2	1
1:B:152:ILE:CG2	1:B:175:LYS:HG3	0.59	2.28	2	1
1:B:302:MET:N	1:B:342:LEU:HD21	0.59	2.12	2	1
1:A:68:GLU:CD	1:A:68:GLU:H	0.59	2.06	1	1
1:A:394:ILE:HG22	1:A:432:THR:HG21	0.59	1.73	1	1
1:B:172:ASN:O	1:B:176:VAL:HG12	0.59	1.98	2	2
1:B:438:ILE:HG22	1:B:438:ILE:O	0.59	1.98	2	1
1:B:456:LEU:HD13	1:B:456:LEU:C	0.59	2.21	1	1
1:B:467:ASN:ND2	1:B:470:ILE:HG12	0.59	2.13	1	1
1:B:453:THR:HA	1:B:456:LEU:HD12	0.58	1.74	1	1
1:A:304:ARG:HE	1:A:306:ALA:C	0.58	2.05	2	1
1:A:530:ILE:HG23	1:A:531:PRO:HD3	0.58	1.74	2	1
1:B:58:LYS:HB2	1:B:73:PHE:CD2	0.58	2.33	2	1
1:B:350:GLU:OE1	1:B:357:TRP:NE1	0.58	2.36	2	1
1:A:431:GLU:CG	1:A:455:ASP:CB	0.58	2.78	1	1
1:A:449:PHE:CE1	1:A:451:ILE:CB	0.58	2.86	1	1
1:A:302:MET:HG2	1:A:342:LEU:CG	0.58	2.28	2	1
1:A:456:LEU:HD13	1:A:456:LEU:C	0.58	2.21	1	1
1:A:107:VAL:CG2	1:A:108:ILE:N	0.58	2.66	2	1
1:A:53:GLN:O	1:A:56:THR:OG1	0.58	2.21	2	2
1:A:89:ILE:CD1	1:A:90:ILE:HG23	0.58	2.29	1	1
1:B:79:LEU:HD11	2:D:648:PHE:CE1	0.58	2.32	2	2
1:A:152:ILE:CG2	1:A:175:LYS:HG3	0.58	2.28	2	1
1:A:354:PHE:H	1:B:352:ASN:ND2	0.58	1.97	2	1
1:B:72:ILE:HD11	2:D:616:THR:CG2	0.58	2.28	2	1
1:A:79:LEU:HD11	2:C:648:PHE:CE1	0.58	2.34	2	2
1:A:301:PHE:CE1	1:A:304:ARG:CZ	0.58	2.86	2	1
1:B:50:ALA:HB2	1:B:140:ASN:ND2	0.58	2.14	2	1
1:A:421:ASP:OD1	1:A:423:SER:HB2	0.58	1.99	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:449:PHE:CE1	1:B:451:ILE:CB	0.58	2.87	1	1
1:B:456:LEU:HD13	1:B:457:THR:CA	0.58	2.26	1	1
1:B:309:THR:C	1:B:372:ASP:OD2	0.58	2.47	2	1
1:B:358:ARG:HE	1:B:358:ARG:CA	0.58	2.09	2	1
1:B:421:ASP:OD1	1:B:423:SER:HB2	0.58	1.99	1	2
1:B:180:ILE:HD13	1:B:202:ILE:H	0.58	1.59	2	1
1:B:331:VAL:HG11	1:B:377:ILE:HG12	0.58	1.76	2	1
1:B:353:PRO:O	1:B:358:ARG:HD2	0.58	1.98	2	1
1:A:309:THR:C	1:A:372:ASP:OD2	0.58	2.47	2	1
1:B:310:GLU:N	1:B:372:ASP:OD2	0.58	2.37	2	1
1:B:345:MET:HB3	1:B:347:PHE:CE2	0.58	2.34	2	1
1:A:276:GLY:O	1:A:299:PHE:CG	0.57	2.55	1	1
1:A:389:MET:HE2	1:A:428:VAL:O	0.57	1.99	1	1
1:B:282:GLU:O	1:B:285:GLU:HG2	0.57	1.99	1	1
1:B:256:LEU:HG	1:B:257:LYS:N	0.57	2.14	2	1
1:A:70:GLU:CD	1:A:71:ALA:N	0.57	2.62	1	1
1:B:79:LEU:HD21	2:D:648:PHE:CE2	0.57	2.34	1	2
1:A:50:ALA:HB2	1:A:140:ASN:ND2	0.57	2.14	2	1
1:A:331:VAL:HG11	1:A:377:ILE:HG12	0.57	1.76	2	1
1:A:350:GLU:OE1	1:A:357:TRP:NE1	0.57	2.37	2	1
1:B:374:LEU:O	1:B:377:ILE:HG23	0.57	1.98	1	1
1:B:470:ILE:HG22	1:B:473:LEU:HB2	0.57	1.76	2	1
1:B:115:LEU:HD21	2:D:651:GLN:CB	0.57	2.30	1	1
1:B:126:ARG:NH2	2:D:619:ALA:HB1	0.57	2.04	1	1
1:B:276:GLY:C	1:B:299:PHE:CE1	0.57	2.82	1	1
1:A:357:TRP:HD1	1:A:358:ARG:NH2	0.57	1.98	2	1
1:B:5:ILE:C	1:B:6:LEU:HD22	0.57	2.24	2	1
1:B:279:ARG:NH2	2:D:685:GLU:OE2	0.57	2.37	2	1
1:A:232:THR:HG22	1:A:233:ASN:H	0.57	1.35	1	2
1:A:374:LEU:O	1:A:377:ILE:HG23	0.57	1.99	1	1
1:B:389:MET:HE2	1:B:428:VAL:O	0.57	2.00	1	1
1:B:520:LEU:CD2	1:B:521:ASP:N	0.57	2.68	1	1
1:A:180:ILE:HD13	1:A:202:ILE:H	0.57	1.60	2	1
1:B:58:LYS:CD	1:B:58:LYS:C	0.57	2.78	2	1
1:A:82:ASP:OD1	1:A:82:ASP:N	0.57	2.35	2	1
1:A:345:MET:HB3	1:A:347:PHE:CE2	0.57	2.34	2	1
1:A:358:ARG:CA	1:A:358:ARG:HE	0.57	2.09	2	1
1:A:276:GLY:C	1:A:299:PHE:CE1	0.57	2.82	1	1
1:A:456:LEU:C	1:A:456:LEU:CD2	0.57	2.77	1	1
1:B:13:PHE:CD2	1:B:240:ARG:NH1	0.57	2.73	2	2
1:A:58:LYS:C	1:A:58:LYS:CD	0.57	2.78	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:82:ASP:OD1	1:B:82:ASP:N	0.57	2.36	2	1
1:B:428:VAL:CG1	1:B:429:MET:O	0.57	2.52	2	1
1:A:79:LEU:HD21	2:C:648:PHE:CE2	0.57	2.35	1	2
1:A:428:VAL:CG1	1:A:429:MET:O	0.57	2.52	2	1
1:A:13:PHE:CD2	1:A:240:ARG:NH1	0.57	2.73	1	2
1:A:229:VAL:C	1:A:231:PRO:HD3	0.57	2.25	1	2
1:A:260:PRO:CB	1:A:290:GLU:HG3	0.57	2.30	1	1
1:A:520:LEU:HD22	1:A:522:GLU:H	0.57	1.60	1	1
1:B:68:GLU:CD	1:B:68:GLU:H	0.57	2.06	1	1
1:B:89:ILE:CD1	1:B:90:ILE:HG23	0.57	2.30	1	1
1:B:303:ASP:C	1:B:303:ASP:OD1	0.57	2.48	1	1
1:A:310:GLU:N	1:A:372:ASP:OD2	0.57	2.36	2	1
1:A:470:ILE:C	1:A:473:LEU:HD22	0.57	2.10	1	1
1:B:314:PHE:CZ	1:B:375:ARG:O	0.57	2.57	1	1
1:B:394:ILE:HG22	1:B:432:THR:HG21	0.57	1.76	1	1
1:A:89:ILE:CG2	1:A:90:ILE:N	0.57	2.67	2	1
1:A:520:LEU:CD2	1:A:521:ASP:N	0.56	2.68	1	1
1:A:314:PHE:CZ	1:A:375:ARG:O	0.56	2.57	1	1
1:A:486:LYS:HD2	1:A:553:LEU:HD13	0.56	1.76	1	2
1:B:229:VAL:C	1:B:231:PRO:HD3	0.56	2.25	2	2
1:B:520:LEU:HD22	1:B:522:GLU:H	0.56	1.60	1	1
1:A:5:ILE:C	1:A:6:LEU:HD22	0.56	2.25	2	1
1:B:255:LYS:O	1:B:256:LEU:O	0.56	2.23	1	1
1:B:389:MET:HE1	1:B:450:SER:CB	0.56	2.31	1	1
1:B:486:LYS:HD2	1:B:553:LEU:HD13	0.56	1.75	1	2
1:A:253:LEU:O	1:A:257:LYS:NZ	0.56	2.35	2	1
1:A:261:ALA:C	1:A:537:ILE:CD1	0.56	2.78	2	1
1:A:336:ILE:N	1:A:336:ILE:CD1	0.56	2.68	2	1
1:A:515:LEU:CB	1:A:520:LEU:HD11	0.56	2.29	2	1
1:B:261:ALA:C	1:B:537:ILE:CD1	0.56	2.79	2	1
1:A:467:ASN:OD1	1:A:467:ASN:O	0.56	2.23	1	1
1:A:221:ASP:OD1	1:A:222:ALA:N	0.56	2.38	2	1
1:A:353:PRO:O	1:A:358:ARG:HD2	0.56	1.98	2	1
1:B:301:PHE:C	1:B:342:LEU:CD2	0.56	2.78	2	1
1:B:341:GLU:H	1:B:341:GLU:CD	0.56	2.09	2	1
1:B:176:VAL:HG13	1:B:176:VAL:O	0.56	2.00	1	2
1:A:72:ILE:HD11	2:C:616:THR:CG2	0.56	2.28	2	1
1:A:271:VAL:O	1:A:271:VAL:CG2	0.56	2.54	2	1
1:B:89:ILE:CG2	1:B:90:ILE:N	0.56	2.68	2	1
1:B:467:ASN:ND2	1:B:470:ILE:HG13	0.56	2.15	1	1
1:B:429:MET:SD	1:B:450:SER:OG	0.56	2.64	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:515:LEU:CB	1:B:520:LEU:HD11	0.56	2.30	2	1
1:B:70:GLU:CD	1:B:71:ALA:N	0.56	2.63	1	1
1:B:412:GLU:O	1:B:416:GLU:HG3	0.56	2.01	1	2
1:B:464:ASP:O	1:B:467:ASN:OD1	0.56	2.23	1	2
1:A:301:PHE:O	1:A:342:LEU:CD2	0.56	2.54	2	1
1:A:438:ILE:HG22	1:A:438:ILE:O	0.56	2.00	2	1
1:A:451:ILE:HD13	1:A:485:ILE:HG12	0.56	1.76	1	1
1:A:58:LYS:HB2	1:A:73:PHE:CD2	0.56	2.35	2	1
1:A:341:GLU:CD	1:A:341:GLU:H	0.56	2.09	2	1
1:A:360:ILE:CD1	1:A:390:PHE:CD2	0.56	2.86	2	1
1:A:470:ILE:HG22	1:A:473:LEU:HB2	0.56	1.77	2	1
1:A:115:LEU:HD21	2:C:651:GLN:CB	0.56	2.31	1	1
1:A:176:VAL:HG13	1:A:176:VAL:O	0.56	2.01	1	2
1:B:451:ILE:HD13	1:B:485:ILE:HG12	0.56	1.76	1	1
1:B:177:LEU:C	1:B:177:LEU:CD1	0.56	2.78	2	1
1:A:11:ILE:CG2	1:A:239:MET:HE3	0.56	2.31	2	2
1:A:70:GLU:HG3	1:A:71:ALA:N	0.56	2.14	1	1
1:A:352:ASN:HD21	1:B:354:PHE:N	0.56	1.97	1	1
1:B:431:GLU:CG	1:B:455:ASP:HB2	0.56	2.31	1	1
1:B:463:VAL:HG21	1:B:473:LEU:HD21	0.56	1.77	1	1
1:A:13:PHE:CD1	1:A:13:PHE:N	0.55	2.74	2	2
1:A:464:ASP:O	1:A:467:ASN:OD1	0.55	2.24	1	2
1:B:467:ASN:OD1	1:B:467:ASN:O	0.55	2.23	1	1
1:A:302:MET:CG	1:A:342:LEU:HG	0.55	2.31	2	1
1:B:530:ILE:HG23	1:B:531:PRO:HD3	0.55	1.76	2	1
1:A:292:VAL:CG2	1:A:329:VAL:CG1	0.55	2.81	1	1
1:A:377:ILE:C	1:A:377:ILE:CD1	0.55	2.77	1	1
1:B:337:GLY:C	1:B:358:ARG:HG2	0.55	2.27	1	1
1:B:398:GLU:OE1	1:B:398:GLU:N	0.55	2.39	1	1
1:B:456:LEU:C	1:B:456:LEU:CD2	0.55	2.78	1	1
1:A:429:MET:SD	1:A:450:SER:OG	0.55	2.64	2	1
1:B:157:ILE:HG12	1:B:177:LEU:HD11	0.55	1.78	2	1
1:B:221:ASP:OD1	1:B:222:ALA:N	0.55	2.38	2	1
1:A:412:GLU:O	1:A:416:GLU:HG3	0.55	2.01	1	2
1:B:11:ILE:CG2	1:B:239:MET:HE3	0.55	2.31	1	2
1:B:117:GLU:N	1:B:117:GLU:OE1	0.55	2.39	2	1
1:B:261:ALA:HA	1:B:537:ILE:HD11	0.55	1.77	2	1
1:B:271:VAL:CG2	1:B:271:VAL:O	0.55	2.54	2	1
1:B:357:TRP:HD1	1:B:358:ARG:NH2	0.55	1.98	2	1
1:A:167:GLU:OE1	1:A:167:GLU:N	0.55	2.40	1	1
1:A:258:ASP:OD1	1:A:258:ASP:N	0.55	2.39	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:474:TYR:O	1:A:474:TYR:CD2	0.55	2.59	2	2
1:B:377:ILE:C	1:B:377:ILE:CD1	0.55	2.77	1	1
1:B:449:PHE:HZ	1:B:451:ILE:HB	0.55	1.50	1	1
1:B:58:LYS:CG	1:B:73:PHE:CD2	0.55	2.90	2	1
1:A:451:ILE:HG22	1:A:501:MET:HG2	0.55	1.79	1	1
1:B:455:ASP:OD1	1:B:459:TYR:CE1	0.55	2.59	1	1
1:B:125:GLU:N	1:B:125:GLU:OE1	0.55	2.38	2	1
1:A:301:PHE:C	1:A:342:LEU:CD2	0.55	2.79	2	1
1:A:355:LEU:HD13	1:B:462:ALA:HA	0.55	1.78	2	1
1:A:484:LEU:HD23	1:A:485:ILE:N	0.55	2.16	1	1
1:B:339:ASP:OD2	1:B:465:ARG:NH2	0.55	2.39	1	1
2:D:650:LEU:O	2:D:652:THR:N	0.55	2.40	1	2
1:B:474:TYR:O	1:B:474:TYR:CD2	0.55	2.60	2	1
1:A:467:ASN:ND2	1:A:470:ILE:HG13	0.55	2.16	1	1
1:A:157:ILE:HG12	1:A:177:LEU:HD11	0.55	1.78	2	1
1:A:389:MET:SD	1:A:450:SER:OG	0.55	2.65	2	1
1:A:522:GLU:OE1	1:A:523:PHE:N	0.55	2.39	2	1
1:A:354:PHE:N	1:B:352:ASN:HD21	0.55	1.96	1	1
1:B:276:GLY:O	1:B:299:PHE:CG	0.55	2.55	1	1
1:B:451:ILE:HG22	1:B:501:MET:HG2	0.55	1.77	1	1
1:A:117:GLU:OE1	1:A:117:GLU:N	0.55	2.40	2	1
1:B:271:VAL:O	1:B:271:VAL:HG23	0.55	2.02	2	1
1:B:272:CYS:SG	1:B:293:GLY:HA3	0.55	2.42	2	1
1:A:456:LEU:HD13	1:A:457:THR:H	0.55	1.58	1	1
1:B:520:LEU:HD23	1:B:521:ASP:N	0.55	2.17	1	1
2:C:650:LEU:O	2:C:652:THR:N	0.55	2.40	2	2
1:B:367:ARG:C	1:B:371:ARG:CG	0.55	2.79	2	1
1:A:337:GLY:C	1:A:358:ARG:HG2	0.54	2.26	1	1
1:A:389:MET:HE1	1:A:450:SER:CB	0.54	2.31	1	1
1:A:431:GLU:CG	1:A:455:ASP:HB2	0.54	2.32	1	1
1:A:467:ASN:CG	1:A:467:ASN:O	0.54	2.50	2	1
1:B:301:PHE:O	1:B:342:LEU:CD2	0.54	2.54	2	1
1:B:13:PHE:N	1:B:13:PHE:CD1	0.54	2.75	1	2
1:B:448:PHE:C	1:B:497:LYS:NZ	0.54	2.66	1	1
1:A:58:LYS:CG	1:A:73:PHE:CD2	0.54	2.91	2	1
1:A:125:GLU:OE1	1:A:125:GLU:N	0.54	2.39	2	1
1:A:520:LEU:HD23	1:A:521:ASP:N	0.54	2.18	1	1
1:B:292:VAL:CG1	1:B:329:VAL:HG13	0.54	2.32	1	1
1:A:177:LEU:C	1:A:177:LEU:CD1	0.54	2.78	2	1
1:A:302:MET:CA	1:A:342:LEU:HD21	0.54	2.32	2	1
1:B:522:GLU:OE1	1:B:523:PHE:N	0.54	2.40	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ARG:NH2	2:C:619:ALA:HB1	0.54	2.05	1	1
1:A:339:ASP:OD2	1:A:465:ARG:NH2	0.54	2.40	1	1
1:A:152:ILE:HG21	1:A:175:LYS:HG3	0.54	1.79	2	1
1:A:448:PHE:C	1:A:497:LYS:NZ	0.54	2.66	1	1
1:B:363:ALA:HB1	1:B:370:LEU:HB2	0.54	1.79	2	2
1:B:484:LEU:HD23	1:B:485:ILE:N	0.54	2.17	1	1
1:A:271:VAL:O	1:A:271:VAL:HG23	0.54	2.02	2	1
1:A:476:PRO:O	1:A:481:VAL:HG23	0.54	2.03	2	1
1:B:74:GLU:OE1	1:B:78:MET:SD	0.54	2.65	2	1
1:A:405:GLU:HG3	1:A:409:TYR:CE1	0.54	2.38	1	2
1:B:126:ARG:HH21	2:D:619:ALA:HB3	0.54	1.49	1	1
1:B:292:VAL:CG2	1:B:329:VAL:CG1	0.54	2.82	1	1
1:B:449:PHE:CD2	1:B:499:THR:HB	0.54	2.38	1	1
1:A:345:MET:CB	1:A:347:PHE:CE2	0.54	2.90	2	1
1:A:374:LEU:HA	1:A:377:ILE:HG23	0.54	1.80	1	1
1:B:167:GLU:N	1:B:167:GLU:OE1	0.54	2.40	1	1
1:B:197:LEU:HD13	1:B:197:LEU:O	0.54	2.03	1	1
1:B:467:ASN:CG	1:B:467:ASN:O	0.54	2.50	2	2
1:B:356:GLY:C	1:B:358:ARG:HG2	0.54	2.28	2	1
1:B:372:ASP:OD1	1:B:373:GLN:N	0.54	2.41	1	1
2:C:679:LYS:NZ	2:C:683:GLU:OE1	0.54	2.36	2	1
1:A:78:MET:HE1	2:C:627:LYS:HB2	0.54	1.80	1	1
1:A:347:PHE:C	1:A:347:PHE:CD2	0.54	2.86	1	1
1:B:456:LEU:HD11	1:B:481:VAL:HG11	0.54	1.78	1	1
1:A:485:ILE:CG2	1:A:518:MET:SD	0.54	2.96	2	1
1:B:152:ILE:HG21	1:B:175:LYS:HG3	0.54	1.80	2	1
1:B:485:ILE:CG2	1:B:518:MET:SD	0.54	2.96	2	1
1:A:46:GLY:O	1:A:140:ASN:ND2	0.53	2.41	1	1
1:B:474:TYR:CD2	1:B:474:TYR:O	0.53	2.60	1	1
1:B:105:HIS:NE2	1:B:109:GLU:OE1	0.53	2.42	1	2
1:B:162:ASP:OD1	1:B:163:LEU:N	0.53	2.41	1	1
1:B:296:ARG:HB3	1:B:299:PHE:CD2	0.53	2.37	1	1
1:A:161:ALA:O	1:A:181:THR:CG2	0.53	2.56	1	1
1:A:197:LEU:O	1:A:197:LEU:HD13	0.53	2.03	1	1
1:A:221:ASP:CA	1:A:239:MET:CE	0.53	2.78	1	2
1:A:74:GLU:HA	1:A:77:ILE:HG22	0.53	1.80	2	1
1:B:5:ILE:HD13	1:B:5:ILE:O	0.53	2.03	2	1
1:B:259:LEU:HB2	1:B:262:ILE:HG12	0.53	1.80	2	1
1:A:221:ASP:OD2	1:A:239:MET:SD	0.53	2.67	1	1
1:B:272:CYS:HG	1:B:273:ALA:N	0.53	2.01	2	1
1:B:345:MET:CB	1:B:347:PHE:CE2	0.53	2.91	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:457:THR:CG2	1:B:458:GLN:N	0.53	2.71	2	1
1:A:296:ARG:HB3	1:A:299:PHE:CD2	0.53	2.38	1	1
1:B:405:GLU:HG3	1:B:409:TYR:CE1	0.53	2.38	1	2
1:A:537:ILE:HG13	1:A:538:ARG:N	0.53	2.19	2	1
1:B:302:MET:CA	1:B:342:LEU:HD21	0.53	2.33	2	1
1:B:336:ILE:N	1:B:336:ILE:CD1	0.53	2.68	2	1
1:A:292:VAL:CG1	1:A:329:VAL:HG13	0.53	2.33	1	1
1:A:363:ALA:HB1	1:A:370:LEU:HB2	0.53	1.79	2	2
1:A:455:ASP:OD1	1:A:459:TYR:CE1	0.53	2.62	1	1
1:A:463:VAL:HG11	1:A:473:LEU:CG	0.53	2.14	1	1
1:B:296:ARG:HB2	1:B:299:PHE:CE2	0.53	2.37	1	1
1:B:317:TYR:CZ	1:B:386:LEU:HD13	0.53	2.39	1	1
1:B:454:ASN:O	1:B:458:GLN:OE1	0.53	2.27	1	1
1:A:74:GLU:OE1	1:A:78:MET:SD	0.53	2.67	2	1
1:A:272:CYS:SG	1:A:293:GLY:HA3	0.53	2.43	2	1
1:A:279:ARG:NH2	2:C:685:GLU:OE2	0.53	2.36	2	1
1:A:287:ASN:HB3	1:A:530:ILE:HG23	0.53	1.81	2	1
1:B:358:ARG:HE	1:B:358:ARG:HA	0.53	1.64	2	1
1:A:221:ASP:C	1:A:223:VAL:N	0.53	2.66	2	2
1:A:449:PHE:CD2	1:A:499:THR:HB	0.53	2.39	1	1
1:B:161:ALA:O	1:B:181:THR:CG2	0.53	2.56	1	1
1:A:51:SER:O	1:A:54:LEU:HG	0.53	2.04	2	1
1:A:296:ARG:HB2	1:A:299:PHE:CE2	0.53	2.38	1	1
1:B:470:ILE:HB	1:B:473:LEU:CD2	0.53	2.34	1	1
1:A:511:ALA:HB1	1:A:515:LEU:HD13	0.53	1.81	2	1
1:A:246:VAL:CG2	1:A:247:ALA:N	0.53	2.72	1	1
1:B:221:ASP:OD2	1:B:239:MET:SD	0.53	2.67	1	1
1:A:301:PHE:O	1:A:304:ARG:HD2	0.53	2.04	2	1
1:A:457:THR:CG2	1:A:458:GLN:N	0.53	2.72	2	1
1:B:51:SER:O	1:B:54:LEU:HG	0.53	2.04	2	1
1:A:161:ALA:O	1:A:181:THR:HG22	0.53	2.04	1	1
1:A:243:GLN:C	1:A:243:GLN:CD	0.53	2.77	1	1
1:B:78:MET:HE1	2:D:627:LYS:HB2	0.53	1.78	1	1
1:B:105:HIS:CE1	1:B:109:GLU:OE1	0.53	2.62	1	1
1:B:199:LEU:O	1:B:199:LEU:CD2	0.53	2.55	1	1
1:B:389:MET:HE3	1:B:429:MET:SD	0.53	2.44	2	1
1:A:88:GLU:N	1:A:88:GLU:OE1	0.52	2.42	1	1
1:A:302:MET:HG2	1:A:342:LEU:HG	0.52	1.80	2	1
1:A:355:LEU:N	1:A:355:LEU:HD23	0.52	2.18	2	1
1:A:367:ARG:C	1:A:371:ARG:CG	0.52	2.78	2	1
1:A:511:ALA:HB1	1:A:515:LEU:CD1	0.52	2.34	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:679:LYS:HZ1	2:C:683:GLU:CD	0.52	2.12	2	1
1:A:79:LEU:O	1:A:82:ASP:OD1	0.52	2.26	2	2
1:A:105:HIS:NE2	1:A:109:GLU:OE1	0.52	2.42	1	2
1:B:263:THR:HG21	1:B:542:PHE:HB3	0.52	1.80	1	1
1:B:74:GLU:CA	1:B:77:ILE:HG22	0.52	2.34	2	1
1:B:287:ASN:HB3	1:B:530:ILE:HG23	0.52	1.80	2	1
1:B:476:PRO:O	1:B:481:VAL:HG23	0.52	2.03	2	1
1:A:162:ASP:OD1	1:A:163:LEU:N	0.52	2.42	1	1
1:A:199:LEU:O	1:A:199:LEU:CD2	0.52	2.54	1	1
1:A:205:THR:OG1	1:A:208:VAL:HG13	0.52	2.04	1	1
1:A:292:VAL:HG13	1:A:329:VAL:HA	0.52	1.81	1	1
1:A:372:ASP:OD1	1:A:373:GLN:N	0.52	2.42	1	1
1:B:116:GLU:OE2	1:B:131:ARG:NH2	0.52	2.42	2	2
1:A:449:PHE:CZ	1:A:451:ILE:CB	0.52	2.84	1	1
1:B:88:GLU:N	1:B:88:GLU:OE1	0.52	2.42	1	1
1:A:5:ILE:HD13	1:A:5:ILE:O	0.52	2.04	2	1
1:A:356:GLY:C	1:A:358:ARG:HG2	0.52	2.28	2	1
1:B:173:LEU:N	1:B:173:LEU:CD2	0.52	2.73	1	1
1:B:205:THR:OG1	1:B:208:VAL:HG13	0.52	2.04	1	1
1:B:292:VAL:HG13	1:B:329:VAL:HA	0.52	1.80	1	1
1:B:347:PHE:C	1:B:347:PHE:CD2	0.52	2.85	1	1
1:A:256:LEU:O	1:A:257:LYS:C	0.52	2.52	2	1
1:A:105:HIS:CE1	1:A:109:GLU:OE1	0.52	2.62	1	1
1:B:243:GLN:C	1:B:243:GLN:CD	0.52	2.78	1	1
1:A:272:CYS:HG	1:A:273:ALA:N	0.52	2.02	2	1
1:B:451:ILE:HD11	1:B:488:VAL:HG21	0.52	1.81	2	1
1:B:515:LEU:CA	1:B:520:LEU:HD11	0.52	2.31	2	1
1:A:173:LEU:N	1:A:173:LEU:CD2	0.52	2.73	1	1
1:A:255:LYS:O	1:A:256:LEU:HB2	0.52	2.04	1	1
1:A:373:GLN:O	1:A:377:ILE:HG22	0.52	2.04	1	1
1:A:58:LYS:HG3	1:A:73:PHE:CD2	0.52	2.40	2	1
1:A:74:GLU:CA	1:A:77:ILE:HG22	0.52	2.34	2	1
1:B:301:PHE:CD1	1:B:342:LEU:HD22	0.52	2.39	2	1
1:A:473:LEU:HD23	1:A:474:TYR:N	0.52	2.20	1	1
1:B:373:GLN:O	1:B:377:ILE:HG22	0.52	2.04	1	1
2:C:675:GLU:O	2:C:678:VAL:HG12	0.52	2.05	1	1
1:B:58:LYS:HG3	1:B:73:PHE:CD2	0.52	2.39	2	1
1:A:263:THR:HG21	1:A:542:PHE:HB3	0.52	1.80	1	1
1:A:492:SER:HA	1:A:497:LYS:CG	0.52	2.35	1	1
2:D:651:GLN:N	2:D:651:GLN:OE1	0.52	2.43	1	2
1:B:126:ARG:NH1	2:D:651:GLN:CD	0.52	2.68	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ARG:HH21	2:C:619:ALA:HB3	0.52	1.49	1	1
1:A:438:ILE:O	1:A:438:ILE:CG2	0.52	2.58	1	1
1:B:161:ALA:O	1:B:181:THR:HG22	0.52	2.04	1	1
1:B:456:LEU:HD13	1:B:457:THR:H	0.52	1.58	1	1
1:A:337:GLY:O	1:A:358:ARG:HD3	0.52	2.04	2	1
1:A:357:TRP:HB3	1:B:470:ILE:HD11	0.52	1.82	2	1
1:B:304:ARG:NH2	1:B:344:TYR:HB3	0.52	2.20	2	1
1:B:337:GLY:O	1:B:358:ARG:HD3	0.52	2.04	2	1
1:B:438:ILE:HG23	1:B:441:HIS:HB2	0.52	1.81	2	1
1:B:492:SER:HA	1:B:497:LYS:CG	0.51	2.35	1	1
1:B:511:ALA:HB1	1:B:515:LEU:CD1	0.51	2.34	2	1
2:C:679:LYS:NZ	2:C:683:GLU:CD	0.51	2.68	2	1
1:A:454:ASN:O	1:A:458:GLN:OE1	0.51	2.27	1	1
1:B:221:ASP:C	1:B:223:VAL:N	0.51	2.66	2	2
1:A:451:ILE:HD11	1:A:488:VAL:HG21	0.51	1.81	2	1
1:B:342:LEU:O	1:B:347:PHE:CE1	0.51	2.63	2	1
1:A:156:VAL:O	1:A:177:LEU:HD12	0.51	2.05	1	1
1:A:520:LEU:CD2	1:A:522:GLU:H	0.51	2.19	1	1
1:B:192:ILE:HG13	1:B:193:MET:N	0.51	2.21	1	1
1:B:557:THR:HB	1:B:560:GLU:OE1	0.51	2.05	1	2
1:A:342:LEU:O	1:A:347:PHE:CE1	0.51	2.62	2	1
1:B:157:ILE:HG13	1:B:177:LEU:HD21	0.51	1.82	2	1
1:B:305:ASP:O	1:B:344:TYR:CD1	0.51	2.63	2	1
1:B:537:ILE:HG13	1:B:538:ARG:N	0.51	2.19	2	1
1:A:177:LEU:H	1:A:177:LEU:CD1	0.51	2.15	1	1
1:A:317:TYR:CZ	1:A:386:LEU:HD13	0.51	2.40	1	1
1:B:473:LEU:HD23	1:B:474:TYR:N	0.51	2.21	1	1
1:B:520:LEU:CD2	1:B:522:GLU:H	0.51	2.18	1	1
1:A:305:ASP:O	1:A:344:TYR:CD1	0.51	2.63	2	1
1:B:511:ALA:HB1	1:B:515:LEU:HD13	0.51	1.81	2	1
1:B:246:VAL:CG2	1:B:247:ALA:N	0.51	2.73	1	1
1:B:304:ARG:NH2	1:B:312:GLU:CD	0.51	2.69	1	1
1:B:157:ILE:HG12	1:B:177:LEU:CG	0.51	2.36	2	1
1:B:394:ILE:H	1:B:394:ILE:CD1	0.51	2.12	2	1
2:C:612:ASN:O	2:C:615:HIS:CE1	0.51	2.64	2	1
1:A:192:ILE:HG13	1:A:193:MET:N	0.51	2.20	1	1
1:A:456:LEU:HD11	1:A:481:VAL:HG11	0.51	1.79	1	1
1:B:156:VAL:O	1:B:177:LEU:HD12	0.51	2.05	1	1
1:B:304:ARG:NH2	1:B:312:GLU:OE2	0.51	2.38	1	1
1:B:438:ILE:O	1:B:438:ILE:CG2	0.51	2.58	1	1
2:C:651:GLN:OE1	2:C:651:GLN:N	0.51	2.43	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:334:MET:HB2	1:A:336:ILE:HD11	0.51	1.82	2	1
1:A:449:PHE:CZ	1:A:451:ILE:N	0.51	2.78	1	1
1:A:301:PHE:CD1	1:A:342:LEU:HD22	0.51	2.41	2	1
1:B:304:ARG:CD	1:B:304:ARG:C	0.51	2.84	2	1
1:A:18:LEU:CD1	1:A:209:THR:OG1	0.51	2.59	1	1
1:A:116:GLU:OE2	1:A:131:ARG:NH2	0.51	2.42	2	2
1:A:179:PHE:C	1:A:179:PHE:CD2	0.51	2.89	1	1
1:B:18:LEU:CD1	1:B:209:THR:OG1	0.51	2.59	1	1
1:B:179:PHE:CD2	1:B:179:PHE:C	0.51	2.89	1	1
1:B:354:PHE:O	1:B:358:ARG:CZ	0.51	2.59	1	1
2:D:675:GLU:O	2:D:678:VAL:HG12	0.51	2.05	1	1
1:A:304:ARG:O	1:A:304:ARG:HD3	0.51	2.05	2	1
1:B:158:LEU:O	1:B:180:ILE:HG23	0.51	2.06	1	1
1:A:264:LEU:C	1:A:264:LEU:CD2	0.51	2.84	2	1
1:A:389:MET:HE3	1:A:429:MET:SD	0.51	2.45	2	1
1:B:51:SER:HA	1:B:54:LEU:CD2	0.51	2.31	2	1
1:B:74:GLU:HA	1:B:77:ILE:HG22	0.51	1.80	2	1
1:A:46:GLY:O	1:A:140:ASN:OD1	0.51	2.29	1	1
1:A:470:ILE:HB	1:A:473:LEU:CD2	0.51	2.35	1	1
1:A:520:LEU:CD2	1:A:520:LEU:C	0.51	2.84	1	1
1:B:126:ARG:HG2	2:D:651:GLN:CG	0.51	2.36	2	1
1:B:294:LEU:C	1:B:294:LEU:HD23	0.51	2.30	2	1
1:B:331:VAL:O	1:B:331:VAL:CG1	0.50	2.59	1	1
1:B:520:LEU:CD2	1:B:520:LEU:C	0.50	2.83	1	1
1:B:520:LEU:HD23	1:B:521:ASP:H	0.50	1.65	1	1
1:A:358:ARG:HE	1:A:358:ARG:HA	0.50	1.64	2	1
1:B:275:ILE:HG22	1:B:280:ASP:CB	0.50	2.35	2	1
2:D:612:ASN:O	2:D:615:HIS:CE1	0.50	2.64	2	1
1:A:354:PHE:O	1:A:358:ARG:CZ	0.50	2.59	1	1
1:A:389:MET:HE1	1:A:450:SER:N	0.50	2.21	1	1
1:B:276:GLY:C	1:B:299:PHE:CD1	0.50	2.84	1	1
1:B:374:LEU:HA	1:B:377:ILE:HG23	0.50	1.81	1	1
1:A:157:ILE:HG12	1:A:177:LEU:CG	0.50	2.36	2	1
1:A:297:THR:HG23	1:A:332:ARG:O	0.50	2.07	2	1
1:A:331:VAL:O	1:A:331:VAL:CG1	0.50	2.59	1	1
1:B:277:THR:O	1:B:278:VAL:C	0.50	2.54	1	2
1:B:389:MET:HE1	1:B:450:SER:N	0.50	2.21	1	1
1:B:449:PHE:CZ	1:B:451:ILE:N	0.50	2.79	1	1
1:A:294:LEU:C	1:A:294:LEU:HD23	0.50	2.31	2	1
1:B:449:PHE:CZ	1:B:451:ILE:CB	0.50	2.84	1	1
1:A:556:PRO:HB3	1:B:441:HIS:CE1	0.50	2.41	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:463:VAL:CG2	1:B:473:LEU:CD2	0.50	2.87	1	1
1:B:105:HIS:CD2	1:B:109:GLU:OE1	0.50	2.65	2	1
1:B:275:ILE:HG22	1:B:280:ASP:HB3	0.50	1.83	2	1
1:B:79:LEU:O	1:B:82:ASP:OD1	0.50	2.28	2	2
1:A:301:PHE:CE1	1:A:304:ARG:NH2	0.50	2.79	2	1
1:A:161:ALA:C	1:A:181:THR:CG2	0.50	2.85	1	1
1:A:520:LEU:HD23	1:A:521:ASP:H	0.50	1.65	1	1
1:A:557:THR:HB	1:A:560:GLU:OE1	0.50	2.05	1	2
1:B:350:GLU:OE1	1:B:357:TRP:CZ2	0.50	2.65	2	1
1:A:192:ILE:C	1:A:192:ILE:CD1	0.49	2.85	1	1
1:B:161:ALA:C	1:B:181:THR:CG2	0.49	2.85	1	1
1:B:449:PHE:CE2	1:B:500:GLY:N	0.49	2.80	1	1
1:A:226:GLN:OE1	1:A:228:TYR:CZ	0.49	2.65	2	1
1:B:80:LEU:HD13	1:B:80:LEU:C	0.49	2.32	2	1
1:B:355:LEU:N	1:B:355:LEU:HD23	0.49	2.22	2	1
1:A:205:THR:OG1	1:A:208:VAL:CG2	0.49	2.57	1	1
1:A:314:PHE:CG	1:A:376:ALA:HA	0.49	2.37	1	1
1:B:46:GLY:O	1:B:140:ASN:ND2	0.49	2.43	1	1
1:B:140:ASN:ND2	1:B:140:ASN:C	0.49	2.68	1	1
1:A:157:ILE:HG13	1:A:177:LEU:HD21	0.49	1.82	2	1
1:A:140:ASN:ND2	1:A:140:ASN:C	0.49	2.70	1	1
1:A:459:TYR:HB3	1:B:459:TYR:O	0.49	2.07	1	2
1:A:126:ARG:NH1	2:C:651:GLN:CD	0.49	2.71	2	1
1:A:314:PHE:HE2	1:A:379:ARG:CB	0.49	2.12	1	1
1:B:78:MET:CE	2:D:627:LYS:HB2	0.49	2.38	1	1
1:B:221:ASP:CA	1:B:239:MET:CE	0.49	2.78	1	2
1:A:126:ARG:HG2	2:C:651:GLN:CG	0.49	2.37	2	1
1:A:350:GLU:OE1	1:A:357:TRP:CZ2	0.49	2.65	2	1
1:A:358:ARG:NE	1:A:358:ARG:CA	0.49	2.76	2	1
1:B:54:LEU:O	1:B:73:PHE:CE1	0.49	2.66	2	1
1:B:297:THR:HG23	1:B:332:ARG:O	0.49	2.07	2	1
1:B:511:ALA:O	1:B:515:LEU:HD13	0.49	2.07	2	1
1:A:277:THR:O	1:A:278:VAL:C	0.49	2.54	1	2
1:A:295:TYR:CD2	1:A:331:VAL:HG23	0.49	2.42	1	1
1:B:89:ILE:HD11	1:B:90:ILE:HG23	0.49	1.85	1	1
1:B:232:THR:HG22	1:B:233:ASN:H	0.49	1.34	1	1
1:A:105:HIS:CD2	1:A:109:GLU:OE1	0.49	2.66	2	1
1:B:51:SER:O	1:B:54:LEU:CD1	0.49	2.61	2	1
1:B:298:GLU:OE2	1:B:342:LEU:HD11	0.49	2.07	2	1
1:A:317:TYR:CE1	1:A:331:VAL:CG2	0.49	2.96	1	1
1:A:463:VAL:CG2	1:A:473:LEU:CD2	0.49	2.86	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:317:TYR:OH	1:B:386:LEU:HB3	0.49	2.07	1	1
1:A:51:SER:O	1:A:54:LEU:CD1	0.49	2.61	2	1
1:A:54:LEU:CD1	1:A:55:GLU:N	0.49	2.69	2	1
1:A:275:ILE:HG22	1:A:280:ASP:CB	0.49	2.36	2	1
1:A:511:ALA:O	1:A:515:LEU:HD13	0.49	2.08	2	1
1:A:86:GLU:O	1:A:90:ILE:CG1	0.49	2.61	1	1
1:B:101:ASP:HB2	1:B:138:LEU:HD21	0.49	1.85	1	1
1:B:263:THR:CG2	1:B:267:HIS:H	0.49	2.14	1	1
1:A:302:MET:HG2	1:A:342:LEU:CD1	0.49	2.37	2	1
1:B:358:ARG:NE	1:B:358:ARG:CA	0.49	2.76	2	1
2:D:679:LYS:NZ	2:D:683:GLU:CD	0.49	2.71	2	1
1:A:101:ASP:HB2	1:A:138:LEU:HD21	0.49	1.84	1	1
1:A:233:ASN:O	1:A:237:ASP:OD2	0.49	2.31	1	2
1:A:342:LEU:HD13	1:A:343:PRO:HD2	0.49	1.85	1	1
1:B:46:GLY:O	1:B:140:ASN:OD1	0.49	2.30	1	1
1:B:285:GLU:HG3	1:B:286:ARG:N	0.49	2.23	1	1
1:B:295:TYR:CD2	1:B:331:VAL:HG23	0.49	2.43	1	1
1:B:342:LEU:HD13	1:B:343:PRO:HD2	0.49	1.84	1	1
1:B:530:ILE:O	1:B:533:ILE:HG12	0.49	2.07	1	1
1:A:80:LEU:HD13	1:A:80:LEU:C	0.49	2.32	2	1
1:A:189:HIS:O	1:A:193:MET:SD	0.49	2.70	2	1
1:A:337:GLY:HA3	1:A:358:ARG:NH2	0.49	2.23	2	1
1:A:470:ILE:HD11	1:B:357:TRP:HB3	0.49	1.84	2	1
1:A:78:MET:CE	2:C:627:LYS:HB2	0.48	2.38	1	1
1:B:140:ASN:ND2	1:B:140:ASN:O	0.48	2.46	1	1
1:B:451:ILE:O	1:B:451:ILE:HG23	0.48	2.08	1	1
2:C:650:LEU:C	2:C:652:THR:N	0.48	2.71	1	2
1:A:54:LEU:O	1:A:73:PHE:CE1	0.48	2.66	2	1
1:B:54:LEU:CD1	1:B:55:GLU:N	0.48	2.69	2	1
1:B:74:GLU:CA	1:B:77:ILE:CG2	0.48	2.90	2	1
1:B:304:ARG:O	1:B:304:ARG:HD3	0.48	2.08	2	1
1:A:89:ILE:HD11	1:A:90:ILE:HG23	0.48	1.83	1	1
1:A:449:PHE:CE2	1:A:500:GLY:N	0.48	2.80	1	1
1:B:86:GLU:O	1:B:90:ILE:CG1	0.48	2.61	1	1
1:B:314:PHE:CD2	1:B:376:ALA:C	0.48	2.88	1	1
2:D:650:LEU:C	2:D:652:THR:N	0.48	2.72	2	2
1:A:126:ARG:CD	2:C:651:GLN:NE2	0.48	2.77	1	1
1:A:530:ILE:O	1:A:533:ILE:HG12	0.48	2.07	1	1
1:B:177:LEU:H	1:B:177:LEU:CD1	0.48	2.16	1	1
1:B:314:PHE:HE2	1:B:379:ARG:CB	0.48	2.12	1	1
1:A:345:MET:HB3	1:A:347:PHE:CZ	0.48	2.44	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:350:GLU:OE1	1:B:357:TRP:CE2	0.48	2.67	2	1
1:B:111:GLN:OE1	2:D:648:PHE:CB	0.48	2.30	1	1
1:A:269:VAL:HG12	1:A:270:GLU:N	0.48	2.23	2	1
1:A:464:ASP:CG	1:A:467:ASN:HB3	0.48	2.33	2	1
1:B:226:GLN:OE1	1:B:228:TYR:CZ	0.48	2.66	2	1
1:B:334:MET:HB2	1:B:336:ILE:HD11	0.48	1.83	2	1
1:A:557:THR:HG22	1:A:560:GLU:H	0.48	1.69	1	2
1:B:233:ASN:O	1:B:237:ASP:OD2	0.48	2.31	2	2
1:B:314:PHE:CE1	1:B:376:ALA:HA	0.48	2.38	1	1
1:B:189:HIS:O	1:B:193:MET:SD	0.48	2.71	2	1
1:A:451:ILE:O	1:A:451:ILE:HG23	0.48	2.08	1	1
1:A:501:MET:CG	1:A:520:LEU:HD11	0.48	2.38	1	1
1:A:530:ILE:C	1:A:530:ILE:CD1	0.48	2.78	2	1
1:B:264:LEU:C	1:B:264:LEU:CD2	0.48	2.84	2	1
1:B:389:MET:CE	1:B:429:MET:SD	0.48	3.02	2	1
1:B:254:ALA:O	1:B:256:LEU:HD12	0.48	2.09	1	1
1:B:489:ILE:CA	1:B:499:THR:HG21	0.48	2.30	1	1
1:A:85:LEU:O	1:A:85:LEU:HD23	0.48	2.09	2	1
1:A:158:LEU:HD21	1:A:163:LEU:HD11	0.48	1.85	1	1
1:A:219:ILE:CD1	1:A:236:ILE:HG12	0.48	2.36	2	2
1:A:314:PHE:CD2	1:A:376:ALA:C	0.48	2.88	1	1
1:A:51:SER:HA	1:A:54:LEU:CD2	0.48	2.31	2	1
1:B:448:PHE:C	1:B:497:LYS:HZ1	0.48	2.17	1	1
1:A:537:ILE:CG1	1:A:538:ARG:N	0.48	2.77	2	1
1:B:337:GLY:HA3	1:B:358:ARG:NH2	0.48	2.24	2	1
1:A:130:VAL:CG2	1:A:131:ARG:N	0.48	2.77	1	1
1:A:260:PRO:CG	1:A:290:GLU:HG3	0.48	2.39	1	1
1:A:292:VAL:HG11	1:A:329:VAL:HG13	0.48	1.85	1	1
1:A:317:TYR:CZ	1:A:331:VAL:CB	0.48	2.96	1	1
1:A:317:TYR:HD2	1:A:317:TYR:O	0.48	1.91	1	1
1:B:181:THR:HG22	1:B:182:ASP:N	0.48	2.24	1	1
1:B:292:VAL:HG11	1:B:329:VAL:HG13	0.48	1.84	1	1
1:B:557:THR:HG22	1:B:560:GLU:H	0.48	1.69	1	2
1:A:462:ALA:HA	1:B:355:LEU:HD13	0.48	1.85	2	1
1:B:301:PHE:O	1:B:304:ARG:HD2	0.48	2.06	2	1
1:A:10:GLY:O	1:A:221:ASP:O	0.47	2.32	1	2
1:A:474:TYR:O	1:A:474:TYR:CG	0.47	2.67	1	1
1:A:562:MET:CE	1:A:562:MET:CG	0.47	2.92	1	1
1:B:126:ARG:CD	2:D:651:GLN:NE2	0.47	2.77	1	1
1:B:219:ILE:CD1	1:B:236:ILE:HG12	0.47	2.36	2	2
1:B:182:ASP:OD1	1:B:182:ASP:N	0.47	2.47	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:269:VAL:HG12	1:B:270:GLU:N	0.47	2.23	2	1
1:A:317:TYR:OH	1:A:386:LEU:HB3	0.47	2.08	1	1
1:B:10:GLY:O	1:B:221:ASP:O	0.47	2.32	2	2
1:B:177:LEU:N	1:B:177:LEU:CD1	0.47	2.74	1	1
1:B:292:VAL:HG11	1:B:329:VAL:CG2	0.47	2.36	1	1
1:A:58:LYS:HB2	1:A:73:PHE:CD1	0.47	2.43	2	1
1:B:464:ASP:CG	1:B:467:ASN:HB3	0.47	2.34	2	1
1:B:537:ILE:CG1	1:B:538:ARG:N	0.47	2.77	2	1
1:A:501:MET:SD	1:A:515:LEU:HD22	0.47	2.50	1	1
1:A:513:LEU:HD22	1:A:513:LEU:N	0.47	2.22	1	1
1:A:360:ILE:HD11	1:A:391:PRO:HD2	0.47	1.86	2	1
1:B:431:GLU:CD	1:B:452:GLY:HA3	0.47	2.35	1	1
1:A:345:MET:CB	1:A:347:PHE:CZ	0.47	2.97	2	1
1:A:438:ILE:HG23	1:A:441:HIS:HB2	0.47	1.86	2	1
1:B:50:ALA:O	1:B:54:LEU:HD23	0.47	2.09	2	1
1:B:345:MET:HB3	1:B:347:PHE:CZ	0.47	2.44	2	1
1:B:158:LEU:HD21	1:B:163:LEU:HD11	0.47	1.85	1	1
1:A:58:LYS:HG3	1:A:73:PHE:CE2	0.47	2.44	2	1
1:B:58:LYS:HG3	1:B:73:PHE:CE2	0.47	2.44	2	1
1:B:146:ILE:HD13	1:B:146:ILE:N	0.47	2.25	2	1
1:B:301:PHE:O	1:B:301:PHE:CD1	0.47	2.67	2	1
1:A:49:LYS:O	1:A:50:ALA:C	0.47	2.57	1	2
1:A:51:SER:OG	1:A:52:ALA:N	0.47	2.47	1	1
1:A:158:LEU:O	1:A:180:ILE:HG23	0.47	2.09	1	1
1:A:431:GLU:CD	1:A:452:GLY:HA3	0.47	2.35	1	1
1:A:463:VAL:HG21	1:A:473:LEU:HD21	0.47	1.75	1	1
1:B:317:TYR:HD2	1:B:317:TYR:O	0.47	1.91	1	1
1:B:501:MET:CG	1:B:520:LEU:HD11	0.47	2.40	1	1
1:A:74:GLU:O	1:A:77:ILE:CG2	0.47	2.63	2	1
1:A:535:LYS:O	1:A:539:ASN:ND2	0.47	2.48	2	1
1:B:562:MET:CE	1:B:562:MET:CG	0.47	2.92	2	1
1:A:10:GLY:O	1:A:11:ILE:CD1	0.47	2.59	1	2
1:A:126:ARG:O	1:A:130:VAL:HG13	0.47	2.09	1	1
1:A:542:PHE:CD1	1:A:542:PHE:C	0.47	2.93	1	1
1:B:43:PHE:CZ	1:B:47:ARG:NE	0.47	2.82	1	1
1:B:259:LEU:CB	1:B:260:PRO:CD	0.47	2.93	1	1
1:B:314:PHE:CG	1:B:376:ALA:HA	0.47	2.37	1	1
1:B:489:ILE:HA	1:B:499:THR:CG2	0.47	2.29	1	1
1:B:492:SER:O	1:B:497:LYS:HG2	0.47	2.10	1	1
1:B:542:PHE:CD1	1:B:542:PHE:C	0.47	2.93	1	1
1:A:182:ASP:OD1	1:A:182:ASP:N	0.47	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:301:PHE:O	1:A:301:PHE:CD1	0.47	2.68	2	1
1:A:304:ARG:HG2	1:A:306:ALA:O	0.47	2.09	2	1
1:B:58:LYS:HB2	1:B:73:PHE:CD1	0.47	2.45	2	1
1:B:243:GLN:C	1:B:243:GLN:OE1	0.47	2.58	2	1
1:B:287:ASN:O	1:B:530:ILE:CG1	0.47	2.63	2	1
1:B:345:MET:CB	1:B:347:PHE:CZ	0.47	2.98	2	1
1:B:360:ILE:CD1	1:B:390:PHE:CG	0.47	2.98	2	1
2:C:674:VAL:O	2:C:678:VAL:HG23	0.47	2.09	2	1
2:D:674:VAL:O	2:D:678:VAL:HG23	0.47	2.10	2	1
1:A:398:GLU:N	1:A:398:GLU:OE1	0.47	2.47	1	1
1:B:269:VAL:HG12	1:B:270:GLU:O	0.47	2.10	2	1
1:A:449:PHE:CE1	1:A:488:VAL:CG1	0.47	2.97	1	1
1:A:463:VAL:CG1	1:A:473:LEU:CG	0.47	2.88	1	1
1:B:181:THR:C	1:B:205:THR:CG2	0.47	2.88	1	1
1:B:157:ILE:HG12	1:B:177:LEU:CD1	0.47	2.40	2	1
1:B:470:ILE:HG22	1:B:470:ILE:O	0.47	2.10	2	1
1:B:515:LEU:CD1	1:B:515:LEU:N	0.47	2.78	2	1
1:A:181:THR:HG22	1:A:182:ASP:N	0.47	2.24	1	1
1:A:221:ASP:O	1:A:223:VAL:N	0.47	2.48	2	2
1:B:149:LEU:HD12	1:B:149:LEU:N	0.47	2.25	1	1
1:B:221:ASP:O	1:B:223:VAL:N	0.47	2.48	2	2
1:A:84:GLU:OE2	2:C:648:PHE:CD1	0.47	2.68	2	1
1:A:123:LEU:CD1	1:A:123:LEU:N	0.47	2.78	2	1
1:A:389:MET:CE	1:A:429:MET:SD	0.47	3.02	2	1
1:B:108:ILE:HG23	1:B:109:GLU:N	0.47	2.25	2	1
1:A:140:ASN:ND2	1:A:140:ASN:O	0.46	2.48	1	1
1:A:149:LEU:N	1:A:149:LEU:HD12	0.46	2.25	1	1
1:A:255:LYS:O	1:A:256:LEU:CB	0.46	2.62	1	1
1:A:369:ILE:O	1:A:372:ASP:OD2	0.46	2.33	1	1
1:B:51:SER:OG	1:B:52:ALA:N	0.46	2.47	1	1
1:B:369:ILE:O	1:B:372:ASP:OD2	0.46	2.33	1	1
1:A:5:ILE:O	1:A:5:ILE:CD1	0.46	2.63	2	1
1:A:146:ILE:N	1:A:146:ILE:HD13	0.46	2.24	2	1
1:A:350:GLU:OE1	1:A:357:TRP:CE2	0.46	2.68	2	1
1:B:6:LEU:N	1:B:6:LEU:CD2	0.46	2.75	2	1
1:B:515:LEU:HB3	1:B:520:LEU:CD2	0.46	2.40	2	1
1:A:43:PHE:CE2	1:A:89:ILE:HD13	0.46	2.46	1	1
1:A:164:THR:OG1	1:A:167:GLU:OE1	0.46	2.33	1	1
1:A:260:PRO:HG2	1:A:268:GLN:HE21	0.46	1.69	1	1
1:A:314:PHE:CE1	1:A:376:ALA:HA	0.46	2.38	1	1
1:A:330:ILE:CD1	1:A:330:ILE:N	0.46	2.78	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:390:PHE:N	1:A:390:PHE:CD2	0.46	2.80	1	1
1:A:492:SER:O	1:A:497:LYS:HG2	0.46	2.10	1	1
1:B:501:MET:SD	1:B:515:LEU:HD22	0.46	2.50	1	1
1:A:243:GLN:C	1:A:243:GLN:OE1	0.46	2.59	2	1
1:A:515:LEU:CD1	1:A:515:LEU:N	0.46	2.79	2	1
1:B:304:ARG:O	1:B:304:ARG:CZ	0.46	2.63	2	1
1:B:457:THR:HG23	1:B:458:GLN:N	0.46	2.26	2	1
1:A:260:PRO:HG3	1:A:290:GLU:HG3	0.46	1.86	1	1
1:B:126:ARG:HD3	2:D:651:GLN:NE2	0.46	2.25	1	1
1:B:147:ILE:HG23	1:B:148:ASP:N	0.46	2.25	1	1
1:B:330:ILE:CD1	1:B:330:ILE:N	0.46	2.78	1	1
1:A:272:CYS:SG	1:A:273:ALA:O	0.46	2.73	2	1
1:A:304:ARG:CD	1:A:304:ARG:C	0.46	2.87	2	1
1:B:74:GLU:O	1:B:77:ILE:CG2	0.46	2.63	2	1
1:A:43:PHE:CZ	1:A:47:ARG:NE	0.46	2.83	1	1
1:A:181:THR:C	1:A:205:THR:CG2	0.46	2.88	1	1
1:A:456:LEU:C	1:A:456:LEU:CD1	0.46	2.86	1	1
1:B:5:ILE:O	1:B:6:LEU:O	0.46	2.34	1	2
1:B:90:ILE:HD12	1:B:90:ILE:C	0.46	2.36	1	1
1:B:192:ILE:C	1:B:192:ILE:CD1	0.46	2.84	1	1
1:A:50:ALA:O	1:A:54:LEU:HD23	0.46	2.09	2	1
2:C:617:ARG:HB3	2:C:618:PRO:HD3	0.46	1.87	2	1
1:A:5:ILE:O	1:A:6:LEU:O	0.46	2.34	1	2
1:A:147:ILE:HG23	1:A:148:ASP:N	0.46	2.25	1	1
1:B:66:GLY:CA	1:B:68:GLU:OE2	0.46	2.64	1	1
1:B:221:ASP:C	1:B:223:VAL:H	0.46	2.19	1	2
1:B:390:PHE:N	1:B:390:PHE:CD2	0.46	2.79	1	1
1:A:113:SER:O	1:A:117:GLU:OE2	0.46	2.34	2	1
1:A:157:ILE:HG12	1:A:177:LEU:CD1	0.46	2.40	2	1
1:A:221:ASP:C	1:A:223:VAL:H	0.46	2.19	1	2
1:B:49:LYS:O	1:B:50:ALA:C	0.46	2.57	1	2
1:A:269:VAL:HG12	1:A:270:GLU:O	0.46	2.09	2	1
1:A:304:ARG:HD3	1:A:304:ARG:C	0.46	2.34	2	1
1:B:485:ILE:CG2	1:B:486:LYS:N	0.46	2.79	2	1
1:B:522:GLU:OE1	1:B:523:PHE:O	0.46	2.34	2	1
1:A:27:ASP:N	1:A:27:ASP:OD1	0.46	2.49	1	2
1:B:27:ASP:OD1	1:B:27:ASP:N	0.46	2.48	2	2
1:A:74:GLU:CA	1:A:77:ILE:CG2	0.46	2.90	2	1
1:B:85:LEU:HD23	1:B:85:LEU:O	0.46	2.10	2	1
1:B:307:LEU:HD23	1:B:307:LEU:C	0.46	2.35	2	1
1:A:66:GLY:CA	1:A:68:GLU:OE2	0.46	2.64	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:GLY:CA	1:A:299:PHE:CZ	0.46	2.95	1	1
1:A:459:TYR:O	1:B:459:TYR:HB3	0.46	2.10	1	2
1:B:332:ARG:NH1	1:B:335:ASP:N	0.46	2.64	1	1
1:A:333:THR:OG1	1:A:390:PHE:CD1	0.46	2.64	2	1
1:A:470:ILE:HG22	1:A:470:ILE:O	0.46	2.10	2	1
1:B:360:ILE:HD11	1:B:391:PRO:HD2	0.46	1.86	2	1
1:A:181:THR:C	1:A:205:THR:HG23	0.46	2.35	1	1
1:B:130:VAL:CG2	1:B:131:ARG:N	0.46	2.79	1	1
1:B:455:ASP:OD1	1:B:459:TYR:CZ	0.46	2.68	1	1
1:A:108:ILE:HG23	1:A:109:GLU:N	0.46	2.25	2	1
1:A:298:GLU:OE2	1:A:342:LEU:HD11	0.46	2.11	2	1
1:A:307:LEU:HD23	1:A:307:LEU:C	0.46	2.35	2	1
1:A:457:THR:HG23	1:A:458:GLN:N	0.46	2.25	2	1
1:B:5:ILE:O	1:B:5:ILE:CD1	0.46	2.63	2	1
1:B:12:ALA:CB	1:B:177:LEU:HD13	0.46	2.33	2	1
1:B:357:TRP:C	1:B:358:ARG:NE	0.46	2.74	2	1
1:B:388:ILE:HD12	1:B:388:ILE:C	0.46	2.34	2	1
1:A:123:LEU:HD12	1:A:123:LEU:N	0.46	2.26	1	1
1:B:449:PHE:CE1	1:B:488:VAL:CG1	0.46	2.97	1	1
1:B:470:ILE:HB	1:B:473:LEU:HD22	0.46	1.86	1	1
1:A:6:LEU:N	1:A:6:LEU:CD2	0.46	2.76	2	1
1:A:121:GLU:O	1:A:125:GLU:CD	0.46	2.59	2	1
1:A:198:GLU:C	1:A:199:LEU:HD22	0.46	2.36	2	1
1:A:354:PHE:C	1:A:355:LEU:CD2	0.46	2.88	2	1
1:B:107:VAL:CG2	1:B:108:ILE:H	0.46	2.24	2	1
1:B:110:GLY:O	1:B:113:SER:OG	0.46	2.31	2	1
1:B:272:CYS:SG	1:B:273:ALA:O	0.46	2.73	2	1
1:B:467:ASN:O	1:B:467:ASN:OD1	0.46	2.34	2	1
1:A:126:ARG:HD3	2:C:651:GLN:NE2	0.45	2.25	1	1
1:A:161:ALA:O	1:A:182:ASP:OD1	0.45	2.34	1	1
1:A:292:VAL:HG11	1:A:329:VAL:CG2	0.45	2.35	1	1
1:B:10:GLY:O	1:B:11:ILE:CD1	0.45	2.61	1	2
1:B:66:GLY:N	1:B:68:GLU:OE2	0.45	2.49	1	1
1:B:181:THR:C	1:B:205:THR:HG23	0.45	2.35	1	1
1:B:317:TYR:CE1	1:B:331:VAL:CG2	0.45	2.98	1	1
1:B:259:LEU:CB	1:B:262:ILE:CG1	0.45	2.90	2	1
1:B:186:ARG:C	1:B:188:SER:H	0.45	2.19	2	2
1:B:277:THR:O	1:B:279:ARG:N	0.45	2.49	1	2
1:A:177:LEU:O	1:A:177:LEU:CD1	0.45	2.60	2	1
1:A:261:ALA:HA	1:A:537:ILE:CD1	0.45	2.41	2	1
1:A:522:GLU:OE1	1:A:523:PHE:O	0.45	2.35	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:535:LYS:O	1:B:539:ASN:ND2	0.45	2.49	2	1
1:A:4:GLY:HA3	1:A:202:ILE:CD1	0.45	2.42	1	1
1:A:470:ILE:HB	1:A:473:LEU:HD22	0.45	1.87	1	1
1:B:43:PHE:CE2	1:B:89:ILE:HD13	0.45	2.46	1	1
1:B:164:THR:OG1	1:B:167:GLU:OE1	0.45	2.33	1	1
1:A:258:ASP:C	1:A:260:PRO:HD3	0.45	2.37	2	1
1:B:121:GLU:O	1:B:125:GLU:CD	0.45	2.60	2	1
1:B:198:GLU:C	1:B:199:LEU:HD22	0.45	2.36	2	1
1:B:388:ILE:C	1:B:388:ILE:CD1	0.45	2.89	2	1
1:A:90:ILE:HD12	1:A:90:ILE:C	0.45	2.36	1	1
1:A:126:ARG:NH2	2:C:616:THR:HA	0.45	2.27	1	1
1:A:367:ARG:O	1:A:368:GLU:C	0.45	2.60	1	2
1:B:123:LEU:N	1:B:123:LEU:HD12	0.45	2.26	1	2
1:B:317:TYR:CZ	1:B:331:VAL:CB	0.45	2.97	1	1
1:B:454:ASN:C	1:B:458:GLN:OE1	0.45	2.60	1	1
1:A:278:VAL:O	1:A:281:VAL:HG13	0.45	2.10	2	1
1:A:360:ILE:CD1	1:A:390:PHE:CG	0.45	3.00	2	1
1:B:123:LEU:CD1	1:B:123:LEU:N	0.45	2.79	2	1
1:A:126:ARG:NE	2:C:651:GLN:NE2	0.45	2.64	1	1
1:A:277:THR:O	1:A:279:ARG:N	0.45	2.49	1	2
1:A:310:GLU:N	1:A:310:GLU:CD	0.45	2.74	1	1
1:B:87:GLN:O	1:B:90:ILE:HG13	0.45	2.11	1	1
1:B:320:VAL:O	1:B:324:CYS:SG	0.45	2.72	1	2
1:A:357:TRP:C	1:A:358:ARG:NE	0.45	2.74	2	1
1:A:365:ASP:OD1	1:A:365:ASP:C	0.45	2.60	2	1
2:D:617:ARG:HB3	2:D:618:PRO:HD3	0.45	1.87	2	1
1:B:118:LEU:N	1:B:118:LEU:CD2	0.45	2.79	1	2
1:B:204:GLY:O	1:B:205:THR:C	0.45	2.59	2	2
1:B:513:LEU:HD22	1:B:513:LEU:N	0.45	2.22	1	1
1:B:521:ASP:OD1	1:B:521:ASP:O	0.45	2.35	1	1
1:B:268:GLN:O	1:B:268:GLN:OE1	0.45	2.35	2	1
1:B:402:LEU:C	1:B:402:LEU:CD1	0.45	2.90	2	1
1:A:204:GLY:O	1:A:205:THR:C	0.45	2.60	1	2
1:A:276:GLY:C	1:A:299:PHE:CD1	0.45	2.83	1	1
1:B:367:ARG:O	1:B:368:GLU:C	0.45	2.60	1	2
1:A:309:THR:HG23	1:A:312:GLU:H	0.45	1.72	2	1
1:B:255:LYS:O	1:B:256:LEU:HB3	0.45	2.12	2	1
1:B:478:SER:HB3	1:B:481:VAL:HG22	0.45	1.88	2	1
1:A:118:LEU:N	1:A:118:LEU:CD2	0.45	2.79	1	2
1:A:182:ASP:OD1	1:A:182:ASP:C	0.45	2.59	1	1
1:A:203:VAL:HG22	1:A:203:VAL:O	0.45	2.12	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:337:GLY:C	1:A:358:ARG:CG	0.45	2.90	1	1
1:B:161:ALA:O	1:B:182:ASP:OD1	0.45	2.35	1	1
1:B:301:PHE:HD2	1:B:342:LEU:HG	0.45	1.72	1	1
1:B:310:GLU:CD	1:B:310:GLU:N	0.45	2.74	1	1
1:B:337:GLY:C	1:B:358:ARG:CG	0.45	2.90	1	1
1:B:436:ALA:HB1	1:B:484:LEU:HG	0.45	1.89	1	1
1:A:12:ALA:HB1	1:A:177:LEU:CD1	0.45	2.34	2	1
1:A:287:ASN:O	1:A:530:ILE:CG1	0.45	2.64	2	1
1:A:515:LEU:CA	1:A:520:LEU:HD11	0.45	2.30	2	1
1:B:294:LEU:HD23	1:B:295:TYR:N	0.45	2.27	2	1
1:B:304:ARG:C	1:B:304:ARG:HD3	0.45	2.36	2	1
1:A:66:GLY:N	1:A:68:GLU:OE2	0.45	2.49	1	1
1:A:162:ASP:HA	1:A:181:THR:CG2	0.45	2.36	1	1
1:A:310:GLU:CD	1:A:311:GLU:H	0.45	2.20	1	1
1:B:85:LEU:O	1:B:89:ILE:HG23	0.45	2.12	1	1
1:A:485:ILE:CG2	1:A:486:LYS:N	0.45	2.79	2	1
1:B:301:PHE:O	1:B:304:ARG:HD3	0.45	2.09	2	1
1:A:301:PHE:HD2	1:A:342:LEU:HG	0.45	1.72	1	1
1:A:317:TYR:OH	1:A:331:VAL:CB	0.45	2.59	1	1
1:A:470:ILE:O	1:A:473:LEU:HD23	0.45	1.94	1	1
1:B:205:THR:OG1	1:B:208:VAL:CG2	0.45	2.58	1	1
1:B:317:TYR:OH	1:B:331:VAL:CB	0.45	2.61	1	1
1:B:484:LEU:HD23	1:B:484:LEU:C	0.45	2.37	1	1
2:D:678:VAL:HG13	2:D:679:LYS:N	0.45	2.26	1	1
1:A:121:GLU:O	1:A:125:GLU:OE2	0.45	2.35	2	1
1:A:268:GLN:OE1	1:A:268:GLN:O	0.45	2.35	2	1
1:B:51:SER:O	1:B:54:LEU:CG	0.45	2.65	2	1
1:A:89:ILE:HG13	1:A:90:ILE:H	0.44	1.73	1	1
1:A:186:ARG:C	1:A:188:SER:H	0.44	2.20	1	2
1:B:90:ILE:CD1	1:B:91:ALA:N	0.44	2.77	1	1
1:B:126:ARG:NE	2:D:651:GLN:NE2	0.44	2.64	1	1
1:B:463:VAL:HG11	1:B:473:LEU:CG	0.44	2.14	1	1
1:A:89:ILE:HD13	1:A:89:ILE:O	0.44	2.12	2	1
1:A:90:ILE:CD1	1:A:91:ALA:N	0.44	2.78	1	1
1:A:332:ARG:NH1	1:A:335:ASP:N	0.44	2.64	1	1
2:D:650:LEU:O	2:D:651:GLN:C	0.44	2.60	2	2
1:A:51:SER:O	1:A:54:LEU:CG	0.44	2.65	2	1
1:B:54:LEU:HD12	1:B:54:LEU:C	0.44	2.36	2	1
1:B:113:SER:O	1:B:117:GLU:OE2	0.44	2.34	2	1
1:B:357:TRP:O	1:B:358:ARG:NH2	0.44	2.50	2	1
1:B:389:MET:SD	1:B:450:SER:OG	0.44	2.65	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:MET:HE2	2:C:627:LYS:HD2	0.44	0.56	1	1
1:A:454:ASN:C	1:A:458:GLN:OE1	0.44	2.60	1	1
1:A:556:PRO:O	1:B:396:VAL:CG2	0.44	2.65	2	2
1:B:182:ASP:OD1	1:B:182:ASP:C	0.44	2.59	1	1
1:B:203:VAL:O	1:B:203:VAL:HG22	0.44	2.12	1	1
1:B:484:LEU:O	1:B:488:VAL:HG23	0.44	2.12	1	2
2:C:678:VAL:HG13	2:C:679:LYS:N	0.44	2.27	1	1
1:B:121:GLU:O	1:B:125:GLU:OE2	0.44	2.36	2	1
1:A:489:ILE:CA	1:A:499:THR:HG21	0.44	2.30	1	1
1:A:504:GLU:C	1:A:504:GLU:CD	0.44	2.86	1	1
1:A:110:GLY:O	1:A:113:SER:OG	0.44	2.32	2	1
1:B:11:ILE:CG2	1:B:239:MET:CE	0.44	2.94	2	1
1:B:269:VAL:CB	1:B:523:PHE:CZ	0.44	3.00	2	1
1:B:431:GLU:O	1:B:431:GLU:OE1	0.44	2.36	2	1
1:A:85:LEU:O	1:A:89:ILE:HG23	0.44	2.12	1	1
1:A:484:LEU:O	1:A:488:VAL:HG23	0.44	2.12	1	2
1:A:521:ASP:O	1:A:521:ASP:OD1	0.44	2.34	1	2
1:B:138:LEU:O	1:B:141:ILE:CG2	0.44	2.65	1	1
1:B:332:ARG:HH12	1:B:334:MET:HA	0.44	1.72	1	1
1:B:470:ILE:O	1:B:473:LEU:HD23	0.44	1.93	1	1
1:A:467:ASN:O	1:A:467:ASN:OD1	0.44	2.34	2	1
1:B:172:ASN:O	1:B:175:LYS:HD2	0.44	2.13	2	1
1:B:521:ASP:O	1:B:521:ASP:OD1	0.44	2.35	2	1
1:A:295:TYR:HB3	1:A:331:VAL:HA	0.44	1.90	2	2
1:B:186:ARG:C	1:B:188:SER:N	0.44	2.76	2	2
1:B:463:VAL:CG1	1:B:473:LEU:CG	0.44	2.89	1	1
2:C:650:LEU:O	2:C:651:GLN:C	0.44	2.60	2	2
2:C:680:LEU:O	2:C:684:LEU:HG	0.44	2.13	1	1
1:A:225:ASN:N	1:A:225:ASN:OD1	0.44	2.51	2	1
1:A:294:LEU:HD23	1:A:295:TYR:N	0.44	2.27	2	1
1:A:527:ALA:C	1:A:530:ILE:HG22	0.44	2.30	2	1
1:B:54:LEU:HD22	1:B:77:ILE:HD13	0.44	1.90	2	1
1:B:365:ASP:C	1:B:365:ASP:OD1	0.44	2.60	2	1
1:B:431:GLU:OE1	1:B:431:GLU:C	0.44	2.61	2	1
1:A:101:ASP:OD1	1:A:101:ASP:N	0.44	2.50	1	1
1:A:455:ASP:OD1	1:A:459:TYR:CZ	0.44	2.70	1	1
1:B:23:GLU:OE1	1:B:23:GLU:N	0.44	2.45	1	1
1:B:449:PHE:CZ	1:B:500:GLY:O	0.44	2.62	1	1
2:D:626:ALA:C	2:D:628:GLY:N	0.44	2.75	2	2
1:A:357:TRP:O	1:A:358:ARG:NH2	0.44	2.50	2	1
1:B:84:GLU:OE2	2:D:648:PHE:CD1	0.44	2.71	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:ARG:C	1:A:188:SER:N	0.44	2.76	2	2
1:A:302:MET:HA	1:A:342:LEU:HD11	0.44	1.90	1	1
1:A:320:VAL:O	1:A:324:CYS:SG	0.44	2.70	1	1
1:B:126:ARG:NH2	2:D:616:THR:HA	0.44	2.27	1	1
1:B:295:TYR:HB3	1:B:331:VAL:HA	0.44	1.90	2	2
2:C:626:ALA:C	2:C:628:GLY:N	0.44	2.75	1	2
1:A:302:MET:HG2	1:A:342:LEU:HD11	0.44	1.88	2	1
1:A:515:LEU:HB3	1:A:520:LEU:CD2	0.44	2.41	2	1
1:B:74:GLU:O	1:B:77:ILE:HG23	0.44	2.13	2	1
1:B:80:LEU:C	1:B:80:LEU:CD1	0.44	2.91	2	1
1:A:85:LEU:O	1:A:89:ILE:CG1	0.44	2.66	1	1
1:A:138:LEU:O	1:A:141:ILE:CG2	0.44	2.66	1	1
1:A:504:GLU:CD	1:A:504:GLU:O	0.44	2.61	2	2
1:B:126:ARG:O	1:B:130:VAL:HG13	0.44	2.12	1	1
2:D:669:ASP:O	2:D:670:GLU:C	0.44	2.60	1	2
1:A:172:ASN:O	1:A:175:LYS:HD2	0.44	2.13	2	1
1:A:357:TRP:CD1	1:A:358:ARG:CZ	0.44	3.01	2	1
1:A:388:ILE:HD12	1:A:388:ILE:C	0.44	2.36	2	1
1:B:225:ASN:N	1:B:225:ASN:OD1	0.44	2.50	2	1
1:B:294:LEU:C	1:B:294:LEU:CD2	0.44	2.91	2	1
1:A:92:LEU:O	1:A:96:LYS:N	0.43	2.50	2	2
1:A:263:THR:CG2	1:A:267:HIS:H	0.43	2.14	1	1
1:B:542:PHE:CD1	1:B:543:GLU:N	0.43	2.87	1	1
1:A:50:ALA:HB2	1:A:140:ASN:HD22	0.43	1.73	2	1
1:A:172:ASN:HB2	1:A:175:LYS:CE	0.43	2.43	2	1
1:A:301:PHE:O	1:A:304:ARG:HD3	0.43	2.10	2	1
1:B:333:THR:OG1	1:B:390:PHE:CD1	0.43	2.63	2	1
1:B:504:GLU:O	1:B:504:GLU:CD	0.43	2.61	2	1
1:A:484:LEU:HD23	1:A:484:LEU:C	0.43	2.37	1	1
1:A:558:THR:O	1:A:559:ASP:C	0.43	2.62	1	2
1:A:261:ALA:CA	1:A:537:ILE:CD1	0.43	2.96	2	1
1:A:301:PHE:CE1	1:A:304:ARG:NE	0.43	2.86	2	1
1:A:516:LEU:CD2	1:A:523:PHE:CZ	0.43	3.01	2	1
1:B:264:LEU:HD23	1:B:264:LEU:O	0.43	2.13	2	1
1:B:515:LEU:N	1:B:515:LEU:HD12	0.43	2.27	2	1
1:A:47:ARG:NH2	1:A:85:LEU:CD2	0.43	2.81	1	1
1:A:87:GLN:O	1:A:90:ILE:HG13	0.43	2.12	1	1
1:A:310:GLU:CG	1:A:311:GLU:N	0.43	2.81	1	1
1:B:4:GLY:HA3	1:B:202:ILE:CD1	0.43	2.41	1	1
1:B:47:ARG:NH2	1:B:85:LEU:CD2	0.43	2.81	1	1
1:B:70:GLU:C	1:B:70:GLU:OE1	0.43	2.61	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:84:GLU:O	1:B:88:GLU:OE2	0.43	2.35	1	1
1:B:453:THR:CA	1:B:456:LEU:HD12	0.43	2.42	1	1
2:C:647:LEU:O	2:C:651:GLN:OE1	0.43	2.36	2	2
2:D:649:LYS:O	2:D:650:LEU:C	0.43	2.62	1	2
1:A:80:LEU:C	1:A:80:LEU:CD1	0.43	2.91	2	1
1:A:304:ARG:NH2	1:A:344:TYR:HB3	0.43	2.28	2	1
1:A:478:SER:HB3	1:A:481:VAL:HG22	0.43	1.88	2	1
1:B:80:LEU:HD23	1:B:133:ILE:CG2	0.43	2.44	2	1
1:B:89:ILE:HD13	1:B:89:ILE:O	0.43	2.13	2	1
1:B:354:PHE:C	1:B:355:LEU:CD2	0.43	2.91	2	1
1:A:332:ARG:HH12	1:A:334:MET:HA	0.43	1.72	1	1
1:A:396:VAL:CG2	1:B:556:PRO:O	0.43	2.66	2	2
1:A:436:ALA:HB1	1:A:484:LEU:HG	0.43	1.89	1	1
1:B:192:ILE:CG1	1:B:193:MET:N	0.43	2.80	1	1
1:B:259:LEU:HB3	1:B:260:PRO:HD2	0.43	1.90	1	1
1:B:310:GLU:CG	1:B:311:GLU:N	0.43	2.81	1	1
1:B:313:GLN:C	1:B:313:GLN:CD	0.43	2.87	1	1
1:B:317:TYR:CE1	1:B:377:ILE:HD13	0.43	2.49	1	1
1:B:456:LEU:C	1:B:456:LEU:CD1	0.43	2.86	1	1
2:C:637:SER:O	2:C:638:ASN:C	0.43	2.62	2	2
1:A:123:LEU:N	1:A:123:LEU:HD12	0.43	2.27	2	1
1:A:515:LEU:N	1:A:515:LEU:HD12	0.43	2.28	2	1
1:A:296:ARG:HB2	1:A:299:PHE:CD2	0.43	2.46	1	1
1:B:276:GLY:CA	1:B:299:PHE:CZ	0.43	2.95	1	1
2:C:669:ASP:O	2:C:670:GLU:C	0.43	2.60	1	2
1:A:388:ILE:C	1:A:388:ILE:CD1	0.43	2.90	2	1
1:A:451:ILE:HB	1:A:501:MET:SD	0.43	2.54	2	1
1:A:473:LEU:CD2	1:B:361:ARG:NE	0.43	2.82	2	1
1:B:82:ASP:OD2	2:D:648:PHE:HE1	0.43	1.97	2	1
1:B:516:LEU:CD2	1:B:523:PHE:CZ	0.43	3.02	2	1
1:A:115:LEU:O	1:A:118:LEU:HB2	0.43	2.14	2	2
1:B:78:MET:CE	2:D:627:LYS:CB	0.43	2.97	1	1
1:B:101:ASP:N	1:B:101:ASP:OD1	0.43	2.49	1	2
1:B:126:ARG:NH2	2:D:619:ALA:HB2	0.43	1.88	1	1
2:D:637:SER:O	2:D:638:ASN:C	0.43	2.62	1	2
1:A:74:GLU:O	1:A:78:MET:HB2	0.43	2.13	2	1
1:A:80:LEU:HD23	1:A:133:ILE:CG2	0.43	2.43	2	1
1:A:107:VAL:CG2	1:A:108:ILE:H	0.43	2.25	2	1
1:A:256:LEU:C	1:A:258:ASP:N	0.43	2.76	2	1
1:B:530:ILE:C	1:B:530:ILE:CD1	0.43	2.77	2	1
1:A:182:ASP:O	1:A:183:ALA:O	0.43	2.37	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:313:GLN:C	1:A:313:GLN:CD	0.43	2.87	1	1
1:B:32:SER:OG	1:B:33:ALA:N	0.43	2.52	2	2
1:B:449:PHE:CZ	1:B:499:THR:OG1	0.43	2.52	1	1
1:B:463:VAL:HB	1:B:473:LEU:HD11	0.43	1.90	1	1
1:A:74:GLU:O	1:A:77:ILE:HG23	0.43	2.13	2	1
1:A:221:ASP:CG	1:A:222:ALA:N	0.43	2.77	2	1
1:A:264:LEU:HD23	1:A:264:LEU:O	0.43	2.13	2	1
1:A:269:VAL:CB	1:A:523:PHE:CZ	0.43	3.01	2	1
1:B:50:ALA:HB2	1:B:140:ASN:HD22	0.43	1.72	2	1
1:B:58:LYS:CB	1:B:73:PHE:CD2	0.43	3.01	2	1
2:D:610:ALA:O	2:D:657:GLN:HB2	0.43	2.14	2	1
1:A:70:GLU:C	1:A:70:GLU:OE1	0.43	2.62	1	1
1:A:84:GLU:O	1:A:88:GLU:OE2	0.43	2.36	1	1
1:A:101:ASP:CB	1:A:138:LEU:HD21	0.43	2.44	1	1
1:A:453:THR:CA	1:A:456:LEU:HD12	0.43	2.42	1	1
1:B:300:LEU:O	1:B:303:ASP:OD1	0.43	2.37	1	1
1:B:504:GLU:C	1:B:504:GLU:CD	0.43	2.86	1	1
2:C:649:LYS:O	2:C:650:LEU:C	0.43	2.62	1	2
2:D:647:LEU:O	2:D:651:GLN:OE1	0.43	2.36	1	2
1:A:294:LEU:C	1:A:294:LEU:CD2	0.43	2.92	2	1
1:B:152:ILE:CG2	1:B:175:LYS:CG	0.43	2.95	2	1
1:B:221:ASP:CA	1:B:239:MET:HE2	0.43	2.30	2	1
1:B:287:ASN:O	1:B:530:ILE:HG12	0.43	2.14	2	1
1:B:301:PHE:CG	1:B:342:LEU:CD2	0.43	2.91	2	1
1:B:360:ILE:HD11	1:B:390:PHE:CG	0.43	2.49	2	1
1:A:287:ASN:ND2	1:A:528:ILE:HA	0.43	2.28	1	1
1:B:8:SER:OG	1:B:199:LEU:O	0.43	2.36	1	2
1:B:182:ASP:O	1:B:183:ALA:O	0.43	2.37	1	2
1:B:310:GLU:CD	1:B:311:GLU:H	0.43	2.21	1	1
1:B:513:LEU:H	1:B:513:LEU:CD2	0.43	2.26	1	1
1:B:547:VAL:O	1:B:551:GLN:HG3	0.43	2.14	1	2
1:B:74:GLU:O	1:B:78:MET:HB2	0.43	2.13	2	1
1:A:192:ILE:CG1	1:A:193:MET:N	0.42	2.80	1	1
1:A:194:ALA:HA	1:A:199:LEU:CD2	0.42	2.45	1	1
1:A:321:ALA:HB2	1:A:386:LEU:HD21	0.42	1.91	1	1
1:A:431:GLU:HG3	1:A:452:GLY:CA	0.42	2.43	1	1
1:A:463:VAL:HB	1:A:473:LEU:HD11	0.42	1.90	1	1
1:A:464:ASP:CG	1:A:467:ASN:CG	0.42	2.87	1	1
1:B:8:SER:CB	1:B:199:LEU:O	0.42	2.67	2	2
1:B:85:LEU:O	1:B:89:ILE:CG1	0.42	2.66	1	1
1:B:92:LEU:O	1:B:96:LYS:N	0.42	2.50	2	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:354:PHE:C	1:A:355:LEU:HD22	0.42	2.39	2	1
1:A:485:ILE:HG22	1:A:518:MET:SD	0.42	2.54	2	1
1:A:179:PHE:CZ	1:A:181:THR:CB	0.42	3.02	1	1
1:A:296:ARG:H	1:A:299:PHE:HE2	0.42	1.56	1	1
1:A:441:HIS:CE1	1:B:556:PRO:HB3	0.42	2.48	1	2
1:B:47:ARG:NH2	1:B:85:LEU:HD21	0.42	2.29	1	1
1:B:296:ARG:H	1:B:299:PHE:HE2	0.42	1.55	1	1
1:B:84:GLU:CG	1:B:85:LEU:N	0.42	2.82	2	1
1:B:302:MET:SD	1:B:342:LEU:HG	0.42	2.54	2	1
1:B:357:TRP:CD1	1:B:358:ARG:CZ	0.42	3.02	2	1
1:A:47:ARG:NH2	1:A:85:LEU:HD21	0.42	2.30	1	1
1:A:542:PHE:CD1	1:A:543:GLU:N	0.42	2.87	1	1
1:B:101:ASP:CB	1:B:138:LEU:HD21	0.42	2.44	1	1
1:B:285:GLU:CG	1:B:286:ARG:N	0.42	2.82	2	1
1:B:451:ILE:HB	1:B:501:MET:SD	0.42	2.54	2	1
1:A:74:GLU:OE1	2:C:624:LYS:CE	0.42	2.66	1	1
1:A:161:ALA:C	1:A:181:THR:HG23	0.42	2.40	1	1
1:A:449:PHE:CZ	1:A:499:THR:OG1	0.42	2.52	1	1
1:B:179:PHE:CZ	1:B:181:THR:CB	0.42	3.02	1	1
1:B:181:THR:O	1:B:203:VAL:C	0.42	2.63	2	2
1:B:371:ARG:O	1:B:375:ARG:HB2	0.42	2.15	1	1
2:D:623:VAL:HG13	2:D:644:ALA:O	0.42	2.14	2	2
1:A:221:ASP:OD1	1:A:226:GLN:N	0.42	2.52	2	1
1:A:498:TRP:CD1	1:A:498:TRP:N	0.42	2.88	2	1
1:B:172:ASN:HB2	1:B:175:LYS:CE	0.42	2.44	2	1
1:B:309:THR:HG23	1:B:312:GLU:H	0.42	1.74	2	1
1:A:8:SER:CB	1:A:199:LEU:O	0.42	2.67	1	2
1:A:181:THR:O	1:A:203:VAL:C	0.42	2.63	1	2
1:A:448:PHE:C	1:A:497:LYS:HZ1	0.42	2.22	1	1
1:A:449:PHE:CD2	1:A:500:GLY:N	0.42	2.87	1	1
1:B:66:GLY:C	1:B:68:GLU:OE2	0.42	2.62	1	1
1:A:54:LEU:CD2	1:A:77:ILE:HD13	0.42	2.44	2	1
1:B:157:ILE:HG12	1:B:177:LEU:HD21	0.42	1.89	2	1
1:B:354:PHE:C	1:B:355:LEU:HD22	0.42	2.40	2	1
1:A:32:SER:OG	1:A:33:ALA:N	0.42	2.52	2	2
1:A:371:ARG:O	1:A:375:ARG:HB2	0.42	2.15	1	1
1:B:179:PHE:O	1:B:201:ALA:HB1	0.42	2.15	1	2
1:B:449:PHE:CD2	1:B:500:GLY:N	0.42	2.88	1	1
1:A:84:GLU:CG	1:A:85:LEU:N	0.42	2.82	2	1
1:A:108:ILE:CG2	1:A:109:GLU:N	0.42	2.82	2	1
1:A:221:ASP:CA	1:A:239:MET:HE2	0.42	2.30	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:221:ASP:CG	1:B:222:ALA:N	0.42	2.77	2	1
1:A:8:SER:OG	1:A:199:LEU:O	0.42	2.37	1	2
1:A:72:ILE:HG13	1:A:73:PHE:N	0.42	2.30	1	1
1:A:455:ASP:O	1:A:458:GLN:HB2	0.42	2.14	1	1
1:B:115:LEU:O	1:B:118:LEU:HB2	0.42	2.14	2	2
1:B:161:ALA:C	1:B:181:THR:HG23	0.42	2.40	1	1
1:B:464:ASP:CG	1:B:467:ASN:CG	0.42	2.88	1	1
1:A:54:LEU:HD22	1:A:77:ILE:HD13	0.42	1.90	2	1
1:A:504:GLU:O	1:A:504:GLU:OE1	0.42	2.38	2	1
1:B:54:LEU:CD2	1:B:77:ILE:HD13	0.42	2.44	2	1
1:B:252:GLU:O	1:B:255:LYS:HG3	0.42	2.14	2	1
1:B:262:ILE:HD12	1:B:262:ILE:O	0.42	2.15	2	1
1:B:269:VAL:CG1	1:B:270:GLU:N	0.42	2.83	2	1
1:B:498:TRP:CD1	1:B:498:TRP:N	0.42	2.88	2	1
1:A:11:ILE:CG2	1:A:239:MET:CE	0.42	2.93	1	2
1:A:449:PHE:CZ	1:A:500:GLY:O	0.42	2.62	1	1
1:A:547:VAL:O	1:A:551:GLN:HG3	0.42	2.14	1	2
1:B:72:ILE:HG13	1:B:73:PHE:N	0.42	2.29	1	1
1:B:520:LEU:HD22	1:B:522:GLU:N	0.42	2.29	1	1
1:B:521:ASP:CG	1:B:522:GLU:OE2	0.42	2.63	1	1
2:C:623:VAL:HG13	2:C:644:ALA:O	0.42	2.14	1	2
1:B:113:SER:O	1:B:117:GLU:CD	0.42	2.63	2	1
1:A:66:GLY:C	1:A:68:GLU:OE2	0.42	2.62	1	1
1:A:275:ILE:C	1:A:299:PHE:CE2	0.42	2.94	1	1
1:A:392:MET:HE1	1:A:455:ASP:OD2	0.42	2.15	1	1
1:B:194:ALA:HA	1:B:199:LEU:CD2	0.42	2.45	1	1
1:B:455:ASP:O	1:B:458:GLN:HB2	0.42	2.14	1	1
1:A:298:GLU:O	1:A:301:PHE:HB3	0.42	2.15	2	1
1:A:301:PHE:CG	1:A:342:LEU:CD2	0.42	2.92	2	1
1:A:489:ILE:CG1	1:A:499:THR:HG21	0.42	2.32	2	1
1:B:298:GLU:O	1:B:301:PHE:HB3	0.42	2.14	2	1
1:B:485:ILE:HG22	1:B:518:MET:SD	0.42	2.54	2	1
1:A:549:ALA:O	1:A:550:GLU:C	0.42	2.63	1	2
1:A:550:GLU:O	1:A:551:GLN:C	0.42	2.62	1	2
1:B:302:MET:HA	1:B:342:LEU:HD11	0.42	1.91	1	1
1:B:314:PHE:CE2	1:B:375:ARG:C	0.42	2.98	1	1
2:D:678:VAL:CG1	2:D:679:LYS:N	0.42	2.82	1	1
1:A:58:LYS:CB	1:A:73:PHE:CD2	0.42	3.03	2	1
1:B:171:LEU:HD23	1:B:175:LYS:NZ	0.42	2.30	2	1
1:B:337:GLY:O	1:B:358:ARG:NH1	0.42	2.52	2	1
1:A:317:TYR:CE1	1:A:331:VAL:CB	0.41	3.02	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:296:ARG:HB2	1:B:299:PHE:CD2	0.41	2.46	1	1
1:B:299:PHE:CD1	1:B:299:PHE:C	0.41	2.97	1	1
1:B:108:ILE:CG2	1:B:109:GLU:N	0.41	2.83	2	1
1:A:78:MET:CE	2:C:627:LYS:CB	0.41	2.98	1	1
1:A:513:LEU:H	1:A:513:LEU:CD2	0.41	2.26	1	1
1:B:89:ILE:HG13	1:B:90:ILE:H	0.41	1.73	1	1
1:B:431:GLU:HG3	1:B:452:GLY:CA	0.41	2.45	1	1
2:C:678:VAL:CG1	2:C:679:LYS:N	0.41	2.82	1	1
1:A:361:ARG:NE	1:B:473:LEU:CD2	0.41	2.84	2	1
1:A:431:GLU:C	1:A:431:GLU:OE1	0.41	2.63	2	1
1:B:177:LEU:O	1:B:177:LEU:CD1	0.41	2.60	2	1
1:A:111:GLN:OE1	2:C:648:PHE:CB	0.41	2.31	1	1
1:B:453:THR:HG21	1:B:505:LEU:HB2	0.41	1.92	1	1
1:B:504:GLU:CD	1:B:504:GLU:O	0.41	2.62	1	1
1:B:558:THR:O	1:B:559:ASP:C	0.41	2.61	1	2
1:A:262:ILE:O	1:A:262:ILE:HD12	0.41	2.15	2	1
1:A:337:GLY:O	1:A:358:ARG:NH1	0.41	2.52	2	1
1:A:337:GLY:CA	1:A:358:ARG:NH2	0.41	2.83	2	1
1:A:356:GLY:C	1:A:358:ARG:HD2	0.41	2.41	2	1
1:B:270:GLU:N	1:B:270:GLU:OE1	0.41	2.54	2	1
1:B:350:GLU:HB3	1:B:357:TRP:CH2	0.41	2.50	2	1
1:B:527:ALA:C	1:B:530:ILE:HG22	0.41	2.31	2	1
1:A:257:LYS:HG3	1:A:257:LYS:O	0.41	2.14	1	1
1:A:458:GLN:CD	1:A:465:ARG:HB2	0.41	2.41	1	1
1:B:74:GLU:OE1	2:D:624:LYS:CE	0.41	2.68	1	1
1:B:302:MET:CB	1:B:342:LEU:HD21	0.41	2.37	1	1
1:B:347:PHE:CE1	1:B:348:PRO:O	0.41	2.74	1	1
1:B:352:ASN:O	1:B:353:PRO:C	0.41	2.63	1	2
1:B:549:ALA:O	1:B:550:GLU:C	0.41	2.63	1	2
1:A:113:SER:O	1:A:117:GLU:CD	0.41	2.63	2	1
1:B:304:ARG:HG2	1:B:306:ALA:O	0.41	2.10	2	1
1:A:23:GLU:OE1	1:A:23:GLU:N	0.41	2.44	1	1
1:A:489:ILE:HA	1:A:499:THR:CG2	0.41	2.30	1	1
1:A:504:GLU:C	1:A:504:GLU:OE1	0.41	2.64	1	1
1:A:521:ASP:CG	1:A:522:GLU:OE2	0.41	2.64	1	1
1:A:269:VAL:CG1	1:A:270:GLU:N	0.41	2.83	2	1
1:A:431:GLU:OE1	1:A:431:GLU:O	0.41	2.39	2	1
1:B:337:GLY:CA	1:B:358:ARG:NH2	0.41	2.84	2	1
1:B:372:ASP:OD1	1:B:372:ASP:O	0.41	2.38	2	1
1:A:179:PHE:O	1:A:201:ALA:HB1	0.41	2.15	2	2
1:A:316:ALA:O	1:A:320:VAL:HG23	0.41	2.16	1	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:321:ALA:HB2	1:B:386:LEU:HD21	0.41	1.91	1	1
1:A:79:LEU:HD22	2:C:647:LEU:HD23	0.41	1.93	2	1
1:A:171:LEU:HD23	1:A:175:LYS:NZ	0.41	2.30	2	1
1:A:438:ILE:CG2	1:A:438:ILE:O	0.41	2.69	2	1
1:A:455:ASP:O	1:A:458:GLN:HB3	0.41	2.15	2	1
1:A:484:LEU:CD1	1:B:437:THR:CG2	0.41	2.97	2	1
1:B:12:ALA:HB1	1:B:177:LEU:CD1	0.41	2.33	2	1
1:A:299:PHE:CD1	1:A:299:PHE:C	0.41	2.96	1	1
1:B:405:GLU:O	1:B:406:ILE:C	0.41	2.62	1	2
2:D:679:LYS:O	2:D:683:GLU:N	0.41	2.54	1	2
1:A:77:ILE:HG23	1:A:78:MET:N	0.41	2.30	2	1
1:A:82:ASP:OD2	2:C:648:PHE:HE1	0.41	1.98	2	1
1:A:157:ILE:HG12	1:A:177:LEU:HD21	0.41	1.89	2	1
1:A:476:PRO:C	1:A:481:VAL:CG2	0.41	2.89	2	1
1:A:197:LEU:O	1:A:197:LEU:CD1	0.41	2.68	1	1
1:A:214:ASN:OD1	1:A:214:ASN:O	0.41	2.38	2	2
1:A:556:PRO:O	1:B:396:VAL:CG1	0.41	2.68	1	1
1:A:287:ASN:O	1:A:530:ILE:HG12	0.41	2.15	2	1
1:B:356:GLY:C	1:B:358:ARG:HD2	0.41	2.40	2	1
2:D:617:ARG:CB	2:D:618:PRO:HD3	0.41	2.46	2	1
1:A:5:ILE:O	1:A:5:ILE:HG22	0.41	2.15	1	1
1:A:470:ILE:O	1:A:471:SER:C	0.41	2.64	1	2
1:B:197:LEU:O	1:B:197:LEU:CD1	0.41	2.68	1	1
1:B:387:ARG:NH1	1:B:425:GLU:OE2	0.41	2.54	1	1
2:C:679:LYS:O	2:C:683:GLU:N	0.41	2.54	2	2
1:A:270:GLU:N	1:A:270:GLU:OE1	0.41	2.54	2	1
1:A:499:THR:O	1:A:499:THR:HG23	0.41	2.16	2	1
1:B:214:ASN:OD1	1:B:214:ASN:O	0.41	2.38	2	1
1:B:261:ALA:CA	1:B:537:ILE:CD1	0.41	2.98	2	1
1:B:271:VAL:HG12	1:B:523:PHE:CD1	0.41	2.50	2	1
1:B:455:ASP:O	1:B:458:GLN:HB3	0.41	2.16	2	1
2:D:618:PRO:HB3	2:D:684:LEU:HD22	0.41	1.92	2	1
1:A:123:LEU:N	1:A:123:LEU:CD1	0.41	2.84	1	1
1:B:162:ASP:HA	1:B:181:THR:CG2	0.41	2.36	1	1
1:B:235:VAL:C	1:B:237:ASP:N	0.41	2.79	1	1
1:B:260:PRO:HG3	1:B:290:GLU:HG3	0.41	1.92	1	1
1:B:317:TYR:CE1	1:B:331:VAL:CB	0.41	3.04	1	1
1:B:458:GLN:CD	1:B:465:ARG:HB2	0.41	2.41	1	1
1:B:58:LYS:HB2	1:B:73:PHE:CE2	0.41	2.51	2	1
1:B:438:ILE:CG2	1:B:438:ILE:O	0.41	2.67	2	1
1:A:352:ASN:O	1:A:353:PRO:C	0.40	2.63	1	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:316:ALA:O	1:B:320:VAL:HG23	0.40	2.16	1	1
1:A:232:THR:HG22	1:A:234:GLU:N	0.40	2.27	2	1
1:A:235:VAL:C	1:A:237:ASP:N	0.40	2.79	2	1
1:A:252:GLU:O	1:A:255:LYS:HG2	0.40	2.16	2	1
1:A:485:ILE:HG22	1:A:486:LYS:N	0.40	2.31	2	1
1:A:515:LEU:CA	1:A:520:LEU:CD1	0.40	2.97	2	1
1:B:283:GLY:O	1:B:287:ASN:ND2	0.40	2.53	2	1
1:B:388:ILE:O	1:B:388:ILE:HG13	0.40	2.15	2	1
1:A:314:PHE:CZ	1:A:379:ARG:HB2	0.40	2.49	1	1
1:A:453:THR:HG21	1:A:505:LEU:HB2	0.40	1.92	1	1
1:B:243:GLN:O	1:B:246:VAL:CG2	0.40	2.42	1	1
1:A:350:GLU:HB3	1:A:357:TRP:CH2	0.40	2.50	2	1
1:B:476:PRO:CA	1:B:481:VAL:HG21	0.40	2.46	2	1
1:B:485:ILE:HG22	1:B:486:LYS:N	0.40	2.31	2	1
1:A:180:ILE:HD11	1:A:208:VAL:HG21	0.40	1.92	1	1
1:A:292:VAL:CG1	1:A:329:VAL:CG2	0.40	2.83	1	1
1:B:214:ASN:O	1:B:214:ASN:OD1	0.40	2.39	1	1
1:B:175:LYS:HD3	1:B:176:VAL:CA	0.40	2.46	2	1
1:B:294:LEU:HD23	1:B:296:ARG:N	0.40	2.31	2	1
1:A:130:VAL:HG23	1:A:131:ARG:N	0.40	2.32	1	1
1:A:145:LYS:HG3	1:A:146:ILE:N	0.40	2.32	1	1
1:A:246:VAL:HG23	1:A:247:ALA:N	0.40	2.31	1	1
1:A:473:LEU:HD23	1:A:473:LEU:C	0.40	2.41	1	1
1:B:305:ASP:HA	1:B:344:TYR:CZ	0.40	2.52	1	1
1:B:393:ILE:O	1:B:393:ILE:CG2	0.40	2.68	1	1
1:A:354:PHE:CG	1:A:458:GLN:OE1	0.40	2.75	2	1
1:A:360:ILE:HD11	1:A:390:PHE:CG	0.40	2.52	2	1
1:B:67:GLU:OE1	1:B:70:GLU:OE1	0.40	2.39	2	1
1:A:347:PHE:CE1	1:A:348:PRO:O	0.40	2.75	1	1
1:A:405:GLU:O	1:A:406:ILE:C	0.40	2.62	1	2
1:A:470:ILE:CG2	1:A:473:LEU:HD13	0.40	2.46	1	1
1:B:173:LEU:CD2	1:B:173:LEU:H	0.40	2.29	1	1
1:B:504:GLU:C	1:B:504:GLU:OE1	0.40	2.65	1	1
1:B:302:MET:O	1:B:302:MET:HG3	0.40	2.16	2	1
1:B:354:PHE:CG	1:B:458:GLN:OE1	0.40	2.75	2	1
2:C:657:GLN:HG3	2:C:657:GLN:O	0.40	2.17	2	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	571/573 (100%)	538±0 (94±0%)	26±0 (5±0%)	7±0 (1±0%)	13	61
1	B	571/573 (100%)	538±2 (94±0%)	26±2 (5±0%)	7±0 (1±0%)	13	61
2	C	83/85 (98%)	76±0 (92±0%)	6±0 (7±0%)	1±0 (1±0%)	13	61
2	D	83/85 (98%)	76±0 (92±0%)	6±0 (7±0%)	1±0 (1±0%)	13	61
All	All	2616/2632 (99%)	2455 (94%)	129 (5%)	32 (1%)	13	61

All 19 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	6	LEU	2
1	A	148	ASP	2
1	A	183	ALA	2
1	A	232	THR	2
1	A	260	PRO	2
1	A	278	VAL	2
1	B	6	LEU	2
1	B	148	ASP	2
1	B	183	ALA	2
1	B	232	THR	2
1	B	278	VAL	2
2	C	651	GLN	2
2	D	651	GLN	2
1	A	256	LEU	1
1	B	256	LEU	1
1	B	260	PRO	1
1	A	257	LYS	1
1	B	254	ALA	1
1	B	255	LYS	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/474 (100%)	406±9 (86±2%)	68±9 (14±2%)	5	44
1	B	474/474 (100%)	406±10 (86±2%)	68±10 (14±2%)	5	44
2	C	70/70 (100%)	62±2 (89±3%)	8±2 (11±3%)	8	50
2	D	70/70 (100%)	62±2 (89±3%)	8±2 (11±3%)	8	50
All	All	2176/2176 (100%)	1872 (86%)	304 (14%)	5	44

All 240 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	27	ASP	2
1	A	28	ARG	2
1	A	32	SER	2
1	A	58	LYS	2
1	A	77	ILE	2
1	A	80	LEU	2
1	A	209	THR	2
1	A	213	LYS	2
1	A	215	ASP	2
1	A	216	ASP	2
1	A	223	VAL	2
1	A	246	VAL	2
1	A	307	LEU	2
1	A	334	MET	2
1	A	347	PHE	2
1	A	388	ILE	2
1	A	396	VAL	2
1	A	402	LEU	2
1	A	404	LYS	2
1	A	411	GLN	2
1	A	423	SER	2
1	A	455	ASP	2
1	A	464	ASP	2
1	A	486	LYS	2
1	A	520	LEU	2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	557	THR	2
1	A	561	LEU	2
1	B	27	ASP	2
1	B	28	ARG	2
1	B	32	SER	2
1	B	58	LYS	2
1	B	77	ILE	2
1	B	80	LEU	2
1	B	209	THR	2
1	B	213	LYS	2
1	B	215	ASP	2
1	B	216	ASP	2
1	B	223	VAL	2
1	B	246	VAL	2
1	B	259	LEU	2
1	B	307	LEU	2
1	B	334	MET	2
1	B	347	PHE	2
1	B	388	ILE	2
1	B	396	VAL	2
1	B	404	LYS	2
1	B	411	GLN	2
1	B	423	SER	2
1	B	455	ASP	2
1	B	464	ASP	2
1	B	486	LYS	2
1	B	520	LEU	2
1	B	557	THR	2
1	B	561	LEU	2
2	C	601	MET	2
2	C	630	THR	2
2	C	641	SER	2
2	C	643	SER	2
2	C	651	GLN	2
2	D	601	MET	2
2	D	630	THR	2
2	D	641	SER	2
2	D	643	SER	2
2	D	651	GLN	2
1	A	70	GLU	1
1	A	88	GLU	1
1	A	130	VAL	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	138	LEU	1
1	A	140	ASN	1
1	A	150	SER	1
1	A	180	ILE	1
1	A	192	ILE	1
1	A	197	LEU	1
1	A	199	LEU	1
1	A	205	THR	1
1	A	243	GLN	1
1	A	258	ASP	1
1	A	277	THR	1
1	A	281	VAL	1
1	A	292	VAL	1
1	A	299	PHE	1
1	A	330	ILE	1
1	A	344	TYR	1
1	A	360	ILE	1
1	A	377	ILE	1
1	A	398	GLU	1
1	A	438	ILE	1
1	A	449	PHE	1
1	A	456	LEU	1
1	A	463	VAL	1
1	A	470	ILE	1
1	A	473	LEU	1
1	A	484	LEU	1
1	A	499	THR	1
1	A	513	LEU	1
1	A	529	SER	1
1	B	70	GLU	1
1	B	88	GLU	1
1	B	130	VAL	1
1	B	138	LEU	1
1	B	140	ASN	1
1	B	150	SER	1
1	B	180	ILE	1
1	B	192	ILE	1
1	B	197	LEU	1
1	B	199	LEU	1
1	B	205	THR	1
1	B	243	GLN	1
1	B	281	VAL	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	292	VAL	1
1	B	299	PHE	1
1	B	302	MET	1
1	B	330	ILE	1
1	B	344	TYR	1
1	B	360	ILE	1
1	B	377	ILE	1
1	B	398	GLU	1
1	B	438	ILE	1
1	B	449	PHE	1
1	B	456	LEU	1
1	B	463	VAL	1
1	B	470	ILE	1
1	B	473	LEU	1
1	B	484	LEU	1
1	B	499	THR	1
1	B	513	LEU	1
1	B	529	SER	1
2	C	683	GLU	1
2	D	683	GLU	1
1	A	5	ILE	1
1	A	47	ARG	1
1	A	72	ILE	1
1	A	73	PHE	1
1	A	78	MET	1
1	A	85	LEU	1
1	A	89	ILE	1
1	A	92	LEU	1
1	A	111	GLN	1
1	A	117	GLU	1
1	A	125	GLU	1
1	A	137	LEU	1
1	A	144	LEU	1
1	A	146	ILE	1
1	A	163	LEU	1
1	A	171	LEU	1
1	A	175	LYS	1
1	A	182	ASP	1
1	A	187	THR	1
1	A	189	HIS	1
1	A	193	MET	1
1	A	253	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	262	ILE	1
1	A	268	GLN	1
1	A	272	CYS	1
1	A	300	LEU	1
1	A	304	ARG	1
1	A	309	THR	1
1	A	336	ILE	1
1	A	341	GLU	1
1	A	350	GLU	1
1	A	355	LEU	1
1	A	358	ARG	1
1	A	371	ARG	1
1	A	372	ASP	1
1	A	390	PHE	1
1	A	392	MET	1
1	A	394	ILE	1
1	A	431	GLU	1
1	A	432	THR	1
1	A	451	ILE	1
1	A	453	THR	1
1	A	474	TYR	1
1	A	480	SER	1
1	A	485	ILE	1
1	A	501	MET	1
1	A	502	CYS	1
1	A	523	PHE	1
1	A	530	ILE	1
1	A	537	ILE	1
1	B	5	ILE	1
1	B	47	ARG	1
1	B	72	ILE	1
1	B	73	PHE	1
1	B	78	MET	1
1	B	85	LEU	1
1	B	89	ILE	1
1	B	92	LEU	1
1	B	117	GLU	1
1	B	125	GLU	1
1	B	137	LEU	1
1	B	144	LEU	1
1	B	146	ILE	1
1	B	163	LEU	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	B	171	LEU	1
1	B	175	LYS	1
1	B	182	ASP	1
1	B	187	THR	1
1	B	189	HIS	1
1	B	193	MET	1
1	B	256	LEU	1
1	B	262	ILE	1
1	B	268	GLN	1
1	B	272	CYS	1
1	B	300	LEU	1
1	B	304	ARG	1
1	B	309	THR	1
1	B	326	SER	1
1	B	336	ILE	1
1	B	341	GLU	1
1	B	350	GLU	1
1	B	355	LEU	1
1	B	358	ARG	1
1	B	371	ARG	1
1	B	372	ASP	1
1	B	390	PHE	1
1	B	392	MET	1
1	B	394	ILE	1
1	B	402	LEU	1
1	B	431	GLU	1
1	B	432	THR	1
1	B	451	ILE	1
1	B	453	THR	1
1	B	474	TYR	1
1	B	480	SER	1
1	B	485	ILE	1
1	B	501	MET	1
1	B	502	CYS	1
1	B	523	PHE	1
1	B	530	ILE	1
1	B	537	ILE	1
2	C	606	VAL	1
2	C	607	THR	1
2	C	612	ASN	1
2	C	614	LEU	1
2	C	676	HIS	1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
2	D	606	VAL	1
2	D	607	THR	1
2	D	614	LEU	1
2	D	676	HIS	1
2	D	684	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided