



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:57 PM GMT

PDB ID : 4GPD  
Title : THE STRUCTURE OF LOBSTER APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE AT 3.0 ANGSTROMS RESOLUTION  
Authors : Griffith, J.P.; Song, S.; Rossmann, M.G.  
Deposited on : 1988-01-04  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

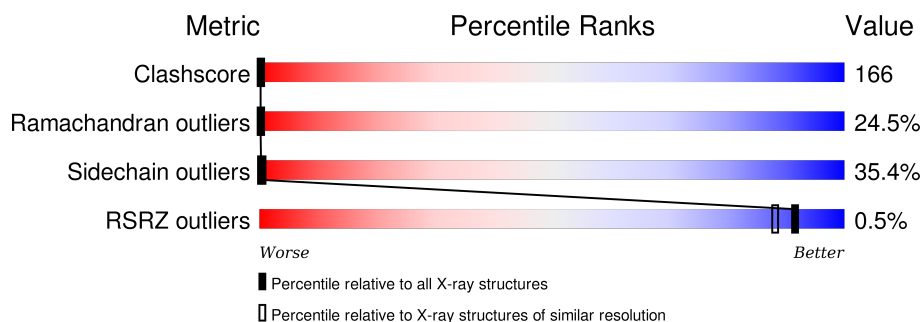
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	333	<div> <div>9%</div> <div>27%</div> <div>39%</div> <div>25%</div> </div>
1	2	333	<div> <div>6%</div> <div>33%</div> <div>38%</div> <div>23%</div> </div>
1	3	333	<div> <div>6%</div> <div>28%</div> <div>39%</div> <div>28%</div> </div>
1	4	333	<div> <div>7%</div> <div>30%</div> <div>37%</div> <div>26%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10150 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			
1	2	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			
1	3	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			
1	4	333	Total	C	N	O	S	0	0	0
			2507	1591	419	482	15			

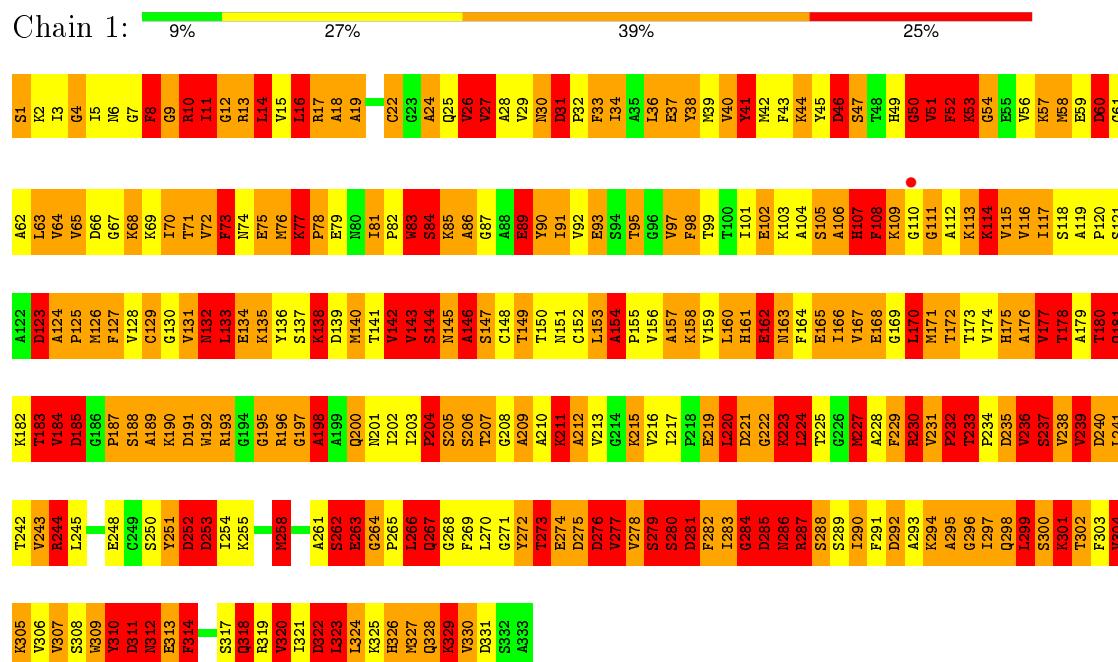
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	23	Total	O	0	0
			23	23		
2	2	28	Total	O	0	0
			28	28		
2	3	27	Total	O	0	0
			27	27		
2	4	44	Total	O	0	0
			44	44		

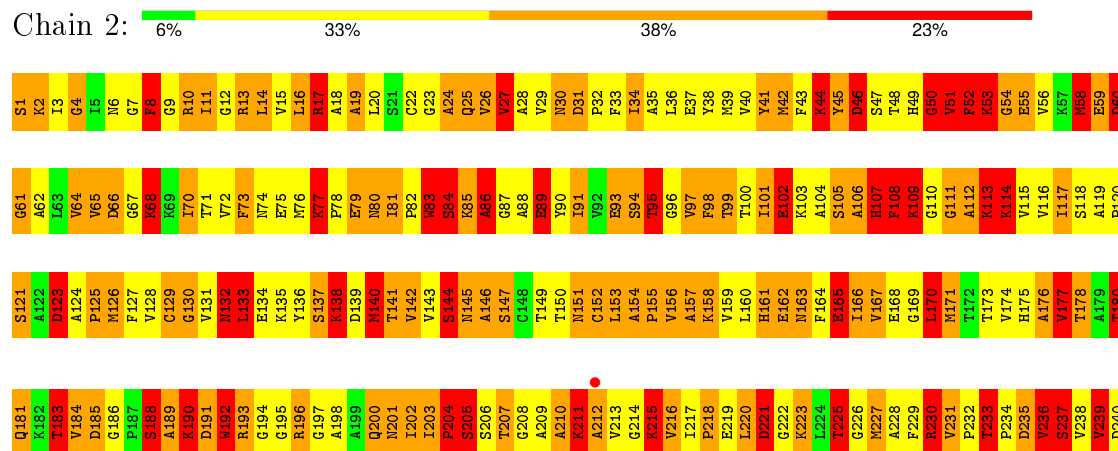
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

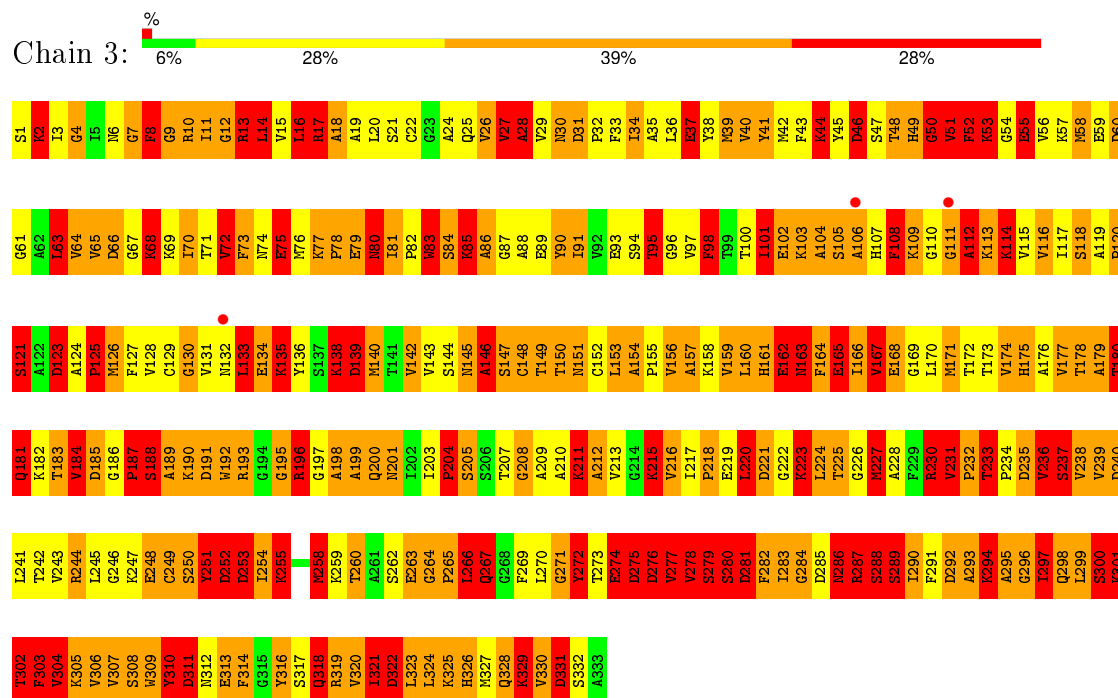


#### • Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

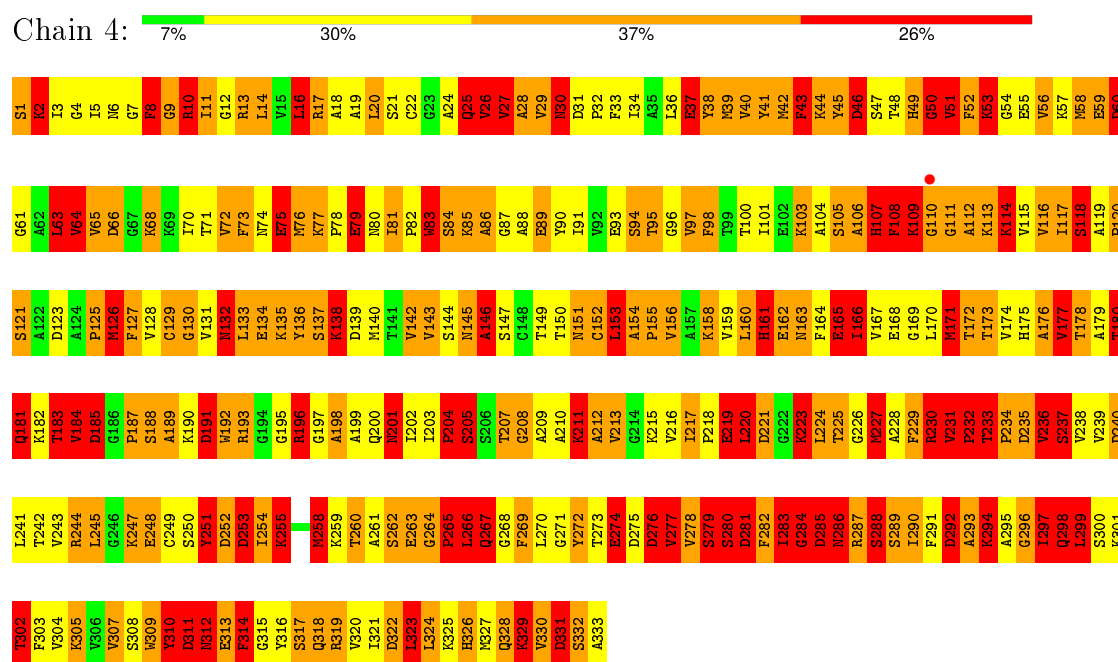




• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



• Molecule 1: APO-D-GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.02Å 80.96Å 82.55Å 110.85° 71.47° 116.86°	Depositor
Resolution (Å)	6.00 – 2.80 45.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.80) 57.9 (45.95-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.51Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.218 , (Not available) (Not available) , (Not available)	Depositor DCC
$R_{free}$ test set	NotAvailable	DCC
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.6	EDS
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 37668 reflections	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	10150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 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 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	1	1.55	19/2553 (0.7%)	2.75	238/3451 (6.9%)
1	2	1.61	27/2553 (1.1%)	2.88	223/3451 (6.5%)
1	3	1.63	29/2553 (1.1%)	2.93	257/3451 (7.4%)
1	4	1.61	26/2553 (1.0%)	3.05	259/3451 (7.5%)
All	All	1.60	101/10212 (1.0%)	2.90	977/13804 (7.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	3	0	2

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	296	GLY	N-CA	10.32	1.61	1.46
1	2	205	SER	CB-OG	8.01	1.52	1.42
1	3	50	GLY	N-CA	-7.68	1.34	1.46
1	4	50	GLY	N-CA	-7.47	1.34	1.46
1	1	300	SER	CA-CB	-7.33	1.42	1.52
1	2	50	GLY	N-CA	-7.23	1.35	1.46
1	3	280	SER	CB-OG	7.09	1.51	1.42
1	1	296	GLY	N-CA	7.05	1.56	1.46
1	3	162	GLU	CD-OE1	-7.03	1.18	1.25
1	2	144	SER	CB-OG	7.01	1.51	1.42
1	4	137	SER	CB-OG	6.92	1.51	1.42
1	2	235	ASP	C-O	6.90	1.36	1.23
1	4	234	PRO	N-CD	6.89	1.57	1.47
1	2	287	ARG	NE-CZ	-6.84	1.24	1.33
1	1	50	GLY	N-CA	-6.82	1.35	1.46
1	4	262	SER	CB-OG	-6.75	1.33	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	234	PRO	N-CD	6.73	1.57	1.47
1	3	246	GLY	N-CA	6.62	1.55	1.46
1	1	1	SER	CB-OG	-6.52	1.33	1.42
1	3	236	VAL	N-CA	6.48	1.59	1.46
1	1	237	SER	CB-OG	-6.47	1.33	1.42
1	2	284	GLY	CA-C	6.46	1.62	1.51
1	4	244	ARG	CD-NE	-6.42	1.35	1.46
1	3	84	SER	CB-OG	6.42	1.50	1.42
1	4	134	GLU	CB-CG	6.40	1.64	1.52
1	4	205	SER	CB-OG	6.33	1.50	1.42
1	3	223	LYS	C-O	6.32	1.35	1.23
1	2	280	SER	CB-OG	6.30	1.50	1.42
1	4	284	GLY	N-CA	6.27	1.55	1.46
1	2	165	GLU	CD-OE1	-6.24	1.18	1.25
1	2	236	VAL	N-CA	6.15	1.58	1.46
1	3	322	ASP	C-O	6.12	1.34	1.23
1	4	168	GLU	CD-OE2	6.10	1.32	1.25
1	2	300	SER	CA-CB	-6.08	1.43	1.52
1	2	94	SER	CB-OG	6.08	1.50	1.42
1	3	263	GLU	CD-OE2	6.05	1.32	1.25
1	4	193	ARG	CG-CD	-6.02	1.36	1.51
1	2	102	GLU	CD-OE1	-5.96	1.19	1.25
1	4	162	GLU	CD-OE1	-5.95	1.19	1.25
1	4	59	GLU	CD-OE1	-5.92	1.19	1.25
1	4	233	THR	CB-OG1	5.83	1.54	1.43
1	3	201	ASN	CA-CB	5.80	1.68	1.53
1	2	234	PRO	N-CD	5.79	1.55	1.47
1	2	315	GLY	N-CA	5.78	1.54	1.46
1	2	303	PHE	C-O	5.76	1.34	1.23
1	1	149	THR	CB-OG1	5.76	1.54	1.43
1	4	37	GLU	CB-CG	5.68	1.62	1.52
1	3	17	ARG	CD-NE	-5.67	1.36	1.46
1	3	244	ARG	CZ-NH2	5.67	1.40	1.33
1	3	233	THR	CB-OG1	5.67	1.54	1.43
1	1	188	SER	CA-CB	-5.64	1.44	1.52
1	3	83	TRP	CA-CB	-5.64	1.41	1.53
1	4	223	LYS	C-O	5.64	1.34	1.23
1	3	85	LYS	N-CA	5.60	1.57	1.46
1	3	138	LYS	C-O	5.59	1.33	1.23
1	3	205	SER	CB-OG	5.57	1.49	1.42
1	1	284	GLY	N-CA	5.56	1.54	1.46
1	2	196	ARG	CB-CG	-5.55	1.37	1.52

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	178	THR	CA-CB	5.52	1.67	1.53
1	2	37	GLU	CD-OE1	-5.51	1.19	1.25
1	3	188	SER	CB-OG	5.50	1.49	1.42
1	2	137	SER	CB-OG	5.50	1.49	1.42
1	4	237	SER	CB-OG	-5.50	1.35	1.42
1	1	147	SER	CA-CB	5.48	1.61	1.52
1	3	187	PRO	N-CD	5.47	1.55	1.47
1	4	193	ARG	CD-NE	-5.46	1.37	1.46
1	4	288	SER	CA-CB	-5.42	1.44	1.52
1	4	286	ASN	C-O	5.42	1.33	1.23
1	2	194	GLY	CA-C	5.35	1.60	1.51
1	3	267	GLN	C-O	5.35	1.33	1.23
1	2	147	SER	CB-OG	5.33	1.49	1.42
1	1	205	SER	CB-OG	5.33	1.49	1.42
1	4	315	GLY	N-CA	5.33	1.54	1.46
1	2	89	GLU	CD-OE1	-5.31	1.19	1.25
1	1	196	ARG	CD-NE	5.29	1.55	1.46
1	2	118	SER	CB-OG	-5.28	1.35	1.42
1	3	198	ALA	CA-CB	5.27	1.63	1.52
1	3	274	GLU	CB-CG	-5.27	1.42	1.52
1	4	262	SER	CA-CB	-5.25	1.45	1.52
1	3	84	SER	C-O	5.23	1.33	1.23
1	3	287	ARG	C-O	5.22	1.33	1.23
1	4	232	PRO	C-O	5.21	1.33	1.23
1	4	180	THR	CB-OG1	5.21	1.53	1.43
1	2	233	THR	CB-OG1	5.19	1.53	1.43
1	1	102	GLU	CD-OE1	-5.19	1.20	1.25
1	1	162	GLU	CD-OE1	-5.18	1.20	1.25
1	3	63	LEU	CA-CB	-5.17	1.41	1.53
1	2	188	SER	CB-OG	5.16	1.49	1.42
1	4	136	TYR	CA-CB	5.16	1.65	1.53
1	1	201	ASN	N-CA	-5.14	1.36	1.46
1	3	287	ARG	CD-NE	-5.14	1.37	1.46
1	2	41	TYR	CG-CD1	5.13	1.45	1.39
1	4	227	MET	CB-CG	-5.10	1.35	1.51
1	1	114	LYS	N-CA	5.09	1.56	1.46
1	1	222	GLY	C-O	5.08	1.31	1.23
1	1	273	THR	CB-OG1	5.07	1.53	1.43
1	1	263	GLU	CB-CG	-5.07	1.42	1.52
1	4	184	VAL	C-N	-5.07	1.22	1.34
1	3	274	GLU	CG-CD	-5.04	1.44	1.51
1	1	224	LEU	C-O	5.02	1.32	1.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	61	GLY	N-CA	-5.01	1.38	1.46

All (977) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	227	MET	CA-CB-CG	39.23	179.99	113.30
1	2	287	ARG	CD-NE-CZ	33.00	169.80	123.60
1	2	10	ARG	NE-CZ-NH1	32.49	136.55	120.30
1	2	10	ARG	NE-CZ-NH2	-30.94	104.83	120.30
1	4	244	ARG	CD-NE-CZ	30.59	166.43	123.60
1	4	319	ARG	NE-CZ-NH1	-21.83	109.39	120.30
1	3	319	ARG	NE-CZ-NH2	20.07	130.33	120.30
1	3	287	ARG	CD-NE-CZ	19.49	150.88	123.60
1	3	63	LEU	CA-CB-CG	19.15	159.35	115.30
1	3	17	ARG	NE-CZ-NH1	18.87	129.74	120.30
1	3	13	ARG	NE-CZ-NH2	-18.61	110.99	120.30
1	3	17	ARG	CD-NE-CZ	18.54	149.56	123.60
1	4	10	ARG	NE-CZ-NH1	18.40	129.50	120.30
1	4	244	ARG	NE-CZ-NH1	18.25	129.43	120.30
1	1	310	TYR	CA-CB-CG	18.20	147.98	113.40
1	1	287	ARG	CD-NE-CZ	17.45	148.03	123.60
1	3	281	ASP	CB-CG-OD1	17.18	133.76	118.30
1	4	322	ASP	CB-CG-OD1	16.93	133.53	118.30
1	4	253	ASP	CB-CG-OD2	-16.59	103.37	118.30
1	2	230	ARG	NE-CZ-NH1	16.12	128.36	120.30
1	4	13	ARG	NE-CZ-NH2	-16.09	112.25	120.30
1	1	244	ARG	NE-CZ-NH1	15.92	128.26	120.30
1	1	300	SER	CA-CB-OG	15.64	153.43	111.20
1	4	235	ASP	CB-CG-OD1	15.59	132.33	118.30
1	2	196	ARG	NE-CZ-NH2	15.37	127.99	120.30
1	1	10	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	4	193	ARG	CG-CD-NE	15.15	143.61	111.80
1	3	31	ASP	CB-CG-OD1	15.14	131.93	118.30
1	1	322	ASP	CB-CG-OD2	-15.08	104.73	118.30
1	4	300	SER	CA-CB-OG	15.00	151.71	111.20
1	2	300	SER	CA-CB-OG	14.79	151.13	111.20
1	2	46	ASP	CB-CG-OD1	14.65	131.48	118.30
1	3	244	ARG	NE-CZ-NH1	14.64	127.62	120.30
1	3	287	ARG	NE-CZ-NH2	14.28	127.44	120.30
1	4	39	MET	CA-CB-CG	14.23	137.50	113.30
1	3	252	ASP	CB-CG-OD2	-14.17	105.54	118.30
1	4	49	HIS	C-N-CA	14.09	151.90	122.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	252	ASP	CB-CG-OD2	-13.99	105.70	118.30
1	2	281	ASP	CB-CG-OD1	13.99	130.89	118.30
1	3	17	ARG	CA-CB-CG	13.80	143.77	113.40
1	1	10	ARG	NE-CZ-NH2	-13.68	113.46	120.30
1	3	310	TYR	CA-CB-CG	13.46	138.98	113.40
1	4	46	ASP	CB-CG-OD1	-13.45	106.20	118.30
1	1	31	ASP	CB-CG-OD1	13.15	130.14	118.30
1	4	196	ARG	NE-CZ-NH1	-13.13	113.73	120.30
1	3	274	GLU	CB-CG-CD	13.00	149.29	114.20
1	2	44	LYS	CA-CB-CG	12.88	141.73	113.40
1	3	310	TYR	CB-CG-CD1	12.87	128.72	121.00
1	4	252	ASP	CB-CG-OD1	-12.82	106.77	118.30
1	4	287	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	4	252	ASP	OD1-CG-OD2	12.71	147.45	123.30
1	4	319	ARG	NE-CZ-NH2	12.66	126.63	120.30
1	4	37	GLU	OE1-CD-OE2	12.44	138.23	123.30
1	4	322	ASP	CB-CG-OD2	-12.40	107.14	118.30
1	1	275	ASP	CB-CG-OD1	12.31	129.38	118.30
1	3	83	TRP	CA-CB-CG	12.29	137.04	113.70
1	3	316	TYR	CB-CG-CD2	12.27	128.36	121.00
1	3	311	ASP	CB-CG-OD2	12.01	129.11	118.30
1	2	83	TRP	CA-CB-CG	12.00	136.51	113.70
1	1	196	ARG	NE-CZ-NH2	11.80	126.20	120.30
1	4	73	PHE	CA-CB-CG	11.78	142.17	113.90
1	2	252	ASP	CB-CG-OD1	11.63	128.77	118.30
1	1	50	GLY	N-CA-C	11.63	142.16	113.10
1	1	287	ARG	NE-CZ-NH2	11.62	126.11	120.30
1	3	196	ARG	CD-NE-CZ	-11.56	107.42	123.60
1	3	316	TYR	CB-CG-CD1	-11.54	114.08	121.00
1	3	49	HIS	C-N-CA	11.43	146.31	122.30
1	2	196	ARG	CB-CG-CD	11.41	141.27	111.60
1	4	196	ARG	NE-CZ-NH2	11.39	126.00	120.30
1	4	240	ASP	CB-CG-OD1	11.38	128.54	118.30
1	1	49	HIS	C-N-CA	11.36	146.16	122.30
1	4	17	ARG	CD-NE-CZ	11.22	139.31	123.60
1	2	287	ARG	NE-CZ-NH2	11.18	125.89	120.30
1	4	17	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	4	109	LYS	N-CA-CB	11.06	130.50	110.60
1	3	280	SER	N-CA-CB	-11.01	93.99	110.50
1	2	235	ASP	CB-CG-OD1	10.91	128.12	118.30
1	3	157	ALA	CB-CA-C	10.90	126.45	110.10
1	3	50	GLY	N-CA-C	10.74	139.96	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	240	ASP	CB-CG-OD2	-10.66	108.70	118.30
1	3	220	LEU	CA-CB-CG	10.64	139.78	115.30
1	1	329	LYS	N-CA-CB	10.60	129.68	110.60
1	2	185	ASP	CB-CG-OD1	-10.59	108.77	118.30
1	1	196	ARG	NE-CZ-NH1	-10.59	115.00	120.30
1	4	311	ASP	N-CA-CB	10.56	129.60	110.60
1	2	285	ASP	CB-CG-OD1	10.55	127.79	118.30
1	4	331	ASP	CB-CG-OD1	10.53	127.78	118.30
1	3	168	GLU	CA-CB-CG	10.52	136.54	113.40
1	4	13	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	4	230	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	1	207	THR	CA-CB-CG2	10.42	126.98	112.40
1	3	300	SER	C-N-CA	10.38	147.65	121.70
1	1	83	TRP	CA-CB-CG	10.36	133.38	113.70
1	4	196	ARG	CD-NE-CZ	-10.36	109.10	123.60
1	2	46	ASP	OD1-CG-OD2	-10.34	103.65	123.30
1	1	323	LEU	CA-CB-CG	10.34	139.07	115.30
1	2	310	TYR	CA-CB-CG	10.32	133.02	113.40
1	2	200	GLN	CB-CG-CD	10.30	138.38	111.60
1	2	311	ASP	CB-CG-OD1	10.27	127.54	118.30
1	1	310	TYR	CB-CG-CD1	10.27	127.16	121.00
1	4	285	ASP	CB-CG-OD1	10.23	127.51	118.30
1	2	236	VAL	CB-CA-C	10.23	130.83	111.40
1	3	41	TYR	CB-CG-CD1	-10.02	114.99	121.00
1	4	10	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	4	185	ASP	CB-CG-OD1	-9.97	109.33	118.30
1	3	300	SER	CB-CA-C	9.95	129.00	110.10
1	1	252	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	2	252	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	4	171	MET	CG-SD-CE	9.73	115.77	100.20
1	2	162	GLU	CA-CB-CG	9.71	134.76	113.40
1	1	244	ARG	NE-CZ-NH2	-9.69	115.46	120.30
1	4	188	SER	N-CA-CB	9.64	124.96	110.50
1	4	323	LEU	CA-CB-CG	9.62	137.41	115.30
1	1	323	LEU	CB-CA-C	9.61	128.46	110.20
1	2	221	ASP	CB-CG-OD1	-9.60	109.66	118.30
1	3	278	VAL	CB-CA-C	9.52	129.48	111.40
1	2	162	GLU	OE1-CD-OE2	9.49	134.69	123.30
1	2	211	LYS	CA-CB-CG	9.44	134.17	113.40
1	3	193	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	2	322	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	1	307	VAL	CA-CB-CG2	9.41	125.01	110.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	201	ASN	N-CA-CB	-9.41	93.67	110.60
1	4	299	LEU	CB-CA-C	9.31	127.90	110.20
1	3	123	ASP	CB-CG-OD1	9.30	126.67	118.30
1	3	49	HIS	CA-CB-CG	-9.29	97.80	113.60
1	2	196	ARG	CD-NE-CZ	-9.28	110.61	123.60
1	3	133	LEU	N-CA-CB	-9.21	91.98	110.40
1	1	322	ASP	CB-CG-OD1	9.21	126.59	118.30
1	3	84	SER	CB-CA-C	9.19	127.56	110.10
1	4	111	GLY	O-C-N	9.18	137.39	122.70
1	1	200	GLN	C-N-CA	9.14	144.56	121.70
1	2	114	LYS	N-CA-CB	-9.13	94.16	110.60
1	2	314	PHE	CA-CB-CG	9.13	135.81	113.90
1	4	233	THR	N-CA-CB	-9.12	92.96	110.30
1	3	280	SER	CB-CA-C	9.12	127.43	110.10
1	3	133	LEU	CB-CA-C	9.11	127.51	110.20
1	3	236	VAL	CB-CA-C	9.08	128.66	111.40
1	4	192	TRP	CA-CB-CG	9.00	130.79	113.70
1	4	193	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	3	319	ARG	NE-CZ-NH1	-8.95	115.82	120.30
1	4	244	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	3	224	LEU	CA-CB-CG	8.95	135.88	115.30
1	4	44	LYS	CA-CB-CG	8.93	133.05	113.40
1	4	258	MET	O-C-N	8.93	136.99	122.70
1	3	17	ARG	NE-CZ-NH2	-8.93	115.83	120.30
1	1	196	ARG	CD-NE-CZ	-8.89	111.16	123.60
1	2	235	ASP	OD1-CG-OD2	-8.88	106.43	123.30
1	4	310	TYR	CA-CB-CG	8.86	130.24	113.40
1	3	13	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	4	310	TYR	CB-CG-CD1	8.78	126.27	121.00
1	1	72	VAL	CB-CA-C	8.78	128.07	111.40
1	2	196	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	3	73	PHE	CA-CB-CG	8.77	134.94	113.90
1	4	26	VAL	CA-C-O	-8.76	101.71	120.10
1	4	51	VAL	CB-CA-C	8.73	127.99	111.40
1	4	153	LEU	CA-CB-CG	8.70	135.31	115.30
1	3	233	THR	N-CA-CB	-8.68	93.81	110.30
1	2	60	ASP	CB-CG-OD1	8.65	126.08	118.30
1	4	251	TYR	CA-CB-CG	-8.61	97.04	113.40
1	1	263	GLU	CA-CB-CG	8.56	132.23	113.40
1	2	230	ARG	CD-NE-CZ	8.54	135.56	123.60
1	3	281	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	2	17	ARG	O-C-N	8.53	136.34	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	212	ALA	N-CA-CB	8.52	122.03	110.10
1	1	230	ARG	CD-NE-CZ	-8.52	111.67	123.60
1	3	331	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	4	224	LEU	O-C-N	8.46	136.24	122.70
1	2	322	ASP	CB-CG-OD1	8.45	125.90	118.30
1	3	244	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	3	134	GLU	N-CA-CB	8.39	125.71	110.60
1	2	210	ALA	CB-CA-C	-8.37	97.55	110.10
1	2	176	ALA	N-CA-CB	-8.36	98.40	110.10
1	2	300	SER	N-CA-CB	8.33	122.99	110.50
1	1	240	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	1	286	ASN	CA-C-O	-8.29	102.69	120.10
1	3	37	GLU	OE1-CD-OE2	8.29	133.25	123.30
1	3	212	ALA	CA-C-O	-8.25	102.78	120.10
1	4	208	GLY	N-CA-C	8.22	133.66	113.10
1	4	274	GLU	OE1-CD-OE2	8.22	133.17	123.30
1	1	14	LEU	CA-CB-CG	8.21	134.19	115.30
1	1	300	SER	CB-CA-C	8.21	125.69	110.10
1	3	244	ARG	CD-NE-CZ	8.21	135.09	123.60
1	3	300	SER	O-C-N	-8.20	109.58	122.70
1	3	10	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	2	216	VAL	CA-CB-CG2	8.18	123.17	110.90
1	2	280	SER	N-CA-CB	-8.14	98.28	110.50
1	1	162	GLU	CG-CD-OE1	8.13	134.56	118.30
1	1	224	LEU	CA-CB-CG	8.12	133.97	115.30
1	3	210	ALA	CB-CA-C	-8.10	97.94	110.10
1	4	51	VAL	CA-CB-CG1	8.09	123.04	110.90
1	1	1	SER	CA-CB-OG	8.08	133.01	111.20
1	3	177	VAL	C-N-CA	8.06	141.85	121.70
1	3	134	GLU	OE1-CD-OE2	-8.05	113.64	123.30
1	2	163	ASN	CB-CG-OD1	-8.02	105.55	121.60
1	2	311	ASP	N-CA-CB	8.02	125.03	110.60
1	3	313	GLU	CG-CD-OE1	8.00	134.30	118.30
1	1	307	VAL	CA-CB-CG1	-7.99	98.92	110.90
1	3	10	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	1	93	GLU	OE1-CD-OE2	7.96	132.85	123.30
1	2	192	TRP	N-CA-C	7.95	132.47	111.00
1	2	235	ASP	CB-CG-OD2	7.95	125.45	118.30
1	4	45	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	4	283	ILE	CB-CG1-CD1	7.93	136.10	113.90
1	2	303	PHE	O-C-N	7.91	135.35	122.70
1	4	233	THR	CA-CB-OG1	-7.90	92.41	109.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	237	SER	CA-CB-OG	7.90	132.52	111.20
1	2	176	ALA	CB-CA-C	7.88	121.92	110.10
1	2	27	VAL	N-CA-CB	-7.87	94.18	111.50
1	4	111	GLY	N-CA-C	-7.87	93.43	113.10
1	3	307	VAL	CA-CB-CG1	-7.86	99.11	110.90
1	4	313	GLU	CA-CB-CG	7.86	130.69	113.40
1	1	286	ASN	O-C-N	7.85	135.26	122.70
1	3	201	ASN	N-CA-C	7.84	132.17	111.00
1	4	114	LYS	CB-CA-C	7.83	126.06	110.40
1	2	266	LEU	CA-CB-CG	7.83	133.30	115.30
1	2	230	ARG	NH1-CZ-NH2	-7.83	110.79	119.40
1	1	146	ALA	C-N-CA	7.81	141.22	121.70
1	4	89	GLU	OE1-CD-OE2	7.80	132.66	123.30
1	2	13	ARG	CD-NE-CZ	-7.80	112.68	123.60
1	3	235	ASP	CA-C-N	7.80	134.35	117.20
1	4	311	ASP	CB-CG-OD1	7.79	125.31	118.30
1	3	251	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	2	114	LYS	CB-CA-C	7.77	125.94	110.40
1	4	230	ARG	O-C-N	7.73	135.07	122.70
1	1	24	ALA	CB-CA-C	7.72	121.69	110.10
1	3	319	ARG	CD-NE-CZ	-7.72	112.80	123.60
1	4	235	ASP	OD1-CG-OD2	-7.69	108.68	123.30
1	3	311	ASP	OD1-CG-OD2	-7.67	108.73	123.30
1	1	180	THR	CA-CB-CG2	7.66	123.12	112.40
1	3	31	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	1	275	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	4	313	GLU	CG-CD-OE2	7.63	133.57	118.30
1	3	302	THR	CA-CB-CG2	7.62	123.08	112.40
1	4	281	ASP	CB-CG-OD1	7.62	125.16	118.30
1	4	263	GLU	N-CA-CB	7.62	124.31	110.60
1	3	79	GLU	CA-CB-CG	7.61	130.15	113.40
1	4	253	ASP	OD1-CG-OD2	7.59	137.71	123.30
1	2	313	GLU	N-CA-CB	7.57	124.23	110.60
1	1	252	ASP	CA-CB-CG	-7.57	96.75	113.40
1	1	31	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	3	230	ARG	C-N-CA	7.55	140.59	121.70
1	2	235	ASP	CA-C-N	7.55	133.81	117.20
1	2	60	ASP	C-N-CA	7.52	138.09	122.30
1	2	280	SER	CB-CA-C	7.52	124.38	110.10
1	3	18	ALA	CB-CA-C	7.51	121.36	110.10
1	1	185	ASP	CA-CB-CG	-7.50	96.90	113.40
1	4	233	THR	CA-CB-CG2	7.50	122.90	112.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	296	GLY	N-CA-C	-7.49	94.38	113.10
1	4	251	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	3	176	ALA	N-CA-CB	-7.47	99.65	110.10
1	2	247	LYS	N-CA-CB	7.46	124.04	110.60
1	2	165	GLU	N-CA-CB	-7.46	97.17	110.60
1	4	302	THR	CA-CB-CG2	7.45	122.82	112.40
1	2	323	LEU	CA-CB-CG	7.43	132.39	115.30
1	2	66	ASP	N-CA-CB	-7.42	97.23	110.60
1	1	40	VAL	CA-CB-CG2	7.40	122.00	110.90
1	3	258	MET	CA-CB-CG	-7.40	100.72	113.30
1	4	201	ASN	N-CA-CB	-7.40	97.28	110.60
1	3	253	ASP	CB-CG-OD2	7.39	124.95	118.30
1	2	236	VAL	CA-C-N	7.39	133.46	117.20
1	2	190	LYS	N-CA-CB	7.39	123.89	110.60
1	1	162	GLU	CA-CB-CG	7.37	129.61	113.40
1	3	80	ASN	CB-CG-OD1	-7.34	106.93	121.60
1	2	93	GLU	CG-CD-OE1	7.33	132.96	118.30
1	1	178	THR	CA-CB-OG1	-7.33	93.62	109.00
1	1	191	ASP	CB-CG-OD2	7.31	124.88	118.30
1	1	287	ARG	NH1-CZ-NH2	-7.31	111.36	119.40
1	3	302	THR	C-N-CA	7.30	139.96	121.70
1	2	46	ASP	CB-CG-OD2	7.29	124.86	118.30
1	1	135	LYS	CG-CD-CE	7.29	133.76	111.90
1	1	142	VAL	N-CA-CB	-7.29	95.47	111.50
1	1	285	ASP	CB-CG-OD1	7.28	124.85	118.30
1	3	313	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	4	126	MET	O-C-N	7.27	134.34	122.70
1	2	328	GLN	CA-CB-CG	7.26	129.37	113.40
1	4	322	ASP	CA-CB-CG	7.25	129.34	113.40
1	3	236	VAL	CA-C-O	-7.24	104.89	120.10
1	1	301	LYS	CD-CE-NZ	7.24	128.35	111.70
1	1	51	VAL	CB-CA-C	7.24	125.15	111.40
1	4	37	GLU	CG-CD-OE1	-7.24	103.83	118.30
1	4	252	ASP	CA-CB-CG	-7.23	97.49	113.40
1	3	28	ALA	CB-CA-C	7.23	120.94	110.10
1	1	280	SER	N-CA-CB	-7.20	99.71	110.50
1	1	235	ASP	CB-CG-OD1	7.19	124.77	118.30
1	3	46	ASP	O-C-N	7.17	134.17	122.70
1	2	279	SER	CB-CA-C	7.17	123.72	110.10
1	1	114	LYS	N-CA-CB	-7.16	97.71	110.60
1	1	183	THR	N-CA-CB	7.16	123.91	110.30
1	4	50	GLY	N-CA-C	7.16	131.00	113.10

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	65	VAL	CB-CA-C	7.16	125.00	111.40
1	2	64	VAL	CA-CB-CG1	7.16	121.63	110.90
1	3	247	LYS	CB-CA-C	7.15	124.70	110.40
1	2	68	LYS	N-CA-CB	7.15	123.47	110.60
1	1	181	GLN	N-CA-CB	-7.14	97.74	110.60
1	1	220	LEU	CA-CB-CG	7.12	131.69	115.30
1	2	109	LYS	N-CA-CB	7.12	123.42	110.60
1	2	141	THR	CA-CB-CG2	7.12	122.36	112.40
1	4	46	ASP	CA-CB-CG	-7.11	97.75	113.40
1	2	142	VAL	CA-CB-CG1	7.10	121.54	110.90
1	2	167	VAL	CA-CB-CG2	7.08	121.53	110.90
1	3	191	ASP	N-CA-CB	-7.08	97.86	110.60
1	1	163	ASN	CB-CG-OD1	-7.07	107.45	121.60
1	1	287	ARG	N-CA-CB	7.06	123.31	110.60
1	1	300	SER	CA-C-O	7.06	134.92	120.10
1	1	185	ASP	CB-CG-OD1	-7.05	111.95	118.30
1	3	329	LYS	N-CA-CB	7.04	123.28	110.60
1	2	259	LYS	O-C-N	7.04	133.96	122.70
1	4	269	PHE	CB-CA-C	7.03	124.46	110.40
1	4	193	ARG	CB-CG-CD	7.03	129.87	111.60
1	3	188	SER	CA-C-O	7.02	134.84	120.10
1	4	193	ARG	CD-NE-CZ	7.01	133.42	123.60
1	3	199	ALA	N-CA-CB	-7.01	100.28	110.10
1	2	50	GLY	N-CA-C	7.01	130.63	113.10
1	2	102	GLU	OE1-CD-OE2	7.01	131.71	123.30
1	4	132	ASN	CA-CB-CG	7.01	128.82	113.40
1	4	265	PRO	CB-CA-C	7.00	129.50	112.00
1	4	162	GLU	CG-CD-OE2	-7.00	104.31	118.30
1	1	201	ASN	N-CA-CB	-6.99	98.02	110.60
1	3	121	SER	N-CA-CB	6.99	120.98	110.50
1	2	84	SER	O-C-N	6.97	133.84	122.70
1	2	225	THR	CA-CB-CG2	-6.96	102.65	112.40
1	2	177	VAL	CA-CB-CG1	6.96	121.34	110.90
1	4	79	GLU	CA-CB-CG	6.96	128.71	113.40
1	3	251	TYR	CA-CB-CG	-6.94	100.22	113.40
1	2	253	ASP	N-CA-CB	6.93	123.08	110.60
1	3	163	ASN	N-CA-CB	-6.93	98.13	110.60
1	3	233	THR	CA-CB-CG2	6.93	122.10	112.40
1	4	267	GLN	OE1-CD-NE2	6.92	137.81	121.90
1	1	175	HIS	CA-CB-CG	6.91	125.35	113.60
1	1	311	ASP	CB-CG-OD1	6.91	124.52	118.30
1	2	231	VAL	CB-CA-C	6.91	124.53	111.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	310	TYR	CB-CG-CD2	-6.90	116.86	121.00
1	3	147	SER	CB-CA-C	-6.90	96.99	110.10
1	1	133	LEU	CB-CA-C	6.90	123.31	110.20
1	3	253	ASP	N-CA-CB	6.89	123.00	110.60
1	1	138	LYS	CA-C-N	6.88	132.33	117.20
1	4	155	PRO	C-N-CA	6.88	138.89	121.70
1	4	300	SER	N-CA-CB	6.88	120.81	110.50
1	3	200	GLN	C-N-CA	6.87	138.88	121.70
1	4	111	GLY	CA-C-O	-6.87	108.23	120.60
1	1	211	LYS	CA-CB-CG	6.87	128.51	113.40
1	4	312	ASN	CA-CB-CG	6.87	128.51	113.40
1	3	236	VAL	CA-C-N	6.86	132.29	117.20
1	3	231	VAL	CA-CB-CG1	6.85	121.18	110.90
1	3	177	VAL	CA-C-O	6.85	134.48	120.10
1	1	167	VAL	CB-CA-C	6.84	124.40	111.40
1	1	311	ASP	N-CA-CB	6.84	122.92	110.60
1	1	237	SER	CA-CB-OG	6.84	129.67	111.20
1	1	304	VAL	CA-CB-CG1	-6.84	100.65	110.90
1	1	143	VAL	CA-CB-CG2	-6.83	100.65	110.90
1	4	127	PHE	C-N-CA	6.83	138.77	121.70
1	1	177	VAL	CA-C-O	6.82	134.43	120.10
1	4	309	TRP	CA-CB-CG	6.82	126.67	113.70
1	3	300	SER	CA-C-O	6.82	134.43	120.10
1	3	165	GLU	CG-CD-OE1	6.81	131.91	118.30
1	3	179	ALA	N-CA-CB	6.80	119.63	110.10
1	1	162	GLU	CG-CD-OE2	-6.80	104.70	118.30
1	2	286	ASN	CA-C-O	-6.79	105.84	120.10
1	2	29	VAL	CA-C-O	-6.79	105.84	120.10
1	3	210	ALA	O-C-N	6.79	133.56	122.70
1	4	41	TYR	CB-CG-CD2	6.79	125.07	121.00
1	1	275	ASP	CB-CA-C	6.78	123.97	110.40
1	2	320	VAL	CB-CA-C	6.78	124.28	111.40
1	3	147	SER	N-CA-CB	-6.78	100.34	110.50
1	4	14	LEU	CA-CB-CG	6.77	130.88	115.30
1	1	111	GLY	N-CA-C	-6.75	96.22	113.10
1	2	311	ASP	OD1-CG-OD2	-6.75	110.48	123.30
1	1	45	TYR	CB-CG-CD1	-6.74	116.95	121.00
1	4	73	PHE	CB-CA-C	6.74	123.88	110.40
1	1	275	ASP	C-N-CA	6.74	138.55	121.70
1	3	254	ILE	CB-CA-C	6.73	125.06	111.60
1	1	183	THR	CA-CB-CG2	6.73	121.82	112.40
1	4	43	PHE	O-C-N	6.72	133.46	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	284	GLY	N-CA-C	-6.70	96.36	113.10
1	2	296	GLY	O-C-N	6.69	133.41	122.70
1	1	167	VAL	CA-CB-CG2	6.68	120.92	110.90
1	4	16	LEU	O-C-N	6.68	133.39	122.70
1	1	37	GLU	CA-CB-CG	6.67	128.08	113.40
1	1	207	THR	CA-CB-OG1	-6.66	95.00	109.00
1	2	221	ASP	OD1-CG-OD2	6.66	135.95	123.30
1	3	240	ASP	CB-CG-OD1	-6.66	112.31	118.30
1	4	298	GLN	CB-CG-CD	6.65	128.90	111.60
1	1	123	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	1	133	LEU	N-CA-CB	-6.65	97.10	110.40
1	4	38	TYR	CB-CG-CD1	6.65	124.99	121.00
1	4	285	ASP	N-CA-CB	6.65	122.57	110.60
1	3	258	MET	CG-SD-CE	6.64	110.83	100.20
1	3	331	ASP	CB-CG-OD1	6.64	124.28	118.30
1	2	207	THR	CA-CB-CG2	6.64	121.70	112.40
1	1	193	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	3	212	ALA	O-C-N	6.64	133.32	122.70
1	1	276	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	2	157	ALA	CB-CA-C	6.63	120.05	110.10
1	3	79	GLU	CG-CD-OE1	6.63	131.56	118.30
1	4	242	THR	OG1-CB-CG2	6.62	125.22	110.00
1	2	49	HIS	C-N-CA	6.61	136.18	122.30
1	1	263	GLU	OE1-CD-OE2	-6.60	115.38	123.30
1	4	185	ASP	CB-CG-OD2	6.60	124.24	118.30
1	2	313	GLU	CA-CB-CG	6.59	127.91	113.40
1	3	272	TYR	CB-CG-CD1	6.58	124.95	121.00
1	1	229	PHE	N-CA-CB	6.57	122.43	110.60
1	3	233	THR	CA-CB-OG1	-6.57	95.20	109.00
1	2	126	MET	CB-CA-C	6.57	123.54	110.40
1	1	240	ASP	CB-CA-C	6.56	123.52	110.40
1	2	303	PHE	CA-C-O	-6.56	106.33	120.10
1	1	276	ASP	CA-CB-CG	-6.55	99.00	113.40
1	3	183	THR	CB-CA-C	-6.55	93.92	111.60
1	3	196	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	2	52	PHE	CB-CA-C	6.54	123.47	110.40
1	1	108	PHE	CA-CB-CG	6.53	129.57	113.90
1	2	191	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	4	183	THR	O-C-N	6.53	133.15	122.70
1	1	285	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	1	191	ASP	C-N-CA	6.52	138.00	121.70
1	3	142	VAL	CB-CA-C	6.52	123.78	111.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	215	LYS	CA-CB-CG	6.52	127.74	113.40
1	1	277	VAL	CA-CB-CG2	-6.52	101.13	110.90
1	2	183	THR	CB-CA-C	-6.52	94.01	111.60
1	3	73	PHE	CB-CA-C	6.51	123.43	110.40
1	1	9	GLY	N-CA-C	-6.51	96.82	113.10
1	1	313	GLU	CA-C-N	6.51	131.51	117.20
1	4	42	MET	O-C-N	6.50	133.11	122.70
1	1	193	ARG	CD-NE-CZ	-6.50	114.50	123.60
1	4	25	GLN	N-CA-CB	6.50	122.30	110.60
1	2	240	ASP	CB-CA-C	6.49	123.38	110.40
1	4	66	ASP	CB-CG-OD2	6.49	124.14	118.30
1	4	114	LYS	N-CA-CB	-6.49	98.93	110.60
1	3	9	GLY	O-C-N	6.48	133.07	122.70
1	4	254	ILE	CB-CA-C	6.48	124.56	111.60
1	2	163	ASN	N-CA-CB	-6.47	98.96	110.60
1	1	209	ALA	N-CA-CB	6.46	119.15	110.10
1	4	163	ASN	CA-CB-CG	6.46	127.61	113.40
1	2	8	PHE	CA-CB-CG	6.45	129.39	113.90
1	1	192	TRP	N-CA-C	6.45	128.40	111.00
1	3	139	ASP	CA-CB-CG	6.44	127.57	113.40
1	2	201	ASN	N-CA-C	6.43	128.37	111.00
1	3	274	GLU	CB-CA-C	-6.43	97.54	110.40
1	1	274	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	2	235	ASP	CA-C-O	-6.43	106.60	120.10
1	4	220	LEU	CA-CB-CG	6.43	130.08	115.30
1	2	323	LEU	CB-CA-C	6.42	122.41	110.20
1	4	245	LEU	CA-C-N	6.42	129.05	116.20
1	3	139	ASP	CB-CA-C	6.42	123.24	110.40
1	2	251	TYR	CB-CG-CD2	-6.42	117.15	121.00
1	1	244	ARG	N-CA-C	-6.41	93.70	111.00
1	4	276	ASP	CB-CG-OD1	6.40	124.06	118.30
1	1	236	VAL	CB-CA-C	6.39	123.54	111.40
1	3	176	ALA	CA-C-N	6.38	131.24	117.20
1	1	83	TRP	CA-C-O	6.38	133.49	120.10
1	4	75	GLU	OE1-CD-OE2	6.37	130.94	123.30
1	2	275	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	2	284	GLY	CA-C-N	-6.37	103.19	117.20
1	2	284	GLY	N-CA-C	-6.37	97.19	113.10
1	3	35	ALA	N-CA-CB	-6.37	101.19	110.10
1	3	183	THR	CA-CB-OG1	-6.36	95.65	109.00
1	3	2	LYS	CA-C-O	-6.36	106.75	120.10
1	1	191	ASP	CA-CB-CG	6.35	127.37	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	183	THR	CB-CA-C	-6.35	94.46	111.60
1	2	31	ASP	CB-CG-OD1	6.35	124.01	118.30
1	4	168	GLU	CA-CB-CG	6.35	127.36	113.40
1	1	172	THR	O-C-N	6.34	132.85	122.70
1	3	248	GLU	OE1-CD-OE2	6.33	130.90	123.30
1	2	330	VAL	CA-CB-CG1	6.33	120.40	110.90
1	1	263	GLU	CB-CG-CD	6.32	131.27	114.20
1	3	45	TYR	CB-CG-CD2	6.32	124.79	121.00
1	4	260	THR	N-CA-CB	6.32	122.30	110.30
1	4	142	VAL	CA-CB-CG1	6.31	120.36	110.90
1	2	46	ASP	N-CA-CB	6.30	121.94	110.60
1	3	201	ASN	N-CA-CB	-6.30	99.26	110.60
1	1	198	ALA	CB-CA-C	-6.29	100.66	110.10
1	4	281	ASP	CA-CB-CG	6.29	127.24	113.40
1	2	273	THR	CA-CB-CG2	6.29	121.20	112.40
1	2	196	ARG	CA-CB-CG	6.27	127.20	113.40
1	3	111	GLY	CA-C-O	-6.27	109.32	120.60
1	3	85	LYS	CA-CB-CG	6.26	127.18	113.40
1	1	147	SER	CA-C-O	6.25	133.23	120.10
1	2	227	MET	O-C-N	6.25	132.70	122.70
1	2	293	ALA	CA-C-O	-6.25	106.98	120.10
1	2	17	ARG	CD-NE-CZ	6.25	132.35	123.60
1	2	239	VAL	CB-CA-C	6.25	123.27	111.40
1	4	262	SER	CA-CB-OG	6.25	128.07	111.20
1	1	192	TRP	CB-CA-C	-6.25	97.91	110.40
1	1	275	ASP	CA-CB-CG	6.23	127.11	113.40
1	4	138	LYS	CD-CE-NZ	6.23	126.03	111.70
1	3	301	LYS	CA-C-O	-6.23	107.02	120.10
1	4	198	ALA	CB-CA-C	-6.23	100.76	110.10
1	2	27	VAL	N-CA-C	6.22	127.81	111.00
1	3	7	GLY	CA-C-O	-6.22	109.40	120.60
1	1	176	ALA	N-CA-CB	-6.22	101.39	110.10
1	2	185	ASP	CB-CG-OD2	6.22	123.90	118.30
1	4	46	ASP	OD1-CG-OD2	6.22	135.12	123.30
1	2	25	GLN	O-C-N	6.22	132.65	122.70
1	4	212	ALA	O-C-N	6.22	132.65	122.70
1	2	236	VAL	CA-C-O	-6.21	107.05	120.10
1	4	135	LYS	CD-CE-NZ	-6.21	97.41	111.70
1	1	310	TYR	CB-CG-CD2	-6.21	117.27	121.00
1	2	41	TYR	CB-CG-CD1	-6.21	117.28	121.00
1	2	140	MET	CB-CA-C	6.20	122.81	110.40
1	3	260	THR	CA-CB-CG2	-6.20	103.72	112.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	271	GLY	CA-C-O	-6.20	109.44	120.60
1	3	286	ASN	CA-C-O	-6.20	107.08	120.10
1	3	230	ARG	CB-CA-C	6.19	122.79	110.40
1	1	304	VAL	CG1-CB-CG2	6.18	120.78	110.90
1	2	207	THR	CA-CB-OG1	-6.17	96.03	109.00
1	1	279	SER	CB-CA-C	6.17	121.83	110.10
1	3	168	GLU	CB-CG-CD	6.17	130.86	114.20
1	4	10	ARG	CB-CA-C	6.17	122.73	110.40
1	2	212	ALA	O-C-N	6.16	132.55	122.70
1	3	191	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	3	248	GLU	N-CA-CB	6.15	121.67	110.60
1	3	267	GLN	CA-C-O	-6.15	107.18	120.10
1	4	162	GLU	O-C-N	6.15	132.54	122.70
1	4	199	ALA	CB-CA-C	-6.14	100.89	110.10
1	1	46	ASP	O-C-N	6.14	132.52	122.70
1	4	266	LEU	CB-CA-C	6.13	121.85	110.20
1	2	301	LYS	CA-CB-CG	-6.13	99.92	113.40
1	3	148	CYS	CA-CB-SG	6.12	125.02	114.00
1	3	318	GLN	CG-CD-OE1	-6.12	109.37	121.60
1	1	126	MET	O-C-N	6.12	132.49	122.70
1	2	170	LEU	CB-CA-C	6.12	121.82	110.20
1	3	296	GLY	C-N-CA	6.12	136.99	121.70
1	2	295	ALA	C-N-CA	-6.11	109.47	122.30
1	4	94	SER	N-CA-CB	-6.11	101.33	110.50
1	3	275	ASP	C-N-CA	6.11	136.97	121.70
1	3	68	LYS	CA-CB-CG	6.10	126.82	113.40
1	4	235	ASP	CA-C-N	6.10	130.62	117.20
1	4	185	ASP	CB-CA-C	6.10	122.60	110.40
1	2	65	VAL	CA-CB-CG2	6.09	120.03	110.90
1	3	181	GLN	CA-CB-CG	-6.09	100.00	113.40
1	4	236	VAL	CB-CA-C	6.09	122.96	111.40
1	2	319	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	2	170	LEU	N-CA-CB	-6.08	98.25	110.40
1	1	143	VAL	CA-CB-CG1	6.07	120.01	110.90
1	1	207	THR	N-CA-CB	6.07	121.84	110.30
1	1	327	MET	CA-CB-CG	-6.07	102.98	113.30
1	4	307	VAL	CA-CB-CG1	-6.07	101.80	110.90
1	3	307	VAL	CA-CB-CG2	6.07	120.00	110.90
1	3	159	VAL	CG1-CB-CG2	6.06	120.60	110.90
1	1	198	ALA	CA-C-O	-6.06	107.37	120.10
1	3	83	TRP	CA-C-N	-6.06	103.87	117.20
1	4	17	ARG	CA-CB-CG	6.06	126.73	113.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	42	MET	CA-C-O	-6.06	107.38	120.10
1	1	83	TRP	CA-C-N	-6.05	103.89	117.20
1	4	137	SER	CB-CA-C	6.05	121.59	110.10
1	4	26	VAL	CA-C-N	6.04	130.49	117.20
1	2	274	GLU	CB-CA-C	-6.03	98.33	110.40
1	1	41	TYR	N-CA-CB	6.03	121.45	110.60
1	1	154	ALA	O-C-N	6.03	132.55	121.10
1	1	299	LEU	CA-CB-CG	6.02	129.14	115.30
1	1	234	PRO	N-CD-CG	-6.00	94.20	103.20
1	4	292	ASP	CB-CG-OD1	6.00	123.70	118.30
1	2	162	GLU	CG-CD-OE2	-5.99	106.31	118.30
1	2	23	GLY	O-C-N	5.99	132.28	122.70
1	4	258	MET	CB-CG-SD	-5.99	94.44	112.40
1	2	191	ASP	C-N-CA	5.98	136.66	121.70
1	3	281	ASP	O-C-N	5.98	132.27	122.70
1	4	319	ARG	CD-NE-CZ	-5.98	115.22	123.60
1	1	115	VAL	CB-CA-C	-5.98	100.04	111.40
1	4	297	ILE	CB-CA-C	5.97	123.55	111.60
1	1	41	TYR	CB-CG-CD2	5.96	124.58	121.00
1	3	104	ALA	N-CA-CB	5.96	118.44	110.10
1	3	313	GLU	CA-CB-CG	5.96	126.50	113.40
1	4	293	ALA	CA-C-O	-5.96	107.59	120.10
1	2	233	THR	CA-CB-OG1	-5.95	96.52	109.00
1	2	183	THR	OG1-CB-CG2	5.94	123.67	110.00
1	4	123	ASP	CB-CA-C	5.94	122.28	110.40
1	4	263	GLU	CG-CD-OE2	-5.94	106.42	118.30
1	3	234	PRO	CA-N-CD	-5.94	103.19	111.50
1	4	191	ASP	C-N-CA	5.94	136.54	121.70
1	1	73	PHE	CA-CB-CG	5.93	128.14	113.90
1	3	276	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	4	187	PRO	N-CD-CG	-5.91	94.33	103.20
1	1	181	GLN	O-C-N	-5.91	113.25	122.70
1	1	212	ALA	CB-CA-C	5.91	118.96	110.10
1	4	178	THR	CA-CB-OG1	-5.91	96.60	109.00
1	2	203	ILE	CA-C-O	-5.90	107.70	120.10
1	1	172	THR	N-CA-CB	5.90	121.51	110.30
1	1	281	ASP	CB-CG-OD2	5.90	123.61	118.30
1	2	107	HIS	N-CA-CB	5.90	121.22	110.60
1	1	313	GLU	CA-C-O	-5.89	107.74	120.10
1	4	10	ARG	CD-NE-CZ	5.89	131.84	123.60
1	2	123	ASP	CB-CG-OD1	5.88	123.60	118.30
1	2	133	LEU	N-CA-CB	-5.88	98.63	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	245	LEU	CA-CB-CG	5.88	128.83	115.30
1	2	244	ARG	N-CA-C	-5.87	95.15	111.00
1	1	63	LEU	O-C-N	5.87	132.09	122.70
1	2	287	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	1	84	SER	N-CA-C	-5.86	95.17	111.00
1	1	266	LEU	CB-CG-CD2	-5.86	101.04	111.00
1	3	98	PHE	CA-CB-CG	5.86	127.97	113.90
1	4	198	ALA	O-C-N	5.86	132.07	122.70
1	4	212	ALA	N-CA-CB	5.86	118.30	110.10
1	4	309	TRP	O-C-N	5.86	132.07	122.70
1	3	45	TYR	N-CA-CB	-5.85	100.06	110.60
1	1	170	LEU	CB-CG-CD1	5.85	120.95	111.00
1	4	242	THR	CA-CB-CG2	-5.85	104.21	112.40
1	3	318	GLN	CA-CB-CG	5.85	126.26	113.40
1	4	225	THR	CA-C-O	-5.85	107.82	120.10
1	3	151	ASN	CA-CB-CG	5.84	126.26	113.40
1	4	37	GLU	CB-CG-CD	-5.84	98.42	114.20
1	3	197	GLY	C-N-CA	5.84	136.31	121.70
1	4	26	VAL	CA-CB-CG2	5.84	119.66	110.90
1	2	328	GLN	OE1-CD-NE2	5.84	135.33	121.90
1	4	244	ARG	N-CA-C	-5.84	95.23	111.00
1	2	83	TRP	CB-CA-C	5.84	122.07	110.40
1	1	154	ALA	N-CA-CB	5.83	118.27	110.10
1	3	192	TRP	N-CA-C	5.83	126.74	111.00
1	3	65	VAL	CA-CB-CG2	5.83	119.64	110.90
1	1	111	GLY	O-C-N	5.82	132.01	122.70
1	4	288	SER	CA-CB-OG	5.82	126.90	111.20
1	3	149	THR	CA-CB-OG1	-5.81	96.80	109.00
1	4	181	GLN	CB-CA-C	5.80	122.00	110.40
1	1	40	VAL	CG1-CB-CG2	-5.80	101.62	110.90
1	3	178	THR	CB-CA-C	-5.79	95.96	111.60
1	2	46	ASP	O-C-N	5.79	131.97	122.70
1	1	52	PHE	CB-CA-C	5.79	121.97	110.40
1	4	28	ALA	O-C-N	5.78	131.95	122.70
1	2	274	GLU	CA-CB-CG	5.78	126.12	113.40
1	2	42	MET	CA-CB-CG	-5.78	103.47	113.30
1	2	281	ASP	OD1-CG-OD2	-5.78	112.32	123.30
1	4	2	LYS	CA-CB-CG	5.78	126.11	113.40
1	4	275	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	3	196	ARG	CB-CA-C	5.78	121.95	110.40
1	4	207	THR	CA-CB-OG1	-5.78	96.87	109.00
1	4	263	GLU	CG-CD-OE1	5.77	129.84	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	147	SER	N-CA-CB	-5.77	101.85	110.50
1	4	229	PHE	N-CA-CB	5.76	120.98	110.60
1	1	262	SER	N-CA-CB	-5.75	101.87	110.50
1	3	293	ALA	CA-C-O	-5.75	108.02	120.10
1	3	297	ILE	N-CA-CB	-5.75	97.57	110.80
1	2	167	VAL	CB-CA-C	5.75	122.32	111.40
1	2	55	GLU	CG-CD-OE2	-5.75	106.81	118.30
1	2	102	GLU	CG-CD-OE2	-5.74	106.81	118.30
1	3	162	GLU	CA-CB-CG	5.74	126.03	113.40
1	4	146	ALA	CB-CA-C	-5.74	101.49	110.10
1	4	331	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	2	52	PHE	CA-CB-CG	5.74	127.67	113.90
1	1	306	VAL	CG1-CB-CG2	5.73	120.08	110.90
1	4	307	VAL	CG1-CB-CG2	5.73	120.07	110.90
1	2	126	MET	CA-CB-CG	5.72	123.03	113.30
1	2	279	SER	N-CA-C	-5.71	95.57	111.00
1	3	244	ARG	CA-CB-CG	5.71	125.97	113.40
1	2	276	ASP	CA-C-N	-5.71	104.63	117.20
1	2	307	VAL	CA-CB-CG2	5.71	119.47	110.90
1	1	191	ASP	CB-CA-C	5.71	121.81	110.40
1	1	176	ALA	CA-C-N	5.71	129.75	117.20
1	4	314	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	2	274	GLU	OE1-CD-OE2	5.70	130.14	123.30
1	4	114	LYS	CB-CG-CD	5.70	126.42	111.60
1	4	285	ASP	O-C-N	5.70	131.82	122.70
1	2	298	GLN	CA-CB-CG	5.70	125.94	113.40
1	2	270	LEU	C-N-CA	5.70	134.26	122.30
1	2	225	THR	N-CA-CB	5.70	121.12	110.30
1	4	311	ASP	OD1-CG-OD2	-5.69	112.48	123.30
1	3	304	VAL	CA-CB-CG2	5.69	119.44	110.90
1	2	209	ALA	C-N-CA	5.68	135.91	121.70
1	4	176	ALA	CB-CA-C	5.67	118.61	110.10
1	1	37	GLU	N-CA-CB	5.67	120.81	110.60
1	2	178	THR	OG1-CB-CG2	5.67	123.05	110.00
1	2	320	VAL	CG1-CB-CG2	-5.67	101.83	110.90
1	3	244	ARG	N-CA-C	-5.66	95.71	111.00
1	2	59	GLU	CB-CA-C	-5.66	99.08	110.40
1	3	196	ARG	CA-CB-CG	5.66	125.85	113.40
1	3	266	LEU	O-C-N	5.66	131.75	122.70
1	1	27	VAL	N-CA-C	5.66	126.27	111.00
1	4	196	ARG	CG-CD-NE	-5.66	99.92	111.80
1	2	275	ASP	C-N-CA	5.65	135.84	121.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	79	GLU	CA-CB-CG	5.65	125.83	113.40
1	1	244	ARG	CB-CA-C	5.65	121.70	110.40
1	4	255	LYS	C-N-CA	5.65	135.82	121.70
1	2	83	TRP	N-CA-C	-5.64	95.76	111.00
1	2	45	TYR	N-CA-CB	-5.64	100.45	110.60
1	3	83	TRP	N-CA-CB	5.64	120.75	110.60
1	3	149	THR	O-C-N	5.63	131.72	122.70
1	4	107	HIS	N-CA-CB	5.63	120.74	110.60
1	4	263	GLU	CB-CG-CD	5.63	129.40	114.20
1	1	60	ASP	CB-CA-C	5.62	121.64	110.40
1	2	259	LYS	CA-CB-CG	5.62	125.77	113.40
1	2	251	TYR	CA-CB-CG	-5.62	102.72	113.40
1	2	85	LYS	N-CA-C	-5.62	95.83	111.00
1	2	236	VAL	CA-CB-CG1	5.62	119.33	110.90
1	2	147	SER	CA-C-O	5.62	131.89	120.10
1	3	272	TYR	CB-CG-CD2	-5.62	117.63	121.00
1	4	281	ASP	OD1-CG-OD2	-5.61	112.63	123.30
1	4	89	GLU	CG-CD-OE2	-5.61	107.08	118.30
1	1	253	ASP	N-CA-CB	5.61	120.69	110.60
1	1	132	ASN	CA-CB-CG	5.60	125.73	113.40
1	4	64	VAL	CA-CB-CG1	5.60	119.31	110.90
1	3	163	ASN	N-CA-C	5.60	126.13	111.00
1	4	181	GLN	O-C-N	-5.60	113.74	122.70
1	4	231	VAL	CG1-CB-CG2	5.59	119.85	110.90
1	4	220	LEU	CB-CG-CD1	5.59	120.50	111.00
1	3	208	GLY	CA-C-O	5.59	130.66	120.60
1	1	241	LEU	CA-CB-CG	5.58	128.14	115.30
1	3	235	ASP	CB-CG-OD2	5.58	123.32	118.30
1	1	36	LEU	CA-CB-CG	5.58	128.12	115.30
1	1	170	LEU	CB-CG-CD2	-5.58	101.52	111.00
1	1	233	THR	CA-CB-OG1	-5.58	97.29	109.00
1	2	133	LEU	CB-CA-C	5.58	120.79	110.20
1	1	188	SER	N-CA-CB	5.57	118.85	110.50
1	3	164	PHE	O-C-N	5.57	131.61	122.70
1	3	183	THR	CA-C-O	-5.57	108.40	120.10
1	3	227	MET	CG-SD-CE	5.57	109.11	100.20
1	3	311	ASP	N-CA-CB	5.57	120.62	110.60
1	2	83	TRP	CA-C-O	5.57	131.79	120.10
1	1	16	LEU	CB-CA-C	5.56	120.77	110.20
1	3	47	SER	CB-CA-C	5.56	120.67	110.10
1	2	97	VAL	CA-C-O	-5.56	108.43	120.10
1	3	235	ASP	CA-C-O	-5.55	108.44	120.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	26	VAL	CB-CA-C	5.54	121.93	111.40
1	1	27	VAL	N-CA-CB	-5.54	99.31	111.50
1	1	144	SER	CB-CA-C	-5.54	99.58	110.10
1	4	313	GLU	CB-CA-C	5.54	121.47	110.40
1	4	314	PHE	N-CA-C	5.54	125.94	111.00
1	1	191	ASP	N-CA-CB	-5.53	100.64	110.60
1	3	308	SER	O-C-N	5.53	131.55	122.70
1	3	4	GLY	N-CA-C	-5.53	99.28	113.10
1	3	46	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	2	165	GLU	OE1-CD-OE2	5.53	129.93	123.30
1	3	41	TYR	CB-CG-CD2	5.52	124.31	121.00
1	1	296	GLY	CA-C-N	-5.52	105.05	117.20
1	1	233	THR	CA-CB-CG2	5.52	120.13	112.40
1	1	306	VAL	CB-CA-C	5.52	121.89	111.40
1	1	89	GLU	N-CA-CB	-5.52	100.67	110.60
1	4	286	ASN	N-CA-CB	-5.52	100.67	110.60
1	2	45	TYR	CA-C-N	5.52	129.34	117.20
1	1	168	GLU	CG-CD-OE2	-5.51	107.27	118.30
1	2	152	CYS	O-C-N	5.51	131.52	122.70
1	1	267	GLN	OE1-CD-NE2	5.51	134.57	121.90
1	1	258	MET	CB-CG-SD	-5.51	95.88	112.40
1	1	244	ARG	CD-NE-CZ	5.50	131.30	123.60
1	3	252	ASP	CA-CB-CG	-5.50	101.30	113.40
1	4	162	GLU	CB-CG-CD	-5.50	99.35	114.20
1	2	86	ALA	N-CA-CB	-5.50	102.40	110.10
1	3	151	ASN	CB-CG-OD1	5.50	132.59	121.60
1	4	83	TRP	N-CA-CB	5.50	120.50	110.60
1	1	40	VAL	CB-CA-C	5.49	121.84	111.40
1	1	69	LYS	CA-CB-CG	5.48	125.46	113.40
1	3	295	ALA	CA-C-N	-5.48	105.24	116.20
1	4	177	VAL	CB-CA-C	5.48	121.81	111.40
1	3	151	ASN	CB-CA-C	5.48	121.35	110.40
1	4	129	CYS	N-CA-CB	5.47	120.45	110.60
1	2	83	TRP	CA-C-N	-5.47	105.16	117.20
1	3	201	ASN	CA-CB-CG	-5.47	101.36	113.40
1	2	19	ALA	CB-CA-C	5.47	118.30	110.10
1	3	102	GLU	CB-CA-C	-5.47	99.46	110.40
1	1	240	ASP	N-CA-CB	-5.46	100.77	110.60
1	2	193	ARG	CA-CB-CG	5.46	125.42	113.40
1	3	114	LYS	N-CA-CB	-5.46	100.77	110.60
1	1	306	VAL	CA-CB-CG1	-5.46	102.71	110.90
1	3	181	GLN	N-CA-CB	-5.46	100.77	110.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	192	TRP	CA-CB-CG	5.45	124.06	113.70
1	4	180	THR	CA-CB-CG2	5.45	120.03	112.40
1	4	258	MET	CA-CB-CG	-5.45	104.03	113.30
1	4	188	SER	CA-C-N	-5.45	105.21	117.20
1	3	134	GLU	CB-CA-C	-5.45	99.50	110.40
1	1	132	ASN	C-N-CA	5.45	135.32	121.70
1	3	116	VAL	CA-CB-CG1	5.45	119.07	110.90
1	1	142	VAL	CG1-CB-CG2	5.44	119.61	110.90
1	2	265	PRO	N-CD-CG	-5.44	95.04	103.20
1	3	230	ARG	CG-CD-NE	-5.44	100.38	111.80
1	3	192	TRP	CB-CA-C	-5.43	99.53	110.40
1	4	293	ALA	O-C-N	5.43	131.39	122.70
1	1	304	VAL	N-CA-CB	-5.43	99.55	111.50
1	4	274	GLU	CA-C-N	-5.43	105.25	117.20
1	3	55	GLU	N-CA-C	-5.43	96.34	111.00
1	4	333	ALA	N-CA-CB	-5.43	102.50	110.10
1	1	147	SER	N-CA-C	5.42	125.64	111.00
1	1	273	THR	CA-CB-CG2	5.42	119.99	112.40
1	1	263	GLU	CG-CD-OE1	5.41	129.12	118.30
1	4	181	GLN	C-N-CA	5.41	135.23	121.70
1	1	138	LYS	CD-CE-NZ	-5.41	99.26	111.70
1	1	195	GLY	N-CA-C	-5.41	99.58	113.10
1	3	289	SER	CA-CB-OG	5.41	125.80	111.20
1	2	267	GLN	OE1-CD-NE2	5.41	134.33	121.90
1	2	95	THR	CA-CB-OG1	-5.40	97.65	109.00
1	2	111	GLY	CA-C-O	-5.40	110.88	120.60
1	1	296	GLY	N-CA-C	-5.40	99.60	113.10
1	3	72	VAL	N-CA-CB	-5.39	99.64	111.50
1	3	120	PRO	N-CD-CG	-5.39	95.12	103.20
1	4	275	ASP	C-N-CA	5.38	135.16	121.70
1	1	89	GLU	OE1-CD-OE2	5.38	129.76	123.30
1	1	11	ILE	CA-C-N	5.38	126.95	116.20
1	2	97	VAL	CA-C-N	5.38	129.03	117.20
1	1	230	ARG	CG-CD-NE	-5.37	100.52	111.80
1	4	132	ASN	OD1-CG-ND2	-5.37	109.54	121.90
1	1	163	ASN	OD1-CG-ND2	5.37	134.24	121.90
1	3	146	ALA	C-N-CA	5.37	135.12	121.70
1	2	202	ILE	N-CA-C	-5.36	96.54	111.00
1	4	281	ASP	N-CA-C	-5.35	96.55	111.00
1	3	66	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	4	233	THR	CB-CA-C	5.35	126.05	111.60
1	4	225	THR	CA-C-N	5.35	126.89	116.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	248	GLU	CG-CD-OE2	-5.35	107.61	118.30
1	1	175	HIS	CB-CA-C	5.34	121.09	110.40
1	2	303	PHE	N-CA-CB	5.34	120.22	110.60
1	3	175	HIS	C-N-CA	5.34	135.05	121.70
1	4	121	SER	N-CA-CB	5.34	118.51	110.50
1	1	227	MET	CA-CB-CG	5.34	122.37	113.30
1	4	60	ASP	CB-CG-OD1	5.33	123.10	118.30
1	4	183	THR	N-CA-CB	5.33	120.43	110.30
1	2	310	TYR	C-N-CA	5.33	135.02	121.70
1	2	314	PHE	N-CA-CB	-5.33	101.01	110.60
1	3	231	VAL	CA-CB-CG2	-5.33	102.91	110.90
1	4	162	GLU	OE1-CD-OE2	5.33	129.69	123.30
1	1	281	ASP	N-CA-C	-5.32	96.62	111.00
1	1	313	GLU	N-CA-CB	5.32	120.18	110.60
1	4	161	HIS	CA-CB-CG	5.32	122.65	113.60
1	1	4	GLY	N-CA-C	-5.32	99.80	113.10
1	1	252	ASP	OD1-CG-OD2	5.32	133.40	123.30
1	3	263	GLU	OE1-CD-OE2	5.32	129.68	123.30
1	3	279	SER	N-CA-C	-5.32	96.64	111.00
1	4	161	HIS	O-C-N	5.32	131.21	122.70
1	3	44	LYS	CB-CA-C	-5.31	99.78	110.40
1	4	281	ASP	CB-CA-C	5.31	121.03	110.40
1	4	165	GLU	N-CA-C	5.31	125.34	111.00
1	1	149	THR	CA-CB-CG2	5.31	119.83	112.40
1	1	178	THR	CB-CA-C	-5.31	97.27	111.60
1	3	180	THR	CA-CB-CG2	5.31	119.83	112.40
1	3	165	GLU	CG-CD-OE2	-5.30	107.69	118.30
1	4	84	SER	O-C-N	5.30	131.18	122.70
1	3	225	THR	C-N-CA	-5.30	111.17	122.30
1	1	178	THR	CA-CB-CG2	5.29	119.81	112.40
1	2	141	THR	CB-CA-C	-5.29	97.31	111.60
1	2	111	GLY	O-C-N	5.29	131.17	122.70
1	1	146	ALA	CB-CA-C	-5.29	102.17	110.10
1	1	223	LYS	CA-CB-CG	5.29	125.03	113.40
1	1	18	ALA	CA-C-N	-5.29	105.57	117.20
1	1	196	ARG	CB-CG-CD	5.28	125.34	111.60
1	4	185	ASP	CA-CB-CG	-5.28	101.78	113.40
1	4	43	PHE	N-CA-CB	5.28	120.10	110.60
1	3	301	LYS	CA-CB-CG	5.28	125.01	113.40
1	3	48	THR	CA-CB-CG2	5.28	119.78	112.40
1	2	183	THR	CA-CB-OG1	-5.27	97.92	109.00
1	2	59	GLU	CG-CD-OE2	-5.27	107.75	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	120	PRO	CB-CA-C	5.27	125.17	112.00
1	4	191	ASP	CA-CB-CG	5.26	124.98	113.40
1	4	313	GLU	CG-CD-OE1	-5.26	107.77	118.30
1	2	185	ASP	CA-CB-CG	-5.26	101.83	113.40
1	3	281	ASP	N-CA-CB	5.26	120.07	110.60
1	3	209	ALA	CB-CA-C	-5.26	102.21	110.10
1	4	165	GLU	CB-CA-C	-5.26	99.89	110.40
1	3	178	THR	N-CA-C	5.26	125.19	111.00
1	1	139	ASP	CB-CG-OD2	5.25	123.03	118.30
1	1	134	GLU	CA-CB-CG	5.25	124.95	113.40
1	1	124	ALA	N-CA-CB	-5.25	102.75	110.10
1	1	41	TYR	O-C-N	5.25	131.09	122.70
1	1	314	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	3	160	LEU	CA-CB-CG	5.25	127.37	115.30
1	4	30	ASN	O-C-N	5.25	131.10	122.70
1	4	219	GLU	CA-CB-CG	5.25	124.94	113.40
1	1	295	ALA	C-N-CA	-5.24	111.29	122.30
1	1	239	VAL	CA-C-N	-5.24	105.68	117.20
1	3	275	ASP	CB-CA-C	5.24	120.87	110.40
1	3	177	VAL	O-C-N	-5.23	114.33	122.70
1	2	300	SER	CA-C-O	5.23	131.09	120.10
1	3	279	SER	O-C-N	5.23	131.07	122.70
1	4	38	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	4	245	LEU	N-CA-C	5.23	125.12	111.00
1	2	314	PHE	N-CA-C	5.23	125.11	111.00
1	3	240	ASP	OD1-CG-OD2	5.22	133.22	123.30
1	3	252	ASP	OD1-CG-OD2	5.22	133.22	123.30
1	3	287	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
1	3	14	LEU	CA-CB-CG	5.22	127.30	115.30
1	3	83	TRP	N-CA-C	-5.22	96.92	111.00
1	2	66	ASP	CA-CB-CG	-5.21	101.93	113.40
1	4	85	LYS	CA-CB-CG	5.21	124.87	113.40
1	1	266	LEU	CB-CA-C	5.21	120.10	110.20
1	4	292	ASP	CA-C-O	5.21	131.04	120.10
1	4	127	PHE	CB-CA-C	5.21	120.81	110.40
1	1	323	LEU	N-CA-C	-5.20	96.95	111.00
1	3	78	PRO	CA-N-CD	-5.20	104.22	111.50
1	4	279	SER	CB-CA-C	5.19	119.97	110.10
1	1	196	ARG	CA-CB-CG	5.19	124.83	113.40
1	3	51	VAL	CA-CB-CG1	5.19	118.69	110.90
1	4	274	GLU	CA-C-O	5.19	131.00	120.10
1	2	289	SER	CA-CB-OG	5.18	125.19	111.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	313	GLU	CG-CD-OE1	5.18	128.66	118.30
1	3	191	ASP	C-N-CA	5.18	134.65	121.70
1	1	243	VAL	O-C-N	5.18	130.99	122.70
1	3	52	PHE	CB-CG-CD1	-5.18	117.18	120.80
1	4	230	ARG	NH1-CZ-NH2	-5.18	113.71	119.40
1	3	112	ALA	N-CA-CB	5.17	117.34	110.10
1	1	4	GLY	O-C-N	5.17	130.97	122.70
1	3	248	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	1	41	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	1	26	VAL	CB-CA-C	5.17	121.22	111.40
1	4	247	LYS	CB-CG-CD	5.17	125.03	111.60
1	1	67	GLY	O-C-N	5.16	130.96	122.70
1	4	296	GLY	O-C-N	5.16	130.96	122.70
1	2	327	MET	CG-SD-CE	5.16	108.45	100.20
1	1	138	LYS	CB-CA-C	-5.16	100.09	110.40
1	1	127	PHE	C-N-CA	5.15	134.57	121.70
1	3	281	ASP	N-CA-C	-5.15	97.10	111.00
1	3	319	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	2	144	SER	CB-CA-C	-5.14	100.34	110.10
1	4	2	LYS	CA-C-O	-5.13	109.32	120.10
1	4	103	LYS	N-CA-CB	5.13	119.83	110.60
1	3	75	GLU	N-CA-CB	5.12	119.82	110.60
1	1	154	ALA	CB-CA-C	-5.12	102.42	110.10
1	3	250	SER	O-C-N	5.12	130.89	122.70
1	3	280	SER	CA-CB-OG	-5.12	97.38	111.20
1	4	300	SER	C-N-CA	5.12	134.49	121.70
1	2	165	GLU	CA-C-N	5.12	128.45	117.20
1	2	66	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	3	9	GLY	N-CA-C	-5.11	100.32	113.10
1	1	320	VAL	O-C-N	5.11	130.88	122.70
1	2	4	GLY	N-CA-C	-5.11	100.32	113.10
1	3	195	GLY	N-CA-C	-5.11	100.32	113.10
1	4	235	ASP	CA-C-O	-5.11	109.37	120.10
1	2	204	PRO	O-C-N	-5.11	114.53	122.70
1	3	303	PHE	CB-CG-CD1	5.11	124.37	120.80
1	4	63	LEU	CB-CA-C	5.10	119.90	110.20
1	1	163	ASN	CA-CB-CG	-5.10	102.17	113.40
1	4	266	LEU	CA-CB-CG	5.10	127.03	115.30
1	3	277	VAL	CA-CB-CG2	-5.10	103.26	110.90
1	2	113	LYS	N-CA-C	5.09	124.75	111.00
1	3	271	GLY	CA-C-N	5.09	128.41	117.20
1	4	142	VAL	O-C-N	-5.09	114.55	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	24	ALA	CB-CA-C	5.09	117.73	110.10
1	3	167	VAL	CA-CB-CG1	-5.09	103.27	110.90
1	2	44	LYS	N-CA-CB	5.09	119.76	110.60
1	1	107	HIS	N-CA-CB	5.09	119.76	110.60
1	1	135	LYS	CD-CE-NZ	5.08	123.39	111.70
1	2	163	ASN	N-CA-C	5.08	124.72	111.00
1	3	204	PRO	O-C-N	-5.08	114.57	122.70
1	3	275	ASP	CB-CG-OD1	5.08	122.87	118.30
1	3	138	LYS	N-CA-C	5.08	124.72	111.00
1	1	139	ASP	N-CA-CB	5.08	119.74	110.60
1	1	75	GLU	CB-CA-C	-5.08	100.25	110.40
1	2	68	LYS	CA-CB-CG	5.08	124.57	113.40
1	1	222	GLY	N-CA-C	5.07	125.78	113.10
1	3	191	ASP	CB-CG-OD2	5.07	122.86	118.30
1	3	303	PHE	O-C-N	5.07	130.81	122.70
1	4	280	SER	N-CA-CB	-5.07	102.90	110.50
1	1	300	SER	O-C-N	-5.07	114.60	122.70
1	4	152	CYS	CA-C-O	-5.07	109.46	120.10
1	4	244	ARG	CA-C-O	-5.06	109.47	120.10
1	4	258	MET	N-CA-CB	5.06	119.72	110.60
1	3	306	VAL	CB-CA-C	5.06	121.01	111.40
1	4	315	GLY	N-CA-C	-5.06	100.45	113.10
1	3	276	ASP	CA-C-N	-5.06	106.07	117.20
1	4	79	GLU	N-CA-CB	5.06	119.70	110.60
1	4	8	PHE	CA-CB-CG	5.05	126.03	113.90
1	3	183	THR	OG1-CB-CG2	5.05	121.62	110.00
1	3	46	ASP	CA-CB-CG	-5.05	102.29	113.40
1	1	73	PHE	CB-CA-C	5.05	120.49	110.40
1	1	193	ARG	CA-CB-CG	5.05	124.50	113.40
1	2	68	LYS	O-C-N	5.05	130.78	122.70
1	1	184	VAL	CB-CA-C	5.04	120.99	111.40
1	2	252	ASP	CA-CB-CG	-5.04	102.31	113.40
1	4	224	LEU	CA-CB-CG	5.04	126.90	115.30
1	2	304	VAL	N-CA-CB	-5.04	100.41	111.50
1	4	288	SER	CB-CA-C	5.04	119.68	110.10
1	3	79	GLU	CG-CD-OE2	-5.04	108.22	118.30
1	4	204	PRO	CB-CA-C	5.04	124.59	112.00
1	4	27	VAL	N-CA-CB	-5.03	100.42	111.50
1	4	178	THR	CB-CA-C	-5.03	98.01	111.60
1	3	238	VAL	CA-CB-CG1	5.03	118.45	110.90
1	1	185	ASP	OD1-CG-OD2	5.03	132.86	123.30
1	2	58	MET	CA-CB-CG	-5.03	104.75	113.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	17	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
1	4	51	VAL	CG1-CB-CG2	-5.03	102.86	110.90
1	2	44	LYS	CD-CE-NZ	-5.02	100.14	111.70
1	1	196	ARG	CG-CD-NE	-5.02	101.25	111.80
1	2	93	GLU	CG-CD-OE2	-5.02	108.26	118.30
1	1	314	PHE	CA-C-N	5.02	126.24	116.20
1	2	151	ASN	CB-CA-C	5.02	120.44	110.40
1	4	208	GLY	CA-C-O	5.02	129.63	120.60
1	2	244	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	1	201	ASN	N-CA-C	5.01	124.53	111.00
1	1	318	GLN	CA-CB-CG	5.01	124.42	113.40
1	3	16	LEU	CA-CB-CG	5.01	126.82	115.30
1	2	191	ASP	CA-C-N	5.01	128.21	117.20
1	4	9	GLY	N-CA-C	-5.01	100.59	113.10
1	2	163	ASN	CA-CB-CG	-5.00	102.39	113.40
1	3	114	LYS	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	3	13	ARG	Sidechain
1	3	196	ARG	Sidechain

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2507	0	2519	903	2
1	2	2507	0	2523	875	25
1	3	2507	0	2519	901	13
1	4	2507	0	2520	887	13
2	1	23	0	0	12	0
2	2	28	0	0	26	4
2	3	27	0	0	28	2
2	4	44	0	0	32	3
All	All	10150	0	10081	3343	31

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 166.

All (3343) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:32:PRO:HA	1:4:74:ASN:ND2	1.32	1.40
1:2:277:VAL:HG21	1:4:41:TYR:CE1	1.58	1.39
1:2:32:PRO:HA	1:2:74:ASN:ND2	1.38	1.34
1:1:220:LEU:HA	1:1:223:LYS:NZ	1.43	1.32
1:1:126:MET:HB2	1:1:215:LYS:NZ	1.45	1.30
1:3:138:LYS:NZ	1:3:330:VAL:HG13	1.42	1.30
1:2:97:VAL:O	1:2:98:PHE:CD1	1.82	1.30
1:4:75:GLU:N	2:4:347:HOH:O	1.62	1.30
1:1:292:ASP:OD1	1:1:295:ALA:HB3	1.32	1.28
1:4:32:PRO:CA	1:4:74:ASN:HD21	1.51	1.24
1:4:270:LEU:HD23	1:4:271:GLY:N	1.50	1.23
1:1:188:SER:O	1:1:190:LYS:N	1.70	1.23
1:1:128:VAL:O	1:1:132:ASN:HB3	1.38	1.23
1:3:52:PHE:N	2:3:370:HOH:O	1.70	1.22
1:1:276:ASP:O	1:1:278:VAL:HG13	1.38	1.22
1:1:169:GLY:O	1:1:170:LEU:HD23	1.38	1.22
1:3:113:LYS:HB3	1:3:114:LYS:CD	1.69	1.22
1:2:52:PHE:N	2:2:400:HOH:O	1.67	1.22
1:2:251:TYR:N	1:2:299:LEU:HD12	1.53	1.21
1:4:119:ALA:HB1	1:4:120:PRO:CD	1.70	1.21
1:2:41:TYR:CE1	1:4:277:VAL:HG21	1.75	1.21
1:1:127:PHE:CB	1:1:132:ASN:HB2	1.72	1.20
1:2:236:VAL:O	1:2:237:SER:HB2	1.39	1.19
1:1:127:PHE:CE2	1:1:136:TYR:HB2	1.76	1.19
1:4:74:ASN:O	1:4:75:GLU:HG2	1.42	1.19
1:1:292:ASP:CG	1:1:295:ALA:HB3	1.63	1.18
1:3:17:ARG:HG2	1:3:43:PHE:HE2	1.09	1.17
1:3:65:VAL:HG22	1:3:66:ASP:OD2	1.40	1.17
1:1:295:ALA:HB2	1:4:193:ARG:HH22	1.08	1.17
1:3:127:PHE:HB3	1:3:132:ASN:CB	1.75	1.17
1:4:220:LEU:HA	1:4:223:LYS:HZ3	1.09	1.17
1:3:270:LEU:HD23	1:3:271:GLY:N	1.58	1.16
1:3:276:ASP:OD1	1:3:277:VAL:HG13	1.45	1.16
1:1:299:LEU:HD23	1:1:304:VAL:HG23	1.23	1.15
1:1:1:SER:OG	1:1:25:GLN:HB2	1.44	1.15
1:2:295:ALA:CB	1:3:193:ARG:HH12	1.60	1.15
1:2:183:THR:HG22	2:2:413:HOH:O	1.47	1.15

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:181:GLN:HE21	1:4:203:ILE:HD12	1.06	1.15
1:1:17:ARG:HG2	1:1:43:PHE:HE2	1.09	1.14
1:3:131:VAL:HG12	1:3:158:LYS:HZ2	1.05	1.14
1:2:225:THR:HG21	1:3:298:GLN:NE2	1.59	1.14
1:2:297:ILE:H	1:2:297:ILE:HD13	1.07	1.14
1:3:131:VAL:HG12	1:3:158:LYS:NZ	1.61	1.14
1:2:11:ILE:HD12	1:2:11:ILE:H	1.04	1.14
1:4:113:LYS:HD3	1:4:114:LYS:HZ2	0.99	1.14
1:2:26:VAL:O	1:2:27:VAL:HB	1.40	1.14
1:2:77:LYS:N	2:2:408:HOH:O	1.78	1.14
1:3:211:LYS:CE	1:3:211:LYS:HA	1.77	1.14
1:1:208:GLY:HA3	1:1:211:LYS:HG2	1.17	1.14
1:1:90:TYR:CE2	1:1:328:GLN:NE2	2.16	1.13
1:1:8:PHE:CD2	1:1:8:PHE:O	2.02	1.13
1:1:41:TYR:CE1	1:3:277:VAL:HG21	1.83	1.13
1:3:4:GLY:HA2	1:3:27:VAL:CG2	1.78	1.13
1:2:128:VAL:O	1:2:132:ASN:HB3	1.48	1.12
1:1:113:LYS:HB3	1:1:114:LYS:HD2	1.29	1.12
1:2:212:ALA:O	1:2:216:VAL:HB	1.48	1.12
1:1:193:ARG:HH22	1:4:295:ALA:HB2	0.99	1.12
1:1:71:THR:HG21	1:1:73:PHE:CE1	1.84	1.11
1:1:8:PHE:O	1:1:8:PHE:HD2	1.29	1.11
1:2:41:TYR:CZ	1:4:277:VAL:HG21	1.84	1.11
1:3:30:ASN:OD1	1:3:81:ILE:HG13	1.50	1.11
1:3:113:LYS:CB	1:3:114:LYS:HD2	1.80	1.11
1:1:297:ILE:H	1:1:297:ILE:CD1	1.64	1.11
1:2:27:VAL:HG13	1:2:28:ALA:H	1.14	1.11
1:1:277:VAL:HG21	1:3:41:TYR:CE1	1.85	1.11
1:3:161:HIS:ND1	1:3:165:GLU:O	1.84	1.10
1:2:30:ASN:OD1	1:2:81:ILE:HG13	1.51	1.10
1:4:73:PHE:O	2:4:335:HOH:O	1.68	1.10
1:4:26:VAL:C	1:4:27:VAL:HG12	1.71	1.10
1:3:101:ILE:HB	1:3:123:ASP:OD1	1.50	1.10
1:3:127:PHE:CB	1:3:132:ASN:HB2	1.81	1.10
1:2:193:ARG:HH22	1:3:295:ALA:HB2	0.96	1.10
1:4:154:ALA:HB3	1:4:155:PRO:CD	1.82	1.09
1:1:4:GLY:HA2	1:1:27:VAL:HG21	1.29	1.09
1:4:28:ALA:HB3	1:4:83:TRP:HZ3	1.15	1.09
1:2:297:ILE:CD1	1:2:297:ILE:H	1.64	1.09
1:4:78:PRO:HG3	1:4:98:PHE:CE2	1.87	1.09
1:4:58:MET:CE	1:4:58:MET:H	1.64	1.09

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:216:VAL:HG13	1:4:217:ILE:HG22	1.17	1.09
1:1:127:PHE:HB3	1:1:132:ASN:CB	1.81	1.09
1:3:27:VAL:HG22	1:3:28:ALA:H	1.03	1.09
1:1:220:LEU:CA	1:1:223:LYS:HZ2	1.66	1.09
1:4:125:PRO:HG2	1:4:140:MET:CE	1.83	1.08
1:4:113:LYS:HD3	1:4:114:LYS:NZ	1.67	1.08
1:1:52:PHE:C	1:1:53:LYS:HE2	1.72	1.08
1:3:307:VAL:O	1:3:307:VAL:HG13	1.41	1.08
1:3:154:ALA:HB3	1:3:155:PRO:CD	1.82	1.08
1:3:211:LYS:HE2	1:3:211:LYS:HA	1.22	1.08
1:1:202:ILE:CD1	1:4:233:THR:HG21	1.83	1.08
1:1:270:LEU:HD23	1:1:271:GLY:N	1.68	1.08
1:1:44:LYS:NZ	1:1:44:LYS:HB3	1.67	1.08
1:1:6:ASN:HA	1:1:30:ASN:HD21	1.16	1.07
1:1:277:VAL:HA	1:4:193:ARG:HG3	1.29	1.07
1:3:78:PRO:HG3	1:3:98:PHE:CE2	1.89	1.07
1:2:1:SER:O	1:2:2:LYS:HG2	1.54	1.07
1:1:154:ALA:HB3	1:1:155:PRO:CD	1.85	1.07
1:4:27:VAL:HG22	1:4:28:ALA:H	0.98	1.07
1:4:44:LYS:HG3	1:4:56:VAL:HG21	1.30	1.07
1:4:161:HIS:ND1	1:4:165:GLU:O	1.85	1.07
1:1:113:LYS:HB3	1:1:114:LYS:CD	1.85	1.07
1:2:17:ARG:HG3	1:2:43:PHE:CE2	1.90	1.07
1:4:113:LYS:HB3	1:4:114:LYS:HD2	1.36	1.07
1:4:161:HIS:O	1:4:165:GLU:N	1.88	1.07
1:2:91:ILE:HD13	1:2:115:VAL:HG22	1.33	1.06
1:1:208:GLY:CA	1:1:211:LYS:HG2	1.85	1.06
1:1:27:VAL:HG13	1:1:28:ALA:H	1.19	1.06
1:1:307:VAL:HG13	1:1:307:VAL:O	1.53	1.06
1:4:154:ALA:HB3	1:4:155:PRO:HD2	1.08	1.06
1:2:248:GLU:HA	1:2:302:THR:CG2	1.85	1.06
1:4:258:MET:HG2	1:4:270:LEU:HD11	1.37	1.05
1:3:113:LYS:C	1:3:114:LYS:HE3	1.75	1.05
1:2:75:GLU:C	2:2:408:HOH:O	1.93	1.05
1:3:81:ILE:HD13	1:3:82:PRO:HD2	1.38	1.05
1:2:11:ILE:H	1:2:11:ILE:CD1	1.67	1.05
1:2:27:VAL:HG13	1:2:28:ALA:N	1.65	1.05
1:1:113:LYS:C	1:1:114:LYS:HE3	1.77	1.05
1:1:297:ILE:H	1:1:297:ILE:HD13	1.20	1.05
1:3:85:LYS:O	1:3:86:ALA:HB2	1.52	1.05
1:1:32:PRO:HA	1:1:74:ASN:ND2	1.71	1.05

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:3:ILE:HG22	1:2:4:GLY:H	1.19	1.05
1:2:78:PRO:HG3	1:2:98:PHE:CE2	1.92	1.04
1:1:208:GLY:HA3	1:1:211:LYS:CG	1.86	1.04
1:1:17:ARG:HG2	1:1:43:PHE:CE2	1.92	1.04
1:2:251:TYR:H	1:2:299:LEU:CD1	1.68	1.04
1:3:27:VAL:HG22	1:3:28:ALA:N	1.69	1.04
1:1:202:ILE:HD11	1:4:233:THR:HG21	1.32	1.04
1:2:220:LEU:O	1:2:222:GLY:N	1.91	1.04
1:1:211:LYS:NZ	1:1:211:LYS:HA	1.73	1.04
1:2:255:LYS:HE2	1:2:293:ALA:HB1	1.36	1.03
1:4:27:VAL:CG2	1:4:28:ALA:H	1.70	1.03
1:3:11:ILE:HD13	1:3:11:ILE:H	1.18	1.03
1:3:138:LYS:HZ2	1:3:330:VAL:CG1	1.69	1.03
1:3:251:TYR:H	1:3:299:LEU:HD12	1.13	1.03
1:2:11:ILE:HD12	1:2:11:ILE:N	1.73	1.03
1:2:281:ASP:O	1:2:283:ILE:N	1.92	1.03
1:3:138:LYS:NZ	1:3:330:VAL:CG1	2.22	1.03
1:4:53:LYS:HB3	1:4:53:LYS:HZ3	1.22	1.03
1:1:277:VAL:HA	1:4:193:ARG:CD	1.88	1.03
1:4:1:SER:HB3	1:4:25:GLN:HE21	1.19	1.03
1:1:225:THR:OG1	1:4:298:GLN:OE1	1.76	1.02
1:2:295:ALA:HB1	1:3:193:ARG:HH12	1.21	1.02
1:4:8:PHE:HD2	1:4:8:PHE:O	1.42	1.02
1:2:131:VAL:HG12	1:2:158:LYS:NZ	1.75	1.02
1:3:127:PHE:HB3	1:3:132:ASN:HB2	1.04	1.02
1:1:101:ILE:HG23	1:1:142:VAL:HG11	1.38	1.02
1:1:31:ASP:O	1:1:34:ILE:HG23	1.59	1.02
1:1:193:ARG:HH12	1:4:295:ALA:HB1	1.20	1.02
1:4:284:GLY:HA2	1:4:314:PHE:CE1	1.95	1.02
1:4:51:VAL:C	2:4:340:HOH:O	1.97	1.02
1:1:270:LEU:HD23	1:1:271:GLY:H	1.25	1.01
1:1:169:GLY:C	1:1:170:LEU:HD23	1.79	1.01
1:4:32:PRO:CA	1:4:74:ASN:ND2	2.16	1.01
1:2:277:VAL:HG23	1:2:278:VAL:H	1.23	1.01
1:4:113:LYS:HB3	1:4:114:LYS:CD	1.89	1.01
1:3:32:PRO:HA	1:3:74:ASN:ND2	1.75	1.01
1:4:129:CYS:HA	1:4:132:ASN:HD22	1.22	1.01
1:4:138:LYS:HE2	1:4:330:VAL:HG13	1.42	1.01
1:2:113:LYS:HG2	1:2:114:LYS:HE3	1.42	1.01
1:1:27:VAL:HG22	1:1:28:ALA:N	1.72	1.00
1:4:119:ALA:CB	1:4:120:PRO:HD2	1.88	1.00

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:277:VAL:HA	1:4:193:ARG:CG	1.89	1.00
1:1:252:ASP:O	1:1:255:LYS:N	1.94	1.00
1:4:284:GLY:HA2	1:4:314:PHE:HE1	1.22	1.00
1:1:193:ARG:NH2	1:4:295:ALA:HB2	1.77	1.00
1:1:2:LYS:CG	1:1:89:GLU:HG3	1.90	1.00
1:1:211:LYS:HZ3	1:1:211:LYS:HA	1.24	1.00
1:1:243:VAL:HG22	1:1:304:VAL:HG12	1.44	1.00
1:3:4:GLY:HA2	1:3:27:VAL:HG21	1.43	1.00
1:1:154:ALA:HB3	1:1:155:PRO:HD3	1.39	0.99
1:3:276:ASP:CG	1:3:277:VAL:HG22	1.82	0.99
1:2:225:THR:HG23	1:2:226:GLY:N	1.75	0.99
1:3:196:ARG:NH1	1:3:196:ARG:HG2	1.75	0.99
1:1:7:GLY:O	1:1:8:PHE:HB3	1.59	0.99
1:1:236:VAL:O	1:1:237:SER:HB3	1.60	0.99
1:1:30:ASN:OD1	1:1:81:ILE:HG13	1.60	0.99
1:2:10:ARG:NH1	1:2:46:ASP:OD1	1.96	0.99
1:1:171:MET:SD	1:1:209:ALA:HB2	2.02	0.99
1:4:77:LYS:C	2:4:348:HOH:O	2.01	0.99
1:4:280:SER:O	2:4:357:HOH:O	1.79	0.99
1:3:17:ARG:HG2	1:3:43:PHE:CE2	1.97	0.99
1:1:127:PHE:HB3	1:1:132:ASN:HB2	1.02	0.98
1:1:2:LYS:HG3	1:1:89:GLU:HG3	0.99	0.98
1:2:175:HIS:CD2	1:2:230:ARG:NH2	2.30	0.98
1:2:328:GLN:HA	1:2:328:GLN:HE21	1.27	0.98
1:4:311:ASP:O	1:4:313:GLU:N	1.96	0.98
1:4:89:GLU:HG3	1:4:90:TYR:CD1	1.97	0.98
1:2:193:ARG:HB2	1:3:277:VAL:HG12	1.45	0.98
1:3:201:ASN:HD22	1:3:201:ASN:N	1.53	0.98
1:3:138:LYS:HZ2	1:3:330:VAL:HG13	1.21	0.98
1:1:188:SER:O	1:1:191:ASP:N	1.96	0.98
1:3:131:VAL:CG1	1:3:158:LYS:NZ	2.26	0.98
1:1:6:ASN:HA	1:1:30:ASN:ND2	1.76	0.98
1:4:251:TYR:HH	1:4:291:PHE:HZ	1.04	0.98
1:2:203:ILE:HG22	1:2:203:ILE:O	1.61	0.98
1:3:28:ALA:HA	1:3:71:THR:O	1.64	0.98
1:3:2:LYS:HG3	1:3:89:GLU:HG3	1.46	0.98
1:2:17:ARG:HG3	1:2:43:PHE:HE2	1.22	0.98
1:1:17:ARG:CG	1:1:43:PHE:HE2	1.77	0.98
1:1:44:LYS:HZ2	1:1:44:LYS:HB3	1.20	0.98
1:3:243:VAL:HG22	1:3:304:VAL:HG12	1.42	0.97
1:3:32:PRO:HD3	2:3:377:HOH:O	1.63	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:113:LYS:O	1:1:114:LYS:HE3	1.64	0.97
1:1:2:LYS:HG3	1:1:89:GLU:CG	1.93	0.97
1:4:119:ALA:HB1	1:4:120:PRO:HD2	0.99	0.97
1:4:113:LYS:HB3	1:4:114:LYS:CE	1.92	0.97
1:2:161:HIS:ND1	1:2:165:GLU:O	1.95	0.97
1:3:121:SER:OG	1:3:124:ALA:HB3	1.63	0.97
1:1:292:ASP:OD2	1:1:295:ALA:HB3	1.64	0.97
1:4:283:ILE:HD11	2:4:358:HOH:O	1.63	0.97
1:2:188:SER:HB3	1:2:192:TRP:N	1.78	0.97
1:2:244:ARG:HG3	1:3:244:ARG:HH12	1.28	0.97
1:2:145:ASN:O	1:2:145:ASN:ND2	1.98	0.97
1:3:76:MET:O	1:3:77:LYS:HD2	1.65	0.97
1:1:236:VAL:O	1:1:237:SER:CB	2.09	0.97
1:2:127:PHE:CE2	1:2:136:TYR:HB2	2.00	0.97
1:4:108:PHE:O	1:4:109:LYS:C	2.03	0.97
1:1:53:LYS:HD2	1:1:54:GLY:H	1.30	0.96
1:1:4:GLY:CA	1:1:27:VAL:HG21	1.94	0.96
1:2:232:PRO:O	1:2:233:THR:O	1.83	0.96
1:3:175:HIS:CD2	1:3:230:ARG:NH2	2.34	0.96
1:3:8:PHE:CD1	1:3:29:VAL:HG11	2.01	0.96
1:2:8:PHE:O	1:2:8:PHE:HD2	1.46	0.96
1:3:11:ILE:CD1	1:3:11:ILE:N	2.28	0.96
1:3:307:VAL:CG1	1:3:307:VAL:O	2.14	0.96
1:1:95:THR:HG22	1:1:97:VAL:H	1.30	0.96
1:1:26:VAL:CG1	1:1:70:ILE:HG21	1.95	0.96
1:2:276:ASP:O	1:2:278:VAL:HG13	1.64	0.96
1:4:188:SER:O	1:4:190:LYS:N	1.98	0.96
1:4:8:PHE:CD2	1:4:8:PHE:O	2.18	0.96
1:1:244:ARG:HH12	1:4:244:ARG:HG3	1.31	0.95
1:2:32:PRO:CA	1:2:74:ASN:ND2	2.29	0.95
1:4:52:PHE:N	2:4:340:HOH:O	1.97	0.95
1:2:65:VAL:HG22	1:2:66:ASP:OD2	1.66	0.95
1:4:52:PHE:O	1:4:53:LYS:HB3	1.64	0.95
1:3:104:ALA:O	1:3:107:HIS:N	1.99	0.95
1:3:113:LYS:O	1:3:114:LYS:HE3	1.63	0.95
1:2:41:TYR:OH	1:4:277:VAL:HG11	1.66	0.95
1:2:52:PHE:O	1:2:53:LYS:NZ	1.99	0.95
1:1:71:THR:HG22	1:1:72:VAL:N	1.78	0.95
1:3:129:CYS:HA	1:3:132:ASN:ND2	1.81	0.95
1:1:193:ARG:HH12	1:4:295:ALA:CB	1.79	0.95
1:1:295:ALA:HB2	1:4:193:ARG:NH2	1.81	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:188:SER:O	1:2:191:ASP:N	1.99	0.95
1:1:97:VAL:O	1:1:98:PHE:CD1	2.19	0.95
1:2:248:GLU:HA	1:2:302:THR:HG22	1.46	0.95
1:4:58:MET:H	1:4:58:MET:HE1	1.28	0.95
1:1:121:SER:CB	1:1:124:ALA:HB3	1.97	0.94
1:1:293:ALA:O	1:1:294:LYS:HB3	1.67	0.94
1:1:299:LEU:CD2	1:1:304:VAL:HG23	1.96	0.94
1:4:2:LYS:NZ	1:4:88:ALA:HA	1.82	0.94
1:3:90:TYR:CE2	1:3:328:GLN:NE2	2.35	0.94
1:3:101:ILE:O	1:3:105:SER:OG	1.84	0.94
1:2:193:ARG:NH2	1:3:295:ALA:HB2	1.80	0.94
1:1:298:GLN:NE2	1:4:225:THR:CG2	2.31	0.94
1:2:1:SER:HB3	1:2:25:GLN:HB2	1.49	0.94
1:3:295:ALA:C	1:3:297:ILE:HG23	1.88	0.94
1:1:190:LYS:HD2	2:1:397:HOH:O	1.66	0.94
1:1:298:GLN:HE22	1:4:225:THR:CG2	1.81	0.94
1:2:295:ALA:HB1	1:3:193:ARG:NH1	1.83	0.94
1:4:132:ASN:ND2	1:4:133:LEU:CD2	2.31	0.94
1:4:181:GLN:NE2	1:4:203:ILE:HD12	1.83	0.93
1:2:277:VAL:O	1:2:278:VAL:O	1.86	0.93
1:2:95:THR:HG22	1:2:97:VAL:H	1.34	0.93
1:1:130:GLY:O	1:1:133:LEU:HD12	1.69	0.93
1:2:127:PHE:HD1	1:2:143:VAL:CG2	1.82	0.93
1:4:276:ASP:OD1	1:4:277:VAL:HG22	1.69	0.93
1:3:6:ASN:HA	1:3:30:ASN:ND2	1.81	0.93
1:4:28:ALA:HB3	1:4:83:TRP:CZ3	2.04	0.93
1:1:292:ASP:OD1	1:1:295:ALA:CB	2.16	0.93
1:4:279:SER:O	1:4:281:ASP:N	2.02	0.93
1:3:3:ILE:O	1:3:88:ALA:HB1	1.67	0.93
1:1:132:ASN:HD21	1:1:133:LEU:HD21	1.34	0.92
1:4:17:ARG:NH2	2:4:339:HOH:O	2.01	0.92
1:4:31:ASP:O	1:4:34:ILE:HG22	1.69	0.92
1:3:19:ALA:O	1:3:22:CYS:HB2	1.69	0.92
1:3:252:ASP:O	1:3:255:LYS:HG2	1.69	0.92
1:3:236:VAL:O	1:3:237:SER:HB2	1.65	0.92
1:4:270:LEU:HD23	1:4:270:LEU:C	1.89	0.92
1:1:101:ILE:HG22	1:1:105:SER:OG	1.70	0.92
1:1:183:THR:O	1:1:184:VAL:HB	1.67	0.92
1:2:113:LYS:CG	1:2:114:LYS:HE3	1.99	0.92
1:3:252:ASP:O	1:3:255:LYS:N	2.01	0.92
1:4:211:LYS:N	1:4:211:LYS:HE2	1.84	0.92

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:131:VAL:CG1	1:3:158:LYS:HZ2	1.81	0.92
1:2:244:ARG:CB	1:3:244:ARG:HH22	1.81	0.92
1:1:251:TYR:HB2	1:1:299:LEU:HG	1.51	0.92
1:2:277:VAL:HG21	1:4:41:TYR:HE1	1.10	0.92
1:3:32:PRO:HA	1:3:74:ASN:HD21	1.35	0.92
1:1:126:MET:SD	1:1:146:ALA:HB2	2.10	0.92
1:1:126:MET:CB	1:1:215:LYS:HZ2	1.82	0.92
1:2:297:ILE:N	1:2:297:ILE:HD13	1.75	0.92
1:4:74:ASN:OD1	1:4:75:GLU:N	2.02	0.92
1:3:138:LYS:HZ1	1:3:330:VAL:HG13	1.32	0.92
1:3:277:VAL:HG23	1:3:278:VAL:H	1.34	0.92
1:4:208:GLY:HA3	1:4:211:LYS:HG2	1.52	0.92
1:2:6:ASN:ND2	1:2:93:GLU:OE1	2.01	0.92
1:4:4:GLY:HA2	1:4:27:VAL:CG2	2.00	0.92
1:2:33:PHE:HZ	1:2:76:MET:CE	1.83	0.91
1:1:119:ALA:HB1	1:1:120:PRO:CD	2.00	0.91
1:2:266:LEU:HD23	1:2:270:LEU:HD12	1.49	0.91
1:4:97:VAL:O	1:4:98:PHE:CD1	2.24	0.91
1:4:173:THR:HG23	1:4:228:ALA:HB2	1.51	0.91
1:4:292:ASP:OD2	1:4:295:ALA:HB3	1.70	0.91
1:3:26:VAL:C	1:3:27:VAL:HG12	1.90	0.91
1:2:66:ASP:O	1:2:68:LYS:HD3	1.70	0.91
1:3:201:ASN:ND2	1:3:201:ASN:N	2.12	0.91
1:1:32:PRO:HA	1:1:74:ASN:HD21	1.35	0.91
1:2:293:ALA:O	1:2:294:LYS:HB3	1.70	0.91
1:4:136:TYR:O	1:4:137:SER:OG	1.88	0.91
1:1:276:ASP:OD1	1:1:277:VAL:N	2.03	0.91
1:3:276:ASP:OD1	1:3:277:VAL:CG1	2.17	0.91
1:1:136:TYR:OH	1:1:331:ASP:OD2	1.88	0.91
1:3:251:TYR:O	1:3:254:ILE:HB	1.71	0.91
1:4:125:PRO:HG2	1:4:140:MET:HE3	1.48	0.91
1:1:158:LYS:O	1:1:162:GLU:HG2	1.68	0.91
1:1:298:GLN:NE2	1:4:225:THR:OG1	2.04	0.91
1:4:27:VAL:HG22	1:4:28:ALA:N	1.83	0.91
1:2:17:ARG:NE	2:2:399:HOH:O	1.62	0.91
1:4:216:VAL:HG13	1:4:217:ILE:CG2	2.00	0.91
1:1:273:THR:HG22	1:1:290:ILE:HD11	1.51	0.91
1:1:266:LEU:O	1:1:267:GLN:O	1.89	0.91
1:4:211:LYS:NZ	1:4:211:LYS:HA	1.85	0.91
1:1:193:ARG:NE	1:4:277:VAL:HA	1.85	0.90
1:2:152:CYS:SG	1:2:239:VAL:HG11	2.11	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:34:ILE:HD11	1:2:39:MET:HG2	1.53	0.90
1:4:278:VAL:HA	1:4:281:ASP:OD2	1.71	0.90
1:3:299:LEU:HD22	1:3:300:SER:H	1.37	0.90
1:3:65:VAL:CG2	1:3:66:ASP:OD2	2.20	0.90
1:4:208:GLY:HA3	1:4:211:LYS:CG	2.01	0.90
1:1:126:MET:HB2	1:1:215:LYS:HZ2	1.01	0.90
1:1:216:VAL:HG13	1:1:217:ILE:HG22	1.50	0.90
1:4:129:CYS:HA	1:4:132:ASN:ND2	1.86	0.90
1:1:101:ILE:CG2	1:1:142:VAL:HG11	2.01	0.90
1:4:43:PHE:HA	2:4:452:HOH:O	1.72	0.90
1:4:53:LYS:HD2	1:4:54:GLY:N	1.86	0.90
1:4:243:VAL:HG23	1:4:304:VAL:HG12	1.53	0.90
1:3:8:PHE:CD2	1:3:8:PHE:O	2.24	0.90
1:2:251:TYR:H	1:2:299:LEU:HD12	0.76	0.90
1:3:83:TRP:HD1	1:3:112:ALA:HB2	1.37	0.90
1:4:30:ASN:O	1:4:30:ASN:ND2	2.05	0.90
1:3:294:LYS:C	1:3:297:ILE:HD12	1.93	0.90
1:2:26:VAL:O	1:2:27:VAL:CB	2.19	0.89
1:3:4:GLY:CA	1:3:27:VAL:HG21	2.02	0.89
1:2:99:THR:O	1:2:121:SER:OG	1.91	0.89
1:1:54:GLY:HA3	1:1:66:ASP:OD2	1.72	0.89
1:1:66:ASP:O	1:1:68:LYS:HD3	1.71	0.89
1:4:6:ASN:HA	1:4:30:ASN:HD21	1.34	0.89
1:2:298:GLN:NE2	1:3:225:THR:HG21	1.87	0.89
1:1:121:SER:HB2	1:1:124:ALA:HB3	1.54	0.89
1:1:27:VAL:HG13	1:1:28:ALA:N	1.87	0.89
1:1:286:ASN:OD1	1:1:318:GLN:NE2	2.06	0.89
1:3:8:PHE:HD2	1:3:8:PHE:O	1.53	0.89
1:4:17:ARG:CZ	2:4:339:HOH:O	2.21	0.89
1:2:170:LEU:HD22	1:2:225:THR:HG22	1.54	0.89
1:2:59:GLU:O	1:2:60:ASP:C	2.11	0.89
1:1:145:ASN:HB2	1:1:323:LEU:CD2	2.03	0.89
1:2:34:ILE:HD11	1:2:39:MET:CG	2.01	0.89
1:2:76:MET:N	2:2:408:HOH:O	2.05	0.89
1:3:211:LYS:CA	1:3:211:LYS:HE2	2.01	0.89
1:1:258:MET:HG2	1:1:270:LEU:HD11	1.53	0.89
1:1:273:THR:HG22	1:1:290:ILE:CD1	2.02	0.89
1:2:283:ILE:O	1:2:284:GLY:O	1.90	0.89
1:2:328:GLN:CA	1:2:328:GLN:HE21	1.81	0.89
1:4:154:ALA:CB	1:4:155:PRO:HD2	1.98	0.89
1:3:83:TRP:CD1	1:3:112:ALA:HB2	2.08	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:318:GLN:O	1:3:321:ILE:HB	1.72	0.89
1:3:220:LEU:O	1:3:222:GLY:N	2.06	0.89
1:1:216:VAL:CG1	1:1:217:ILE:HG22	2.03	0.89
1:1:219:GLU:O	1:1:223:LYS:NZ	2.06	0.89
1:3:154:ALA:CB	1:3:155:PRO:CD	2.48	0.88
1:3:2:LYS:HB3	1:3:2:LYS:HZ3	1.36	0.88
1:3:6:ASN:HA	1:3:30:ASN:HD21	1.35	0.88
1:1:298:GLN:HE22	1:4:225:THR:CB	1.86	0.88
1:2:152:CYS:SG	1:2:239:VAL:CG1	2.60	0.88
1:2:295:ALA:CB	1:3:193:ARG:NH1	2.36	0.88
1:4:112:ALA:O	1:4:113:LYS:HB2	1.71	0.88
1:1:207:THR:OG1	1:1:208:GLY:N	2.02	0.88
1:2:6:ASN:HA	1:2:30:ASN:ND2	1.87	0.88
1:2:8:PHE:CZ	1:2:39:MET:HG2	2.08	0.88
1:4:44:LYS:O	1:4:51:VAL:HA	1.72	0.88
1:3:154:ALA:CB	1:3:155:PRO:HD3	2.02	0.88
1:3:295:ALA:N	1:3:297:ILE:HD12	1.89	0.88
1:1:277:VAL:HG23	1:1:278:VAL:H	1.37	0.88
1:2:108:PHE:O	1:2:111:GLY:N	2.05	0.88
1:2:132:ASN:ND2	1:2:133:LEU:CD2	2.36	0.88
1:2:193:ARG:HH22	1:3:295:ALA:CB	1.83	0.88
1:3:81:ILE:CD1	1:3:82:PRO:HD2	2.02	0.88
1:4:220:LEU:HA	1:4:223:LYS:NZ	1.88	0.88
1:1:113:LYS:HB3	1:1:114:LYS:CE	2.04	0.88
1:2:91:ILE:HD12	1:2:114:LYS:O	1.73	0.88
1:2:299:LEU:CD2	1:2:304:VAL:HG23	2.04	0.88
1:2:32:PRO:HA	1:2:74:ASN:HD21	1.08	0.88
1:3:11:ILE:HD13	1:3:11:ILE:N	1.84	0.88
1:3:294:LYS:C	1:3:297:ILE:CD1	2.42	0.88
1:4:131:VAL:HG12	1:4:158:LYS:NZ	1.89	0.88
1:1:63:LEU:HB2	1:1:72:VAL:HG11	1.55	0.88
1:4:164:PHE:O	1:4:165:GLU:HB2	1.74	0.88
1:3:200:GLN:OE1	1:4:48:THR:HG22	1.72	0.88
1:2:127:PHE:CD1	1:2:143:VAL:CG2	2.57	0.88
1:2:244:ARG:NH2	1:3:244:ARG:HG3	1.89	0.88
1:4:211:LYS:CE	1:4:211:LYS:HA	2.04	0.88
1:2:210:ALA:O	1:2:211:LYS:O	1.91	0.88
1:1:176:ALA:HB1	1:1:233:THR:O	1.73	0.87
1:2:319:ARG:HA	1:2:322:ASP:OD2	1.73	0.87
1:4:255:LYS:HD3	1:4:293:ALA:HB1	1.56	0.87
1:1:14:LEU:HA	1:1:17:ARG:HG3	1.55	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:220:LEU:HA	1:1:223:LYS:HZ2	0.74	0.87
1:2:217:ILE:HG12	1:2:220:LEU:HD22	1.57	0.87
1:1:297:ILE:CD1	1:1:297:ILE:N	2.36	0.87
1:3:145:ASN:O	1:3:146:ALA:O	1.91	0.87
1:2:318:GLN:HA	1:2:318:GLN:OE1	1.71	0.87
1:1:298:GLN:NE2	1:4:225:THR:HG21	1.88	0.87
1:3:175:HIS:CG	1:3:230:ARG:HH21	1.92	0.87
1:2:66:ASP:O	1:2:68:LYS:CD	2.23	0.87
1:1:212:ALA:O	1:1:216:VAL:HB	1.74	0.87
1:1:27:VAL:CG1	1:1:28:ALA:H	1.74	0.87
1:4:25:GLN:O	1:4:26:VAL:O	1.92	0.87
1:3:161:HIS:O	1:3:162:GLU:C	2.12	0.87
1:1:66:ASP:HB3	2:1:432:HOH:O	1.74	0.87
1:2:113:LYS:HE2	1:2:114:LYS:HZ1	1.38	0.87
1:1:8:PHE:HA	1:1:12:GLY:HA3	1.57	0.87
1:1:145:ASN:O	1:1:145:ASN:ND2	2.08	0.86
1:2:294:LYS:C	1:2:297:ILE:CD1	2.43	0.86
1:2:296:GLY:O	1:2:307:VAL:HG23	1.74	0.86
1:3:85:LYS:O	1:3:86:ALA:CB	2.20	0.86
1:4:132:ASN:ND2	1:4:133:LEU:HD21	1.90	0.86
1:1:53:LYS:HZ3	1:1:53:LYS:HB3	1.39	0.86
1:3:154:ALA:HB3	1:3:155:PRO:HD2	1.55	0.86
1:1:298:GLN:OE1	1:4:226:GLY:N	2.09	0.86
1:1:243:VAL:HG22	1:1:304:VAL:CG1	2.04	0.86
1:1:3:ILE:HG22	1:1:4:GLY:H	1.38	0.86
1:4:154:ALA:CB	1:4:155:PRO:CD	2.52	0.86
1:4:321:ILE:O	1:4:325:LYS:HG2	1.74	0.86
1:1:220:LEU:O	1:1:221:ASP:C	2.13	0.86
1:1:126:MET:CB	1:1:215:LYS:NZ	2.35	0.86
1:1:220:LEU:O	1:1:222:GLY:N	2.08	0.86
1:2:216:VAL:CG1	1:2:217:ILE:HG22	2.05	0.86
1:3:276:ASP:O	1:3:278:VAL:HG13	1.75	0.86
1:3:3:ILE:HG22	1:3:4:GLY:H	1.38	0.86
1:1:243:VAL:CG2	1:1:304:VAL:HG12	2.03	0.86
1:1:83:TRP:HA	1:1:86:ALA:HB3	1.58	0.86
1:3:292:ASP:CG	1:3:295:ALA:HB3	1.96	0.86
1:3:55:GLU:O	1:3:65:VAL:HA	1.76	0.86
1:3:66:ASP:O	1:3:68:LYS:HD3	1.73	0.86
1:3:75:GLU:O	2:3:378:HOH:O	1.92	0.86
1:1:251:TYR:H	1:1:299:LEU:HD12	1.40	0.86
1:3:291:PHE:HA	1:3:308:SER:OG	1.75	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:319:ARG:O	1:3:320:VAL:C	2.13	0.86
1:1:282:PHE:CZ	1:1:290:ILE:HD13	2.11	0.86
1:2:294:LYS:O	1:2:297:ILE:HD11	1.75	0.86
1:3:71:THR:HG21	1:3:73:PHE:CZ	2.10	0.86
1:1:244:ARG:HH22	1:4:244:ARG:HB2	1.40	0.85
1:1:75:GLU:N	2:1:437:HOH:O	2.09	0.85
1:2:3:ILE:C	1:2:27:VAL:HG23	1.96	0.85
1:4:277:VAL:O	1:4:278:VAL:O	1.93	0.85
1:3:208:GLY:HA3	1:3:211:LYS:HG2	1.58	0.85
1:1:220:LEU:CA	1:1:223:LYS:NZ	2.33	0.85
1:2:113:LYS:HE2	1:2:114:LYS:NZ	1.90	0.85
1:4:2:LYS:HB3	1:4:2:LYS:HZ3	1.41	0.85
1:3:291:PHE:HA	1:3:308:SER:HG	1.41	0.85
1:1:126:MET:HB2	1:1:215:LYS:HZ3	1.37	0.85
1:3:84:SER:OG	1:3:111:GLY:HA3	1.76	0.85
1:2:153:LEU:O	1:2:153:LEU:HD23	1.75	0.85
1:4:276:ASP:O	1:4:278:VAL:HG13	1.76	0.85
1:1:297:ILE:N	1:1:297:ILE:HD13	1.84	0.85
1:1:101:ILE:O	1:1:105:SER:OG	1.95	0.85
1:1:11:ILE:HG22	1:1:15:VAL:HG21	1.57	0.85
1:2:243:VAL:HG23	1:2:245:LEU:HD23	1.58	0.85
1:4:53:LYS:HB3	1:4:53:LYS:NZ	1.91	0.85
1:2:3:ILE:CG2	1:2:4:GLY:H	1.87	0.85
1:4:8:PHE:HZ	1:4:39:MET:HB2	1.41	0.85
1:3:17:ARG:NE	2:3:369:HOH:O	1.91	0.85
1:3:292:ASP:OD2	1:3:295:ALA:HB3	1.76	0.85
1:3:53:LYS:HB3	1:3:53:LYS:NZ	1.91	0.85
1:2:296:GLY:HA3	1:2:307:VAL:HG21	1.59	0.85
1:2:32:PRO:O	1:2:33:PHE:HB2	1.74	0.85
1:4:183:THR:O	1:4:184:VAL:HB	1.76	0.85
1:4:1:SER:HB3	1:4:25:GLN:HB2	1.58	0.85
1:3:2:LYS:NZ	1:3:87:GLY:O	2.08	0.85
1:1:129:CYS:O	1:1:133:LEU:HD11	1.77	0.85
1:1:53:LYS:NZ	1:1:53:LYS:HB3	1.92	0.85
1:2:27:VAL:CG1	1:2:28:ALA:N	2.34	0.85
1:3:53:LYS:HZ3	1:3:53:LYS:HB3	1.42	0.85
1:2:170:LEU:CD2	1:2:225:THR:HG22	2.07	0.85
1:2:244:ARG:HH22	1:3:244:ARG:HG3	1.41	0.85
1:2:298:GLN:HE22	1:3:225:THR:HG21	1.39	0.84
1:2:127:PHE:CD1	1:2:143:VAL:HG21	2.11	0.84
1:2:91:ILE:HD12	1:2:91:ILE:H	1.41	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:239:VAL:CG1	1:4:310:TYR:HE1	1.90	0.84
1:3:56:VAL:HG13	1:3:56:VAL:O	1.78	0.84
1:1:1:SER:HG	1:1:25:GLN:HB2	1.41	0.84
1:1:251:TYR:H	1:1:299:LEU:CD1	1.90	0.84
1:3:105:SER:O	1:3:107:HIS:N	2.10	0.84
1:3:50:GLY:O	1:3:51:VAL:HG23	1.76	0.84
1:2:175:HIS:CD2	1:2:230:ARG:HH21	1.93	0.84
1:2:3:ILE:O	1:2:88:ALA:HB1	1.78	0.84
1:2:196:ARG:HG2	1:2:196:ARG:NH1	1.90	0.84
1:3:8:PHE:CZ	1:3:39:MET:HG2	2.12	0.84
1:2:244:ARG:CG	1:3:244:ARG:HH22	1.89	0.84
1:4:26:VAL:C	1:4:27:VAL:CG1	2.39	0.84
1:4:6:ASN:HA	1:4:30:ASN:ND2	1.92	0.84
1:3:251:TYR:H	1:3:299:LEU:CD1	1.89	0.84
1:1:193:ARG:NH1	1:1:204:PRO:HG2	1.91	0.84
1:2:113:LYS:HB3	1:2:114:LYS:CD	2.08	0.84
1:4:251:TYR:HB2	1:4:299:LEU:CB	2.06	0.84
1:3:154:ALA:HB3	1:3:155:PRO:HD3	1.55	0.84
1:1:168:GLU:CG	1:1:244:ARG:HD2	2.06	0.84
1:4:173:THR:HG23	1:4:228:ALA:CB	2.08	0.84
1:4:273:THR:HG22	1:4:290:ILE:HD11	1.60	0.84
1:3:134:GLU:O	1:3:136:TYR:N	2.10	0.84
1:3:27:VAL:CG2	1:3:28:ALA:N	2.36	0.84
1:2:10:ARG:O	1:2:14:LEU:HD22	1.77	0.84
1:1:161:HIS:ND1	1:1:165:GLU:O	2.09	0.84
1:1:307:VAL:CG1	1:1:307:VAL:O	2.25	0.84
1:2:188:SER:HB3	1:2:191:ASP:C	1.96	0.84
1:3:75:GLU:N	2:3:377:HOH:O	2.02	0.84
1:2:15:VAL:O	1:2:18:ALA:HB3	1.77	0.84
1:4:89:GLU:HG3	1:4:90:TYR:HD1	1.38	0.84
1:3:128:VAL:O	1:3:132:ASN:ND2	2.10	0.84
1:3:161:HIS:HB2	1:3:166:ILE:HD12	1.60	0.84
1:3:207:THR:OG1	1:3:208:GLY:N	2.08	0.84
1:4:183:THR:HB	1:4:184:VAL:HG12	1.59	0.84
1:4:25:GLN:C	1:4:26:VAL:O	2.15	0.84
1:4:78:PRO:CG	1:4:98:PHE:CE2	2.61	0.84
1:4:329:LYS:NZ	1:4:329:LYS:C	2.31	0.84
1:1:205:SER:HB3	1:1:228:ALA:HB3	1.60	0.84
1:4:11:ILE:CD1	1:4:11:ILE:H	1.91	0.83
1:1:53:LYS:HD2	1:1:54:GLY:N	1.92	0.83
1:4:297:ILE:C	1:4:297:ILE:HD13	1.98	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:251:TYR:CZ	1:4:297:ILE:HG12	2.13	0.83
1:1:193:ARG:HH22	1:4:295:ALA:CB	1.87	0.83
1:2:8:PHE:HA	1:2:12:GLY:HA3	1.59	0.83
1:4:104:ALA:O	1:4:107:HIS:N	2.12	0.83
1:1:95:THR:CG2	1:1:97:VAL:HG23	2.07	0.83
1:1:161:HIS:O	1:1:162:GLU:C	2.17	0.83
1:4:58:MET:SD	1:4:58:MET:N	2.50	0.83
1:3:27:VAL:HG22	1:3:28:ALA:O	1.78	0.83
1:1:95:THR:HG22	1:1:97:VAL:N	1.93	0.83
1:3:205:SER:HB3	1:3:228:ALA:HB3	1.59	0.83
1:2:11:ILE:HG22	1:2:15:VAL:CG2	2.08	0.83
1:1:65:VAL:O	1:1:68:LYS:HG2	1.78	0.83
1:2:299:LEU:HD23	1:2:304:VAL:HG23	1.60	0.83
1:1:277:VAL:HG11	1:3:41:TYR:OH	1.77	0.83
1:3:10:ARG:O	1:3:14:LEU:HD22	1.78	0.83
1:1:244:ARG:HH22	1:4:244:ARG:CB	1.90	0.83
1:2:3:ILE:C	1:2:27:VAL:CG2	2.47	0.83
1:4:30:ASN:OD1	1:4:81:ILE:HG13	1.77	0.83
1:2:188:SER:O	1:2:190:LYS:N	2.12	0.83
1:1:137:SER:O	1:1:140:MET:HG3	1.79	0.83
1:4:2:LYS:NZ	1:4:87:GLY:O	2.12	0.83
1:3:11:ILE:CD1	1:3:11:ILE:H	1.86	0.83
1:2:244:ARG:HB2	1:3:244:ARG:NH2	1.94	0.83
1:3:167:VAL:HG13	1:3:245:LEU:O	1.78	0.83
1:1:277:VAL:O	1:1:278:VAL:HG22	1.79	0.83
1:1:9:GLY:O	1:1:13:ARG:HG3	1.78	0.83
1:2:1:SER:C	1:2:2:LYS:HG2	1.95	0.83
1:4:40:VAL:HG11	1:4:58:MET:SD	2.18	0.83
1:2:54:GLY:HA2	1:2:66:ASP:OD1	1.77	0.83
1:1:202:ILE:HD11	1:4:233:THR:CG2	2.08	0.82
1:4:276:ASP:CG	1:4:277:VAL:HG22	1.99	0.82
1:3:4:GLY:CA	1:3:27:VAL:CG2	2.55	0.82
1:1:11:ILE:HD12	1:1:11:ILE:H	1.45	0.82
1:4:293:ALA:O	1:4:294:LYS:HB3	1.78	0.82
1:4:219:GLU:O	1:4:223:LYS:NZ	2.12	0.82
1:2:64:VAL:O	1:2:64:VAL:HG22	1.77	0.82
1:1:128:VAL:O	1:1:132:ASN:CB	2.26	0.82
1:1:277:VAL:HG21	1:3:41:TYR:HE1	1.41	0.82
1:2:294:LYS:C	1:2:297:ILE:HD11	2.00	0.82
1:2:293:ALA:O	1:2:294:LYS:CB	2.26	0.82
1:4:196:ARG:HG3	1:4:197:GLY:H	1.43	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:51:VAL:C	2:2:400:HOH:O	2.03	0.82
1:1:6:ASN:CA	1:1:30:ASN:HD21	1.92	0.82
1:2:27:VAL:CG1	1:2:28:ALA:H	1.74	0.82
1:2:311:ASP:O	1:2:312:ASN:C	2.18	0.82
1:3:104:ALA:O	1:3:105:SER:C	2.17	0.82
1:2:277:VAL:HG21	1:4:41:TYR:CZ	2.15	0.82
1:2:225:THR:HG21	1:3:298:GLN:CD	1.98	0.82
1:2:173:THR:CG2	1:2:228:ALA:HB2	2.10	0.82
1:4:188:SER:O	1:4:191:ASP:N	2.12	0.82
1:1:276:ASP:OD1	1:1:277:VAL:HG22	1.80	0.82
1:1:71:THR:O	1:1:72:VAL:HG12	1.79	0.82
1:2:97:VAL:O	1:2:98:PHE:CG	2.32	0.82
1:3:97:VAL:O	1:3:98:PHE:CB	2.25	0.82
1:1:243:VAL:CG2	1:1:304:VAL:CG1	2.57	0.82
1:2:105:SER:O	1:2:108:PHE:CD1	2.32	0.82
1:2:251:TYR:HB2	1:2:299:LEU:HB2	1.60	0.82
1:2:244:ARG:HG3	1:3:244:ARG:NH1	1.93	0.82
1:2:329:LYS:C	1:2:329:LYS:HZ3	1.82	0.82
1:1:129:CYS:SG	1:1:269:PHE:HE1	2.02	0.82
1:2:225:THR:CG2	1:3:298:GLN:NE2	2.43	0.82
1:1:22:CYS:SG	1:1:321:ILE:HG21	2.19	0.82
1:1:244:ARG:NH2	1:4:244:ARG:HB2	1.94	0.82
1:2:137:SER:HB3	1:2:138:LYS:NZ	1.95	0.82
1:3:284:GLY:HA2	1:3:314:PHE:HE1	1.45	0.81
1:2:212:ALA:O	1:2:216:VAL:CB	2.29	0.81
1:2:217:ILE:HG12	1:2:220:LEU:CD2	2.11	0.81
1:3:40:VAL:O	1:3:44:LYS:HG3	1.80	0.81
1:1:169:GLY:O	1:1:170:LEU:CD2	2.25	0.81
1:1:127:PHE:CE2	1:1:136:TYR:CB	2.61	0.81
1:1:193:ARG:NH1	1:4:295:ALA:HB1	1.94	0.81
1:1:124:ALA:O	1:1:125:PRO:O	1.97	0.81
1:1:284:GLY:HA2	1:1:314:PHE:CE1	2.15	0.81
1:2:277:VAL:C	1:2:278:VAL:O	2.18	0.81
1:2:296:GLY:H	1:2:297:ILE:CD1	1.94	0.81
1:4:3:ILE:HG22	1:4:4:GLY:H	1.43	0.81
1:2:13:ARG:O	1:2:16:LEU:N	2.13	0.81
1:1:281:ASP:O	1:1:283:ILE:N	2.14	0.81
1:4:26:VAL:O	1:4:27:VAL:HB	1.80	0.81
1:1:4:GLY:HA2	1:1:27:VAL:CG2	2.08	0.81
1:1:41:TYR:HE1	1:3:277:VAL:HG21	1.41	0.81
1:3:284:GLY:HA2	1:3:314:PHE:CE1	2.15	0.81

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:132:ASN:ND2	1:1:133:LEU:CD2	2.44	0.81
1:1:1:SER:O	1:1:25:GLN:HG2	1.80	0.81
1:4:8:PHE:HA	1:4:12:GLY:HA3	1.62	0.81
1:3:286:ASN:ND2	1:3:314:PHE:CZ	2.48	0.81
1:3:71:THR:HG21	1:3:73:PHE:CE1	2.15	0.81
1:3:129:CYS:HA	1:3:132:ASN:HD21	1.43	0.81
1:2:276:ASP:OD1	1:2:277:VAL:HG13	1.81	0.81
1:4:3:ILE:O	1:4:27:VAL:HG23	1.81	0.81
1:4:287:ARG:O	1:4:288:SER:HB2	1.81	0.81
1:2:137:SER:HB3	1:2:138:LYS:HZ2	1.46	0.81
1:2:26:VAL:HG23	1:2:27:VAL:H	1.44	0.80
1:3:97:VAL:O	1:3:98:PHE:CG	2.34	0.80
1:1:231:VAL:HG11	1:4:231:VAL:HG11	1.63	0.80
1:1:66:ASP:CB	2:1:432:HOH:O	2.29	0.80
1:4:52:PHE:C	1:4:53:LYS:HZ3	1.85	0.80
1:3:44:LYS:O	1:3:51:VAL:HA	1.80	0.80
1:1:219:GLU:C	1:1:223:LYS:HZ1	1.85	0.80
1:2:14:LEU:O	1:2:18:ALA:HB2	1.81	0.80
1:2:105:SER:O	1:2:108:PHE:HD1	1.63	0.80
1:2:297:ILE:N	1:2:297:ILE:CD1	2.35	0.80
1:3:173:THR:HG23	1:3:228:ALA:HB2	1.63	0.80
1:2:3:ILE:HG22	1:2:4:GLY:N	1.97	0.80
1:2:74:ASN:OD1	1:2:74:ASN:C	2.20	0.80
1:4:252:ASP:C	1:4:252:ASP:OD1	2.14	0.80
1:4:85:LYS:O	1:4:86:ALA:HB2	1.79	0.80
1:3:91:ILE:HG21	1:3:107:HIS:NE2	1.97	0.80
1:3:113:LYS:HB3	1:3:114:LYS:HD2	0.86	0.80
1:4:321:ILE:HG22	1:4:325:LYS:HE3	1.63	0.80
1:3:180:THR:OG1	1:3:181:GLN:N	2.14	0.80
1:4:150:THR:CG2	1:4:212:ALA:HB3	2.11	0.80
1:2:244:ARG:CG	1:3:244:ARG:HH12	1.93	0.80
1:1:17:ARG:HB3	1:1:43:PHE:CZ	2.16	0.80
1:4:307:VAL:HG13	1:4:307:VAL:O	1.79	0.80
1:3:97:VAL:O	1:3:98:PHE:HB2	1.82	0.80
1:4:138:LYS:CE	1:4:330:VAL:HG13	2.11	0.80
1:1:161:HIS:CD2	1:1:162:GLU:N	2.49	0.80
1:2:8:PHE:CD2	1:2:8:PHE:O	2.33	0.80
1:4:273:THR:OG1	1:4:274:GLU:N	2.13	0.80
1:4:208:GLY:CA	1:4:211:LYS:HG2	2.11	0.80
1:4:187:PRO:HG2	1:4:187:PRO:O	1.79	0.80
1:3:138:LYS:CE	1:3:330:VAL:HG13	2.11	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:277:VAL:HA	1:3:193:ARG:CD	2.12	0.79
1:2:76:MET:O	1:2:77:LYS:HD3	1.81	0.79
1:4:180:THR:HG23	1:4:181:GLN:H	1.47	0.79
1:4:26:VAL:O	1:4:27:VAL:CB	2.30	0.79
1:1:250:SER:O	1:1:252:ASP:N	2.15	0.79
1:1:276:ASP:OD1	1:1:277:VAL:HG13	1.81	0.79
1:1:323:LEU:HD12	1:1:327:MET:SD	2.22	0.79
1:2:78:PRO:CG	1:2:98:PHE:CE2	2.65	0.79
1:4:44:LYS:HB3	1:4:44:LYS:HZ2	1.45	0.79
1:3:4:GLY:HA2	1:3:27:VAL:HG23	1.62	0.79
1:3:251:TYR:N	1:3:299:LEU:HD12	1.96	0.79
1:3:81:ILE:HD13	1:3:82:PRO:O	1.81	0.79
1:3:216:VAL:CG1	1:3:217:ILE:N	2.45	0.79
1:1:58:MET:SD	1:1:58:MET:N	2.55	0.79
1:1:129:CYS:O	1:1:133:LEU:CD1	2.30	0.79
1:1:277:VAL:HA	1:4:193:ARG:HD3	1.63	0.79
1:4:83:TRP:CA	1:4:86:ALA:HB3	2.12	0.79
1:2:185:ASP:C	1:2:195:GLY:O	2.21	0.79
1:1:117:ILE:HD13	1:1:121:SER:OG	1.82	0.79
1:1:40:VAL:O	1:1:44:LYS:HG3	1.82	0.79
1:3:8:PHE:HA	1:3:12:GLY:HA3	1.64	0.79
1:4:132:ASN:ND2	1:4:133:LEU:HD23	1.97	0.79
1:4:105:SER:O	1:4:108:PHE:HD1	1.65	0.79
1:1:26:VAL:HG12	1:1:70:ILE:HG21	1.62	0.79
1:1:188:SER:HB3	1:1:191:ASP:C	2.03	0.79
1:1:270:LEU:CD2	1:1:271:GLY:N	2.46	0.79
1:1:132:ASN:ND2	1:1:133:LEU:HD21	1.96	0.79
1:1:295:ALA:CB	1:4:193:ARG:HH12	1.96	0.79
1:4:11:ILE:HD12	1:4:11:ILE:N	1.96	0.79
1:3:175:HIS:CD2	1:3:230:ARG:HH21	1.98	0.79
1:3:188:SER:HB3	1:3:191:ASP:C	2.03	0.79
1:3:270:LEU:HD23	1:3:270:LEU:C	2.03	0.79
1:2:318:GLN:O	1:2:321:ILE:HB	1.82	0.79
1:4:265:PRO:N	2:4:453:HOH:O	2.16	0.79
1:1:318:GLN:OE1	1:1:318:GLN:HA	1.81	0.79
1:1:104:ALA:O	1:1:107:HIS:N	2.16	0.78
1:4:52:PHE:CE1	1:4:53:LYS:HE3	2.17	0.78
1:3:212:ALA:O	1:3:216:VAL:HB	1.82	0.78
1:4:89:GLU:OE1	1:4:90:TYR:HE1	1.67	0.78
1:2:295:ALA:HB2	1:3:193:ARG:HH22	1.46	0.78
1:2:320:VAL:O	1:2:324:LEU:HB2	1.84	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:50:GLY:C	1:3:51:VAL:HG23	2.03	0.78
1:3:277:VAL:O	1:3:278:VAL:O	2.02	0.78
1:2:232:PRO:HG2	1:3:232:PRO:HB2	1.63	0.78
1:4:74:ASN:O	1:4:75:GLU:CG	2.27	0.78
1:1:59:GLU:O	1:1:60:ASP:C	2.21	0.78
1:2:132:ASN:ND2	1:2:133:LEU:HD21	1.98	0.78
1:2:203:ILE:CG2	1:2:203:ILE:O	2.27	0.78
1:3:117:ILE:HB	1:3:144:SER:HA	1.63	0.78
1:4:305:LYS:HB2	1:4:305:LYS:HZ3	1.49	0.78
1:1:273:THR:OG1	1:1:274:GLU:N	2.17	0.78
1:2:181:GLN:HG2	1:2:198:ALA:CB	2.14	0.78
1:1:225:THR:CG2	1:4:298:GLN:OE1	2.31	0.78
1:4:3:ILE:O	1:4:88:ALA:HB1	1.83	0.78
1:3:100:THR:H	1:3:103:LYS:HB2	1.49	0.78
1:1:213:VAL:O	1:1:216:VAL:HG12	1.82	0.78
1:2:277:VAL:O	1:3:193:ARG:HD3	1.84	0.78
1:1:131:VAL:HG12	1:1:158:LYS:HE2	1.66	0.78
1:2:113:LYS:CB	1:2:114:LYS:HE3	2.14	0.78
1:2:4:GLY:N	1:2:27:VAL:HG21	1.99	0.78
1:2:292:ASP:OD2	1:2:295:ALA:HB3	1.84	0.78
1:2:251:TYR:N	1:2:299:LEU:CD1	2.35	0.78
1:4:38:TYR:O	1:4:42:MET:N	2.17	0.78
1:1:127:PHE:CD1	1:1:143:VAL:HG21	2.19	0.77
1:1:168:GLU:HG2	1:1:244:ARG:HD2	1.64	0.77
1:1:8:PHE:N	1:1:31:ASP:OD2	2.17	0.77
1:4:26:VAL:O	1:4:27:VAL:HG12	1.84	0.77
1:4:51:VAL:HB	2:4:340:HOH:O	1.83	0.77
1:3:127:PHE:HZ	1:3:140:MET:HE1	1.48	0.77
1:3:294:LYS:O	1:3:297:ILE:HD11	1.84	0.77
1:3:8:PHE:N	1:3:31:ASP:OD2	2.16	0.77
1:1:160:LEU:HD21	1:1:254:ILE:HD12	1.65	0.77
1:1:276:ASP:O	1:1:278:VAL:N	2.17	0.77
1:2:276:ASP:O	1:2:278:VAL:N	2.17	0.77
1:2:41:TYR:CE1	1:4:277:VAL:CG2	2.63	0.77
1:2:81:ILE:HD12	1:2:83:TRP:CE2	2.19	0.77
1:3:276:ASP:O	1:3:278:VAL:HG22	1.83	0.77
1:1:320:VAL:O	1:1:324:LEU:N	2.16	0.77
1:1:51:VAL:C	2:1:430:HOH:O	2.22	0.77
1:3:13:ARG:O	1:3:16:LEU:N	2.15	0.77
1:3:252:ASP:O	1:3:254:ILE:N	2.17	0.77
1:2:244:ARG:HG3	1:3:244:ARG:HH22	1.47	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:112:ALA:O	1:2:113:LYS:HB2	1.83	0.77
1:2:261:ALA:HB1	1:2:266:LEU:HD22	1.67	0.77
1:2:3:ILE:HD13	1:2:324:LEU:CD1	2.15	0.77
1:3:258:MET:HG2	1:3:270:LEU:HD11	1.65	0.77
1:1:261:ALA:O	1:1:262:SER:C	2.21	0.77
1:1:8:PHE:C	1:1:8:PHE:HD2	1.88	0.77
1:4:78:PRO:C	1:4:80:ASN:H	1.87	0.77
1:3:330:VAL:HG12	1:3:331:ASP:N	1.99	0.77
1:3:216:VAL:CG1	1:3:217:ILE:H	1.97	0.77
1:2:141:THR:OG1	1:2:142:VAL:N	2.18	0.77
1:2:250:SER:O	1:2:252:ASP:N	2.18	0.77
1:2:277:VAL:HG23	1:2:278:VAL:N	1.98	0.77
1:4:44:LYS:HE3	1:4:45:TYR:CE2	2.20	0.77
1:3:292:ASP:OD1	1:3:295:ALA:HB3	1.84	0.77
1:2:46:ASP:HB3	1:2:50:GLY:H	1.49	0.77
1:2:78:PRO:HG3	1:2:98:PHE:HE2	1.43	0.77
1:3:78:PRO:HG3	1:3:98:PHE:HE2	1.46	0.77
1:2:75:GLU:N	2:2:407:HOH:O	1.76	0.77
1:3:145:ASN:O	1:3:145:ASN:ND2	2.18	0.77
1:4:210:ALA:O	1:4:211:LYS:O	2.03	0.77
1:1:272:TYR:OH	1:1:274:GLU:CD	2.24	0.77
1:1:277:VAL:O	1:1:278:VAL:O	2.03	0.77
1:2:138:LYS:HE3	1:2:330:VAL:HG13	1.67	0.77
1:1:175:HIS:N	1:1:229:PHE:O	2.17	0.76
1:4:32:PRO:HA	1:4:74:ASN:HD21	0.67	0.76
1:1:258:MET:CG	1:1:270:LEU:HD11	2.15	0.76
1:2:129:CYS:O	1:2:133:LEU:HD11	1.85	0.76
1:4:75:GLU:CA	2:4:347:HOH:O	2.14	0.76
1:3:216:VAL:HG12	1:3:217:ILE:H	1.50	0.76
1:2:101:ILE:O	1:2:105:SER:OG	2.03	0.76
1:2:85:LYS:O	1:2:86:ALA:HB2	1.85	0.76
1:2:52:PHE:CA	2:2:400:HOH:O	2.21	0.76
1:4:97:VAL:O	1:4:98:PHE:CG	2.38	0.76
1:4:113:LYS:CB	1:4:114:LYS:HE3	2.15	0.76
1:1:90:TYR:CZ	1:1:328:GLN:NE2	2.52	0.76
1:3:129:CYS:O	1:3:132:ASN:ND2	2.18	0.76
1:3:272:TYR:CE2	1:3:293:ALA:HB2	2.21	0.76
1:1:284:GLY:HA2	1:1:314:PHE:HE1	1.50	0.76
1:2:161:HIS:HA	1:2:166:ILE:HG13	1.67	0.76
1:2:295:ALA:N	1:2:297:ILE:HD12	2.00	0.76
1:4:27:VAL:HG22	1:4:28:ALA:O	1.85	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:83:TRP:CA	1:1:86:ALA:HB3	2.15	0.76
1:2:175:HIS:CG	1:2:230:ARG:HH21	2.03	0.76
1:2:6:ASN:OD1	1:2:30:ASN:ND2	2.18	0.76
1:3:16:LEU:HD21	1:3:70:ILE:CD1	2.16	0.76
1:2:244:ARG:CB	1:3:244:ARG:NH2	2.47	0.76
1:1:298:GLN:HE22	1:4:225:THR:HG21	1.49	0.76
1:2:278:VAL:HA	1:2:281:ASP:OD2	1.84	0.76
1:4:76:MET:O	1:4:77:LYS:HD3	1.85	0.76
1:1:217:ILE:HG12	1:1:220:LEU:CD2	2.16	0.76
1:4:55:GLU:O	1:4:65:VAL:HA	1.85	0.76
1:3:66:ASP:O	1:3:68:LYS:CD	2.34	0.76
1:1:276:ASP:CG	1:1:277:VAL:N	2.28	0.76
1:2:116:VAL:HG11	1:2:324:LEU:HD23	1.68	0.76
1:2:129:CYS:O	1:2:133:LEU:CD1	2.34	0.76
1:2:277:VAL:HA	1:3:193:ARG:NE	2.00	0.76
1:3:330:VAL:O	1:3:332:SER:N	2.18	0.76
1:4:270:LEU:C	1:4:270:LEU:CD2	2.53	0.75
1:4:258:MET:CG	1:4:270:LEU:HD11	2.15	0.75
1:3:277:VAL:O	1:3:278:VAL:C	2.24	0.75
1:3:281:ASP:O	1:3:283:ILE:N	2.18	0.75
1:2:65:VAL:CG2	1:2:66:ASP:OD2	2.33	0.75
1:2:124:ALA:O	1:2:125:PRO:O	2.04	0.75
1:2:117:ILE:HD11	1:2:142:VAL:O	1.85	0.75
1:1:244:ARG:NH1	1:4:244:ARG:HG3	2.01	0.75
1:4:329:LYS:HZ2	1:4:330:VAL:N	1.83	0.75
1:2:232:PRO:O	1:2:233:THR:C	2.23	0.75
1:3:91:ILE:HG21	1:3:107:HIS:CE1	2.21	0.75
1:1:71:THR:CG2	1:1:72:VAL:N	2.46	0.75
1:2:299:LEU:HD22	1:2:300:SER:H	1.51	0.75
1:1:44:LYS:HG2	1:1:56:VAL:HG11	1.69	0.75
1:3:251:TYR:HB2	1:3:299:LEU:HB2	1.66	0.75
1:4:182:LYS:HE3	1:4:187:PRO:HG2	1.69	0.75
1:2:58:MET:N	1:2:58:MET:SD	2.55	0.75
1:4:113:LYS:CD	1:4:114:LYS:NZ	2.47	0.75
1:2:193:ARG:NE	1:3:277:VAL:HA	2.01	0.75
1:2:10:ARG:HH12	1:2:46:ASP:CG	1.88	0.75
1:4:182:LYS:HE3	1:4:187:PRO:CG	2.17	0.75
1:1:27:VAL:CG2	1:1:28:ALA:H	1.98	0.75
1:4:34:ILE:CD1	1:4:42:MET:SD	2.74	0.75
1:3:129:CYS:O	1:3:133:LEU:HG	1.87	0.75
1:1:277:VAL:HG12	1:4:193:ARG:HA	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:281:ASP:C	1:2:283:ILE:H	1.90	0.75
1:4:14:LEU:HA	1:4:17:ARG:HB2	1.69	0.75
1:4:136:TYR:OH	1:4:331:ASP:OD2	2.05	0.75
1:1:174:VAL:CG1	1:1:231:VAL:HG21	2.17	0.74
1:1:129:CYS:SG	1:1:269:PHE:CE1	2.79	0.74
1:4:253:ASP:HB2	2:4:355:HOH:O	1.86	0.74
1:2:269:PHE:O	1:2:288:SER:HB3	1.87	0.74
1:3:252:ASP:HA	1:3:255:LYS:HG3	1.69	0.74
1:3:76:MET:O	1:3:77:LYS:CD	2.34	0.74
1:4:118:SER:O	1:4:316:TYR:OH	2.03	0.74
1:1:27:VAL:HG22	1:1:28:ALA:H	1.52	0.74
1:4:272:TYR:CE2	1:4:293:ALA:HB2	2.22	0.74
1:4:53:LYS:CB	1:4:53:LYS:HZ3	1.99	0.74
1:2:126:MET:CB	1:2:215:LYS:HZ2	2.00	0.74
1:4:188:SER:C	1:4:190:LYS:H	1.91	0.74
1:2:329:LYS:NZ	1:2:329:LYS:C	2.40	0.74
1:1:236:VAL:O	1:1:237:SER:HB2	1.87	0.74
1:4:203:ILE:O	1:4:204:PRO:O	2.06	0.74
1:3:131:VAL:CG1	1:3:158:LYS:HZ3	2.00	0.74
1:3:277:VAL:C	1:3:278:VAL:O	2.22	0.74
1:3:283:ILE:O	1:3:284:GLY:O	2.05	0.74
1:4:319:ARG:O	1:4:320:VAL:C	2.25	0.74
1:1:101:ILE:HG23	1:1:142:VAL:CG1	2.17	0.74
1:4:262:SER:O	1:4:267:GLN:HA	1.86	0.74
1:1:174:VAL:O	1:1:237:SER:HA	1.88	0.74
1:2:142:VAL:O	1:2:142:VAL:HG22	1.86	0.74
1:2:319:ARG:NH2	2:2:419:HOH:O	2.20	0.74
1:2:32:PRO:O	1:2:33:PHE:CB	2.35	0.74
1:3:159:VAL:O	1:3:163:ASN:HB2	1.88	0.74
1:4:106:ALA:O	1:4:107:HIS:O	2.06	0.74
1:4:113:LYS:HB3	1:4:114:LYS:HE3	1.69	0.74
1:2:220:LEU:O	1:2:221:ASP:C	2.25	0.74
1:2:278:VAL:O	1:2:279:SER:OG	2.06	0.74
1:3:232:PRO:O	1:3:233:THR:C	2.25	0.74
1:4:182:LYS:CE	1:4:187:PRO:HG2	2.18	0.74
1:4:4:GLY:HA2	1:4:27:VAL:HG23	1.68	0.73
1:1:152:CYS:SG	1:1:239:VAL:CG1	2.76	0.73
1:1:11:ILE:HG22	1:1:15:VAL:CG2	2.17	0.73
1:1:131:VAL:HG12	1:1:158:LYS:CE	2.18	0.73
1:1:251:TYR:CB	1:1:299:LEU:HG	2.18	0.73
1:1:34:ILE:HD11	1:1:39:MET:HG2	1.68	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:287:ARG:O	1:2:319:ARG:NH1	2.22	0.73
1:3:175:HIS:O	1:3:231:VAL:HG23	1.87	0.73
1:3:161:HIS:HA	1:3:166:ILE:HG13	1.68	0.73
1:3:248:GLU:HG2	1:3:302:THR:HG22	1.70	0.73
1:1:329:LYS:NZ	1:1:330:VAL:N	2.36	0.73
1:2:175:HIS:N	1:2:229:PHE:O	2.21	0.73
1:2:33:PHE:CZ	1:2:76:MET:CE	2.70	0.73
1:4:4:GLY:CA	1:4:27:VAL:CG2	2.66	0.73
1:4:77:LYS:N	2:4:348:HOH:O	2.03	0.73
1:3:294:LYS:HA	1:3:297:ILE:HG13	1.70	0.73
1:4:216:VAL:CG1	1:4:217:ILE:HG22	2.10	0.73
1:4:207:THR:OG1	1:4:208:GLY:N	2.20	0.73
1:1:124:ALA:C	1:1:125:PRO:O	2.24	0.73
1:2:235:ASP:CG	1:2:235:ASP:O	2.25	0.73
1:2:31:ASP:OD1	1:2:32:PRO:O	2.06	0.73
1:1:8:PHE:CD2	1:1:8:PHE:C	2.60	0.73
1:3:293:ALA:O	1:3:294:LYS:HB3	1.87	0.73
1:3:329:LYS:HZ2	1:3:329:LYS:HB3	1.52	0.73
1:3:17:ARG:CG	1:3:43:PHE:HE2	1.97	0.73
1:4:129:CYS:CA	1:4:132:ASN:HD22	2.01	0.73
1:2:132:ASN:HD21	1:2:133:LEU:CD2	2.00	0.73
1:2:277:VAL:CG2	1:4:41:TYR:CE1	2.55	0.73
1:3:251:TYR:CE1	1:3:255:LYS:HD3	2.24	0.73
1:3:295:ALA:CA	1:3:297:ILE:HD12	2.19	0.73
1:4:11:ILE:CD1	1:4:11:ILE:N	2.51	0.73
1:2:138:LYS:HE3	1:2:330:VAL:CG1	2.18	0.73
1:3:152:CYS:SG	1:3:239:VAL:HG13	2.27	0.73
1:3:272:TYR:HA	1:3:291:PHE:O	1.88	0.73
1:4:329:LYS:HZ3	1:4:329:LYS:C	1.89	0.73
1:4:211:LYS:CE	1:4:211:LYS:CA	2.66	0.73
1:1:193:ARG:HH11	1:1:204:PRO:HG2	1.53	0.73
1:1:327:MET:O	1:1:331:ASP:HB2	1.88	0.73
1:2:159:VAL:CG2	1:2:266:LEU:HD21	2.18	0.73
1:3:276:ASP:OD1	1:3:277:VAL:HG22	1.88	0.73
1:2:248:GLU:HA	1:2:302:THR:HG21	1.69	0.73
1:2:81:ILE:HD13	1:2:82:PRO:O	1.89	0.73
1:3:53:LYS:HE2	1:3:53:LYS:N	2.02	0.73
1:1:180:THR:OG1	1:1:181:GLN:N	2.22	0.73
1:1:272:TYR:HA	1:1:291:PHE:O	1.88	0.73
1:2:311:ASP:O	1:2:313:GLU:N	2.21	0.73
1:3:129:CYS:CA	1:3:132:ASN:ND2	2.51	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:262:SER:O	1:3:267:GLN:HA	1.89	0.73
1:3:7:GLY:O	1:3:8:PHE:HB3	1.88	0.73
1:2:135:LYS:HD2	1:2:135:LYS:O	1.89	0.73
1:4:248:GLU:HG2	1:4:302:THR:HG22	1.69	0.73
1:1:127:PHE:CA	1:1:132:ASN:HB2	2.18	0.72
1:1:161:HIS:CG	1:1:162:GLU:N	2.52	0.72
1:1:292:ASP:OD2	1:1:295:ALA:CB	2.35	0.72
1:2:266:LEU:CD2	1:2:270:LEU:HD12	2.19	0.72
1:4:75:GLU:HB2	2:4:347:HOH:O	1.89	0.72
1:4:138:LYS:H	1:4:138:LYS:CD	2.00	0.72
1:4:288:SER:HB2	1:4:319:ARG:NH1	2.03	0.72
1:4:190:LYS:HD2	2:4:367:HOH:O	1.87	0.72
1:2:284:GLY:HA2	1:2:314:PHE:CE1	2.24	0.72
1:3:294:LYS:O	1:3:297:ILE:CD1	2.37	0.72
1:3:81:ILE:HD12	1:3:83:TRP:CE2	2.24	0.72
1:1:145:ASN:HB2	1:1:323:LEU:HD21	1.70	0.72
1:4:44:LYS:HG3	1:4:56:VAL:CG2	2.12	0.72
1:2:266:LEU:HD23	1:2:270:LEU:CD1	2.20	0.72
1:4:294:LYS:H	1:4:297:ILE:HG21	1.54	0.72
1:2:196:ARG:HG2	1:2:196:ARG:HH11	1.52	0.72
1:3:81:ILE:HD13	1:3:82:PRO:CD	2.18	0.72
1:4:113:LYS:CB	1:4:114:LYS:CE	2.67	0.72
1:3:220:LEU:HB3	1:3:223:LYS:HG2	1.71	0.72
1:1:145:ASN:CG	1:1:323:LEU:HD23	2.08	0.72
1:1:276:ASP:O	1:1:278:VAL:CG1	2.28	0.72
1:3:150:THR:HG22	1:3:151:ASN:N	2.04	0.72
1:3:200:GLN:C	1:3:201:ASN:HD22	1.93	0.72
1:4:173:THR:CG2	1:4:228:ALA:HB2	2.19	0.72
1:3:200:GLN:OE1	1:4:48:THR:CG2	2.38	0.72
1:3:101:ILE:HG21	2:3:380:HOH:O	1.89	0.72
1:1:51:VAL:O	1:1:52:PHE:HB2	1.89	0.72
1:1:65:VAL:CG1	1:1:70:ILE:HD13	2.19	0.72
1:2:76:MET:O	1:2:77:LYS:CD	2.37	0.72
1:1:277:VAL:HG21	1:3:41:TYR:CZ	2.25	0.72
1:2:19:ALA:HA	1:2:24:ALA:HB3	1.72	0.72
1:1:295:ALA:N	1:1:297:ILE:HD12	2.04	0.72
1:2:251:TYR:CE1	1:2:255:LYS:HD3	2.23	0.72
1:2:296:GLY:H	1:2:297:ILE:HD13	1.55	0.72
1:2:95:THR:HG22	1:2:97:VAL:HG23	1.71	0.72
1:4:200:GLN:O	2:4:448:HOH:O	2.07	0.72
1:1:193:ARG:CD	1:4:277:VAL:HA	2.20	0.72

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:127:PHE:HB3	1:4:132:ASN:HB2	1.71	0.72
1:3:180:THR:O	1:3:181:GLN:C	2.26	0.72
1:1:11:ILE:CD1	1:1:11:ILE:H	2.03	0.72
1:4:131:VAL:HG12	1:4:158:LYS:HZ3	1.54	0.72
1:3:239:VAL:HG12	1:3:310:TYR:HE1	1.55	0.72
1:2:132:ASN:HD21	1:2:133:LEU:HD21	1.55	0.71
1:3:46:ASP:HB3	1:3:50:GLY:N	2.05	0.71
1:2:11:ILE:HG22	1:2:15:VAL:HG21	1.71	0.71
1:4:118:SER:O	1:4:118:SER:OG	2.08	0.71
1:2:244:ARG:CD	1:3:244:ARG:NH1	2.53	0.71
1:2:126:MET:HB3	1:2:215:LYS:HD2	1.72	0.71
1:1:273:THR:CG2	1:1:290:ILE:HD11	2.20	0.71
1:2:106:ALA:O	1:2:107:HIS:C	2.27	0.71
1:3:78:PRO:CG	1:3:98:PHE:CE2	2.70	0.71
1:4:101:ILE:HG23	1:4:142:VAL:HG11	1.71	0.71
1:2:177:VAL:HG13	1:2:232:PRO:O	1.91	0.71
1:2:292:ASP:CG	1:2:295:ALA:HB3	2.11	0.71
1:3:161:HIS:O	1:3:163:ASN:N	2.24	0.71
1:4:164:PHE:O	1:4:165:GLU:CB	2.38	0.71
1:1:319:ARG:O	1:1:322:ASP:N	2.23	0.71
1:2:189:ALA:O	1:2:190:LYS:NZ	2.22	0.71
1:4:138:LYS:CE	1:4:330:VAL:CG1	2.69	0.71
1:4:104:ALA:O	1:4:105:SER:C	2.29	0.71
1:2:244:ARG:NH1	1:3:244:ARG:HG3	2.04	0.71
1:2:145:ASN:O	1:2:146:ALA:O	2.08	0.71
1:1:280:SER:O	1:1:281:ASP:O	2.08	0.71
1:2:235:ASP:OD1	1:2:235:ASP:O	2.09	0.71
1:1:167:VAL:CG2	1:1:244:ARG:HG2	2.20	0.71
1:1:277:VAL:CA	1:4:193:ARG:HG3	2.15	0.71
1:4:282:PHE:CE1	1:4:290:ILE:HD13	2.26	0.71
1:4:142:VAL:HG22	1:4:142:VAL:O	1.91	0.71
1:3:167:VAL:CG1	1:3:245:LEU:O	2.38	0.71
1:4:273:THR:N	1:4:291:PHE:O	2.20	0.71
1:4:8:PHE:CZ	1:4:39:MET:HB2	2.25	0.71
1:4:105:SER:O	1:4:108:PHE:CD1	2.43	0.71
1:1:265:PRO:HG2	2:1:442:HOH:O	1.90	0.71
1:1:26:VAL:O	1:1:27:VAL:HB	1.90	0.71
1:1:320:VAL:O	1:1:324:LEU:HB2	1.91	0.71
1:2:269:PHE:O	1:2:288:SER:CB	2.39	0.71
1:2:270:LEU:HD23	1:2:271:GLY:H	1.54	0.71
1:4:78:PRO:HG3	1:4:98:PHE:HE2	1.54	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:78:PRO:CD	1:4:98:PHE:CE2	2.74	0.71
1:3:126:MET:HE2	1:3:212:ALA:HA	1.71	0.71
1:1:138:LYS:CD	1:1:138:LYS:H	2.04	0.70
1:1:2:LYS:CE	1:1:87:GLY:O	2.38	0.70
1:2:232:PRO:CG	1:3:232:PRO:HB2	2.20	0.70
1:4:146:ALA:CB	1:4:150:THR:HG21	2.21	0.70
1:2:244:ARG:HG3	1:3:244:ARG:NH2	2.06	0.70
1:3:196:ARG:HD2	1:4:47:SER:OG	1.89	0.70
1:3:14:LEU:O	1:3:18:ALA:N	2.24	0.70
1:1:2:LYS:HB2	1:1:89:GLU:HB2	1.73	0.70
1:2:30:ASN:OD1	1:2:81:ILE:CG1	2.35	0.70
1:4:131:VAL:HG21	1:4:216:VAL:HG22	1.74	0.70
1:3:239:VAL:HG12	1:3:310:TYR:CE1	2.26	0.70
1:1:44:LYS:HD2	1:1:56:VAL:CG1	2.21	0.70
1:2:125:PRO:HD2	1:2:143:VAL:HA	1.73	0.70
1:2:161:HIS:HB2	1:2:166:ILE:HD12	1.71	0.70
1:4:26:VAL:O	1:4:27:VAL:CG1	2.38	0.70
1:3:71:THR:CG2	1:3:73:PHE:CE1	2.75	0.70
1:3:94:SER:O	1:3:95:THR:C	2.29	0.70
1:4:137:SER:HB3	1:4:138:LYS:NZ	2.06	0.70
1:2:145:ASN:HD22	1:2:145:ASN:C	1.93	0.70
1:2:329:LYS:HB3	1:2:329:LYS:HZ2	1.55	0.70
1:1:108:PHE:O	1:1:111:GLY:N	2.25	0.70
1:2:220:LEU:HA	1:2:223:LYS:HZ2	1.55	0.70
1:1:261:ALA:O	1:1:263:GLU:N	2.24	0.70
1:1:95:THR:HA	2:1:436:HOH:O	1.90	0.70
1:1:277:VAL:C	1:1:278:VAL:O	2.30	0.70
1:2:301:LYS:O	1:2:302:THR:HG23	1.90	0.70
1:3:94:SER:O	1:3:96:GLY:N	2.24	0.70
1:3:51:VAL:O	1:3:52:PHE:HB2	1.90	0.70
1:4:137:SER:HA	1:4:138:LYS:HE3	1.72	0.70
1:2:211:LYS:NZ	1:2:211:LYS:HA	2.07	0.70
1:2:156:VAL:HG22	1:2:258:MET:CE	2.22	0.70
1:1:3:ILE:O	1:1:27:VAL:HG23	1.91	0.70
1:2:159:VAL:O	1:2:163:ASN:HB2	1.90	0.70
1:2:4:GLY:N	1:2:27:VAL:CG2	2.55	0.70
1:2:81:ILE:HD12	1:2:83:TRP:CZ2	2.26	0.70
1:3:37:GLU:HA	1:3:40:VAL:CG1	2.21	0.70
1:1:1:SER:CB	1:1:25:GLN:HB2	2.22	0.70
1:1:311:ASP:O	1:1:312:ASN:C	2.30	0.70
1:1:75:GLU:O	2:1:438:HOH:O	2.09	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:1:SER:HB3	1:4:25:GLN:NE2	2.00	0.70
1:4:76:MET:O	1:4:77:LYS:CD	2.40	0.70
1:3:286:ASN:OD1	1:3:318:GLN:NE2	2.25	0.70
1:2:298:GLN:NE2	1:3:225:THR:CG2	2.54	0.70
1:4:264:GLY:C	2:4:453:HOH:O	2.29	0.70
1:1:71:THR:HG21	1:1:73:PHE:CD1	2.26	0.70
1:3:232:PRO:O	1:3:233:THR:O	2.08	0.70
1:4:277:VAL:C	1:4:278:VAL:O	2.29	0.70
1:3:105:SER:O	1:3:108:PHE:HD1	1.74	0.70
1:2:54:GLY:CA	1:2:66:ASP:OD1	2.39	0.70
1:4:270:LEU:HD23	1:4:271:GLY:H	1.53	0.70
1:2:173:THR:O	1:2:228:ALA:HA	1.92	0.70
1:1:47:SER:OG	1:2:185:ASP:OD2	2.10	0.70
1:3:265:PRO:C	1:3:267:GLN:H	1.93	0.70
1:2:168:GLU:OE2	1:2:244:ARG:CZ	2.40	0.70
1:4:318:GLN:OE1	1:4:318:GLN:HA	1.90	0.70
1:1:171:MET:SD	1:1:209:ALA:CB	2.78	0.69
1:1:325:LYS:O	1:1:326:HIS:C	2.30	0.69
1:2:128:VAL:H	1:2:132:ASN:CB	2.05	0.69
1:3:279:SER:C	1:3:281:ASP:H	1.96	0.69
1:3:27:VAL:O	1:3:28:ALA:HB2	1.92	0.69
1:4:150:THR:HG21	1:4:212:ALA:HB3	1.74	0.69
1:1:145:ASN:OD1	1:1:323:LEU:HD23	1.92	0.69
1:1:203:ILE:O	1:1:204:PRO:O	2.10	0.69
1:2:235:ASP:OD2	1:2:311:ASP:OD1	2.10	0.69
1:3:8:PHE:CD1	1:3:29:VAL:CG1	2.74	0.69
1:2:52:PHE:C	1:2:53:LYS:HZ3	1.95	0.69
1:3:59:GLU:O	1:3:60:ASP:C	2.30	0.69
1:1:297:ILE:HD13	1:1:297:ILE:O	1.91	0.69
1:2:244:ARG:CG	1:3:244:ARG:NH2	2.55	0.69
1:2:127:PHE:HD1	1:2:143:VAL:HG23	1.57	0.69
1:1:298:GLN:OE1	1:4:225:THR:HG23	1.92	0.69
1:1:272:TYR:CE2	1:1:293:ALA:HB2	2.27	0.69
1:1:325:LYS:O	1:1:327:MET:N	2.25	0.69
1:1:44:LYS:O	1:1:51:VAL:HA	1.92	0.69
1:2:113:LYS:HB3	1:2:114:LYS:HG2	1.73	0.69
1:2:296:GLY:N	1:2:297:ILE:CD1	2.55	0.69
1:4:204:PRO:HG3	1:4:229:PHE:HE2	1.57	0.69
1:4:276:ASP:CG	1:4:277:VAL:N	2.44	0.69
1:2:95:THR:HG22	1:2:97:VAL:N	2.08	0.69
1:1:119:ALA:HB1	1:1:120:PRO:HD3	1.72	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:216:VAL:HG12	1:2:217:ILE:HG22	1.75	0.69
1:2:74:ASN:HA	2:2:407:HOH:O	1.92	0.69
1:3:19:ALA:HB1	1:3:24:ALA:HB3	1.73	0.69
1:1:97:VAL:O	1:1:98:PHE:CG	2.45	0.69
1:1:17:ARG:HB3	1:1:43:PHE:CE2	2.28	0.69
1:1:319:ARG:HA	1:1:322:ASP:OD2	1.93	0.69
1:1:54:GLY:CA	1:1:66:ASP:OD2	2.40	0.69
1:2:277:VAL:CG2	1:4:41:TYR:HE1	1.97	0.69
1:4:44:LYS:HG2	1:4:56:VAL:HG11	1.75	0.69
1:2:244:ARG:CZ	1:3:244:ARG:HG3	2.22	0.69
1:2:84:SER:O	1:2:86:ALA:HB3	1.93	0.69
1:3:255:LYS:HB3	1:3:255:LYS:NZ	2.08	0.69
1:3:296:GLY:N	1:3:297:ILE:CD1	2.56	0.69
1:3:296:GLY:N	1:3:297:ILE:HD12	2.07	0.69
1:4:211:LYS:HE2	1:4:211:LYS:CA	2.22	0.69
1:3:212:ALA:O	1:3:216:VAL:N	2.26	0.69
1:2:113:LYS:HB3	1:2:114:LYS:CG	2.23	0.68
1:2:255:LYS:CE	1:2:293:ALA:HB1	2.19	0.68
1:3:9:GLY:O	1:3:13:ARG:HB2	1.93	0.68
1:4:325:LYS:O	1:4:327:MET:N	2.25	0.68
1:2:284:GLY:HA2	1:2:314:PHE:HE1	1.58	0.68
1:1:225:THR:CB	1:4:298:GLN:OE1	2.40	0.68
1:3:8:PHE:CE1	1:3:29:VAL:HG11	2.29	0.68
1:1:13:ARG:O	1:1:16:LEU:N	2.25	0.68
1:1:292:ASP:OD1	1:1:292:ASP:O	2.10	0.68
1:1:9:GLY:HA2	1:1:13:ARG:HH21	1.56	0.68
1:1:295:ALA:HB1	1:4:193:ARG:HH12	1.56	0.68
1:1:193:ARG:NH1	1:4:295:ALA:CB	2.53	0.68
1:4:125:PRO:HG2	1:4:140:MET:HE1	1.74	0.68
1:1:145:ASN:HD22	1:1:145:ASN:C	1.96	0.68
1:2:34:ILE:HD11	1:2:39:MET:HG3	1.75	0.68
1:4:297:ILE:C	1:4:297:ILE:CD1	2.62	0.68
1:1:294:LYS:C	1:1:297:ILE:CD1	2.62	0.68
1:3:115:VAL:HB	1:3:142:VAL:HG23	1.75	0.68
1:4:301:LYS:HZ3	1:4:301:LYS:HB2	1.59	0.68
1:1:129:CYS:O	1:1:133:LEU:CG	2.42	0.68
1:2:131:VAL:HG12	1:2:158:LYS:HZ1	1.54	0.68
1:4:73:PHE:HB2	1:4:81:ILE:HD11	1.75	0.68
1:3:105:SER:O	1:3:106:ALA:C	2.31	0.68
1:3:328:GLN:O	1:3:329:LYS:C	2.31	0.68
1:1:213:VAL:HA	1:1:216:VAL:HG12	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:26:VAL:HG11	1:1:70:ILE:HG21	1.76	0.68
1:1:71:THR:HG22	1:1:72:VAL:H	1.55	0.68
1:2:149:THR:O	1:2:152:CYS:HB3	1.93	0.68
1:2:216:VAL:HG13	1:2:217:ILE:HG22	1.74	0.68
1:2:296:GLY:N	1:2:297:ILE:HD12	2.09	0.68
1:4:236:VAL:O	1:4:237:SER:OG	2.11	0.68
1:4:53:LYS:HE2	1:4:53:LYS:N	2.07	0.68
1:4:58:MET:CE	1:4:58:MET:N	2.48	0.68
1:2:11:ILE:HG22	1:2:15:VAL:HG23	1.76	0.68
1:4:188:SER:C	1:4:190:LYS:N	2.44	0.68
1:1:225:THR:HG21	1:4:298:GLN:NE2	2.09	0.68
1:2:6:ASN:CB	1:2:30:ASN:HD21	2.07	0.68
1:4:236:VAL:HG12	1:4:237:SER:H	1.59	0.68
1:4:2:LYS:NZ	1:4:2:LYS:HB3	1.99	0.68
1:2:193:ARG:HH12	1:3:295:ALA:HB1	1.59	0.68
1:1:276:ASP:CG	1:1:277:VAL:HG22	2.14	0.68
1:2:31:ASP:O	1:2:34:ILE:HG23	1.93	0.68
1:4:209:ALA:O	1:4:213:VAL:HB	1.94	0.68
1:4:34:ILE:O	1:4:34:ILE:HG23	1.94	0.68
1:1:11:ILE:N	1:1:11:ILE:HD12	2.09	0.68
1:1:329:LYS:HZ1	1:1:330:VAL:N	1.91	0.68
1:4:232:PRO:O	1:4:233:THR:C	2.32	0.68
1:2:277:VAL:HB	1:4:41:TYR:OH	1.94	0.68
1:3:318:GLN:HA	1:3:318:GLN:OE1	1.93	0.68
1:4:51:VAL:CA	2:4:340:HOH:O	2.38	0.67
1:1:41:TYR:CZ	1:3:277:VAL:HG21	2.28	0.67
1:3:113:LYS:HB3	1:3:114:LYS:CE	2.24	0.67
1:4:127:PHE:HD1	1:4:143:VAL:CG2	2.07	0.67
1:2:126:MET:HB2	1:2:215:LYS:HZ2	1.58	0.67
1:2:3:ILE:HD13	1:2:324:LEU:HD12	1.75	0.67
1:3:183:THR:HG22	2:3:383:HOH:O	1.93	0.67
1:3:173:THR:HG22	1:3:227:MET:O	1.93	0.67
1:3:81:ILE:HG23	1:3:83:TRP:NE1	2.08	0.67
1:2:168:GLU:OE2	1:2:244:ARG:NE	2.27	0.67
1:2:112:ALA:O	1:2:113:LYS:CB	2.41	0.67
1:2:283:ILE:O	1:2:284:GLY:C	2.33	0.67
1:4:273:THR:CG2	1:4:290:ILE:HD11	2.24	0.67
1:3:243:VAL:CG2	1:3:304:VAL:HG12	2.19	0.67
1:2:244:ARG:HD3	1:3:244:ARG:NH1	2.09	0.67
1:1:251:TYR:O	1:1:254:ILE:HB	1.95	0.67
1:1:129:CYS:HG	1:1:269:PHE:HE1	1.36	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:158:LYS:O	1:2:162:GLU:HG2	1.94	0.67
1:4:17:ARG:NE	2:4:339:HOH:O	2.23	0.67
1:3:127:PHE:CE2	1:3:136:TYR:HB2	2.29	0.67
1:1:297:ILE:H	1:1:297:ILE:HD12	1.55	0.67
1:1:314:PHE:HB2	1:1:317:SER:HB2	1.74	0.67
1:1:44:LYS:HD2	1:1:56:VAL:HG13	1.77	0.67
1:1:36:LEU:HD11	1:1:62:ALA:C	2.14	0.67
1:3:81:ILE:CG2	1:3:83:TRP:NE1	2.57	0.67
1:4:329:LYS:NZ	1:4:330:VAL:N	2.42	0.67
1:4:105:SER:O	1:4:107:HIS:N	2.27	0.67
1:3:211:LYS:NZ	1:3:211:LYS:HA	2.10	0.67
1:1:138:LYS:HD3	1:1:138:LYS:H	1.58	0.67
1:1:177:VAL:HA	1:1:181:GLN:OE1	1.94	0.67
1:1:277:VAL:HG23	1:1:278:VAL:N	2.07	0.67
1:1:71:THR:C	1:1:72:VAL:CG1	2.62	0.67
1:2:236:VAL:O	1:2:312:ASN:OD1	2.13	0.67
1:3:273:THR:O	1:3:293:ALA:HB3	1.95	0.67
1:4:135:LYS:HD2	1:4:135:LYS:O	1.94	0.67
1:1:178:THR:OG1	1:1:180:THR:N	2.28	0.67
1:2:220:LEU:O	1:2:223:LYS:HG2	1.95	0.67
1:2:250:SER:O	1:2:251:TYR:C	2.33	0.67
1:1:78:PRO:HD3	1:1:98:PHE:CZ	2.29	0.67
1:4:211:LYS:HZ3	1:4:211:LYS:HA	1.59	0.67
1:1:59:GLU:HB3	1:1:64:VAL:CG1	2.24	0.67
1:1:71:THR:HG21	1:1:73:PHE:CZ	2.29	0.67
1:2:74:ASN:HB2	2:2:395:HOH:O	1.95	0.67
1:4:54:GLY:O	1:4:56:VAL:HG12	1.93	0.67
1:2:185:ASP:OD2	1:2:196:ARG:HD2	1.95	0.67
1:3:131:VAL:HG13	1:3:158:LYS:HZ3	1.59	0.67
1:2:225:THR:CG2	1:3:298:GLN:CD	2.62	0.67
1:2:181:GLN:HE22	1:2:230:ARG:HB2	1.60	0.67
1:2:93:GLU:OE2	1:2:98:PHE:HB2	1.95	0.67
1:4:237:SER:OG	1:4:312:ASN:OD1	2.12	0.67
1:3:251:TYR:O	1:3:254:ILE:CB	2.43	0.67
1:2:126:MET:HB2	1:2:215:LYS:NZ	2.10	0.67
1:1:129:CYS:O	1:1:133:LEU:HG	1.94	0.67
1:2:124:ALA:C	1:2:125:PRO:O	2.26	0.67
1:2:252:ASP:O	1:2:255:LYS:N	2.25	0.67
1:3:32:PRO:HG3	1:3:75:GLU:O	1.94	0.67
1:4:113:LYS:CD	1:4:114:LYS:HZ2	1.91	0.67
1:2:64:VAL:O	1:2:64:VAL:CG2	2.42	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:O	1:1:105:SER:CB	2.43	0.66
1:2:178:THR:OG1	1:2:180:THR:HG23	1.94	0.66
1:2:180:THR:OG1	1:2:181:GLN:N	2.27	0.66
1:4:276:ASP:O	1:4:278:VAL:N	2.28	0.66
1:1:2:LYS:HE2	1:1:87:GLY:O	1.95	0.66
1:1:41:TYR:OH	1:2:196:ARG:NH1	2.26	0.66
1:1:131:VAL:CG1	1:1:158:LYS:HE2	2.24	0.66
1:1:287:ARG:O	1:1:319:ARG:NH1	2.27	0.66
1:2:41:TYR:OH	1:4:277:VAL:CG1	2.42	0.66
1:3:297:ILE:HA	1:3:305:LYS:O	1.94	0.66
1:4:150:THR:HG21	1:4:212:ALA:CB	2.25	0.66
1:3:69:LYS:O	1:3:69:LYS:HG2	1.94	0.66
1:2:250:SER:O	1:2:253:ASP:N	2.29	0.66
1:2:328:GLN:CA	1:2:328:GLN:NE2	2.58	0.66
1:2:33:PHE:CZ	1:2:76:MET:SD	2.88	0.66
1:2:232:PRO:HB2	1:3:232:PRO:HG2	1.77	0.66
1:4:239:VAL:HG13	1:4:310:TYR:HE1	1.60	0.66
1:4:156:VAL:HG21	1:4:308:SER:OG	1.95	0.66
1:3:164:PHE:CE2	1:3:249:CYS:CB	2.78	0.66
1:3:220:LEU:O	1:3:221:ASP:C	2.33	0.66
1:1:14:LEU:O	1:1:18:ALA:HB2	1.95	0.66
1:4:39:MET:CE	1:4:72:VAL:HB	2.26	0.66
1:4:78:PRO:C	1:4:80:ASN:N	2.47	0.66
1:4:113:LYS:CB	1:4:114:LYS:HD2	2.18	0.66
1:1:53:LYS:HE2	1:1:53:LYS:N	2.10	0.66
1:2:113:LYS:HB3	1:2:114:LYS:HD2	1.76	0.66
1:2:281:ASP:O	1:2:283:ILE:HB	1.94	0.66
1:3:173:THR:CG2	1:3:228:ALA:HB2	2.25	0.66
1:4:292:ASP:OD1	1:4:307:VAL:HG11	1.95	0.66
1:3:252:ASP:HA	1:3:255:LYS:CG	2.25	0.66
1:2:59:GLU:O	1:2:61:GLY:N	2.28	0.66
1:1:149:THR:HG23	1:1:310:TYR:OH	1.94	0.66
1:2:131:VAL:HG12	1:2:158:LYS:HZ3	1.60	0.66
1:4:53:LYS:HD2	1:4:53:LYS:C	2.16	0.66
1:3:3:ILE:CD1	1:3:24:ALA:HB1	2.26	0.66
1:3:287:ARG:O	1:3:288:SER:HB2	1.96	0.66
1:3:117:ILE:C	1:3:119:ALA:H	1.97	0.66
1:1:52:PHE:N	2:1:430:HOH:O	2.28	0.66
1:2:3:ILE:O	1:2:27:VAL:HG23	1.96	0.66
1:2:295:ALA:HB2	1:3:193:ARG:NH2	2.10	0.66
1:2:332:SER:O	1:2:333:ALA:HB2	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:30:ASN:OD1	1:4:81:ILE:CG1	2.44	0.66
1:3:1:SER:HB3	1:3:25:GLN:NE2	2.11	0.66
1:4:133:LEU:O	1:4:136:TYR:HB3	1.95	0.66
1:1:128:VAL:HG23	1:1:216:VAL:HG21	1.78	0.66
1:2:108:PHE:O	1:2:109:LYS:C	2.33	0.66
1:4:8:PHE:HZ	1:4:39:MET:CB	2.08	0.66
1:3:101:ILE:HG23	2:3:381:HOH:O	1.96	0.66
1:2:66:ASP:HB2	1:2:68:LYS:HE2	1.77	0.66
1:4:127:PHE:HD1	1:4:143:VAL:HG23	1.60	0.66
1:2:127:PHE:CD1	1:2:143:VAL:HG23	2.30	0.66
1:2:33:PHE:HZ	1:2:76:MET:HE3	1.60	0.66
1:3:216:VAL:HG13	1:3:217:ILE:N	2.11	0.66
1:2:55:GLU:OE2	1:2:55:GLU:HA	1.94	0.66
1:1:59:GLU:O	1:1:61:GLY:N	2.29	0.65
1:3:128:VAL:N	1:3:132:ASN:HB3	2.10	0.65
1:3:276:ASP:CG	1:3:277:VAL:N	2.47	0.65
1:3:297:ILE:HD13	1:3:297:ILE:N	2.11	0.65
1:3:173:THR:HG23	1:3:228:ALA:CB	2.25	0.65
1:4:277:VAL:O	1:4:278:VAL:C	2.35	0.65
1:4:34:ILE:HD11	1:4:42:MET:SD	2.36	0.65
1:4:295:ALA:N	1:4:297:ILE:HG23	2.10	0.65
1:4:66:ASP:O	1:4:68:LYS:CD	2.45	0.65
1:3:127:PHE:CZ	1:3:140:MET:HE1	2.30	0.65
1:3:277:VAL:HG23	1:3:278:VAL:N	2.10	0.65
1:1:277:VAL:HG11	1:3:41:TYR:CZ	2.31	0.65
1:2:181:GLN:HG2	1:2:198:ALA:HB2	1.77	0.65
1:2:94:SER:O	1:2:95:THR:C	2.34	0.65
1:3:322:ASP:O	1:3:323:LEU:C	2.34	0.65
1:3:328:GLN:O	1:3:329:LYS:O	2.14	0.65
1:4:170:LEU:CD2	1:4:225:THR:CG2	2.74	0.65
1:1:132:ASN:HD21	1:1:133:LEU:CD2	2.05	0.65
1:2:185:ASP:HA	1:2:196:ARG:HA	1.78	0.65
1:1:319:ARG:HH11	1:1:319:ARG:HG2	1.61	0.65
1:2:213:VAL:O	1:2:216:VAL:HG12	1.96	0.65
1:1:303:PHE:HE2	1:4:303:PHE:CE2	2.14	0.65
1:1:127:PHE:HB3	1:1:132:ASN:CG	2.17	0.65
1:1:250:SER:C	1:1:252:ASP:N	2.47	0.65
1:2:155:PRO:O	1:2:159:VAL:HG23	1.96	0.65
1:2:4:GLY:HA2	1:2:27:VAL:CG2	2.26	0.65
1:4:44:LYS:CE	1:4:45:TYR:CE2	2.79	0.65
1:4:83:TRP:HA	1:4:86:ALA:CB	2.26	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:84:SER:OG	1:3:111:GLY:CA	2.43	0.65
1:4:224:LEU:HD21	1:4:241:LEU:HD11	1.79	0.65
1:4:108:PHE:O	1:4:111:GLY:N	2.29	0.65
1:1:142:VAL:O	1:1:142:VAL:HG13	1.95	0.65
1:1:309:TRP:CD1	1:1:309:TRP:N	2.63	0.65
1:1:76:MET:O	1:1:77:LYS:HB2	1.96	0.65
1:2:292:ASP:OD1	1:2:295:ALA:HB3	1.97	0.65
1:4:33:PHE:HZ	1:4:76:MET:SD	2.19	0.65
1:3:243:VAL:HG22	1:3:304:VAL:CG1	2.24	0.65
1:4:130:GLY:HA3	1:4:158:LYS:NZ	2.12	0.65
1:1:164:PHE:O	1:1:165:GLU:CB	2.46	0.65
1:1:276:ASP:O	1:1:277:VAL:C	2.35	0.65
1:3:188:SER:HB2	1:3:195:GLY:HA3	1.79	0.65
1:3:188:SER:O	1:3:190:LYS:N	2.30	0.65
1:1:189:ALA:O	1:1:190:LYS:HD3	1.97	0.65
1:1:101:ILE:CG1	1:1:142:VAL:HG11	2.27	0.64
1:1:129:CYS:O	1:1:132:ASN:ND2	2.28	0.64
1:1:17:ARG:CG	1:1:43:PHE:CE2	2.67	0.64
1:3:175:HIS:CB	1:3:230:ARG:HH21	2.10	0.64
1:4:82:PRO:HB2	1:4:85:LYS:O	1.96	0.64
1:3:252:ASP:O	1:3:255:LYS:CG	2.45	0.64
1:3:78:PRO:C	1:3:80:ASN:H	2.01	0.64
1:2:193:ARG:CB	1:3:277:VAL:HG12	2.25	0.64
1:3:66:ASP:HB2	1:3:68:LYS:HD3	1.77	0.64
1:4:128:VAL:O	1:4:132:ASN:HB3	1.97	0.64
1:4:307:VAL:CG1	1:4:307:VAL:O	2.44	0.64
1:2:204:PRO:HA	1:2:228:ALA:O	1.97	0.64
1:3:8:PHE:CD2	1:3:8:PHE:C	2.70	0.64
1:2:53:LYS:NZ	1:2:53:LYS:HB3	2.12	0.64
1:1:244:ARG:CZ	1:4:244:ARG:CZ	2.76	0.64
1:3:131:VAL:N	1:3:158:LYS:NZ	2.45	0.64
1:3:127:PHE:CG	1:3:132:ASN:HB2	2.33	0.64
1:4:328:GLN:O	1:4:332:SER:N	2.29	0.64
1:4:185:ASP:N	1:4:185:ASP:OD1	2.30	0.64
1:3:146:ALA:CB	1:3:150:THR:HG21	2.27	0.64
1:1:325:LYS:O	1:1:328:GLN:N	2.30	0.64
1:3:276:ASP:O	1:3:278:VAL:CG1	2.45	0.64
1:1:27:VAL:CG2	1:1:28:ALA:N	2.38	0.64
1:4:4:GLY:CA	1:4:27:VAL:HG23	2.28	0.64
1:4:71:THR:HG21	1:4:73:PHE:CE1	2.31	0.64
1:3:127:PHE:HB2	1:3:323:LEU:HD21	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:275:ASP:C	1:3:276:ASP:OD2	2.35	0.64
1:3:46:ASP:CB	1:3:50:GLY:HA2	2.28	0.64
1:4:217:ILE:HG12	1:4:220:LEU:HD22	1.80	0.64
1:3:196:ARG:HH11	1:3:196:ARG:CG	2.08	0.64
1:4:250:SER:O	1:4:252:ASP:N	2.31	0.64
1:2:117:ILE:HD12	1:2:144:SER:HB3	1.79	0.64
1:4:146:ALA:HB1	1:4:150:THR:HG21	1.79	0.64
1:4:108:PHE:HA	1:4:112:ALA:HB3	1.79	0.64
1:2:244:ARG:HH12	1:3:244:ARG:HG3	1.60	0.64
1:3:175:HIS:CG	1:3:230:ARG:NH2	2.61	0.64
1:2:173:THR:HG23	1:2:228:ALA:CB	2.28	0.64
1:3:127:PHE:CB	1:3:132:ASN:CB	2.57	0.64
1:3:14:LEU:O	1:3:18:ALA:CB	2.46	0.64
1:3:235:ASP:OD2	1:3:313:GLU:HB2	1.98	0.64
1:3:83:TRP:CA	1:3:86:ALA:HB3	2.28	0.64
1:1:266:LEU:O	1:1:267:GLN:C	2.37	0.64
1:3:168:GLU:HG2	1:3:244:ARG:HD2	1.79	0.64
1:1:196:ARG:NH2	1:4:281:ASP:OD2	2.31	0.63
1:1:277:VAL:O	1:1:278:VAL:CG2	2.45	0.63
1:1:71:THR:C	1:1:72:VAL:HG12	2.18	0.63
1:4:131:VAL:O	1:4:132:ASN:C	2.36	0.63
1:4:217:ILE:CD1	1:4:220:LEU:CD2	2.75	0.63
1:1:211:LYS:HZ2	1:1:211:LYS:HA	1.62	0.63
1:1:105:SER:O	1:1:106:ALA:C	2.34	0.63
1:1:253:ASP:C	1:1:255:LYS:N	2.45	0.63
1:2:105:SER:O	1:2:106:ALA:C	2.36	0.63
1:2:236:VAL:O	1:2:237:SER:CB	2.28	0.63
1:2:277:VAL:O	1:2:278:VAL:C	2.33	0.63
1:2:294:LYS:C	1:2:297:ILE:HD12	2.16	0.63
1:2:6:ASN:HD22	1:2:93:GLU:CD	2.01	0.63
1:4:283:ILE:O	1:4:284:GLY:O	2.17	0.63
1:4:95:THR:CG2	1:4:97:VAL:HG23	2.28	0.63
1:3:134:GLU:C	1:3:136:TYR:N	2.52	0.63
1:3:81:ILE:HD12	1:3:83:TRP:CD2	2.33	0.63
1:4:136:TYR:C	1:4:137:SER:OG	2.35	0.63
1:1:121:SER:OG	1:1:124:ALA:HB3	1.97	0.63
1:1:129:CYS:HA	1:1:132:ASN:ND2	2.12	0.63
1:1:252:ASP:O	1:1:255:LYS:CB	2.46	0.63
1:4:17:ARG:HG2	1:4:43:PHE:HE2	1.62	0.63
1:1:193:ARG:NE	1:4:277:VAL:CA	2.60	0.63
1:2:193:ARG:CD	1:3:277:VAL:HA	2.28	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:14:LEU:HA	1:2:17:ARG:HB2	1.79	0.63
1:4:126:MET:HG3	1:4:146:ALA:HB2	1.81	0.63
1:4:13:ARG:O	1:4:16:LEU:N	2.30	0.63
1:1:129:CYS:HB3	1:1:269:PHE:CE1	2.34	0.63
1:4:52:PHE:O	1:4:53:LYS:NZ	2.27	0.63
1:4:7:GLY:O	1:4:8:PHE:HB3	1.98	0.63
1:3:127:PHE:CD2	1:3:132:ASN:HB2	2.33	0.63
1:2:66:ASP:CB	1:2:68:LYS:HE2	2.28	0.63
1:1:150:THR:OG1	1:1:212:ALA:HB3	1.98	0.63
1:1:65:VAL:HG11	1:1:70:ILE:HD13	1.79	0.63
1:1:85:LYS:O	1:1:85:LYS:HG3	1.99	0.63
1:2:41:TYR:OH	1:4:277:VAL:HG21	1.98	0.63
1:3:184:VAL:O	1:3:184:VAL:CG1	2.45	0.63
1:4:78:PRO:HD3	1:4:98:PHE:CE2	2.33	0.63
1:3:6:ASN:CA	1:3:30:ASN:HD21	2.08	0.63
1:3:8:PHE:C	1:3:8:PHE:HD2	2.01	0.63
1:2:10:ARG:O	1:2:14:LEU:CD2	2.47	0.63
1:4:248:GLU:HG2	1:4:302:THR:CG2	2.28	0.63
1:1:145:ASN:CB	1:1:323:LEU:HD23	2.28	0.63
1:3:98:PHE:HA	1:3:103:LYS:HB3	1.81	0.63
1:3:127:PHE:HD2	1:3:132:ASN:CA	2.12	0.63
1:4:127:PHE:CD1	1:4:143:VAL:HG23	2.32	0.63
1:2:244:ARG:CG	1:3:244:ARG:NH1	2.58	0.63
1:2:26:VAL:HG23	1:2:27:VAL:N	2.12	0.63
1:4:239:VAL:CG1	1:4:310:TYR:CE1	2.79	0.63
1:3:276:ASP:OD1	1:3:277:VAL:CG2	2.47	0.63
1:1:131:VAL:O	1:1:132:ASN:C	2.36	0.63
1:1:9:GLY:HA2	1:1:13:ARG:NH2	2.14	0.63
1:2:117:ILE:HD11	1:2:142:VAL:HG22	1.81	0.63
1:2:131:VAL:HG12	1:2:158:LYS:CE	2.28	0.63
1:2:175:HIS:HA	1:2:237:SER:OG	1.99	0.63
1:2:272:TYR:HA	1:2:291:PHE:O	1.98	0.63
1:4:55:GLU:O	1:4:66:ASP:N	2.30	0.63
1:3:91:ILE:HD11	1:3:112:ALA:HB1	1.81	0.63
1:3:113:LYS:C	1:3:114:LYS:CE	2.60	0.63
1:3:65:VAL:O	1:3:68:LYS:HG2	1.99	0.63
1:1:294:LYS:O	1:1:297:ILE:HD11	1.99	0.63
1:1:54:GLY:HA2	1:1:66:ASP:OD1	1.99	0.63
1:4:239:VAL:HG12	1:4:310:TYR:HE1	1.60	0.63
1:4:208:GLY:HA3	1:4:211:LYS:HG3	1.81	0.63
1:3:180:THR:O	1:3:182:LYS:N	2.32	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:305:LYS:HB2	1:1:305:LYS:NZ	2.12	0.62
1:2:104:ALA:O	1:2:105:SER:C	2.37	0.62
1:3:81:ILE:HD12	1:3:83:TRP:CZ2	2.34	0.62
1:2:100:THR:O	1:2:103:LYS:N	2.32	0.62
1:1:161:HIS:CD2	1:1:162:GLU:H	2.15	0.62
1:1:89:GLU:HB3	1:1:90:TYR:CD1	2.34	0.62
1:2:251:TYR:O	1:2:254:ILE:HB	1.98	0.62
1:2:277:VAL:HA	1:3:193:ARG:CG	2.29	0.62
1:3:188:SER:HB3	1:3:191:ASP:O	1.97	0.62
1:4:251:TYR:HB2	1:4:299:LEU:HB2	1.80	0.62
1:4:52:PHE:C	1:4:53:LYS:NZ	2.52	0.62
1:3:25:GLN:C	1:3:26:VAL:O	2.38	0.62
1:3:287:ARG:O	1:3:319:ARG:NH1	2.32	0.62
1:2:211:LYS:HZ2	1:2:211:LYS:HA	1.63	0.62
1:1:126:MET:HE2	1:1:215:LYS:HD2	1.81	0.62
1:2:132:ASN:CG	1:2:133:LEU:H	2.03	0.62
1:2:84:SER:O	1:2:86:ALA:N	2.32	0.62
1:3:189:ALA:C	1:3:190:LYS:HE2	2.20	0.62
1:4:58:MET:N	1:4:58:MET:HE1	2.08	0.62
1:3:32:PRO:HA	1:3:74:ASN:CG	2.19	0.62
1:1:153:LEU:HD21	1:1:241:LEU:CD2	2.30	0.62
1:1:90:TYR:N	1:1:90:TYR:CD1	2.68	0.62
1:2:161:HIS:O	1:2:162:GLU:C	2.38	0.62
1:2:83:TRP:C	1:2:86:ALA:HB3	2.19	0.62
1:4:250:SER:O	1:4:251:TYR:C	2.38	0.62
1:4:6:ASN:OD1	1:4:30:ASN:ND2	2.32	0.62
1:2:161:HIS:O	1:2:165:GLU:N	2.31	0.62
1:2:4:GLY:CA	1:2:27:VAL:HG21	2.29	0.62
1:3:196:ARG:NH1	1:3:196:ARG:CG	2.42	0.62
1:4:200:GLN:C	1:4:201:ASN:HD22	2.03	0.62
1:4:204:PRO:HG3	1:4:229:PHE:CE2	2.32	0.62
1:4:274:GLU:C	1:4:276:ASP:H	2.01	0.62
1:4:292:ASP:CG	1:4:295:ALA:HB3	2.19	0.62
1:2:244:ARG:CZ	1:3:244:ARG:CZ	2.77	0.62
1:4:170:LEU:HD21	1:4:225:THR:CG2	2.30	0.62
1:1:145:ASN:HB2	1:1:323:LEU:HD23	1.80	0.62
1:1:285:ASP:O	1:1:285:ASP:OD2	2.18	0.62
1:1:71:THR:CG2	1:1:72:VAL:H	2.09	0.62
1:4:273:THR:O	1:4:293:ALA:N	2.29	0.62
1:3:253:ASP:HB2	2:3:385:HOH:O	2.00	0.62
1:3:2:LYS:HG3	1:3:89:GLU:CG	2.27	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:89:GLU:HB2	1:3:90:TYR:HD1	1.64	0.62
1:2:16:LEU:C	1:2:18:ALA:N	2.53	0.62
1:2:232:PRO:HB2	1:3:232:PRO:CG	2.30	0.62
1:4:251:TYR:HB2	1:4:299:LEU:HB3	1.82	0.62
1:4:44:LYS:HB3	1:4:44:LYS:NZ	2.10	0.62
1:3:108:PHE:O	1:3:111:GLY:N	2.33	0.62
1:3:71:THR:CG2	1:3:73:PHE:CZ	2.80	0.62
1:1:128:VAL:C	1:1:132:ASN:HB3	2.17	0.62
1:1:295:ALA:CB	1:4:193:ARG:NH1	2.63	0.62
1:1:277:VAL:CA	1:4:193:ARG:CD	2.73	0.62
1:4:52:PHE:CD1	1:4:53:LYS:CE	2.83	0.62
1:4:134:GLU:O	1:4:134:GLU:OE2	2.17	0.62
1:4:220:LEU:CA	1:4:223:LYS:HZ3	2.00	0.62
1:4:11:ILE:HD12	1:4:11:ILE:H	1.59	0.62
1:2:273:THR:HB	1:2:290:ILE:HD11	1.82	0.62
1:1:108:PHE:HA	1:1:112:ALA:HB3	1.81	0.62
1:1:127:PHE:HZ	1:1:140:MET:SD	2.22	0.62
1:1:144:SER:OG	1:1:145:ASN:N	2.25	0.62
1:1:181:GLN:O	1:2:183:THR:HG23	2.00	0.62
1:1:4:GLY:N	1:1:27:VAL:HG21	2.15	0.62
1:1:57:LYS:O	1:1:64:VAL:HG13	1.99	0.62
1:4:3:ILE:CG2	1:4:4:GLY:H	2.10	0.62
1:2:193:ARG:NH1	1:2:204:PRO:HG2	2.14	0.62
1:3:74:ASN:OD1	1:3:75:GLU:N	2.33	0.62
1:1:188:SER:C	1:1:190:LYS:N	2.51	0.62
1:4:118:SER:C	1:4:316:TYR:HH	2.00	0.62
1:1:52:PHE:O	1:1:53:LYS:HB3	2.00	0.62
1:2:252:ASP:C	1:2:252:ASP:OD1	2.38	0.62
1:2:28:ALA:HA	1:2:71:THR:O	1.99	0.62
1:4:250:SER:O	1:4:253:ASP:N	2.33	0.62
1:4:3:ILE:C	1:4:27:VAL:HG23	2.20	0.62
1:3:196:ARG:CD	1:4:47:SER:OG	2.47	0.62
1:3:49:HIS:CD2	1:3:313:GLU:OE1	2.53	0.62
1:4:170:LEU:CD2	1:4:225:THR:HG22	2.29	0.62
1:4:266:LEU:O	1:4:267:GLN:C	2.38	0.62
1:1:193:ARG:HH11	1:1:204:PRO:CG	2.11	0.61
1:2:220:LEU:HA	1:2:223:LYS:NZ	2.14	0.61
1:4:73:PHE:CD2	1:4:81:ILE:CD1	2.82	0.61
1:3:252:ASP:O	1:3:253:ASP:C	2.39	0.61
1:1:248:GLU:HG2	1:1:302:THR:CG2	2.30	0.61
1:1:165:GLU:OE1	1:1:167:VAL:HG12	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:243:VAL:HG23	1:2:245:LEU:CD2	2.28	0.61
1:3:128:VAL:O	1:3:132:ASN:HB3	1.99	0.61
1:3:241:LEU:O	1:3:305:LYS:HA	2.00	0.61
1:1:303:PHE:CE2	1:4:303:PHE:CE2	2.89	0.61
1:1:1:SER:C	1:1:25:GLN:HG2	2.19	0.61
1:1:209:ALA:O	1:1:213:VAL:HB	2.01	0.61
1:4:183:THR:HG22	1:4:183:THR:O	1.99	0.61
1:1:193:ARG:HE	1:4:277:VAL:HA	1.66	0.61
1:4:138:LYS:HD3	1:4:330:VAL:HG12	1.83	0.61
1:4:108:PHE:O	1:4:110:GLY:N	2.33	0.61
1:1:303:PHE:CE2	1:4:303:PHE:HE2	2.17	0.61
1:1:131:VAL:HG12	1:1:158:LYS:NZ	2.16	0.61
1:1:324:LEU:HD12	1:1:324:LEU:O	2.00	0.61
1:1:81:ILE:CG2	1:1:83:TRP:NE1	2.63	0.61
1:3:6:ASN:OD1	1:3:30:ASN:ND2	2.33	0.61
1:3:152:CYS:HA	1:3:289:SER:HB2	1.80	0.61
1:2:276:ASP:OD1	1:2:277:VAL:CG1	2.48	0.61
1:3:11:ILE:HG22	1:3:15:VAL:CG2	2.30	0.61
1:3:53:LYS:CB	1:3:53:LYS:NZ	2.59	0.61
1:2:16:LEU:C	1:2:18:ALA:H	2.02	0.61
1:4:109:LYS:O	1:4:110:GLY:C	2.39	0.61
1:1:165:GLU:O	1:1:166:ILE:O	2.17	0.61
1:1:282:PHE:CZ	1:1:290:ILE:CD1	2.84	0.61
1:2:132:ASN:ND2	1:2:133:LEU:HG	2.15	0.61
1:2:127:PHE:CZ	1:2:136:TYR:HB2	2.35	0.61
1:4:83:TRP:CA	1:4:86:ALA:CB	2.78	0.61
1:3:83:TRP:CA	1:3:86:ALA:CB	2.79	0.61
1:2:66:ASP:N	1:2:66:ASP:OD2	2.33	0.61
1:4:321:ILE:CG2	1:4:325:LYS:HE3	2.31	0.61
1:1:127:PHE:CE1	1:1:143:VAL:HG21	2.34	0.61
1:2:243:VAL:CG2	1:2:245:LEU:HD23	2.28	0.61
1:3:153:LEU:O	1:3:154:ALA:C	2.39	0.61
1:3:270:LEU:CD2	1:3:271:GLY:N	2.51	0.61
1:3:172:THR:O	1:3:240:ASP:N	2.30	0.61
1:1:128:VAL:CG2	1:1:216:VAL:HG21	2.31	0.61
1:1:193:ARG:HA	1:4:277:VAL:HG12	1.83	0.61
1:4:185:ASP:HA	1:4:196:ARG:HA	1.81	0.61
1:4:66:ASP:C	1:4:68:LYS:HD3	2.20	0.61
1:2:65:VAL:C	1:2:66:ASP:OD2	2.39	0.61
1:1:272:TYR:CE2	1:1:293:ALA:CB	2.83	0.61
1:2:127:PHE:CB	1:2:132:ASN:HB2	2.31	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:281:ASP:O	1:4:283:ILE:N	2.33	0.61
1:4:74:ASN:C	2:4:347:HOH:O	2.12	0.61
1:1:188:SER:O	1:1:189:ALA:C	2.39	0.61
1:4:127:PHE:HB2	1:4:323:LEU:HD21	1.83	0.61
1:4:325:LYS:O	1:4:326:HIS:C	2.39	0.61
1:4:161:HIS:O	1:4:165:GLU:HA	2.01	0.61
1:1:243:VAL:CG2	1:1:304:VAL:HG11	2.30	0.61
1:2:319:ARG:HG2	1:2:319:ARG:NH1	2.15	0.61
1:4:227:MET:CE	1:4:229:PHE:CZ	2.84	0.61
1:4:281:ASP:HA	2:4:357:HOH:O	2.00	0.61
1:3:278:VAL:O	1:3:279:SER:OG	2.17	0.61
1:3:2:LYS:HB3	1:3:2:LYS:NZ	2.10	0.61
1:3:33:PHE:CZ	1:3:76:MET:SD	2.94	0.61
1:4:161:HIS:O	1:4:165:GLU:CA	2.49	0.61
1:4:318:GLN:CA	1:4:318:GLN:OE1	2.47	0.61
1:1:285:ASP:OD2	1:1:285:ASP:C	2.38	0.60
1:1:17:ARG:HB3	1:1:43:PHE:HZ	1.62	0.60
1:4:311:ASP:O	1:4:312:ASN:C	2.40	0.60
1:4:46:ASP:O	1:4:50:GLY:HA2	2.00	0.60
1:4:65:VAL:O	1:4:68:LYS:HD3	2.01	0.60
1:4:85:LYS:O	1:4:86:ALA:CB	2.47	0.60
1:3:296:GLY:H	1:3:297:ILE:CD1	2.14	0.60
1:3:239:VAL:CG1	1:3:310:TYR:CE1	2.83	0.60
1:1:273:THR:HG22	1:1:290:ILE:HD12	1.81	0.60
1:2:154:ALA:HB3	1:2:155:PRO:HD3	1.83	0.60
1:4:292:ASP:O	1:4:294:LYS:N	2.34	0.60
1:3:136:TYR:CD2	1:3:140:MET:SD	2.94	0.60
1:3:283:ILE:HD11	2:3:388:HOH:O	2.01	0.60
1:3:33:PHE:HZ	1:3:76:MET:SD	2.23	0.60
1:3:125:PRO:O	1:3:144:SER:HB3	2.01	0.60
1:4:145:ASN:C	1:4:145:ASN:HD22	2.04	0.60
1:1:293:ALA:O	1:1:294:LYS:CB	2.47	0.60
1:1:321:ILE:O	1:1:325:LYS:HG3	2.00	0.60
1:2:91:ILE:HD12	1:2:91:ILE:N	2.14	0.60
1:1:295:ALA:HB1	1:4:193:ARG:NH1	2.15	0.60
1:4:53:LYS:C	1:4:53:LYS:CD	2.69	0.60
1:4:8:PHE:HD2	1:4:8:PHE:C	2.04	0.60
1:2:173:THR:CG2	1:2:228:ALA:CB	2.79	0.60
1:3:113:LYS:HG2	1:3:114:LYS:HZ2	1.65	0.60
1:3:11:ILE:O	1:3:15:VAL:HG23	2.00	0.60
1:3:272:TYR:HE1	1:3:274:GLU:OE2	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:146:ALA:O	1:3:316:TYR:HE1	1.84	0.60
1:3:119:ALA:HB1	1:3:120:PRO:CD	2.31	0.60
1:3:216:VAL:O	1:3:218:PRO:CD	2.50	0.60
1:1:59:GLU:HB3	1:1:64:VAL:HG11	1.84	0.60
1:1:90:TYR:HA	1:1:114:LYS:O	2.00	0.60
1:3:275:ASP:O	1:3:275:ASP:OD2	2.18	0.60
1:3:294:LYS:CA	1:3:297:ILE:HG13	2.30	0.60
1:3:250:SER:HA	1:3:299:LEU:CD1	2.30	0.60
1:2:208:GLY:HA3	1:2:211:LYS:HG2	1.83	0.60
1:3:32:PRO:HG3	1:3:75:GLU:C	2.22	0.60
1:1:196:ARG:HG3	1:1:197:GLY:H	1.66	0.60
1:1:19:ALA:CA	1:1:24:ALA:HB3	2.31	0.60
1:2:25:GLN:O	1:2:26:VAL:O	2.20	0.60
1:2:4:GLY:CA	1:2:27:VAL:CG2	2.80	0.60
1:3:127:PHE:CB	1:3:323:LEU:HD21	2.30	0.60
1:4:127:PHE:HE1	1:4:140:MET:CE	2.15	0.60
1:3:178:THR:OG1	1:3:181:GLN:HB2	2.01	0.60
1:1:319:ARG:NH1	1:1:319:ARG:HG2	2.15	0.60
1:3:132:ASN:OD1	1:3:133:LEU:HD23	2.02	0.60
1:1:106:ALA:O	1:1:107:HIS:C	2.39	0.60
1:2:89:GLU:O	1:2:114:LYS:HG3	2.02	0.60
1:4:2:LYS:HZ1	1:4:88:ALA:HA	1.66	0.60
1:3:11:ILE:HD12	1:3:11:ILE:N	2.16	0.60
1:3:4:GLY:CA	1:3:27:VAL:HG23	2.29	0.60
1:4:243:VAL:HG23	1:4:304:VAL:CG1	2.28	0.60
1:1:163:ASN:OD1	1:1:163:ASN:O	2.20	0.60
1:1:8:PHE:CE1	1:1:39:MET:SD	2.95	0.60
1:3:131:VAL:O	1:3:131:VAL:HG23	2.02	0.60
1:4:116:VAL:HG11	1:4:324:LEU:HD22	1.82	0.60
1:4:150:THR:HG23	1:4:212:ALA:HB3	1.83	0.60
1:4:113:LYS:CG	1:4:114:LYS:HE3	2.32	0.60
1:1:119:ALA:HB1	1:1:120:PRO:HD2	1.84	0.60
1:1:83:TRP:HA	1:1:86:ALA:CB	2.30	0.60
1:2:104:ALA:CB	1:2:142:VAL:HG21	2.32	0.60
1:2:127:PHE:HB3	1:2:132:ASN:HB2	1.84	0.60
1:4:8:PHE:CZ	1:4:39:MET:CB	2.84	0.60
1:4:127:PHE:CZ	1:4:135:LYS:NZ	2.70	0.60
1:1:1:SER:OG	1:1:25:GLN:CB	2.36	0.59
1:1:90:TYR:CZ	1:1:328:GLN:CD	2.76	0.59
1:3:101:ILE:HD13	2:3:380:HOH:O	2.02	0.59
1:3:26:VAL:HB	1:3:70:ILE:CG2	2.32	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:200:GLN:OE1	1:2:48:THR:HG23	2.02	0.59
1:1:112:ALA:O	1:1:113:LYS:HG3	2.01	0.59
1:1:193:ARG:NH1	1:1:204:PRO:CG	2.65	0.59
1:2:125:PRO:HB2	1:2:143:VAL:HG23	1.84	0.59
1:2:216:VAL:CG1	1:2:217:ILE:N	2.65	0.59
1:2:277:VAL:CG2	1:2:278:VAL:H	2.08	0.59
1:4:66:ASP:O	1:4:68:LYS:HD3	2.01	0.59
1:3:22:CYS:SG	1:3:321:ILE:HG21	2.41	0.59
1:3:52:PHE:CA	2:3:370:HOH:O	2.29	0.59
1:2:54:GLY:O	1:2:56:VAL:N	2.34	0.59
1:1:295:ALA:CA	1:1:297:ILE:HD12	2.33	0.59
1:1:31:ASP:HB3	1:1:34:ILE:CG2	2.32	0.59
1:1:74:ASN:OD1	1:1:75:GLU:N	2.35	0.59
1:4:1:SER:CB	1:4:25:GLN:HE21	2.04	0.59
1:4:77:LYS:O	2:4:348:HOH:O	2.11	0.59
1:4:8:PHE:C	1:4:8:PHE:CD2	2.75	0.59
1:3:173:THR:O	1:3:228:ALA:HA	2.02	0.59
1:4:53:LYS:CB	1:4:53:LYS:NZ	2.52	0.59
1:3:74:ASN:HB2	2:3:365:HOH:O	2.01	0.59
1:2:16:LEU:O	1:2:18:ALA:N	2.35	0.59
1:1:281:ASP:O	1:1:283:ILE:HB	2.01	0.59
1:2:154:ALA:HB3	1:2:155:PRO:CD	2.33	0.59
1:2:165:GLU:O	1:2:166:ILE:HB	2.02	0.59
1:3:78:PRO:O	1:3:81:ILE:HG22	2.02	0.59
1:4:64:VAL:HG22	1:4:64:VAL:O	2.01	0.59
1:1:113:LYS:CB	1:1:114:LYS:HD2	2.18	0.59
1:1:153:LEU:O	1:1:154:ALA:C	2.41	0.59
1:1:294:LYS:C	1:1:297:ILE:HD12	2.23	0.59
1:1:30:ASN:ND2	1:1:30:ASN:O	2.35	0.59
1:4:160:LEU:HD22	1:4:245:LEU:HD21	1.85	0.59
1:4:153:LEU:HD21	1:4:241:LEU:HD13	1.84	0.59
1:4:44:LYS:CG	1:4:56:VAL:HG11	2.32	0.59
1:4:101:ILE:HG23	1:4:142:VAL:CG1	2.32	0.59
1:2:298:GLN:HE22	1:3:225:THR:CG2	2.14	0.59
1:3:126:MET:CE	1:3:212:ALA:HA	2.32	0.59
1:1:244:ARG:HH22	1:4:244:ARG:CG	2.16	0.59
1:1:251:TYR:CD2	1:1:254:ILE:HG21	2.37	0.59
1:2:242:THR:HA	1:2:304:VAL:O	2.02	0.59
1:4:156:VAL:HA	1:4:258:MET:HE2	1.84	0.59
1:3:287:ARG:HH11	1:3:290:ILE:HG21	1.66	0.59
1:3:325:LYS:O	1:3:328:GLN:N	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:78:PRO:HG3	1:3:98:PHE:CD2	2.38	0.59
1:4:320:VAL:O	1:4:324:LEU:HB2	2.02	0.59
1:1:311:ASP:O	1:1:313:GLU:N	2.35	0.59
1:2:127:PHE:CE2	1:2:136:TYR:CB	2.82	0.59
1:2:127:PHE:CA	1:2:132:ASN:HB2	2.33	0.59
1:2:40:VAL:HG22	1:2:41:TYR:N	2.18	0.59
1:4:270:LEU:CD2	1:4:271:GLY:N	2.44	0.59
1:4:251:TYR:OH	1:4:291:PHE:HZ	1.78	0.59
1:4:3:ILE:HG22	1:4:4:GLY:N	2.17	0.59
1:1:41:TYR:CE1	1:3:277:VAL:CG2	2.74	0.59
1:3:156:VAL:HG22	1:3:258:MET:CE	2.32	0.59
1:2:132:ASN:CG	1:2:133:LEU:N	2.55	0.59
1:2:4:GLY:HA2	1:2:27:VAL:HG22	1.85	0.59
1:4:52:PHE:O	1:4:53:LYS:CB	2.45	0.59
1:4:56:VAL:O	1:4:56:VAL:HG22	2.02	0.59
1:2:297:ILE:HD12	1:2:297:ILE:H	1.64	0.59
1:1:277:VAL:HG12	1:4:193:ARG:HG3	1.85	0.59
1:3:134:GLU:O	1:3:135:LYS:C	2.40	0.59
1:3:329:LYS:C	1:3:329:LYS:HZ3	2.06	0.59
1:4:128:VAL:HG13	1:4:151:ASN:ND2	2.18	0.59
1:1:210:ALA:HB2	1:1:224:LEU:O	2.03	0.58
1:2:293:ALA:O	1:2:294:LYS:CG	2.50	0.58
1:4:53:LYS:CD	1:4:54:GLY:N	2.63	0.58
1:3:49:HIS:HD2	1:3:313:GLU:OE1	1.83	0.58
1:2:44:LYS:CD	1:2:56:VAL:HG21	2.32	0.58
1:4:132:ASN:HD21	1:4:133:LEU:CD2	2.12	0.58
1:2:298:GLN:OE1	1:3:225:THR:HG23	2.03	0.58
1:2:208:GLY:HA3	1:2:211:LYS:CG	2.33	0.58
1:1:112:ALA:O	1:1:113:LYS:CB	2.52	0.58
1:3:132:ASN:ND2	1:3:133:LEU:HG	2.18	0.58
1:3:265:PRO:O	1:3:267:GLN:N	2.36	0.58
1:3:265:PRO:C	1:3:267:GLN:N	2.56	0.58
1:2:250:SER:C	1:2:252:ASP:N	2.55	0.58
1:2:33:PHE:C	1:2:34:ILE:HG22	2.18	0.58
1:4:42:MET:CG	1:4:42:MET:O	2.49	0.58
1:2:185:ASP:HA	1:2:195:GLY:O	2.04	0.58
1:4:325:LYS:O	1:4:328:GLN:N	2.37	0.58
1:1:298:GLN:CD	1:4:225:THR:HG23	2.23	0.58
1:1:212:ALA:O	1:1:216:VAL:CB	2.48	0.58
1:1:276:ASP:OD1	1:1:277:VAL:CG2	2.52	0.58
1:1:296:GLY:N	1:1:297:ILE:HD12	2.18	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:44:LYS:HG2	1:1:56:VAL:HG21	1.85	0.58
1:4:34:ILE:HD12	1:4:42:MET:SD	2.43	0.58
1:3:164:PHE:HZ	1:3:253:ASP:HB3	1.68	0.58
1:3:255:LYS:HB3	1:3:255:LYS:HZ3	1.66	0.58
1:3:78:PRO:HD3	1:3:98:PHE:CZ	2.38	0.58
1:2:44:LYS:O	1:2:51:VAL:HA	2.04	0.58
1:4:132:ASN:HD21	1:4:133:LEU:HD21	1.67	0.58
1:4:126:MET:HB2	1:4:215:LYS:HD3	1.85	0.58
1:1:93:GLU:OE2	1:1:98:PHE:CD2	2.56	0.58
1:1:181:GLN:O	1:2:183:THR:CG2	2.51	0.58
1:2:113:LYS:C	1:2:114:LYS:HG2	2.02	0.58
1:2:3:ILE:HD13	1:2:324:LEU:HD11	1.83	0.58
1:3:134:GLU:C	1:3:136:TYR:H	2.06	0.58
1:3:90:TYR:CD1	1:3:90:TYR:N	2.71	0.58
1:3:119:ALA:HB1	1:3:120:PRO:HD3	1.85	0.58
1:3:220:LEU:HA	1:3:223:LYS:HZ2	1.67	0.58
1:3:118:SER:O	1:3:118:SER:OG	2.20	0.58
1:2:95:THR:CG2	1:2:97:VAL:HG23	2.34	0.58
1:3:188:SER:O	1:3:189:ALA:C	2.41	0.58
1:4:196:ARG:HG3	1:4:197:GLY:N	2.16	0.58
1:3:114:LYS:N	1:3:114:LYS:HE3	2.18	0.58
1:3:20:LEU:C	1:3:22:CYS:H	2.07	0.58
1:3:241:LEU:HG	1:3:243:VAL:HG13	1.85	0.58
1:3:276:ASP:CG	1:3:277:VAL:H	1.88	0.58
1:1:167:VAL:HG22	1:1:244:ARG:HG2	1.84	0.58
1:3:146:ALA:HB1	1:3:150:THR:HG21	1.85	0.58
1:3:155:PRO:O	1:3:159:VAL:HG23	2.03	0.58
1:3:299:LEU:CD2	1:3:300:SER:H	2.14	0.58
1:2:44:LYS:NZ	1:2:45:TYR:CE2	2.69	0.58
1:4:127:PHE:CE2	1:4:135:LYS:HG3	2.38	0.58
1:1:250:SER:O	1:1:251:TYR:C	2.41	0.58
1:1:31:ASP:HB3	1:1:34:ILE:HG23	1.84	0.58
1:4:236:VAL:CG1	1:4:237:SER:H	2.16	0.58
1:3:270:LEU:CD2	1:3:270:LEU:C	2.70	0.58
1:2:10:ARG:NH1	1:2:46:ASP:OD2	2.36	0.58
1:2:44:LYS:HB3	1:2:56:VAL:HG21	1.86	0.58
1:4:127:PHE:CD1	1:4:143:VAL:CG2	2.85	0.58
1:2:244:ARG:CD	1:3:244:ARG:HH12	2.15	0.58
1:1:161:HIS:O	1:1:163:ASN:N	2.35	0.58
1:1:277:VAL:O	1:1:278:VAL:C	2.42	0.58
1:4:53:LYS:HD2	1:4:54:GLY:CA	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:91:ILE:HD13	1:2:115:VAL:CG2	2.22	0.58
1:3:279:SER:O	1:3:281:ASP:N	2.29	0.58
1:3:287:ARG:HH11	1:3:290:ILE:CG2	2.17	0.58
1:3:77:LYS:O	1:3:80:ASN:HB2	2.03	0.58
1:2:36:LEU:HD21	1:2:62:ALA:C	2.25	0.58
1:1:322:ASP:O	1:1:323:LEU:C	2.41	0.57
1:2:150:THR:HG21	1:2:212:ALA:CB	2.34	0.57
1:2:266:LEU:HD13	2:2:412:HOH:O	2.04	0.57
1:2:231:VAL:HB	1:3:231:VAL:HG12	1.86	0.57
1:3:52:PHE:C	1:3:53:LYS:HE2	2.25	0.57
1:1:305:LYS:HD3	1:4:227:MET:SD	2.44	0.57
1:2:128:VAL:H	1:2:132:ASN:HB2	1.69	0.57
1:3:249:CYS:SG	1:3:254:ILE:HD11	2.44	0.57
1:3:279:SER:C	1:3:281:ASP:N	2.57	0.57
1:3:168:GLU:OE2	1:3:244:ARG:NE	2.37	0.57
1:1:28:ALA:HB1	1:1:73:PHE:CE2	2.39	0.57
1:2:128:VAL:H	1:2:132:ASN:HB3	1.69	0.57
1:4:176:ALA:O	1:4:177:VAL:O	2.23	0.57
1:4:261:ALA:O	1:4:262:SER:C	2.43	0.57
1:1:252:ASP:O	1:1:255:LYS:CG	2.53	0.57
1:1:7:GLY:O	1:1:8:PHE:CB	2.40	0.57
1:2:78:PRO:C	1:2:80:ASN:H	2.05	0.57
1:1:232:PRO:HB2	1:4:232:PRO:HB2	1.86	0.57
1:3:26:VAL:C	1:3:27:VAL:CG1	2.57	0.57
1:3:84:SER:O	1:3:85:LYS:C	2.41	0.57
1:4:269:PHE:O	1:4:288:SER:HB3	2.02	0.57
1:4:319:ARG:O	1:4:322:ASP:N	2.36	0.57
1:1:279:SER:C	1:1:281:ASP:H	2.06	0.57
1:3:41:TYR:OH	1:4:196:ARG:NH1	2.37	0.57
1:4:83:TRP:C	1:4:86:ALA:HB3	2.24	0.57
1:4:126:MET:HA	1:4:144:SER:O	2.04	0.57
1:4:159:VAL:O	1:4:160:LEU:C	2.41	0.57
1:4:251:TYR:OH	1:4:291:PHE:CZ	2.55	0.57
1:4:38:TYR:O	1:4:42:MET:HB2	2.04	0.57
1:3:291:PHE:CE2	1:3:306:VAL:HB	2.39	0.57
1:3:296:GLY:N	1:3:297:ILE:HG23	2.20	0.57
1:3:319:ARG:HG2	1:3:319:ARG:NH1	2.19	0.57
1:3:32:PRO:O	1:3:33:PHE:CD1	2.58	0.57
1:3:216:VAL:O	1:3:218:PRO:HD2	2.05	0.57
1:1:205:SER:CB	1:1:228:ALA:HB3	2.33	0.57
1:1:172:THR:O	1:1:240:ASP:N	2.34	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:161:HIS:CA	1:2:166:ILE:HG13	2.35	0.57
1:4:276:ASP:OD1	1:4:277:VAL:N	2.38	0.57
1:1:41:TYR:HE1	1:3:277:VAL:CG2	2.13	0.57
1:3:95:THR:CG2	1:3:97:VAL:HG22	2.34	0.57
1:1:188:SER:HB2	1:1:192:TRP:HA	1.86	0.57
1:4:11:ILE:HD13	1:4:11:ILE:H	1.66	0.57
1:2:193:ARG:HH12	1:3:295:ALA:CB	2.17	0.57
1:3:258:MET:CG	1:3:270:LEU:HD11	2.32	0.57
1:3:330:VAL:O	1:3:331:ASP:C	2.43	0.57
1:1:152:CYS:SG	1:1:239:VAL:HG11	2.43	0.57
1:1:213:VAL:HA	1:1:216:VAL:CG1	2.35	0.57
1:1:52:PHE:O	1:1:53:LYS:HE2	2.05	0.57
1:4:4:GLY:N	1:4:27:VAL:CG2	2.68	0.57
1:4:44:LYS:HE3	1:4:45:TYR:CD2	2.39	0.57
1:3:36:LEU:O	1:3:40:VAL:HG12	2.04	0.57
1:1:213:VAL:C	1:1:216:VAL:HG12	2.25	0.57
1:3:55:GLU:HB2	1:3:66:ASP:HA	1.87	0.57
1:4:104:ALA:O	1:4:106:ALA:N	2.37	0.57
1:2:244:ARG:HG3	1:3:244:ARG:CZ	2.34	0.57
1:1:101:ILE:HG22	1:1:105:SER:HG	1.67	0.56
1:1:128:VAL:H	1:1:132:ASN:HB3	1.70	0.56
1:1:127:PHE:CD2	1:1:136:TYR:HB2	2.36	0.56
1:1:251:TYR:N	1:1:299:LEU:CD1	2.67	0.56
1:1:10:ARG:HH12	1:1:46:ASP:CG	2.07	0.56
1:1:277:VAL:CG1	1:3:41:TYR:OH	2.49	0.56
1:4:193:ARG:O	1:4:203:ILE:CG2	2.53	0.56
1:4:76:MET:HG3	1:4:76:MET:O	2.05	0.56
1:3:138:LYS:HZ2	1:3:330:VAL:HG11	1.63	0.56
1:3:282:PHE:O	1:3:283:ILE:C	2.42	0.56
1:3:90:TYR:CD2	1:3:328:GLN:NE2	2.69	0.56
1:2:65:VAL:O	1:2:68:LYS:HD3	2.04	0.56
1:2:244:ARG:HH22	1:3:244:ARG:CG	2.17	0.56
1:4:22:CYS:SG	1:4:318:GLN:NE2	2.78	0.56
1:1:168:GLU:OE2	1:1:244:ARG:CZ	2.53	0.56
1:1:277:VAL:CA	1:4:193:ARG:HD3	2.34	0.56
1:2:251:TYR:CZ	1:2:297:ILE:HB	2.40	0.56
1:2:188:SER:HB3	1:2:192:TRP:HA	1.86	0.56
1:3:161:HIS:CG	1:3:162:GLU:N	2.72	0.56
1:2:318:GLN:OE1	1:2:318:GLN:CA	2.45	0.56
1:1:26:VAL:HB	1:1:70:ILE:HG22	1.86	0.56
1:2:153:LEU:HD12	1:2:171:MET:SD	2.45	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:216:VAL:O	1:2:218:PRO:HD2	2.04	0.56
1:4:236:VAL:O	1:4:237:SER:CB	2.51	0.56
1:1:17:ARG:CB	1:1:43:PHE:CE2	2.88	0.56
1:4:54:GLY:HA3	1:4:66:ASP:OD2	2.05	0.56
1:2:193:ARG:NH1	1:3:295:ALA:HB1	2.20	0.56
1:3:297:ILE:N	1:3:297:ILE:CD1	2.69	0.56
1:3:282:PHE:CE2	1:3:309:TRP:CG	2.92	0.56
1:3:83:TRP:C	1:3:86:ALA:HB3	2.25	0.56
1:4:79:GLU:OE1	1:4:79:GLU:N	2.39	0.56
1:1:126:MET:CG	1:1:146:ALA:HB2	2.35	0.56
1:1:126:MET:CE	1:1:215:LYS:HZ2	2.17	0.56
1:2:44:LYS:HD3	1:2:56:VAL:HG21	1.88	0.56
1:1:14:LEU:O	1:1:18:ALA:N	2.39	0.56
1:2:161:HIS:CG	1:2:165:GLU:O	2.57	0.56
1:2:243:VAL:HG22	1:2:304:VAL:HG12	1.87	0.56
1:2:30:ASN:HA	1:2:73:PHE:O	2.06	0.56
1:4:276:ASP:CG	1:4:277:VAL:H	2.01	0.56
1:1:193:ARG:CG	1:4:277:VAL:HA	2.36	0.56
1:3:164:PHE:CD2	1:3:249:CYS:HB3	2.40	0.56
1:2:19:ALA:CA	1:2:24:ALA:HB3	2.35	0.56
1:4:117:ILE:HD12	1:4:121:SER:OG	2.04	0.56
1:4:127:PHE:CB	1:4:132:ASN:HB2	2.34	0.56
1:4:328:GLN:O	1:4:332:SER:HB2	2.04	0.56
1:2:137:SER:CB	1:2:138:LYS:NZ	2.67	0.56
1:4:187:PRO:CG	1:4:187:PRO:O	2.53	0.56
1:1:248:GLU:HG2	1:1:302:THR:HG22	1.87	0.56
1:1:8:PHE:HZ	1:1:39:MET:HB3	1.71	0.56
1:2:277:VAL:HA	1:3:193:ARG:HG3	1.87	0.56
1:2:41:TYR:HH	1:4:277:VAL:HG11	1.69	0.56
1:4:314:PHE:HA	1:4:317:SER:OG	2.06	0.56
1:3:154:ALA:HB1	1:3:155:PRO:HD3	1.84	0.56
1:3:271:GLY:O	1:3:272:TYR:HB3	2.05	0.56
1:1:188:SER:C	1:1:190:LYS:H	2.08	0.56
1:4:216:VAL:HG13	1:4:217:ILE:N	2.18	0.56
1:1:216:VAL:CG1	1:1:217:ILE:N	2.69	0.56
1:1:22:CYS:SG	1:1:321:ILE:CG2	2.92	0.56
1:4:255:LYS:CD	1:4:293:ALA:HB1	2.34	0.56
1:4:2:LYS:HZ3	1:4:88:ALA:HA	1.65	0.56
1:3:305:LYS:HG2	1:3:305:LYS:O	2.05	0.56
1:3:66:ASP:C	1:3:68:LYS:HD3	2.25	0.56
1:4:212:ALA:O	1:4:216:VAL:N	2.39	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:175:HIS:CD2	1:1:230:ARG:NH2	2.74	0.56
1:1:253:ASP:O	1:1:254:ILE:C	2.42	0.56
1:1:8:PHE:HD1	1:1:29:VAL:HG11	1.70	0.56
1:2:116:VAL:HA	1:2:143:VAL:O	2.05	0.56
1:4:272:TYR:HA	1:4:291:PHE:O	2.05	0.56
1:4:239:VAL:HG13	1:4:310:TYR:CE1	2.41	0.56
1:3:287:ARG:NH1	1:3:290:ILE:CD1	2.68	0.56
1:3:299:LEU:CD2	1:3:304:VAL:HG23	2.35	0.56
1:3:89:GLU:HB2	1:3:90:TYR:CD1	2.40	0.56
1:4:106:ALA:O	1:4:107:HIS:C	2.43	0.56
1:4:113:LYS:C	1:4:114:LYS:HE3	2.26	0.56
1:2:296:GLY:O	1:2:307:VAL:CG2	2.51	0.56
1:2:11:ILE:O	1:2:15:VAL:HG23	2.05	0.56
1:3:167:VAL:HG22	1:3:168:GLU:H	1.70	0.56
1:1:164:PHE:O	1:1:165:GLU:HB2	2.06	0.56
1:1:213:VAL:CA	1:1:216:VAL:HG12	2.36	0.56
1:1:217:ILE:HG12	1:1:220:LEU:HD22	1.86	0.56
1:1:53:LYS:NZ	1:1:53:LYS:CB	2.60	0.56
1:2:113:LYS:HB3	1:2:114:LYS:HE3	1.86	0.56
1:2:272:TYR:OH	1:2:274:GLU:CD	2.45	0.56
1:3:184:VAL:O	1:3:184:VAL:HG13	2.06	0.56
1:2:277:VAL:CA	1:3:193:ARG:NE	2.68	0.56
1:4:19:ALA:HB1	1:4:24:ALA:HB3	1.87	0.56
1:4:292:ASP:O	1:4:297:ILE:HG21	2.06	0.56
1:4:52:PHE:CD1	1:4:53:LYS:HE3	2.41	0.56
1:3:4:GLY:N	1:3:27:VAL:HG21	2.20	0.56
1:4:133:LEU:HD23	1:4:133:LEU:H	1.71	0.56
1:1:167:VAL:HG13	1:1:245:LEU:O	2.06	0.55
1:1:46:ASP:O	1:1:50:GLY:HA3	2.06	0.55
1:2:91:ILE:CD1	1:2:114:LYS:O	2.50	0.55
1:2:299:LEU:CG	1:2:304:VAL:HG23	2.35	0.55
1:2:93:GLU:OE2	1:2:98:PHE:CD2	2.59	0.55
1:4:232:PRO:O	1:4:233:THR:O	2.24	0.55
1:4:39:MET:HE1	1:4:72:VAL:HB	1.87	0.55
1:2:185:ASP:OD1	1:2:185:ASP:N	2.39	0.55
1:2:14:LEU:H	1:2:14:LEU:HD13	1.70	0.55
1:4:220:LEU:O	1:4:221:ASP:C	2.45	0.55
1:1:95:THR:HG23	1:1:97:VAL:HG23	1.87	0.55
1:3:302:THR:O	1:3:302:THR:OG1	2.24	0.55
1:1:220:LEU:CB	1:1:223:LYS:HZ2	2.19	0.55
1:1:282:PHE:HZ	1:1:290:ILE:HD13	1.64	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:314:PHE:HB2	1:1:317:SER:CB	2.37	0.55
1:1:71:THR:HG22	1:1:72:VAL:O	2.05	0.55
1:4:28:ALA:HB1	1:4:73:PHE:CE2	2.40	0.55
1:3:3:ILE:CG2	1:3:4:GLY:H	2.14	0.55
1:2:126:MET:CB	1:2:215:LYS:NZ	2.66	0.55
1:1:133:LEU:O	1:1:136:TYR:HB3	2.06	0.55
1:3:188:SER:O	1:3:191:ASP:N	2.40	0.55
1:4:17:ARG:NH1	2:4:452:HOH:O	2.39	0.55
1:3:131:VAL:HG12	1:3:158:LYS:CE	2.36	0.55
1:3:128:VAL:O	1:3:132:ASN:CB	2.53	0.55
1:3:259:LYS:HG3	1:3:272:TYR:CD1	2.41	0.55
1:3:44:LYS:O	1:3:51:VAL:CA	2.52	0.55
1:3:50:GLY:C	1:3:51:VAL:CG2	2.70	0.55
1:4:59:GLU:O	1:4:60:ASP:C	2.44	0.55
1:1:116:VAL:HA	1:1:143:VAL:O	2.06	0.55
1:1:251:TYR:O	1:1:252:ASP:C	2.45	0.55
1:1:282:PHE:HD1	1:1:285:ASP:OD1	1.90	0.55
1:2:104:ALA:HB3	1:2:142:VAL:HG21	1.88	0.55
1:2:293:ALA:O	1:2:294:LYS:HG2	2.06	0.55
1:3:128:VAL:C	1:3:132:ASN:HD22	2.08	0.55
1:1:93:GLU:OE2	1:1:98:PHE:HD2	1.88	0.55
1:1:128:VAL:HG11	1:1:154:ALA:HB2	1.88	0.55
1:1:276:ASP:C	1:1:277:VAL:CG2	2.74	0.55
1:1:283:ILE:HG22	1:1:283:ILE:O	2.07	0.55
1:2:83:TRP:HD1	1:2:112:ALA:HB2	1.72	0.55
1:4:26:VAL:CA	1:4:27:VAL:HG12	2.36	0.55
1:1:105:SER:O	1:1:107:HIS:N	2.39	0.55
1:2:295:ALA:HB2	1:3:193:ARG:HH12	1.66	0.55
1:3:127:PHE:CZ	1:3:140:MET:CE	2.89	0.55
1:4:287:ARG:O	1:4:288:SER:CB	2.53	0.55
1:4:182:LYS:HE3	1:4:187:PRO:HG3	1.89	0.55
1:1:112:ALA:O	1:1:113:LYS:HB2	2.07	0.55
1:1:8:PHE:CZ	1:1:39:MET:HB3	2.41	0.55
1:1:83:TRP:CZ2	1:1:91:ILE:HG21	2.41	0.55
1:4:181:GLN:HE21	1:4:203:ILE:CD1	1.99	0.55
1:4:227:MET:HE1	1:4:229:PHE:CE1	2.41	0.55
1:4:292:ASP:HB3	1:4:307:VAL:HG13	1.87	0.55
1:4:251:TYR:H	1:4:299:LEU:HG	1.72	0.55
1:4:313:GLU:O	1:4:317:SER:OG	2.24	0.55
1:2:65:VAL:O	1:2:66:ASP:HB2	2.06	0.55
1:4:132:ASN:CG	1:4:133:LEU:HD23	2.26	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:143:VAL:HG22	1:4:144:SER:N	2.20	0.55
1:1:101:ILE:C	1:1:105:SER:HG	2.07	0.55
1:4:78:PRO:HG3	1:4:98:PHE:CD2	2.39	0.55
1:4:95:THR:HG22	1:4:97:VAL:HG23	1.88	0.55
1:1:270:LEU:C	1:1:270:LEU:CD2	2.73	0.55
1:1:2:LYS:HA	1:1:25:GLN:HG2	1.89	0.55
1:2:294:LYS:HA	1:2:297:ILE:HG13	1.88	0.55
1:2:6:ASN:CG	1:2:30:ASN:HD21	2.10	0.55
1:4:4:GLY:CA	1:4:27:VAL:HG21	2.37	0.55
1:3:1:SER:O	1:3:25:GLN:NE2	2.40	0.55
1:4:287:ARG:O	1:4:319:ARG:NH1	2.40	0.55
1:3:59:GLU:O	1:3:61:GLY:N	2.40	0.55
1:2:132:ASN:ND2	1:2:133:LEU:CG	2.69	0.55
1:2:319:ARG:O	1:2:320:VAL:C	2.46	0.55
1:2:39:MET:O	1:2:42:MET:N	2.40	0.55
1:2:94:SER:O	1:2:96:GLY:N	2.40	0.55
1:4:252:ASP:O	1:4:255:LYS:N	2.40	0.55
1:3:101:ILE:HG22	1:3:102:GLU:N	2.21	0.55
1:3:270:LEU:HD23	1:3:271:GLY:CA	2.36	0.55
1:4:188:SER:HB3	1:4:191:ASP:C	2.27	0.55
1:1:79:GLU:HB2	1:1:109:LYS:HD3	1.89	0.54
1:2:113:LYS:HB3	1:2:114:LYS:CE	2.37	0.54
1:2:3:ILE:HG22	1:2:4:GLY:O	2.06	0.54
1:3:236:VAL:O	1:3:237:SER:CB	2.42	0.54
1:4:201:ASN:HB3	1:4:203:ILE:CG1	2.37	0.54
1:2:188:SER:HB3	1:2:192:TRP:CA	2.37	0.54
1:4:316:TYR:CE2	1:4:320:VAL:HG23	2.42	0.54
1:2:138:LYS:HZ2	1:2:138:LYS:H	1.54	0.54
1:1:3:ILE:CG2	1:1:4:GLY:H	2.10	0.54
1:2:221:ASP:O	1:2:221:ASP:OD2	2.25	0.54
1:3:190:LYS:HE2	1:3:190:LYS:N	2.23	0.54
1:3:150:THR:CG2	1:3:151:ASN:N	2.71	0.54
1:3:266:LEU:O	1:3:267:GLN:O	2.25	0.54
1:3:39:MET:O	1:3:42:MET:N	2.40	0.54
1:3:44:LYS:HG2	1:3:56:VAL:HG21	1.88	0.54
1:3:120:PRO:O	1:3:120:PRO:HD2	2.07	0.54
1:1:19:ALA:O	1:1:24:ALA:HB3	2.06	0.54
1:1:276:ASP:OD1	1:1:277:VAL:CG1	2.54	0.54
1:1:56:VAL:O	1:1:57:LYS:HE2	2.07	0.54
1:1:81:ILE:HG23	1:1:83:TRP:NE1	2.22	0.54
1:3:175:HIS:HB3	1:3:230:ARG:HH21	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:66:ASP:HB3	1:4:68:LYS:HE2	1.89	0.54
1:3:161:HIS:CA	1:3:166:ILE:HG13	2.38	0.54
1:3:249:CYS:SG	1:3:250:SER:N	2.79	0.54
1:3:272:TYR:CE1	1:3:274:GLU:OE2	2.61	0.54
1:1:101:ILE:CB	1:1:142:VAL:HG11	2.37	0.54
1:1:142:VAL:O	1:1:142:VAL:CG1	2.55	0.54
1:1:1:SER:HB3	1:1:25:GLN:HE21	1.73	0.54
1:1:89:GLU:HB3	1:1:90:TYR:HD1	1.69	0.54
1:2:91:ILE:HG21	1:2:107:HIS:NE2	2.23	0.54
1:4:8:PHE:HD1	1:4:29:VAL:HG11	1.72	0.54
1:3:259:LYS:HG3	1:3:272:TYR:CE1	2.43	0.54
1:4:217:ILE:CD1	1:4:220:LEU:HD22	2.38	0.54
1:2:36:LEU:HD12	1:2:36:LEU:O	2.07	0.54
1:1:108:PHE:O	1:1:109:LYS:C	2.46	0.54
1:1:145:ASN:CB	1:1:323:LEU:CD2	2.78	0.54
1:1:3:ILE:HG13	1:1:25:GLN:O	2.08	0.54
1:1:26:VAL:CG1	1:1:70:ILE:CG2	2.80	0.54
1:4:271:GLY:O	1:4:272:TYR:HB3	2.08	0.54
1:3:164:PHE:CE2	1:3:249:CYS:HB2	2.43	0.54
1:1:93:GLU:OE2	1:1:98:PHE:HB2	2.08	0.54
1:1:216:VAL:HG13	1:1:217:ILE:N	2.21	0.54
1:1:272:TYR:OH	1:1:274:GLU:CG	2.56	0.54
1:1:296:GLY:HA2	1:4:227:MET:HG2	1.88	0.54
1:1:30:ASN:N	1:1:30:ASN:HD22	2.04	0.54
1:2:3:ILE:CD1	1:2:324:LEU:HD12	2.36	0.54
1:3:183:THR:O	1:3:184:VAL:HB	2.07	0.54
1:4:185:ASP:C	1:4:195:GLY:O	2.46	0.54
1:4:251:TYR:HB2	1:4:299:LEU:CG	2.38	0.54
1:4:44:LYS:CE	1:4:45:TYR:HE2	2.20	0.54
1:4:78:PRO:CD	1:4:98:PHE:CZ	2.90	0.54
1:1:324:LEU:CD1	1:1:324:LEU:O	2.56	0.54
1:3:282:PHE:CE2	1:3:309:TRP:CD1	2.96	0.54
1:4:329:LYS:HZ2	1:4:329:LYS:C	2.07	0.54
1:1:263:GLU:O	1:1:264:GLY:O	2.26	0.54
1:3:187:PRO:O	1:3:187:PRO:HG2	2.07	0.54
1:1:101:ILE:HG13	1:1:123:ASP:OD1	2.08	0.54
1:1:295:ALA:O	1:1:307:VAL:HG11	2.07	0.54
1:2:294:LYS:CA	1:2:297:ILE:HG13	2.38	0.54
1:4:171:MET:O	1:4:227:MET:N	2.32	0.54
1:3:113:LYS:CG	1:3:114:LYS:HZ2	2.21	0.54
1:3:8:PHE:CZ	1:3:39:MET:CG	2.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:182:LYS:HE2	1:4:187:PRO:HG2	1.90	0.54
1:1:128:VAL:N	1:1:132:ASN:HB3	2.22	0.54
1:1:141:THR:OG1	1:1:142:VAL:HB	2.08	0.54
1:1:154:ALA:CB	1:1:155:PRO:CD	2.65	0.54
1:2:296:GLY:HA2	1:3:227:MET:SD	2.47	0.54
1:4:175:HIS:CG	1:4:230:ARG:HH21	2.26	0.54
1:4:314:PHE:HB2	1:4:317:SER:HB2	1.89	0.54
1:4:6:ASN:O	1:4:94:SER:HB3	2.08	0.54
1:3:8:PHE:HD1	1:3:29:VAL:CG1	2.17	0.54
1:4:126:MET:CG	1:4:146:ALA:HB2	2.37	0.54
1:3:220:LEU:HD12	1:3:223:LYS:HG3	1.89	0.54
1:1:14:LEU:HA	1:1:17:ARG:CG	2.35	0.54
1:1:70:ILE:O	1:1:70:ILE:HG12	2.07	0.54
1:2:217:ILE:HG23	1:2:220:LEU:HD23	1.90	0.54
1:4:152:CYS:SG	1:4:239:VAL:HG13	2.48	0.54
1:3:132:ASN:CG	1:3:133:LEU:H	2.11	0.54
1:4:127:PHE:HD2	1:4:132:ASN:HA	1.72	0.54
1:4:113:LYS:HG2	1:4:114:LYS:HE3	1.90	0.54
1:3:167:VAL:CG2	1:3:168:GLU:N	2.71	0.54
1:1:328:GLN:HA	1:1:328:GLN:HE21	1.73	0.53
1:2:152:CYS:O	1:2:152:CYS:SG	2.66	0.53
1:4:292:ASP:OD1	1:4:295:ALA:HB3	2.08	0.53
1:3:81:ILE:CG2	1:3:83:TRP:CE2	2.92	0.53
1:4:220:LEU:CA	1:4:223:LYS:NZ	2.67	0.53
1:2:58:MET:HA	1:2:62:ALA:O	2.08	0.53
1:1:113:LYS:C	1:1:114:LYS:CE	2.66	0.53
1:4:17:ARG:HG2	1:4:43:PHE:CE2	2.43	0.53
1:4:8:PHE:HD1	1:4:29:VAL:CG1	2.21	0.53
1:3:74:ASN:HA	2:3:377:HOH:O	2.08	0.53
1:3:78:PRO:C	1:3:80:ASN:N	2.59	0.53
1:3:56:VAL:O	1:3:56:VAL:CG1	2.55	0.53
1:4:301:LYS:NZ	1:4:301:LYS:HB2	2.21	0.53
1:3:280:SER:O	2:3:387:HOH:O	2.19	0.53
1:1:129:CYS:CB	1:1:269:PHE:CE1	2.90	0.53
1:1:153:LEU:O	1:1:154:ALA:O	2.25	0.53
1:1:252:ASP:C	1:1:252:ASP:OD1	2.46	0.53
1:2:152:CYS:SG	1:2:239:VAL:HG12	2.48	0.53
1:2:297:ILE:O	1:2:297:ILE:HD13	2.07	0.53
1:2:301:LYS:O	1:2:302:THR:CG2	2.56	0.53
1:4:250:SER:C	1:4:252:ASP:N	2.61	0.53
1:4:1:SER:CB	1:4:25:GLN:HB2	2.36	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:39:MET:O	1:4:43:PHE:N	2.40	0.53
1:1:5:ILE:HG23	1:1:92:VAL:CG1	2.38	0.53
1:4:42:MET:HG2	1:4:42:MET:O	2.07	0.53
1:3:254:ILE:O	1:3:255:LYS:O	2.27	0.53
1:3:83:TRP:HA	1:3:86:ALA:HB1	1.90	0.53
1:4:126:MET:HE2	1:4:212:ALA:HA	1.90	0.53
1:4:259:LYS:C	1:4:261:ALA:N	2.62	0.53
1:1:232:PRO:O	1:1:233:THR:C	2.45	0.53
1:1:296:GLY:N	1:1:297:ILE:CD1	2.71	0.53
1:2:113:LYS:CG	1:2:114:LYS:CE	2.81	0.53
1:2:265:PRO:C	1:2:267:GLN:H	2.12	0.53
1:2:271:GLY:O	1:2:272:TYR:HB3	2.09	0.53
1:3:196:ARG:NE	1:4:47:SER:OG	2.42	0.53
1:3:145:ASN:HD22	1:3:145:ASN:C	2.10	0.53
1:3:155:PRO:HB3	1:3:266:LEU:HD23	1.90	0.53
1:3:292:ASP:OD1	1:3:292:ASP:C	2.47	0.53
1:3:326:HIS:O	1:3:327:MET:C	2.46	0.53
1:2:298:GLN:OE1	1:3:226:GLY:N	2.41	0.53
1:1:8:PHE:CD1	1:1:29:VAL:HG11	2.43	0.53
1:1:44:LYS:CG	1:1:56:VAL:HG11	2.38	0.53
1:2:131:VAL:O	1:2:132:ASN:C	2.47	0.53
1:2:243:VAL:CG2	1:2:245:LEU:CD2	2.87	0.53
1:2:32:PRO:C	1:2:33:PHE:CG	2.74	0.53
1:4:238:VAL:HG22	1:4:307:VAL:HG22	1.91	0.53
1:3:295:ALA:C	1:3:297:ILE:HD12	2.29	0.53
1:1:261:ALA:C	1:1:263:GLU:N	2.59	0.53
1:2:285:ASP:OD2	1:2:285:ASP:C	2.45	0.53
1:1:101:ILE:HG23	1:1:142:VAL:HG21	1.90	0.53
1:1:161:HIS:CG	1:1:162:GLU:H	2.24	0.53
1:1:252:ASP:O	1:1:255:LYS:CA	2.56	0.53
1:3:205:SER:CB	1:3:228:ALA:HB3	2.33	0.53
1:4:276:ASP:OD1	1:4:277:VAL:CG2	2.52	0.53
1:3:274:GLU:C	1:3:276:ASP:H	2.11	0.53
1:2:296:GLY:CA	1:2:307:VAL:HG21	2.37	0.53
1:4:128:VAL:C	1:4:132:ASN:HB3	2.30	0.53
1:4:259:LYS:O	1:4:261:ALA:N	2.41	0.53
1:2:84:SER:O	1:2:85:LYS:C	2.45	0.53
1:4:117:ILE:HG13	1:4:144:SER:HB2	1.91	0.53
1:1:30:ASN:HD22	1:1:30:ASN:C	2.08	0.53
1:1:56:VAL:O	1:1:57:LYS:CE	2.57	0.53
1:2:283:ILE:HG22	1:2:283:ILE:O	2.07	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:171:MET:HA	1:4:240:ASP:O	2.09	0.53
1:3:278:VAL:HA	1:3:281:ASP:OD2	2.08	0.53
1:2:56:VAL:O	1:2:56:VAL:HG22	2.08	0.53
1:2:177:VAL:HA	1:2:181:GLN:OE1	2.09	0.52
1:2:325:LYS:O	1:2:326:HIS:C	2.47	0.52
1:4:177:VAL:HG13	1:4:231:VAL:O	2.08	0.52
1:4:153:LEU:HD13	1:4:213:VAL:HG21	1.90	0.52
1:4:71:THR:CG2	1:4:73:PHE:CE1	2.92	0.52
1:3:129:CYS:O	1:3:133:LEU:CG	2.57	0.52
1:4:131:VAL:O	1:4:132:ASN:O	2.27	0.52
1:1:220:LEU:HA	1:1:223:LYS:CE	2.35	0.52
1:1:44:LYS:HD2	1:1:56:VAL:HG11	1.90	0.52
1:2:216:VAL:HG12	1:2:217:ILE:H	1.74	0.52
1:3:127:PHE:HZ	1:3:140:MET:CE	2.21	0.52
1:3:156:VAL:HA	1:3:258:MET:HE2	1.90	0.52
1:1:265:PRO:CG	2:1:442:HOH:O	2.54	0.52
1:2:41:TYR:CZ	1:4:277:VAL:HG11	2.45	0.52
1:4:4:GLY:N	1:4:27:VAL:HG21	2.24	0.52
1:4:6:ASN:HD22	1:4:93:GLU:CD	2.13	0.52
1:1:11:ILE:N	1:1:11:ILE:CD1	2.72	0.52
1:1:164:PHE:HZ	1:1:253:ASP:HB3	1.74	0.52
1:2:272:TYR:OH	1:2:274:GLU:OE2	2.24	0.52
1:2:327:MET:HB3	1:2:331:ASP:OD2	2.09	0.52
1:2:186:GLY:N	1:2:195:GLY:O	2.43	0.52
1:3:181:GLN:HE21	1:3:203:ILE:HD13	1.74	0.52
1:3:152:CYS:SG	1:3:239:VAL:CG1	2.97	0.52
1:1:193:ARG:NH2	1:4:295:ALA:CB	2.59	0.52
1:2:119:ALA:HB1	1:2:120:PRO:CD	2.39	0.52
1:2:251:TYR:CA	1:2:299:LEU:HD12	2.33	0.52
1:2:231:VAL:HB	1:3:231:VAL:CG1	2.38	0.52
1:3:75:GLU:C	2:3:378:HOH:O	2.43	0.52
1:3:82:PRO:O	1:3:83:TRP:CG	2.62	0.52
1:4:104:ALA:HB3	1:4:142:VAL:HG21	1.92	0.52
1:4:104:ALA:CB	1:4:142:VAL:HG21	2.39	0.52
1:1:109:LYS:O	1:1:110:GLY:C	2.48	0.52
1:4:40:VAL:CG2	1:4:41:TYR:N	2.72	0.52
1:4:137:SER:HB3	1:4:138:LYS:HZ2	1.73	0.52
1:1:298:GLN:CD	1:4:225:THR:CG2	2.78	0.52
1:4:182:LYS:HE2	1:4:187:PRO:O	2.09	0.52
1:1:127:PHE:CD1	1:1:143:VAL:CG2	2.92	0.52
1:1:90:TYR:HD1	1:1:90:TYR:H	1.57	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:269:PHE:O	1:2:288:SER:HB2	2.08	0.52
1:2:3:ILE:O	1:2:27:VAL:CG2	2.54	0.52
1:4:98:PHE:HA	1:4:103:LYS:HB3	1.91	0.52
1:2:227:MET:CE	1:3:296:GLY:HA3	2.40	0.52
1:2:52:PHE:C	1:2:53:LYS:HE2	2.30	0.52
1:2:113:LYS:CB	1:2:114:LYS:HG2	2.39	0.52
1:2:28:ALA:HB1	1:2:73:PHE:CE2	2.44	0.52
1:4:183:THR:HB	1:4:184:VAL:CG1	2.37	0.52
1:4:34:ILE:O	1:4:34:ILE:CG2	2.57	0.52
1:3:14:LEU:O	1:3:18:ALA:HB2	2.09	0.52
1:3:68:LYS:O	1:3:70:ILE:HG23	2.09	0.52
1:2:14:LEU:N	1:2:14:LEU:HD13	2.24	0.52
1:1:193:ARG:CB	1:4:277:VAL:HG12	2.40	0.52
1:1:63:LEU:HD22	1:1:65:VAL:HG12	1.92	0.52
1:1:27:VAL:H	1:1:70:ILE:HB	1.75	0.52
1:2:176:ALA:O	1:2:177:VAL:O	2.28	0.52
1:2:78:PRO:CD	1:2:98:PHE:CE2	2.92	0.52
1:2:81:ILE:HD13	1:2:82:PRO:HD2	1.92	0.52
1:2:270:LEU:HD23	1:2:271:GLY:N	2.25	0.52
1:4:227:MET:HE1	1:4:229:PHE:CZ	2.45	0.52
1:4:231:VAL:O	1:4:232:PRO:C	2.49	0.52
1:2:277:VAL:HG11	1:4:41:TYR:CZ	2.45	0.52
1:4:32:PRO:CB	1:4:74:ASN:HD21	2.20	0.52
1:4:78:PRO:HD3	1:4:98:PHE:HE2	1.75	0.52
1:3:296:GLY:N	1:3:297:ILE:HD13	2.25	0.52
1:2:210:ALA:O	1:2:211:LYS:C	2.48	0.52
1:1:160:LEU:O	1:1:164:PHE:N	2.42	0.51
1:1:244:ARG:CZ	1:4:244:ARG:NE	2.73	0.51
1:1:39:MET:O	1:1:43:PHE:N	2.44	0.51
1:2:276:ASP:C	1:2:277:VAL:HG22	2.31	0.51
1:2:6:ASN:CA	1:2:30:ASN:ND2	2.68	0.51
1:1:225:THR:CG2	1:4:298:GLN:CD	2.79	0.51
1:4:314:PHE:CG	1:4:314:PHE:O	2.63	0.51
1:2:173:THR:HG22	1:2:228:ALA:HB2	1.91	0.51
1:3:83:TRP:N	1:3:86:ALA:CB	2.73	0.51
1:2:51:VAL:CG2	2:2:401:HOH:O	2.57	0.51
1:4:114:LYS:CD	1:4:114:LYS:N	2.70	0.51
1:2:298:GLN:CD	1:3:225:THR:HG23	2.30	0.51
1:1:117:ILE:HB	1:1:144:SER:HB2	1.90	0.51
1:1:128:VAL:HG13	1:1:151:ASN:HD22	1.74	0.51
1:2:113:LYS:HG2	1:2:114:LYS:CE	2.26	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:113:LYS:CE	1:2:114:LYS:NZ	2.69	0.51
1:2:236:VAL:HG22	1:2:311:ASP:HA	1.92	0.51
1:2:267:GLN:CG	1:2:268:GLY:N	2.73	0.51
1:2:277:VAL:CB	1:4:41:TYR:OH	2.56	0.51
1:2:30:ASN:CG	1:2:81:ILE:HG13	2.29	0.51
1:2:97:VAL:O	1:2:98:PHE:CE1	2.54	0.51
1:3:79:GLU:HB2	1:3:109:LYS:HB3	1.91	0.51
1:1:188:SER:OG	1:1:195:GLY:CA	2.58	0.51
1:1:208:GLY:HA3	1:1:211:LYS:HG3	1.85	0.51
1:1:211:LYS:NZ	1:1:211:LYS:CA	2.62	0.51
1:2:135:LYS:NZ	1:2:140:MET:CE	2.72	0.51
1:3:171:MET:CG	1:3:172:THR:N	2.66	0.51
1:4:57:LYS:O	1:4:64:VAL:HG13	2.10	0.51
1:4:89:GLU:HG3	1:4:90:TYR:CE1	2.45	0.51
1:4:89:GLU:CG	1:4:90:TYR:HD1	2.15	0.51
1:2:46:ASP:O	1:2:50:GLY:CA	2.59	0.51
1:2:145:ASN:O	1:2:146:ALA:C	2.49	0.51
1:1:272:TYR:OH	1:1:274:GLU:HG2	2.10	0.51
1:1:309:TRP:H	1:1:309:TRP:HD1	1.55	0.51
1:1:74:ASN:HB2	2:1:425:HOH:O	2.11	0.51
1:3:188:SER:HB2	1:3:195:GLY:CA	2.39	0.51
1:4:89:GLU:OE1	1:4:90:TYR:CE1	2.55	0.51
1:3:145:ASN:O	1:3:146:ALA:C	2.49	0.51
1:3:26:VAL:HG11	1:3:68:LYS:HG3	1.92	0.51
1:3:276:ASP:O	1:3:278:VAL:CG2	2.55	0.51
1:4:125:PRO:CG	1:4:140:MET:HE1	2.41	0.51
1:1:113:LYS:HB3	1:1:114:LYS:NZ	2.26	0.51
1:1:255:LYS:HD2	1:1:293:ALA:HB1	1.93	0.51
1:1:328:GLN:CA	1:1:328:GLN:HE21	2.23	0.51
1:2:85:LYS:O	1:2:86:ALA:CB	2.58	0.51
1:3:3:ILE:HD11	1:3:24:ALA:HB1	1.91	0.51
1:3:252:ASP:C	1:3:254:ILE:N	2.62	0.51
1:3:78:PRO:HD3	1:3:98:PHE:CE2	2.46	0.51
1:2:225:THR:CB	1:3:298:GLN:HE22	2.23	0.51
1:1:270:LEU:HA	1:1:289:SER:O	2.10	0.51
1:1:205:SER:HB3	1:1:228:ALA:CB	2.38	0.51
1:3:172:THR:N	1:3:240:ASP:O	2.36	0.51
1:1:117:ILE:HD11	1:1:142:VAL:O	2.10	0.51
1:1:160:LEU:CD2	1:1:254:ILE:HD12	2.37	0.51
1:2:153:LEU:O	1:2:153:LEU:CD2	2.54	0.51
1:2:153:LEU:CD2	1:2:157:ALA:HB2	2.40	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:251:TYR:CE1	1:4:297:ILE:HG12	2.44	0.51
1:2:188:SER:CB	1:2:192:TRP:HA	2.41	0.51
1:2:196:ARG:NH2	1:3:281:ASP:OD2	2.43	0.51
1:3:82:PRO:HB2	1:3:85:LYS:O	2.11	0.51
1:3:51:VAL:C	2:3:370:HOH:O	2.21	0.51
1:2:54:GLY:O	1:2:56:VAL:HG12	2.10	0.51
1:4:134:GLU:C	1:4:136:TYR:N	2.63	0.51
1:2:137:SER:O	1:2:140:MET:CG	2.58	0.51
1:2:329:LYS:NZ	1:2:330:VAL:N	2.58	0.51
1:1:113:LYS:CB	1:1:114:LYS:CE	2.86	0.51
1:1:236:VAL:HG12	1:1:237:SER:N	2.26	0.51
1:1:288:SER:HB2	1:1:319:ARG:NH1	2.25	0.51
1:2:295:ALA:CA	1:2:297:ILE:HD12	2.40	0.51
1:2:78:PRO:C	1:2:80:ASN:N	2.64	0.51
1:4:27:VAL:CG2	1:4:28:ALA:N	2.45	0.51
1:3:207:THR:HG1	1:3:208:GLY:H	1.54	0.51
1:1:175:HIS:O	1:1:231:VAL:CG2	2.58	0.51
1:4:235:ASP:CG	1:4:311:ASP:OD1	2.49	0.51
1:3:83:TRP:HA	1:3:86:ALA:CB	2.40	0.51
1:2:225:THR:HG21	1:3:298:GLN:HE22	1.66	0.51
1:2:27:VAL:HG13	1:2:28:ALA:O	2.10	0.51
1:2:75:GLU:O	2:2:408:HOH:O	2.18	0.51
1:2:188:SER:HB2	1:2:195:GLY:HA3	1.93	0.51
1:3:153:LEU:HD23	1:3:156:VAL:HG12	1.93	0.51
1:4:105:SER:O	1:4:106:ALA:C	2.49	0.51
1:3:168:GLU:OE2	1:3:244:ARG:CZ	2.59	0.51
1:4:265:PRO:CA	2:4:453:HOH:O	2.57	0.51
1:1:32:PRO:O	1:1:34:ILE:HG22	2.11	0.51
1:1:90:TYR:HD1	1:1:90:TYR:N	2.09	0.51
1:2:127:PHE:HA	1:2:132:ASN:HB2	1.92	0.51
1:2:276:ASP:OD1	1:2:277:VAL:HG22	2.10	0.51
1:2:7:GLY:O	1:2:8:PHE:HB3	2.10	0.51
1:3:184:VAL:O	1:3:185:ASP:O	2.29	0.51
1:4:89:GLU:CG	1:4:90:TYR:CD1	2.86	0.51
1:3:103:LYS:O	1:3:106:ALA:HB3	2.11	0.51
1:3:127:PHE:HD2	1:3:132:ASN:HA	1.74	0.51
1:2:53:LYS:HE2	1:2:53:LYS:N	2.26	0.51
1:4:134:GLU:O	1:4:135:LYS:C	2.48	0.51
1:3:301:LYS:NZ	1:3:301:LYS:HB2	2.25	0.51
1:1:253:ASP:C	1:1:255:LYS:H	2.13	0.50
1:1:44:LYS:O	1:1:51:VAL:CA	2.58	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:281:ASP:O	1:2:283:ILE:CB	2.58	0.50
1:2:32:PRO:O	1:2:34:ILE:HG22	2.10	0.50
1:4:175:HIS:N	1:4:229:PHE:O	2.44	0.50
1:2:303:PHE:HE2	1:3:303:PHE:CE2	2.29	0.50
1:4:127:PHE:HE1	1:4:140:MET:HE2	1.76	0.50
1:2:181:GLN:HE22	1:2:230:ARG:CB	2.25	0.50
1:2:272:TYR:CE2	1:2:293:ALA:HB2	2.46	0.50
1:3:81:ILE:HD12	1:3:83:TRP:CH2	2.47	0.50
1:4:217:ILE:CG1	1:4:220:LEU:HD22	2.40	0.50
1:2:126:MET:HB3	1:2:215:LYS:HZ2	1.77	0.50
1:1:11:ILE:O	1:1:15:VAL:HG23	2.10	0.50
1:2:109:LYS:O	1:2:110:GLY:C	2.50	0.50
1:2:149:THR:O	1:2:152:CYS:N	2.44	0.50
1:4:3:ILE:C	1:4:27:VAL:CG2	2.80	0.50
1:3:9:GLY:HA2	1:3:13:ARG:NH2	2.25	0.50
1:3:14:LEU:HA	1:3:17:ARG:HG3	1.92	0.50
1:3:38:TYR:O	1:3:42:MET:N	2.41	0.50
1:2:9:GLY:O	1:2:10:ARG:C	2.49	0.50
1:4:125:PRO:CG	1:4:140:MET:CE	2.74	0.50
1:3:168:GLU:CG	1:3:244:ARG:HD2	2.41	0.50
1:3:213:VAL:HA	1:3:216:VAL:HG12	1.93	0.50
1:3:178:THR:O	1:3:179:ALA:C	2.49	0.50
1:1:19:ALA:C	1:1:24:ALA:HB3	2.31	0.50
1:1:19:ALA:HA	1:1:24:ALA:HB3	1.91	0.50
1:1:319:ARG:O	1:1:320:VAL:C	2.50	0.50
1:1:66:ASP:O	1:1:68:LYS:CD	2.53	0.50
1:4:180:THR:CG2	1:4:181:GLN:H	2.21	0.50
1:3:129:CYS:O	1:3:133:LEU:CD1	2.59	0.50
1:3:250:SER:HA	1:3:299:LEU:HD12	1.92	0.50
1:4:134:GLU:O	1:4:136:TYR:N	2.45	0.50
1:3:117:ILE:HG22	1:3:119:ALA:O	2.11	0.50
1:4:243:VAL:CG2	1:4:304:VAL:CG1	2.89	0.50
1:1:92:VAL:HG12	1:1:92:VAL:O	2.10	0.50
1:2:6:ASN:HA	1:2:30:ASN:HD22	1.71	0.50
1:4:98:PHE:HA	1:4:103:LYS:CD	2.41	0.50
1:3:116:VAL:HA	1:3:143:VAL:O	2.11	0.50
1:1:112:ALA:O	1:1:113:LYS:CG	2.59	0.50
1:1:115:VAL:CG1	1:1:116:VAL:N	2.75	0.50
1:1:148:CYS:SG	1:1:149:THR:N	2.84	0.50
1:2:276:ASP:O	1:2:277:VAL:C	2.49	0.50
1:2:319:ARG:HH11	1:2:319:ARG:HG2	1.74	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:174:VAL:HG12	1:3:231:VAL:HG21	1.92	0.50
1:3:161:HIS:HB2	1:3:166:ILE:CD1	2.36	0.50
1:3:84:SER:OG	1:3:111:GLY:C	2.49	0.50
1:1:119:ALA:CB	1:1:120:PRO:CD	2.75	0.50
1:3:239:VAL:CG1	1:3:310:TYR:HE1	2.20	0.50
1:2:205:SER:OG	1:2:206:SER:O	2.29	0.50
1:1:175:HIS:CG	1:1:230:ARG:HH21	2.30	0.50
1:1:129:CYS:HB3	1:1:269:PHE:CD1	2.45	0.50
1:2:161:HIS:HB2	1:2:166:ILE:CD1	2.41	0.50
1:4:78:PRO:CG	1:4:98:PHE:HE2	2.16	0.50
1:4:95:THR:HG22	1:4:97:VAL:H	1.76	0.50
1:3:161:HIS:C	1:3:163:ASN:N	2.64	0.50
1:3:156:VAL:HG22	1:3:258:MET:HE2	1.94	0.50
1:3:68:LYS:O	1:3:70:ILE:CG2	2.59	0.50
1:4:243:VAL:CG2	1:4:304:VAL:HG12	2.34	0.50
1:2:117:ILE:HD12	1:2:144:SER:CB	2.41	0.50
1:4:10:ARG:O	1:4:14:LEU:HD23	2.12	0.50
1:3:43:PHE:HE1	1:3:65:VAL:HG21	1.77	0.50
1:2:46:ASP:HB3	1:2:50:GLY:N	2.23	0.50
1:1:173:THR:O	1:1:228:ALA:HA	2.11	0.50
1:1:277:VAL:CG1	1:4:193:ARG:HG3	2.41	0.50
1:1:295:ALA:HB2	1:4:193:ARG:CZ	2.40	0.50
1:2:73:PHE:CE1	1:2:82:PRO:HG2	2.46	0.50
1:4:17:ARG:CG	1:4:43:PHE:HE2	2.24	0.50
1:4:108:PHE:CG	1:4:109:LYS:N	2.80	0.50
1:1:266:LEU:HD23	1:1:270:LEU:HB2	1.92	0.50
1:2:329:LYS:NZ	1:2:329:LYS:HB3	2.23	0.50
1:4:265:PRO:C	2:4:453:HOH:O	2.51	0.50
1:1:134:GLU:OE2	1:1:134:GLU:O	2.30	0.50
1:2:28:ALA:HB1	1:2:73:PHE:HE2	1.77	0.49
1:2:75:GLU:HB3	2:2:408:HOH:O	2.11	0.49
1:4:297:ILE:HD13	1:4:298:GLN:N	2.27	0.49
1:3:105:SER:C	1:3:107:HIS:N	2.63	0.49
1:3:129:CYS:CA	1:3:132:ASN:HD22	2.21	0.49
1:3:145:ASN:O	1:3:316:TYR:OH	2.19	0.49
1:2:156:VAL:HG22	1:2:258:MET:HE2	1.93	0.49
1:1:101:ILE:HG12	1:1:142:VAL:CG1	2.43	0.49
1:1:304:VAL:O	1:1:304:VAL:HG12	2.11	0.49
1:2:322:ASP:O	1:2:323:LEU:C	2.51	0.49
1:2:4:GLY:HA2	1:2:27:VAL:HG21	1.92	0.49
1:4:238:VAL:CG2	1:4:307:VAL:HG22	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:251:TYR:HB2	1:4:299:LEU:HG	1.93	0.49
1:3:135:LYS:HG3	1:3:135:LYS:O	2.11	0.49
1:1:150:THR:HG21	1:1:212:ALA:HB1	1.95	0.49
1:1:225:THR:HG21	1:4:298:GLN:CD	2.32	0.49
1:4:76:MET:O	1:4:76:MET:CG	2.60	0.49
1:3:276:ASP:O	1:3:278:VAL:N	2.45	0.49
1:3:117:ILE:O	1:3:119:ALA:N	2.40	0.49
1:4:170:LEU:CD2	1:4:225:THR:HG23	2.42	0.49
1:1:227:MET:CE	1:4:296:GLY:HA2	2.42	0.49
1:1:227:MET:HE3	1:4:296:GLY:HA2	1.94	0.49
1:1:126:MET:CE	1:1:212:ALA:HA	2.42	0.49
1:1:46:ASP:HB3	1:1:50:GLY:N	2.28	0.49
1:1:50:GLY:C	1:1:51:VAL:HG23	2.33	0.49
1:1:54:GLY:HA2	1:1:66:ASP:CG	2.31	0.49
1:2:149:THR:O	1:2:152:CYS:CB	2.60	0.49
1:4:272:TYR:H	1:4:291:PHE:H	1.58	0.49
1:3:106:ALA:O	1:3:107:HIS:C	2.50	0.49
1:3:115:VAL:HG12	1:3:116:VAL:N	2.27	0.49
1:3:325:LYS:O	1:3:326:HIS:C	2.50	0.49
1:4:127:PHE:HD2	1:4:132:ASN:CA	2.25	0.49
1:3:181:GLN:NE2	1:3:203:ILE:HD13	2.28	0.49
1:1:170:LEU:O	1:1:241:LEU:HA	2.12	0.49
1:2:328:GLN:O	1:2:332:SER:HB2	2.13	0.49
1:3:27:VAL:O	1:3:28:ALA:CB	2.60	0.49
1:3:292:ASP:OD2	1:3:295:ALA:CB	2.54	0.49
1:3:38:TYR:O	1:3:42:MET:HB2	2.12	0.49
1:2:279:SER:O	1:2:281:ASP:N	2.42	0.49
1:4:272:TYR:CD2	1:4:291:PHE:HD1	2.30	0.49
1:4:83:TRP:HA	1:4:86:ALA:HB3	1.84	0.49
1:3:282:PHE:O	1:3:285:ASP:HB3	2.12	0.49
1:3:81:ILE:HG21	1:3:83:TRP:CE2	2.48	0.49
1:2:46:ASP:O	1:2:50:GLY:HA3	2.13	0.49
1:1:81:ILE:HD12	1:1:82:PRO:O	2.12	0.49
1:2:30:ASN:ND2	1:2:30:ASN:O	2.46	0.49
1:2:97:VAL:C	1:2:98:PHE:CD1	2.78	0.49
1:3:199:ALA:HB2	2:3:383:HOH:O	2.12	0.49
1:4:279:SER:C	1:4:281:ASP:N	2.65	0.49
1:3:156:VAL:HG22	1:3:258:MET:HE1	1.94	0.49
1:3:319:ARG:CG	1:3:319:ARG:HH11	2.23	0.49
1:3:84:SER:O	1:3:86:ALA:N	2.45	0.49
1:3:37:GLU:HA	1:3:40:VAL:HG13	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:105:SER:C	1:4:107:HIS:N	2.66	0.49
1:4:165:GLU:O	1:4:166:ILE:HB	2.12	0.49
1:1:193:ARG:CA	1:4:277:VAL:HG12	2.42	0.49
1:2:129:CYS:CB	1:2:269:PHE:CE1	2.96	0.49
1:4:73:PHE:CD2	1:4:81:ILE:HD11	2.47	0.49
1:3:155:PRO:HB3	1:3:266:LEU:CD2	2.43	0.49
1:3:95:THR:HA	2:3:376:HOH:O	2.13	0.49
1:1:132:ASN:ND2	1:1:133:LEU:CG	2.75	0.49
1:1:219:GLU:O	1:1:223:LYS:CE	2.61	0.49
1:1:236:VAL:HG12	1:1:237:SER:H	1.78	0.49
1:1:322:ASP:O	1:1:323:LEU:O	2.30	0.49
1:4:77:LYS:HA	1:4:77:LYS:HD2	1.52	0.49
1:4:81:ILE:CG2	1:4:83:TRP:NE1	2.76	0.49
1:3:159:VAL:O	1:3:163:ASN:CB	2.61	0.49
1:3:241:LEU:HG	1:3:243:VAL:CG1	2.41	0.49
1:3:295:ALA:O	1:3:307:VAL:HG11	2.12	0.49
1:3:314:PHE:CG	1:3:314:PHE:O	2.63	0.49
1:3:319:ARG:CG	1:3:319:ARG:NH1	2.75	0.49
1:3:116:VAL:HG11	1:3:324:LEU:HD22	1.93	0.49
1:4:218:PRO:O	1:4:220:LEU:N	2.46	0.49
1:2:126:MET:CG	1:2:146:ALA:HB2	2.43	0.49
1:2:55:GLU:HB3	1:2:67:GLY:H	1.77	0.49
1:2:129:CYS:SG	1:2:269:PHE:CE1	3.05	0.49
1:4:100:THR:O	1:4:103:LYS:N	2.46	0.49
1:4:282:PHE:HE1	1:4:290:ILE:HD13	1.76	0.49
1:3:235:ASP:CG	1:3:235:ASP:O	2.51	0.49
1:3:273:THR:OG1	1:3:274:GLU:N	2.46	0.49
1:3:290:ILE:O	1:3:308:SER:OG	2.31	0.49
1:3:291:PHE:HE2	1:3:306:VAL:HB	1.78	0.49
1:1:189:ALA:C	1:1:190:LYS:HD3	2.34	0.49
1:2:11:ILE:O	1:2:15:VAL:CG2	2.61	0.49
1:4:131:VAL:HG22	1:4:132:ASN:N	2.28	0.49
1:2:126:MET:HG3	1:2:146:ALA:HB2	1.95	0.49
1:2:298:GLN:OE1	1:3:225:THR:CG2	2.60	0.49
1:2:150:THR:HG21	1:2:212:ALA:HB1	1.94	0.48
1:3:250:SER:O	1:3:253:ASP:N	2.45	0.48
1:3:74:ASN:O	1:3:75:GLU:HG2	2.13	0.48
1:3:37:GLU:HA	1:3:40:VAL:HG11	1.92	0.48
1:2:51:VAL:HB	2:2:400:HOH:O	2.13	0.48
1:2:66:ASP:HB2	1:2:68:LYS:CE	2.42	0.48
1:1:156:VAL:HG22	1:1:258:MET:HE1	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:170:LEU:HD23	1:4:225:THR:HG22	1.95	0.48
1:3:221:ASP:O	1:3:221:ASP:OD2	2.31	0.48
1:4:247:LYS:O	1:4:248:GLU:C	2.49	0.48
1:2:174:VAL:CG2	1:2:238:VAL:HG13	2.43	0.48
1:1:104:ALA:O	1:1:105:SER:C	2.50	0.48
1:1:131:VAL:O	1:1:133:LEU:N	2.46	0.48
1:1:238:VAL:HG23	1:1:309:TRP:CD2	2.48	0.48
1:1:304:VAL:HG13	1:1:305:LYS:N	2.20	0.48
1:2:164:PHE:O	1:2:165:GLU:CB	2.61	0.48
1:2:177:VAL:HG13	1:2:233:THR:O	2.13	0.48
1:2:282:PHE:O	1:2:283:ILE:C	2.51	0.48
1:1:277:VAL:CB	1:3:41:TYR:OH	2.60	0.48
1:4:83:TRP:HA	1:4:86:ALA:HB1	1.95	0.48
1:3:18:ALA:O	1:3:19:ALA:C	2.51	0.48
1:3:55:GLU:O	1:3:66:ASP:N	2.46	0.48
1:1:188:SER:O	1:1:190:LYS:CA	2.56	0.48
1:2:10:ARG:HD3	1:2:10:ARG:HA	1.53	0.48
1:4:161:HIS:O	1:4:162:GLU:C	2.50	0.48
1:3:217:ILE:HG23	1:3:220:LEU:HD23	1.95	0.48
1:4:259:LYS:C	1:4:261:ALA:H	2.15	0.48
1:1:101:ILE:O	1:1:105:SER:HB2	2.13	0.48
1:1:91:ILE:O	1:1:115:VAL:HA	2.12	0.48
1:2:129:CYS:HA	1:2:132:ASN:HD22	1.77	0.48
1:2:213:VAL:O	1:2:214:GLY:C	2.52	0.48
1:2:255:LYS:HZ3	1:2:255:LYS:HB3	1.79	0.48
1:2:40:VAL:CG2	1:2:41:TYR:N	2.76	0.48
1:1:193:ARG:HG3	1:4:277:VAL:HG12	1.95	0.48
1:4:129:CYS:SG	1:4:269:PHE:CE1	3.07	0.48
1:3:117:ILE:C	1:3:119:ALA:N	2.66	0.48
1:3:167:VAL:CG2	1:3:168:GLU:H	2.25	0.48
1:1:248:GLU:HG2	1:1:302:THR:HG21	1.96	0.48
1:3:301:LYS:CB	1:3:301:LYS:NZ	2.76	0.48
1:1:296:GLY:H	1:1:297:ILE:CD1	2.26	0.48
1:2:319:ARG:HH11	1:2:319:ARG:CG	2.27	0.48
1:2:93:GLU:OE2	1:2:98:PHE:CB	2.62	0.48
1:4:155:PRO:O	1:4:159:VAL:HG23	2.13	0.48
1:2:41:TYR:OH	1:4:277:VAL:CB	2.61	0.48
1:4:8:PHE:CD1	1:4:29:VAL:HG11	2.48	0.48
1:3:292:ASP:O	1:3:292:ASP:OD1	2.31	0.48
1:1:282:PHE:CE1	1:1:290:ILE:HD13	2.49	0.48
1:1:34:ILE:HD11	1:1:39:MET:CG	2.40	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:113:LYS:C	1:2:114:LYS:CG	2.73	0.48
1:4:4:GLY:N	1:4:27:VAL:HG23	2.29	0.48
1:4:310:TYR:HB2	1:4:312:ASN:H	1.78	0.48
1:4:32:PRO:HB3	1:4:74:ASN:OD1	2.12	0.48
1:3:52:PHE:C	1:3:53:LYS:HZ3	2.17	0.48
1:4:217:ILE:HD11	1:4:220:LEU:CD2	2.43	0.48
1:3:117:ILE:HB	1:3:144:SER:CA	2.38	0.48
1:1:170:LEU:HA	1:1:170:LEU:HD22	1.51	0.48
1:1:215:LYS:O	1:1:215:LYS:CD	2.62	0.48
1:1:292:ASP:OD1	1:1:295:ALA:CA	2.60	0.48
1:4:236:VAL:HG11	1:4:280:SER:HA	1.96	0.48
1:4:310:TYR:HB2	1:4:311:ASP:H	1.47	0.48
1:1:41:TYR:O	1:1:41:TYR:CG	2.66	0.48
1:3:113:LYS:CE	1:3:114:LYS:HZ2	2.27	0.48
1:3:259:LYS:HD2	1:3:272:TYR:CE1	2.48	0.48
1:3:8:PHE:HZ	1:3:39:MET:HG2	1.71	0.48
1:4:329:LYS:NZ	1:4:330:VAL:CA	2.77	0.48
1:1:292:ASP:HB3	1:1:307:VAL:HG13	1.96	0.48
1:2:104:ALA:O	1:2:107:HIS:N	2.46	0.48
1:2:83:TRP:CD1	1:2:112:ALA:HB2	2.49	0.48
1:2:277:VAL:CG2	1:2:278:VAL:N	2.71	0.48
1:2:173:THR:HG22	1:2:227:MET:O	2.14	0.48
1:2:190:LYS:HD3	2:2:427:HOH:O	2.13	0.48
1:2:196:ARG:HH11	1:2:196:ARG:CG	2.16	0.48
1:3:19:ALA:CB	1:3:24:ALA:HB3	2.42	0.48
1:3:276:ASP:N	1:3:276:ASP:OD2	2.47	0.48
1:1:263:GLU:O	1:1:264:GLY:C	2.52	0.48
1:1:244:ARG:HH22	1:4:244:ARG:HG3	1.78	0.48
1:2:27:VAL:CG2	1:2:28:ALA:H	2.23	0.48
1:4:17:ARG:CG	1:4:43:PHE:CE2	2.97	0.48
1:3:164:PHE:CE2	1:3:249:CYS:HB3	2.49	0.48
1:3:287:ARG:NH1	1:3:290:ILE:HD12	2.28	0.48
1:3:6:ASN:HD22	1:3:93:GLU:CD	2.17	0.48
1:3:53:LYS:HD2	1:3:54:GLY:N	2.29	0.48
1:4:215:LYS:HG2	1:4:215:LYS:O	2.13	0.48
1:4:216:VAL:CG1	1:4:217:ILE:N	2.76	0.48
1:1:79:GLU:HB2	1:1:109:LYS:HB3	1.95	0.48
1:1:34:ILE:HG12	1:1:39:MET:CE	2.43	0.48
1:1:44:LYS:CD	1:1:56:VAL:HG11	2.43	0.48
1:2:27:VAL:HG22	1:2:28:ALA:N	2.29	0.48
1:1:225:THR:HG21	1:4:298:GLN:HE22	1.76	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:201:ASN:HD22	1:2:201:ASN:N	2.10	0.48
1:3:19:ALA:HB1	1:3:24:ALA:CB	2.42	0.48
1:3:81:ILE:HG23	1:3:83:TRP:CE2	2.49	0.48
1:1:5:ILE:HG23	1:1:92:VAL:HG11	1.95	0.48
1:2:70:ILE:O	1:2:70:ILE:HG12	2.13	0.48
1:1:115:VAL:HG12	1:1:116:VAL:N	2.29	0.48
1:1:213:VAL:HG11	1:1:224:LEU:HD13	1.95	0.48
1:1:318:GLN:OE1	1:1:318:GLN:CA	2.53	0.48
1:2:161:HIS:O	1:2:163:ASN:N	2.47	0.48
1:4:66:ASP:O	1:4:68:LYS:CE	2.62	0.48
1:2:184:VAL:O	1:2:185:ASP:HB2	2.13	0.48
1:2:185:ASP:CA	1:2:195:GLY:O	2.62	0.48
1:4:59:GLU:O	1:4:61:GLY:N	2.47	0.48
1:1:32:PRO:HB2	1:1:33:PHE:CE1	2.49	0.47
1:4:180:THR:HG23	1:4:181:GLN:N	2.21	0.47
1:1:305:LYS:CD	1:4:227:MET:SD	3.01	0.47
1:4:6:ASN:ND2	1:4:93:GLU:OE1	2.47	0.47
1:3:129:CYS:O	1:3:130:GLY:C	2.52	0.47
1:3:287:ARG:NH1	1:3:290:ILE:HD13	2.29	0.47
1:4:126:MET:HE3	1:4:212:ALA:HB2	1.95	0.47
1:4:127:PHE:CE2	1:4:136:TYR:HB2	2.48	0.47
1:3:200:GLN:C	1:3:201:ASN:ND2	2.58	0.47
1:1:175:HIS:O	1:1:231:VAL:HG23	2.14	0.47
1:1:294:LYS:C	1:1:297:ILE:HD11	2.34	0.47
1:1:52:PHE:CA	1:1:53:LYS:HE2	2.42	0.47
1:1:53:LYS:CD	1:1:54:GLY:N	2.70	0.47
1:2:1:SER:HB3	1:2:25:GLN:HE21	1.78	0.47
1:2:33:PHE:HZ	1:2:76:MET:HE1	1.71	0.47
1:4:14:LEU:O	1:4:18:ALA:N	2.46	0.47
1:3:130:GLY:O	1:3:133:LEU:HD12	2.15	0.47
1:4:217:ILE:HG12	1:4:217:ILE:O	2.13	0.47
1:3:171:MET:HA	1:3:240:ASP:O	2.14	0.47
1:1:127:PHE:CZ	1:1:140:MET:SD	3.04	0.47
1:1:196:ARG:NH1	1:2:41:TYR:OH	2.47	0.47
1:2:295:ALA:HB2	1:3:193:ARG:NH1	2.24	0.47
1:4:31:ASP:HB3	1:4:34:ILE:CG2	2.43	0.47
1:4:65:VAL:O	1:4:66:ASP:HB2	2.12	0.47
1:4:8:PHE:N	1:4:31:ASP:OD2	2.47	0.47
1:3:104:ALA:O	1:3:106:ALA:N	2.45	0.47
1:3:105:SER:O	1:3:108:PHE:CD1	2.62	0.47
1:3:132:ASN:CG	1:3:133:LEU:N	2.67	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:305:LYS:NZ	1:4:305:LYS:HB2	2.18	0.47
1:1:8:PHE:CD2	1:1:13:ARG:HG2	2.50	0.47
1:1:233:THR:HG21	1:4:202:ILE:HD11	1.96	0.47
1:1:250:SER:O	1:1:253:ASP:N	2.48	0.47
1:1:26:VAL:HB	1:1:70:ILE:CG2	2.43	0.47
1:1:273:THR:O	1:1:293:ALA:HB3	2.15	0.47
1:2:81:ILE:CG2	1:2:83:TRP:NE1	2.77	0.47
1:1:296:GLY:HA2	1:4:227:MET:CG	2.44	0.47
1:2:303:PHE:HE2	1:3:303:PHE:CZ	2.32	0.47
1:3:100:THR:HG23	1:3:103:LYS:HD3	1.95	0.47
1:3:27:VAL:CG2	1:3:28:ALA:O	2.59	0.47
1:4:322:ASP:O	1:4:323:LEU:C	2.52	0.47
1:1:138:LYS:CD	1:1:330:VAL:HG12	2.45	0.47
1:2:201:ASN:HB3	1:2:203:ILE:HG13	1.96	0.47
1:3:299:LEU:HD23	1:3:304:VAL:HG23	1.96	0.47
1:3:97:VAL:O	1:3:97:VAL:HG23	2.13	0.47
1:4:138:LYS:HE3	1:4:330:VAL:CG1	2.45	0.47
1:2:211:LYS:HZ3	1:2:211:LYS:HA	1.80	0.47
1:1:178:THR:O	1:1:179:ALA:C	2.52	0.47
1:1:328:GLN:N	1:1:328:GLN:HE21	2.13	0.47
1:1:26:VAL:HG21	1:1:68:LYS:HG3	1.96	0.47
1:3:283:ILE:CD1	2:3:388:HOH:O	2.59	0.47
1:3:28:ALA:HB1	1:3:73:PHE:CE2	2.49	0.47
1:2:193:ARG:NH2	1:3:295:ALA:CB	2.58	0.47
1:3:32:PRO:HB3	1:3:74:ASN:OD1	2.15	0.47
1:2:66:ASP:HB3	2:2:402:HOH:O	2.13	0.47
1:4:327:MET:O	1:4:328:GLN:C	2.52	0.47
1:2:126:MET:HB3	1:2:215:LYS:CD	2.44	0.47
1:1:301:LYS:O	1:1:302:THR:HG22	2.15	0.47
1:1:174:VAL:CG1	1:1:231:VAL:CG2	2.89	0.47
1:1:276:ASP:C	1:1:277:VAL:HG22	2.32	0.47
1:1:320:VAL:O	1:1:324:LEU:CB	2.62	0.47
1:2:249:CYS:SG	1:2:250:SER:N	2.88	0.47
1:3:231:VAL:HA	1:3:232:PRO:HD2	1.77	0.47
1:1:6:ASN:CB	1:1:30:ASN:HD21	2.28	0.47
1:1:329:LYS:HZ2	1:1:330:VAL:N	2.10	0.47
1:2:117:ILE:C	1:2:119:ALA:H	2.17	0.47
1:2:25:GLN:HB2	1:2:25:GLN:HE21	1.31	0.47
1:4:39:MET:HE3	1:4:72:VAL:HB	1.95	0.47
1:3:130:GLY:HA3	1:3:158:LYS:HZ1	1.80	0.47
1:3:314:PHE:HB2	1:3:317:SER:HB2	1.97	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:2:LYS:NZ	1:3:88:ALA:HA	2.30	0.47
1:3:146:ALA:O	1:3:316:TYR:CE1	2.67	0.47
1:3:34:ILE:HD11	1:3:39:MET:HG2	1.95	0.47
1:4:132:ASN:CG	1:4:133:LEU:H	2.18	0.47
1:4:327:MET:O	1:4:331:ASP:N	2.47	0.47
1:4:108:PHE:O	1:4:109:LYS:O	2.30	0.47
1:1:262:SER:O	1:1:267:GLN:HA	2.15	0.47
1:3:120:PRO:O	1:3:120:PRO:CD	2.62	0.47
1:2:244:ARG:NH2	1:3:244:ARG:CG	2.70	0.47
1:2:167:VAL:HG22	1:2:244:ARG:HG2	1.96	0.47
1:2:36:LEU:C	1:2:36:LEU:HD12	2.35	0.47
1:3:149:THR:O	1:3:152:CYS:HB3	2.15	0.47
1:1:235:ASP:O	1:1:235:ASP:CG	2.52	0.47
1:1:3:ILE:C	1:1:27:VAL:CG2	2.83	0.47
1:1:73:PHE:CD2	1:1:81:ILE:HD11	2.49	0.47
1:2:8:PHE:CZ	1:2:39:MET:CG	2.91	0.47
1:4:175:HIS:O	1:4:231:VAL:HG22	2.15	0.47
1:3:101:ILE:HG12	1:3:142:VAL:HG13	1.96	0.47
1:4:170:LEU:HD21	1:4:225:THR:HG22	1.95	0.47
1:2:298:GLN:CD	1:3:225:THR:CG2	2.83	0.47
1:1:205:SER:O	1:1:206:SER:C	2.53	0.47
1:1:14:LEU:CA	1:1:17:ARG:HG3	2.37	0.47
1:1:59:GLU:HB3	1:1:64:VAL:HG12	1.95	0.47
1:2:294:LYS:N	1:2:297:ILE:HG13	2.29	0.47
1:2:311:ASP:O	1:2:314:PHE:N	2.48	0.47
1:2:33:PHE:CD2	1:2:33:PHE:N	2.77	0.47
1:2:78:PRO:CG	1:2:98:PHE:HE2	2.17	0.47
1:2:17:ARG:CG	1:2:43:PHE:HE2	2.11	0.47
1:1:156:VAL:HA	1:1:258:MET:HE2	1.97	0.47
1:1:298:GLN:OE1	1:4:225:THR:CG2	2.61	0.47
1:2:137:SER:CB	1:2:138:LYS:HZ1	2.28	0.47
1:1:101:ILE:N	1:1:123:ASP:OD1	2.36	0.47
1:1:129:CYS:HB2	1:1:319:ARG:HD3	1.96	0.47
1:1:32:PRO:HA	1:1:74:ASN:CG	2.32	0.47
1:2:73:PHE:CD1	1:2:82:PRO:HG2	2.50	0.47
1:3:188:SER:HB3	1:3:192:TRP:N	2.29	0.47
1:4:66:ASP:O	1:4:68:LYS:HE2	2.15	0.47
1:2:201:ASN:ND2	1:2:201:ASN:N	2.62	0.47
1:3:270:LEU:HD23	1:3:271:GLY:H	1.67	0.47
1:3:26:VAL:CA	1:3:27:VAL:HG12	2.44	0.47
1:3:36:LEU:HD21	1:3:58:MET:HB3	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:218:PRO:C	1:4:220:LEU:H	2.18	0.47
1:1:54:GLY:CA	1:1:66:ASP:CG	2.83	0.46
1:2:133:LEU:O	1:2:136:TYR:HB3	2.15	0.46
1:2:252:ASP:O	1:2:255:LYS:HB2	2.15	0.46
1:2:74:ASN:CA	2:2:407:HOH:O	2.53	0.46
1:4:38:TYR:O	1:4:42:MET:CB	2.63	0.46
1:4:7:GLY:O	1:4:8:PHE:CB	2.63	0.46
1:2:184:VAL:HG13	1:2:184:VAL:O	2.15	0.46
1:2:197:GLY:O	1:2:201:ASN:HB2	2.15	0.46
1:2:200:GLN:C	1:2:201:ASN:HD22	2.18	0.46
1:1:126:MET:CB	1:1:215:LYS:HZ3	2.14	0.46
1:2:242:THR:C	1:2:243:VAL:CG1	2.83	0.46
1:2:251:TYR:HB2	1:2:299:LEU:CB	2.38	0.46
1:2:272:TYR:HH	1:2:274:GLU:CD	2.18	0.46
1:2:71:THR:HG22	1:2:72:VAL:N	2.30	0.46
1:2:83:TRP:CA	1:2:86:ALA:CB	2.93	0.46
1:1:193:ARG:HG3	1:4:277:VAL:HA	1.97	0.46
1:3:321:ILE:O	1:3:324:LEU:CB	2.63	0.46
1:1:188:SER:HB3	1:1:191:ASP:O	2.15	0.46
1:2:44:LYS:HG3	1:2:56:VAL:HG11	1.97	0.46
1:4:131:VAL:HG12	1:4:158:LYS:CE	2.44	0.46
1:1:108:PHE:O	1:1:110:GLY:N	2.48	0.46
1:1:161:HIS:O	1:1:165:GLU:N	2.42	0.46
1:1:126:MET:CE	1:1:215:LYS:HD2	2.44	0.46
1:2:325:LYS:O	1:2:327:MET:N	2.48	0.46
1:2:327:MET:O	1:2:328:GLN:C	2.53	0.46
1:2:332:SER:O	1:2:333:ALA:CB	2.63	0.46
1:2:78:PRO:O	1:2:81:ILE:HG22	2.15	0.46
1:3:151:ASN:O	1:3:155:PRO:HD2	2.15	0.46
1:3:16:LEU:HD21	1:3:70:ILE:HD12	1.97	0.46
1:3:26:VAL:O	1:3:27:VAL:HB	2.14	0.46
1:3:81:ILE:HG21	1:3:83:TRP:CZ2	2.50	0.46
1:4:189:ALA:O	1:4:190:LYS:HD3	2.15	0.46
1:1:11:ILE:HG21	1:1:118:SER:OG	2.15	0.46
1:1:132:ASN:ND2	1:1:133:LEU:HG	2.30	0.46
1:1:160:LEU:HA	1:1:160:LEU:HD23	1.53	0.46
1:1:36:LEU:O	1:1:40:VAL:HG13	2.15	0.46
1:2:127:PHE:HD2	1:2:132:ASN:CB	2.29	0.46
1:2:165:GLU:O	1:2:166:ILE:CB	2.63	0.46
1:2:251:TYR:HE1	1:2:255:LYS:HD3	1.79	0.46
1:3:138:LYS:HZ1	1:3:330:VAL:CG1	2.09	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:156:VAL:HA	1:3:258:MET:CE	2.44	0.46
1:3:78:PRO:HD2	1:3:79:GLU:H	1.80	0.46
1:4:145:ASN:ND2	1:4:145:ASN:O	2.47	0.46
1:1:8:PHE:CA	1:1:12:GLY:HA3	2.39	0.46
1:1:299:LEU:O	1:1:300:SER:HB3	2.16	0.46
1:2:153:LEU:O	1:2:154:ALA:C	2.54	0.46
1:2:90:TYR:CZ	1:2:328:GLN:NE2	2.83	0.46
1:1:295:ALA:HB2	1:4:193:ARG:HH12	1.79	0.46
1:4:235:ASP:OD2	1:4:311:ASP:OD1	2.33	0.46
1:4:251:TYR:O	1:4:254:ILE:HB	2.16	0.46
1:4:52:PHE:CG	1:4:53:LYS:HE2	2.50	0.46
1:4:33:PHE:CZ	1:4:76:MET:SD	3.06	0.46
1:3:16:LEU:HD21	1:3:70:ILE:HD11	1.93	0.46
1:3:250:SER:O	1:3:251:TYR:C	2.54	0.46
1:4:120:PRO:O	1:4:120:PRO:HG2	2.15	0.46
1:4:129:CYS:O	1:4:130:GLY:C	2.53	0.46
1:4:130:GLY:HA3	1:4:158:LYS:HZ1	1.79	0.46
1:4:131:VAL:CG2	1:4:216:VAL:HG22	2.45	0.46
1:1:159:VAL:O	1:1:160:LEU:C	2.52	0.46
1:1:168:GLU:HG3	1:1:244:ARG:HD2	1.94	0.46
1:1:28:ALA:HB1	1:1:73:PHE:HE2	1.77	0.46
1:4:236:VAL:CG1	1:4:237:SER:N	2.77	0.46
1:3:108:PHE:CG	1:3:109:LYS:N	2.84	0.46
1:3:322:ASP:O	1:3:323:LEU:O	2.34	0.46
1:3:329:LYS:HZ3	1:3:330:VAL:N	2.14	0.46
1:3:81:ILE:HD12	1:3:83:TRP:CE3	2.50	0.46
1:1:266:LEU:HD23	1:1:270:LEU:CB	2.45	0.46
1:1:153:LEU:HD21	1:1:241:LEU:HD22	1.98	0.46
1:1:16:LEU:C	1:1:18:ALA:N	2.69	0.46
1:2:128:VAL:N	1:2:132:ASN:HB2	2.30	0.46
1:2:164:PHE:HZ	1:2:253:ASP:HB3	1.80	0.46
1:1:196:ARG:NH2	1:4:281:ASP:CG	2.69	0.46
1:4:251:TYR:CB	1:4:299:LEU:HG	2.46	0.46
1:2:188:SER:O	1:2:190:LYS:C	2.54	0.46
1:3:27:VAL:H	1:3:70:ILE:HB	1.81	0.46
1:3:29:VAL:O	1:3:30:ASN:HB3	2.16	0.46
1:3:6:ASN:CB	1:3:30:ASN:HD21	2.29	0.46
1:4:212:ALA:O	1:4:216:VAL:HG12	2.15	0.46
1:2:36:LEU:HD21	1:2:62:ALA:CA	2.46	0.46
1:1:282:PHE:HZ	1:1:290:ILE:CD1	2.27	0.46
1:1:294:LYS:HA	1:1:297:ILE:HG13	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:318:GLN:O	1:1:321:ILE:HB	2.16	0.46
1:3:148:CYS:SG	1:3:175:HIS:HE1	2.39	0.46
1:4:152:CYS:SG	1:4:239:VAL:CG1	3.04	0.46
1:4:53:LYS:CE	1:4:53:LYS:N	2.77	0.46
1:3:161:HIS:O	1:3:165:GLU:N	2.46	0.46
1:3:255:LYS:CB	1:3:255:LYS:NZ	2.77	0.46
1:3:287:ARG:HH12	1:3:290:ILE:CD1	2.28	0.46
1:3:321:ILE:O	1:3:324:LEU:HB3	2.15	0.46
1:3:81:ILE:CD1	1:3:82:PRO:O	2.59	0.46
1:3:2:LYS:HZ3	1:3:88:ALA:HA	1.81	0.46
1:2:169:GLY:O	1:2:170:LEU:HD23	2.16	0.46
1:1:244:ARG:NH2	1:4:244:ARG:CG	2.78	0.46
1:1:276:ASP:OD1	1:1:277:VAL:CB	2.64	0.46
1:1:292:ASP:OD1	1:1:307:VAL:HG11	2.14	0.46
1:1:318:GLN:O	1:1:322:ASP:OD2	2.34	0.46
1:1:82:PRO:HB2	1:1:85:LYS:O	2.16	0.46
1:2:131:VAL:HG12	1:2:158:LYS:HE2	1.97	0.46
1:2:220:LEU:HA	1:2:223:LYS:HG3	1.98	0.46
1:2:235:ASP:CG	1:2:313:GLU:HG3	2.35	0.46
1:2:136:TYR:CZ	1:2:327:MET:HG2	2.51	0.46
1:2:76:MET:O	1:2:77:LYS:CG	2.64	0.46
1:4:180:THR:OG1	1:4:181:GLN:N	2.46	0.46
1:4:314:PHE:HB2	1:4:317:SER:CB	2.45	0.46
1:2:185:ASP:HA	1:2:196:ARG:CA	2.46	0.46
1:3:142:VAL:HG11	2:3:381:HOH:O	2.16	0.46
1:3:283:ILE:O	1:3:284:GLY:C	2.53	0.46
1:4:127:PHE:HB2	1:4:323:LEU:CD2	2.46	0.46
1:1:145:ASN:O	1:1:146:ALA:C	2.55	0.46
1:1:15:VAL:HA	1:1:18:ALA:HB2	1.98	0.46
1:2:106:ALA:O	1:2:107:HIS:O	2.34	0.46
1:2:295:ALA:O	1:2:307:VAL:HG11	2.16	0.46
1:2:78:PRO:HG3	1:2:98:PHE:CD2	2.47	0.46
1:4:7:GLY:H	1:4:30:ASN:ND2	2.14	0.46
1:3:104:ALA:C	1:3:106:ALA:N	2.64	0.46
1:3:152:CYS:HB3	1:3:239:VAL:HG11	1.96	0.46
1:3:172:THR:HB	1:3:240:ASP:HB3	1.97	0.46
1:1:84:SER:O	1:1:86:ALA:N	2.49	0.45
1:2:292:ASP:O	1:2:292:ASP:OD1	2.33	0.45
1:2:6:ASN:HA	1:2:30:ASN:HD21	1.75	0.45
1:3:190:LYS:HA	1:3:190:LYS:CE	2.45	0.45
1:4:169:GLY:C	1:4:224:LEU:HD23	2.36	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:175:HIS:O	1:4:231:VAL:CG2	2.64	0.45
1:1:202:ILE:HD12	1:4:233:THR:HG21	1.85	0.45
1:4:19:ALA:CA	1:4:24:ALA:HB3	2.46	0.45
1:4:294:LYS:HZ2	1:4:294:LYS:HG3	1.61	0.45
1:4:74:ASN:HB2	2:4:457:HOH:O	2.16	0.45
1:3:138:LYS:HZ2	1:3:138:LYS:HG2	1.41	0.45
1:1:233:THR:HG21	1:4:202:ILE:CD1	2.46	0.45
1:1:277:VAL:O	1:4:193:ARG:HD3	2.16	0.45
1:2:89:GLU:O	1:2:114:LYS:CG	2.65	0.45
1:2:8:PHE:CE2	1:2:34:ILE:CD1	2.99	0.45
1:4:65:VAL:CG2	1:4:66:ASP:OD2	2.64	0.45
1:3:266:LEU:O	1:3:267:GLN:C	2.54	0.45
1:3:299:LEU:O	1:3:300:SER:CB	2.64	0.45
1:3:327:MET:HB3	1:3:327:MET:HE3	1.81	0.45
1:3:329:LYS:NZ	1:3:329:LYS:HB3	2.27	0.45
1:3:216:VAL:O	1:3:218:PRO:HD3	2.15	0.45
1:2:102:GLU:C	1:2:102:GLU:OE1	2.54	0.45
1:1:128:VAL:O	1:1:132:ASN:N	2.49	0.45
1:1:16:LEU:C	1:1:18:ALA:H	2.20	0.45
1:1:220:LEU:O	1:1:223:LYS:HD3	2.17	0.45
1:1:4:GLY:CA	1:1:27:VAL:CG2	2.79	0.45
1:4:292:ASP:HB3	1:4:307:VAL:CG1	2.47	0.45
1:4:77:LYS:O	1:4:80:ASN:HB2	2.17	0.45
1:3:283:ILE:CG1	2:3:388:HOH:O	2.64	0.45
1:3:46:ASP:HB3	1:3:50:GLY:HA2	1.98	0.45
1:4:221:ASP:C	1:4:221:ASP:OD2	2.55	0.45
1:1:328:GLN:O	1:1:329:LYS:O	2.34	0.45
1:1:3:ILE:HG13	1:1:25:GLN:HB3	1.99	0.45
1:1:51:VAL:O	1:1:52:PHE:CB	2.59	0.45
1:1:71:THR:HG22	1:1:72:VAL:C	2.37	0.45
1:2:213:VAL:HA	1:2:216:VAL:HG12	1.98	0.45
1:2:281:ASP:OD1	1:3:196:ARG:NH2	2.49	0.45
1:4:26:VAL:HG21	1:4:68:LYS:HG3	1.99	0.45
1:3:285:ASP:OD2	1:3:287:ARG:HB2	2.17	0.45
1:3:55:GLU:HB3	1:3:67:GLY:H	1.80	0.45
1:4:217:ILE:O	1:4:220:LEU:HB2	2.16	0.45
1:4:164:PHE:CE2	1:4:249:CYS:HB3	2.51	0.45
1:1:126:MET:HE3	1:1:212:ALA:HA	1.97	0.45
1:4:276:ASP:O	1:4:277:VAL:C	2.55	0.45
1:3:11:ILE:HG22	1:3:15:VAL:HG21	1.97	0.45
1:3:282:PHE:HE2	1:3:309:TRP:CD2	2.35	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:143:VAL:HG11	1:3:327:MET:SD	2.57	0.45
1:3:71:THR:C	1:3:72:VAL:HG12	2.36	0.45
1:4:329:LYS:NZ	1:4:329:LYS:O	2.37	0.45
1:3:220:LEU:O	1:3:223:LYS:HD3	2.15	0.45
1:2:137:SER:O	1:2:140:MET:HG2	2.17	0.45
1:4:259:LYS:O	1:4:260:THR:C	2.54	0.45
1:1:153:LEU:HD23	1:1:153:LEU:O	2.17	0.45
1:1:252:ASP:O	1:1:255:LYS:HB2	2.17	0.45
1:1:3:ILE:C	1:1:27:VAL:HG23	2.35	0.45
1:1:85:LYS:O	1:1:86:ALA:HB2	2.17	0.45
1:2:149:THR:HA	1:2:310:TYR:CZ	2.52	0.45
1:2:7:GLY:HA2	1:2:31:ASP:HB2	1.98	0.45
1:2:97:VAL:O	1:2:98:PHE:HD1	1.78	0.45
1:4:160:LEU:HD23	1:4:160:LEU:HA	1.72	0.45
1:1:295:ALA:HB2	1:4:193:ARG:NH1	2.31	0.45
1:3:79:GLU:HG3	1:3:109:LYS:CD	2.47	0.45
1:3:114:LYS:HG2	1:3:114:LYS:H	1.45	0.45
1:3:55:GLU:O	1:3:65:VAL:CA	2.58	0.45
1:3:95:THR:HG21	1:3:97:VAL:CG2	2.47	0.45
1:3:78:PRO:CD	1:3:98:PHE:CE2	2.99	0.45
1:2:215:LYS:O	1:2:215:LYS:HD3	2.16	0.45
1:2:59:GLU:HB2	1:2:64:VAL:CG1	2.47	0.45
1:1:152:CYS:SG	1:1:239:VAL:HG13	2.54	0.45
1:4:36:LEU:CD1	1:4:63:LEU:HB2	2.46	0.45
1:1:113:LYS:HG2	1:1:114:LYS:HZ1	1.82	0.45
1:1:157:ALA:O	1:1:158:LYS:C	2.55	0.45
1:1:176:ALA:O	1:1:177:VAL:C	2.55	0.45
1:1:76:MET:O	1:1:77:LYS:HD3	2.17	0.45
1:2:280:SER:O	1:2:281:ASP:O	2.35	0.45
1:4:201:ASN:HB3	1:4:203:ILE:HG12	1.97	0.45
1:3:170:LEU:O	1:3:241:LEU:HD12	2.16	0.45
1:3:314:PHE:HA	1:3:317:SER:OG	2.16	0.45
1:2:13:ARG:C	1:2:15:VAL:N	2.69	0.45
1:1:253:ASP:O	1:1:255:LYS:N	2.48	0.45
1:1:290:ILE:O	1:1:308:SER:HA	2.16	0.45
1:2:101:ILE:O	1:2:105:SER:CB	2.65	0.45
1:4:272:TYR:CZ	1:4:293:ALA:HB2	2.51	0.45
1:3:33:PHE:HZ	1:3:76:MET:CE	2.30	0.45
1:2:51:VAL:HG23	2:2:401:HOH:O	2.15	0.45
1:1:154:ALA:N	1:1:155:PRO:HD2	2.32	0.45
1:1:174:VAL:HG12	1:1:231:VAL:HG21	1.95	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:19:ALA:HA	1:1:24:ALA:CB	2.46	0.45
1:1:237:SER:O	1:1:310:TYR:CD1	2.70	0.45
1:2:3:ILE:HG13	1:2:25:GLN:O	2.17	0.45
1:2:299:LEU:HG	1:2:304:VAL:HG23	1.99	0.45
1:3:190:LYS:HD3	2:3:337:HOH:O	2.17	0.45
1:4:193:ARG:O	1:4:203:ILE:HG23	2.16	0.45
1:4:201:ASN:HD22	1:4:201:ASN:N	2.15	0.45
1:4:17:ARG:HH22	1:4:46:ASP:HB2	1.81	0.45
1:3:39:MET:O	1:3:43:PHE:N	2.48	0.45
1:3:46:ASP:HB2	1:3:50:GLY:HA2	1.98	0.45
1:4:142:VAL:CG2	1:4:142:VAL:O	2.63	0.45
1:2:117:ILE:HG13	1:2:117:ILE:H	1.44	0.45
1:2:272:TYR:C	1:2:272:TYR:CD1	2.89	0.45
1:3:185:ASP:OD2	1:3:196:ARG:HD3	2.17	0.45
1:3:188:SER:HA	1:3:191:ASP:OD2	2.16	0.45
1:4:238:VAL:HG22	1:4:307:VAL:CG2	2.46	0.45
1:3:269:PHE:O	1:3:288:SER:HB3	2.17	0.45
1:1:129:CYS:HA	1:1:132:ASN:HD22	1.81	0.44
1:1:157:ALA:O	1:1:159:VAL:N	2.50	0.44
1:1:175:HIS:CD2	1:1:230:ARG:HH21	2.35	0.44
1:2:38:TYR:O	1:2:42:MET:HB2	2.16	0.44
1:2:188:SER:O	1:2:189:ALA:C	2.56	0.44
1:3:128:VAL:HG11	1:3:154:ALA:HB1	1.99	0.44
1:4:116:VAL:HG11	1:4:324:LEU:CD2	2.47	0.44
1:1:105:SER:O	1:1:108:PHE:HD1	1.99	0.44
1:1:295:ALA:C	1:1:297:ILE:HD12	2.38	0.44
1:2:117:ILE:CD1	1:2:142:VAL:HG22	2.46	0.44
1:4:14:LEU:HD22	1:4:14:LEU:H	1.82	0.44
1:4:239:VAL:HG22	1:4:308:SER:HB2	1.99	0.44
1:1:225:THR:HG23	1:4:298:GLN:OE1	2.14	0.44
1:4:83:TRP:CE2	1:4:91:ILE:HG12	2.51	0.44
1:3:36:LEU:HD11	1:3:63:LEU:HB2	1.98	0.44
1:4:319:ARG:HG2	1:4:319:ARG:NH1	2.32	0.44
1:2:22:CYS:SG	1:2:321:ILE:HG21	2.57	0.44
1:2:100:THR:OG1	1:2:103:LYS:HD2	2.17	0.44
1:1:181:GLN:O	1:1:182:LYS:C	2.56	0.44
1:4:227:MET:HE3	1:4:229:PHE:CZ	2.51	0.44
1:4:3:ILE:HD12	1:4:24:ALA:HB1	1.99	0.44
1:4:39:MET:O	1:4:42:MET:N	2.50	0.44
1:4:52:PHE:CE1	1:4:53:LYS:CE	2.94	0.44
1:4:97:VAL:O	1:4:98:PHE:CB	2.65	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:98:PHE:HA	1:3:103:LYS:HG2	1.97	0.44
1:2:66:ASP:C	1:2:68:LYS:HD3	2.35	0.44
1:3:171:MET:CA	1:3:240:ASP:O	2.65	0.44
1:1:202:ILE:HD11	1:4:233:THR:CB	2.46	0.44
1:1:242:THR:HA	1:1:304:VAL:O	2.17	0.44
1:2:109:LYS:HG2	1:2:110:GLY:N	2.32	0.44
1:2:77:LYS:O	1:2:80:ASN:HB2	2.17	0.44
1:3:26:VAL:HG11	1:3:68:LYS:CG	2.48	0.44
1:1:168:GLU:CG	1:1:244:ARG:CD	2.88	0.44
1:2:117:ILE:HB	1:2:144:SER:HB2	1.99	0.44
1:2:279:SER:C	1:2:281:ASP:H	2.20	0.44
1:4:172:THR:O	1:4:240:ASP:N	2.41	0.44
1:4:233:THR:HA	1:4:234:PRO:HD2	1.87	0.44
1:4:28:ALA:CB	1:4:83:TRP:CZ3	2.91	0.44
1:3:100:THR:O	1:3:101:ILE:C	2.54	0.44
1:3:329:LYS:NZ	1:3:330:VAL:N	2.66	0.44
1:3:57:LYS:HD3	1:3:57:LYS:HA	1.87	0.44
1:1:11:ILE:CG2	1:1:15:VAL:CG2	2.90	0.44
1:1:295:ALA:O	1:1:307:VAL:HG21	2.18	0.44
1:3:186:GLY:O	1:3:195:GLY:CA	2.66	0.44
1:2:193:ARG:O	1:2:203:ILE:HG23	2.18	0.44
1:3:4:GLY:N	1:3:27:VAL:CG2	2.78	0.44
1:3:319:ARG:O	1:3:320:VAL:O	2.35	0.44
1:1:168:GLU:OE2	1:1:244:ARG:NE	2.50	0.44
1:1:181:GLN:HB3	1:1:198:ALA:CB	2.48	0.44
1:2:261:ALA:O	1:2:262:SER:C	2.56	0.44
1:4:193:ARG:O	1:4:203:ILE:HG21	2.17	0.44
1:4:292:ASP:OD1	1:4:295:ALA:O	2.35	0.44
1:4:30:ASN:HD22	1:4:30:ASN:C	2.10	0.44
1:4:7:GLY:H	1:4:30:ASN:HD22	1.65	0.44
1:4:52:PHE:CE2	1:4:66:ASP:OD2	2.71	0.44
1:4:78:PRO:HD3	1:4:98:PHE:CZ	2.51	0.44
1:3:251:TYR:N	1:3:299:LEU:CD1	2.69	0.44
1:2:9:GLY:O	1:2:10:ARG:O	2.35	0.44
1:3:211:LYS:N	1:3:211:LYS:HE2	2.31	0.44
1:4:267:GLN:HB3	1:4:268:GLY:H	1.43	0.44
1:2:156:VAL:HG22	1:2:258:MET:HE1	1.95	0.44
1:1:138:LYS:N	1:1:138:LYS:HD3	2.29	0.44
1:2:150:THR:C	1:2:152:CYS:N	2.69	0.44
1:2:150:THR:O	1:2:151:ASN:C	2.54	0.44
1:4:75:GLU:CB	2:4:347:HOH:O	2.38	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:73:PHE:HD2	1:4:81:ILE:CD1	2.29	0.44
1:3:273:THR:O	1:3:293:ALA:CB	2.64	0.44
1:3:44:LYS:CG	1:3:56:VAL:HG21	2.46	0.44
1:2:66:ASP:O	1:2:68:LYS:HD2	2.16	0.44
1:4:127:PHE:HZ	1:4:135:LYS:HZ3	1.64	0.44
1:4:330:VAL:O	1:4:331:ASP:C	2.56	0.44
1:3:216:VAL:HG12	1:3:217:ILE:HG22	2.00	0.44
1:1:141:THR:OG1	1:1:142:VAL:N	2.51	0.44
1:2:113:LYS:CE	1:2:114:LYS:HZ1	2.18	0.44
1:2:127:PHE:CD2	1:2:132:ASN:OD1	2.71	0.44
1:2:159:VAL:HG21	1:2:266:LEU:HD21	1.95	0.44
1:2:270:LEU:CD2	1:2:271:GLY:N	2.80	0.44
1:4:281:ASP:CA	2:4:357:HOH:O	2.63	0.44
1:4:298:GLN:HE21	1:4:299:LEU:N	2.16	0.44
1:3:81:ILE:CG1	1:3:82:PRO:HD2	2.48	0.44
1:3:172:THR:O	1:3:240:ASP:HB2	2.17	0.44
1:1:101:ILE:HG23	1:1:142:VAL:CB	2.48	0.43
1:1:183:THR:CG2	1:2:181:GLN:O	2.66	0.43
1:4:19:ALA:CB	1:4:24:ALA:HB3	2.48	0.43
1:4:6:ASN:CA	1:4:30:ASN:HD21	2.19	0.43
1:4:39:MET:O	1:4:40:VAL:C	2.56	0.43
1:4:39:MET:CE	1:4:72:VAL:CG2	2.96	0.43
1:4:83:TRP:N	1:4:86:ALA:CB	2.81	0.43
1:3:146:ALA:HB3	1:3:150:THR:HG21	1.98	0.43
1:3:160:LEU:O	1:3:164:PHE:N	2.51	0.43
1:3:1:SER:HB3	1:3:25:GLN:HE22	1.81	0.43
1:3:46:ASP:HB3	1:3:50:GLY:CA	2.48	0.43
1:2:44:LYS:O	1:2:51:VAL:CA	2.66	0.43
1:2:138:LYS:HE3	1:2:330:VAL:HG12	1.95	0.43
1:1:124:ALA:O	1:1:125:PRO:C	2.53	0.43
1:1:128:VAL:HG11	1:1:154:ALA:CB	2.48	0.43
1:1:16:LEU:O	1:1:18:ALA:N	2.51	0.43
1:2:161:HIS:O	1:2:165:GLU:CA	2.66	0.43
1:4:153:LEU:O	1:4:154:ALA:C	2.56	0.43
1:4:239:VAL:HG12	1:4:310:TYR:CE1	2.47	0.43
1:4:1:SER:C	1:4:25:GLN:HB2	2.38	0.43
1:3:169:GLY:C	1:3:224:LEU:HD23	2.39	0.43
1:3:26:VAL:O	1:3:27:VAL:CB	2.66	0.43
1:3:330:VAL:C	1:3:332:SER:N	2.69	0.43
1:2:13:ARG:O	1:2:17:ARG:N	2.47	0.43
1:3:245:LEU:HD23	1:3:245:LEU:HA	1.84	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:251:TYR:O	1:1:252:ASP:O	2.35	0.43
1:2:262:SER:O	1:2:267:GLN:HA	2.18	0.43
1:4:52:PHE:CD1	1:4:53:LYS:HE2	2.52	0.43
1:3:283:ILE:HG13	2:3:388:HOH:O	2.18	0.43
1:3:311:ASP:O	1:3:314:PHE:N	2.51	0.43
1:3:319:ARG:HG2	1:3:319:ARG:HH11	1.84	0.43
1:4:129:CYS:O	1:4:133:LEU:HG	2.18	0.43
1:4:146:ALA:HB3	1:4:150:THR:HG21	2.00	0.43
1:2:244:ARG:HA	1:3:244:ARG:HH22	1.84	0.43
1:3:126:MET:HG2	1:3:212:ALA:HB2	2.01	0.43
1:1:10:ARG:HA	1:1:10:ARG:HD3	1.62	0.43
1:1:269:PHE:N	1:1:269:PHE:CD2	2.86	0.43
1:1:272:TYR:OH	1:1:274:GLU:OE1	2.35	0.43
1:1:292:ASP:HB2	1:1:309:TRP:HE1	1.82	0.43
1:1:34:ILE:CD1	1:1:39:MET:HG2	2.44	0.43
1:1:50:GLY:O	1:1:51:VAL:HG23	2.18	0.43
1:2:142:VAL:CG2	1:2:142:VAL:O	2.60	0.43
1:3:79:GLU:HG3	1:3:109:LYS:HD2	2.00	0.43
1:3:95:THR:HG21	1:3:97:VAL:HG22	2.00	0.43
1:1:38:TYR:O	1:1:42:MET:N	2.51	0.43
1:1:184:VAL:O	1:1:185:ASP:O	2.37	0.43
1:1:175:HIS:CB	1:1:230:ARG:HH21	2.31	0.43
1:1:170:LEU:O	1:1:241:LEU:HD12	2.18	0.43
1:1:30:ASN:N	1:1:30:ASN:ND2	2.66	0.43
1:2:236:VAL:N	2:2:418:HOH:O	2.52	0.43
1:1:202:ILE:HD11	1:4:233:THR:HB	1.99	0.43
1:3:131:VAL:N	1:3:158:LYS:HZ1	2.14	0.43
1:2:227:MET:HG2	1:3:305:LYS:HE3	2.01	0.43
1:2:36:LEU:CD2	1:2:62:ALA:HA	2.48	0.43
1:1:193:ARG:HD3	1:4:277:VAL:O	2.17	0.43
1:1:220:LEU:CD1	1:1:223:LYS:NZ	2.81	0.43
1:1:251:TYR:CE2	1:1:254:ILE:HG21	2.53	0.43
1:1:286:ASN:HD22	1:1:286:ASN:N	2.14	0.43
1:2:153:LEU:C	1:2:153:LEU:CD2	2.87	0.43
1:2:6:ASN:ND2	1:2:93:GLU:CD	2.68	0.43
1:3:29:VAL:HG12	1:3:30:ASN:N	2.34	0.43
1:4:146:ALA:CB	1:4:212:ALA:HB2	2.49	0.43
1:3:211:LYS:NZ	2:3:384:HOH:O	2.51	0.43
1:3:178:THR:HG1	1:3:181:GLN:HB2	1.84	0.43
1:1:126:MET:HE1	1:1:215:LYS:HZ2	1.84	0.43
1:1:76:MET:O	1:1:77:LYS:CB	2.64	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:113:LYS:CA	1:2:114:LYS:HG2	2.48	0.43
1:2:202:ILE:HD11	1:3:233:THR:HG21	2.00	0.43
1:4:183:THR:C	1:4:184:VAL:HG12	2.38	0.43
1:4:152:CYS:HA	1:4:289:SER:CB	2.49	0.43
1:3:285:ASP:C	1:3:285:ASP:OD2	2.57	0.43
1:3:44:LYS:HD2	1:3:56:VAL:HG11	1.99	0.43
1:2:44:LYS:HZ2	1:2:44:LYS:HG2	1.41	0.43
1:4:190:LYS:HD3	1:4:190:LYS:HA	1.64	0.43
1:1:220:LEU:HD13	1:1:223:LYS:NZ	2.33	0.43
1:1:278:VAL:HG23	1:1:309:TRP:CZ2	2.54	0.43
1:1:310:TYR:HB2	1:1:311:ASP:H	1.22	0.43
1:1:36:LEU:HD11	1:1:62:ALA:CA	2.49	0.43
1:2:133:LEU:HG	1:2:133:LEU:H	1.23	0.43
1:2:34:ILE:HG12	1:2:39:MET:CE	2.49	0.43
1:2:41:TYR:OH	1:4:277:VAL:CG2	2.65	0.43
1:2:71:THR:HG21	1:2:73:PHE:CE1	2.53	0.43
1:4:293:ALA:O	1:4:294:LYS:CB	2.56	0.43
1:4:238:VAL:HB	1:4:309:TRP:CE3	2.53	0.43
1:4:30:ASN:OD1	1:4:81:ILE:HG21	2.18	0.43
1:4:3:ILE:HA	1:4:90:TYR:O	2.19	0.43
1:3:224:LEU:CD2	1:3:241:LEU:HD11	2.49	0.43
1:3:276:ASP:HB3	1:3:294:LYS:HD3	2.00	0.43
1:2:18:ALA:O	1:2:19:ALA:C	2.57	0.43
1:2:50:GLY:C	1:2:51:VAL:O	2.56	0.43
1:2:244:ARG:NE	1:3:244:ARG:CZ	2.82	0.43
1:2:135:LYS:NZ	1:2:140:MET:HE1	2.34	0.43
1:2:319:ARG:O	1:2:322:ASP:N	2.52	0.43
1:4:282:PHE:O	1:4:283:ILE:C	2.56	0.43
1:3:269:PHE:CD2	1:3:269:PHE:N	2.86	0.43
1:3:318:GLN:O	1:3:321:ILE:CB	2.57	0.43
1:3:44:LYS:HE3	1:3:44:LYS:HB3	1.68	0.43
1:1:208:GLY:HA2	1:1:211:LYS:HG2	1.91	0.43
1:4:211:LYS:HA	1:4:211:LYS:HE2	1.84	0.43
1:1:8:PHE:HB2	1:1:12:GLY:C	2.39	0.43
1:1:319:ARG:O	1:1:323:LEU:N	2.49	0.43
1:1:328:GLN:O	1:1:329:LYS:C	2.56	0.43
1:2:101:ILE:HD11	1:2:124:ALA:HA	2.01	0.43
1:2:271:GLY:O	1:2:272:TYR:CB	2.66	0.43
1:2:327:MET:O	1:2:331:ASP:N	2.52	0.43
1:2:84:SER:O	1:2:86:ALA:CB	2.63	0.43
1:2:52:PHE:C	2:2:400:HOH:O	2.55	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:101:ILE:CG1	1:1:142:VAL:CG1	2.95	0.42
1:1:133:LEU:HG	1:1:133:LEU:H	1.30	0.42
1:1:161:HIS:C	1:1:163:ASN:N	2.72	0.42
1:1:57:LYS:HA	1:1:57:LYS:HD3	1.78	0.42
1:2:130:GLY:C	1:2:158:LYS:NZ	2.73	0.42
1:2:252:ASP:O	1:2:255:LYS:CB	2.67	0.42
1:4:119:ALA:CB	1:4:120:PRO:CD	2.50	0.42
1:4:137:SER:CA	1:4:138:LYS:HE3	2.45	0.42
1:2:156:VAL:CG2	1:2:258:MET:HE2	2.49	0.42
1:1:282:PHE:O	1:1:285:ASP:HB3	2.19	0.42
1:2:93:GLU:OE2	1:2:98:PHE:HD2	2.00	0.42
1:4:184:VAL:O	1:4:185:ASP:O	2.37	0.42
1:1:125:PRO:HB2	1:1:127:PHE:CE1	2.54	0.42
1:1:175:HIS:HB3	1:1:230:ARG:HH21	1.83	0.42
1:4:32:PRO:O	1:4:33:PHE:CB	2.68	0.42
1:4:95:THR:HG21	1:4:97:VAL:HG23	2.01	0.42
1:2:66:ASP:CB	2:2:402:HOH:O	2.68	0.42
1:1:134:GLU:O	1:1:135:LYS:C	2.57	0.42
1:1:129:CYS:CA	1:1:132:ASN:HD22	2.33	0.42
1:2:127:PHE:HD2	1:2:132:ASN:CA	2.32	0.42
1:2:131:VAL:N	1:2:158:LYS:NZ	2.67	0.42
1:2:235:ASP:O	1:2:236:VAL:HG23	2.20	0.42
1:2:300:SER:O	1:2:301:LYS:CB	2.66	0.42
1:3:186:GLY:O	1:3:195:GLY:HA3	2.19	0.42
1:4:10:ARG:HD3	1:4:10:ARG:HA	1.57	0.42
1:4:271:GLY:O	1:4:272:TYR:CB	2.67	0.42
1:3:307:VAL:H	1:3:307:VAL:HG12	1.63	0.42
1:3:53:LYS:CE	1:3:53:LYS:N	2.76	0.42
1:1:101:ILE:O	1:1:102:GLU:C	2.57	0.42
1:1:16:LEU:O	1:1:19:ALA:HB3	2.18	0.42
1:1:251:TYR:CD2	1:1:254:ILE:CG2	3.03	0.42
1:2:104:ALA:O	1:2:106:ALA:N	2.51	0.42
1:2:101:ILE:HB	1:2:123:ASP:OD1	2.19	0.42
1:2:326:HIS:O	1:2:327:MET:C	2.57	0.42
1:4:252:ASP:OD1	1:4:252:ASP:O	2.37	0.42
1:3:108:PHE:O	1:3:110:GLY:N	2.52	0.42
1:3:318:GLN:O	1:3:321:ILE:N	2.52	0.42
1:2:135:LYS:CD	1:2:135:LYS:O	2.63	0.42
1:1:160:LEU:CD2	1:1:254:ILE:CD1	2.97	0.42
1:1:329:LYS:NZ	1:1:330:VAL:CA	2.82	0.42
1:2:1:SER:C	1:2:2:LYS:CG	2.77	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:81:ILE:HG23	1:2:83:TRP:NE1	2.34	0.42
1:4:152:CYS:HA	1:4:289:SER:HB3	2.01	0.42
1:4:14:LEU:O	1:4:18:ALA:HB2	2.20	0.42
1:3:11:ILE:O	1:3:12:GLY:C	2.58	0.42
1:3:132:ASN:OD1	1:3:133:LEU:CD2	2.66	0.42
1:3:314:PHE:HB2	1:3:317:SER:CB	2.50	0.42
1:4:130:GLY:HA3	1:4:158:LYS:HZ2	1.82	0.42
1:4:329:LYS:HD2	1:4:329:LYS:HA	1.54	0.42
1:4:208:GLY:HA2	1:4:211:LYS:HG2	1.98	0.42
1:4:178:THR:O	1:4:179:ALA:C	2.58	0.42
1:1:101:ILE:HG12	1:1:142:VAL:HG11	1.97	0.42
1:1:168:GLU:HG3	1:1:244:ARG:CD	2.50	0.42
1:1:282:PHE:O	1:1:285:ASP:CB	2.67	0.42
1:2:232:PRO:HG2	1:3:232:PRO:CB	2.41	0.42
1:2:31:ASP:HA	1:2:32:PRO:HD2	1.73	0.42
1:2:77:LYS:HD2	1:2:77:LYS:HA	1.64	0.42
1:4:8:PHE:CZ	1:4:39:MET:HB3	2.54	0.42
1:3:101:ILE:CB	1:3:123:ASP:OD1	2.42	0.42
1:2:303:PHE:CE2	1:3:303:PHE:CE2	3.08	0.42
1:3:43:PHE:CE1	1:3:65:VAL:HG21	2.54	0.42
1:2:11:ILE:N	1:2:11:ILE:CD1	2.42	0.42
1:2:51:VAL:HG21	2:2:401:HOH:O	2.18	0.42
1:4:115:VAL:HG12	1:4:116:VAL:N	2.33	0.42
1:4:131:VAL:HG12	1:4:158:LYS:HZ1	1.77	0.42
1:4:319:ARG:HA	1:4:322:ASP:OD2	2.20	0.42
1:4:165:GLU:OE1	1:4:167:VAL:HG12	2.19	0.42
1:1:233:THR:HG22	1:1:236:VAL:H	1.85	0.42
1:1:251:TYR:CZ	1:1:255:LYS:HD3	2.55	0.42
1:1:282:PHE:O	1:1:283:ILE:C	2.57	0.42
1:2:150:THR:CG2	1:2:212:ALA:HB3	2.50	0.42
1:2:247:LYS:C	1:2:248:GLU:O	2.57	0.42
1:2:25:GLN:C	1:2:26:VAL:O	2.58	0.42
1:2:27:VAL:HG13	1:2:28:ALA:C	2.39	0.42
1:2:34:ILE:O	1:2:39:MET:HE3	2.19	0.42
1:4:58:MET:HB2	1:4:58:MET:HE2	1.95	0.42
1:3:161:HIS:O	1:3:164:PHE:N	2.47	0.42
1:3:156:VAL:CG2	1:3:258:MET:HE2	2.49	0.42
1:3:272:TYR:CE2	1:3:293:ALA:CB	2.98	0.42
1:3:71:THR:C	1:3:72:VAL:CG1	2.80	0.42
1:1:105:SER:C	1:1:107:HIS:N	2.74	0.42
1:1:101:ILE:HD13	1:1:142:VAL:CG1	2.49	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:167:VAL:HG23	1:1:244:ARG:HG2	2.01	0.42
1:1:68:LYS:O	1:1:70:ILE:HG23	2.20	0.42
1:2:131:VAL:HG22	1:2:132:ASN:H	1.85	0.42
1:3:175:HIS:HA	1:3:237:SER:OG	2.19	0.42
1:4:276:ASP:OD2	1:4:277:VAL:HG22	2.19	0.42
1:3:156:VAL:HG12	1:3:157:ALA:N	2.34	0.42
1:3:295:ALA:O	1:3:297:ILE:HG23	2.17	0.42
1:3:66:ASP:O	1:3:68:LYS:HD2	2.17	0.42
1:4:119:ALA:O	1:4:144:SER:OG	2.33	0.42
1:4:170:LEU:HD23	1:4:170:LEU:HA	1.80	0.42
1:4:9:GLY:HA2	1:4:13:ARG:NH2	2.35	0.42
1:1:1:SER:CB	1:1:25:GLN:HE21	2.33	0.42
1:1:243:VAL:HG23	1:1:304:VAL:HG12	1.94	0.42
1:2:214:GLY:O	1:2:216:VAL:N	2.53	0.42
1:2:235:ASP:O	1:2:236:VAL:CG2	2.67	0.42
1:4:20:LEU:HD21	1:4:26:VAL:HG13	2.01	0.42
1:4:282:PHE:CE2	1:4:309:TRP:CD1	3.08	0.42
1:3:250:SER:O	1:3:252:ASP:N	2.53	0.42
1:3:74:ASN:OD1	1:3:74:ASN:C	2.59	0.42
1:4:138:LYS:CE	1:4:138:LYS:H	2.33	0.42
1:1:165:GLU:OE1	1:1:167:VAL:CG1	2.65	0.41
1:1:279:SER:C	1:1:281:ASP:N	2.72	0.41
1:2:213:VAL:HG13	1:2:217:ILE:CG2	2.49	0.41
1:2:177:VAL:CG1	1:2:232:PRO:O	2.66	0.41
1:2:266:LEU:O	1:2:269:PHE:N	2.51	0.41
1:2:27:VAL:HG22	1:2:28:ALA:H	1.83	0.41
1:2:316:TYR:O	1:2:319:ARG:HB2	2.19	0.41
1:2:76:MET:O	1:2:77:LYS:CB	2.68	0.41
1:3:205:SER:HB3	1:3:228:ALA:CB	2.41	0.41
1:4:66:ASP:CB	1:4:68:LYS:HE2	2.48	0.41
1:2:193:ARG:HG3	1:3:277:VAL:HA	2.01	0.41
1:4:319:ARG:CG	1:4:319:ARG:NH1	2.80	0.41
1:4:138:LYS:CD	1:4:330:VAL:CG1	2.98	0.41
1:4:188:SER:HB3	1:4:191:ASP:CA	2.50	0.41
1:2:20:LEU:HA	1:2:20:LEU:HD23	1.83	0.41
1:1:281:ASP:C	1:1:283:ILE:N	2.73	0.41
1:2:131:VAL:CG2	1:2:132:ASN:N	2.83	0.41
1:2:213:VAL:HA	1:2:216:VAL:CG1	2.50	0.41
1:2:230:ARG:C	1:2:231:VAL:HG13	2.39	0.41
1:2:295:ALA:C	1:2:297:ILE:HD12	2.39	0.41
1:4:17:ARG:HG3	1:4:43:PHE:CD2	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:127:PHE:CA	1:3:132:ASN:HB3	2.50	0.41
1:3:255:LYS:HZ2	1:3:255:LYS:HB3	1.85	0.41
1:4:218:PRO:C	1:4:220:LEU:N	2.72	0.41
1:2:244:ARG:CA	1:3:244:ARG:HH22	2.31	0.41
1:3:126:MET:CE	1:3:212:ALA:HB2	2.51	0.41
1:1:329:LYS:HZ1	1:1:330:VAL:H	1.65	0.41
1:1:43:PHE:CE1	1:1:52:PHE:CE2	3.08	0.41
1:1:32:PRO:CA	1:1:74:ASN:ND2	2.62	0.41
1:2:136:TYR:OH	1:2:331:ASP:OD2	2.32	0.41
1:4:55:GLU:H	1:4:66:ASP:HA	1.85	0.41
1:3:241:LEU:HD21	1:3:243:VAL:HG11	2.02	0.41
1:3:313:GLU:O	1:3:317:SER:OG	2.38	0.41
1:4:117:ILE:HD13	1:4:117:ILE:HG21	1.76	0.41
1:2:170:LEU:HD22	1:2:170:LEU:HA	1.87	0.41
1:1:319:ARG:CG	1:1:319:ARG:HH11	2.27	0.41
1:1:325:LYS:C	1:1:327:MET:N	2.74	0.41
1:1:82:PRO:O	1:1:83:TRP:CG	2.74	0.41
1:2:242:THR:C	1:2:243:VAL:HG13	2.41	0.41
1:2:294:LYS:H	1:2:297:ILE:HG13	1.85	0.41
1:2:295:ALA:HB2	1:3:193:ARG:CZ	2.50	0.41
1:2:74:ASN:CB	2:2:395:HOH:O	2.62	0.41
1:3:185:ASP:C	1:3:195:GLY:O	2.59	0.41
1:3:158:LYS:HE2	1:3:158:LYS:HB2	1.78	0.41
1:3:19:ALA:CA	1:3:24:ALA:HB3	2.50	0.41
1:3:251:TYR:CD1	1:3:255:LYS:HD3	2.55	0.41
1:3:25:GLN:HG3	1:3:26:VAL:N	2.35	0.41
1:3:304:VAL:HG13	1:3:305:LYS:N	2.35	0.41
1:3:97:VAL:O	1:3:98:PHE:CD1	2.73	0.41
1:3:124:ALA:C	1:3:125:PRO:O	2.55	0.41
1:1:279:SER:O	1:1:281:ASP:N	2.52	0.41
1:1:27:VAL:HG22	1:1:28:ALA:CA	2.46	0.41
1:1:282:PHE:CD1	1:1:285:ASP:OD1	2.72	0.41
1:1:187:PRO:HA	1:2:38:TYR:OH	2.20	0.41
1:4:174:VAL:HG12	1:4:231:VAL:HG21	2.03	0.41
1:4:174:VAL:O	1:4:237:SER:HA	2.20	0.41
1:3:128:VAL:H	1:3:132:ASN:HB3	1.84	0.41
1:4:138:LYS:CD	1:4:138:LYS:N	2.78	0.41
1:1:78:PRO:HG3	1:1:98:PHE:CE2	2.56	0.41
1:1:143:VAL:CG2	1:1:144:SER:N	2.79	0.41
1:1:2:LYS:CA	1:1:25:GLN:HG2	2.50	0.41
1:1:312:ASN:O	1:1:313:GLU:C	2.58	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:324:LEU:C	1:1:324:LEU:HD12	2.41	0.41
1:1:66:ASP:CA	2:1:432:HOH:O	2.62	0.41
1:2:242:THR:O	1:2:243:VAL:HG12	2.21	0.41
1:4:149:THR:O	1:4:152:CYS:N	2.54	0.41
1:4:46:ASP:O	1:4:50:GLY:CA	2.69	0.41
1:3:104:ALA:HB3	1:3:142:VAL:HG21	2.02	0.41
1:3:20:LEU:C	1:3:22:CYS:N	2.69	0.41
1:3:224:LEU:HD21	1:3:241:LEU:HD11	2.01	0.41
1:3:3:ILE:CG2	1:3:4:GLY:N	2.82	0.41
1:3:66:ASP:O	1:3:67:GLY:C	2.59	0.41
1:4:113:LYS:CG	1:4:114:LYS:CE	2.97	0.41
1:3:57:LYS:O	1:3:64:VAL:HG13	2.21	0.41
1:1:127:PHE:CZ	1:1:136:TYR:HB2	2.43	0.41
1:1:127:PHE:HD1	1:1:143:VAL:CG2	2.34	0.41
1:1:171:MET:CE	1:1:209:ALA:HB2	2.49	0.41
1:2:128:VAL:N	1:2:132:ASN:CB	2.80	0.41
1:2:276:ASP:OD1	1:2:277:VAL:CG2	2.69	0.41
1:3:188:SER:CB	1:3:192:TRP:HA	2.51	0.41
1:2:188:SER:C	1:2:190:LYS:N	2.69	0.41
1:3:113:LYS:HE2	1:3:114:LYS:NZ	2.36	0.41
1:3:77:LYS:N	2:3:378:HOH:O	1.76	0.41
1:2:225:THR:CB	1:3:298:GLN:NE2	2.84	0.41
1:3:213:VAL:HA	1:3:216:VAL:CG1	2.51	0.41
1:1:294:LYS:CA	1:1:297:ILE:HG13	2.50	0.41
1:1:34:ILE:CG1	1:1:34:ILE:O	2.69	0.41
1:1:33:PHE:CZ	1:1:76:MET:SD	3.13	0.41
1:2:143:VAL:HG22	1:2:144:SER:N	2.36	0.41
1:2:8:PHE:HZ	1:2:39:MET:CB	2.34	0.41
1:4:175:HIS:HB3	1:4:230:ARG:HE	1.85	0.41
1:4:93:GLU:OE2	1:4:98:PHE:HB2	2.20	0.41
1:3:65:VAL:C	1:3:66:ASP:OD2	2.59	0.41
1:3:77:LYS:HA	1:3:78:PRO:HD3	1.85	0.41
1:3:81:ILE:HD12	1:3:83:TRP:CZ3	2.56	0.41
1:2:256:ALA:O	1:2:257:ALA:C	2.57	0.41
1:1:131:VAL:HG13	1:1:131:VAL:H	1.62	0.41
1:1:285:ASP:O	1:1:285:ASP:CG	2.59	0.41
1:1:304:VAL:O	1:1:304:VAL:CG1	2.58	0.41
1:2:231:VAL:HA	1:2:232:PRO:HD2	1.88	0.41
1:2:269:PHE:CE1	1:2:319:ARG:NH2	2.89	0.41
1:2:74:ASN:OD1	1:2:75:GLU:N	2.53	0.41
1:1:244:ARG:NH2	1:4:244:ARG:HG3	2.35	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:2:LYS:O	1:4:3:ILE:HG13	2.21	0.41
1:1:14:LEU:HG	1:1:314:PHE:HB3	2.02	0.41
1:1:182:LYS:HD2	1:1:182:LYS:HA	1.74	0.41
1:1:213:VAL:O	1:1:217:ILE:CG2	2.69	0.41
1:2:149:THR:O	1:2:152:CYS:CA	2.68	0.41
1:2:213:VAL:HG13	1:2:217:ILE:HG23	2.03	0.41
1:2:299:LEU:CD2	1:2:300:SER:H	2.27	0.41
1:3:276:ASP:OD1	1:3:277:VAL:CB	2.68	0.41
1:3:286:ASN:N	1:3:286:ASN:HD22	2.17	0.41
1:3:81:ILE:HG21	1:3:83:TRP:NE1	2.36	0.41
1:3:255:LYS:HG2	1:3:255:LYS:H	1.49	0.41
1:3:264:GLY:HA3	1:3:265:PRO:HD3	1.84	0.41
1:3:316:TYR:O	1:3:319:ARG:HB2	2.21	0.41
1:3:13:ARG:HD3	1:3:42:MET:O	2.21	0.41
1:3:8:PHE:CE1	1:3:39:MET:SD	3.14	0.41
1:4:216:VAL:CG1	1:4:217:ILE:H	2.34	0.41
1:4:101:ILE:HG21	1:4:101:ILE:HD13	1.82	0.41
1:4:107:HIS:O	1:4:108:PHE:C	2.59	0.41
1:4:79:GLU:CD	1:4:79:GLU:H	2.24	0.41
1:1:127:PHE:CE2	1:1:136:TYR:CA	3.03	0.41
1:1:278:VAL:O	1:1:279:SER:OG	2.38	0.41
1:1:272:TYR:H	1:1:291:PHE:H	1.69	0.41
1:1:65:VAL:HG12	1:1:70:ILE:HD13	1.98	0.41
1:1:81:ILE:HG21	1:1:83:TRP:NE1	2.34	0.41
1:2:104:ALA:C	1:2:106:ALA:N	2.74	0.41
1:2:132:ASN:HD21	1:2:133:LEU:HD23	1.82	0.41
1:2:181:GLN:CG	1:2:198:ALA:CB	2.94	0.41
1:2:181:GLN:NE2	1:2:230:ARG:HB2	2.32	0.41
1:2:299:LEU:HA	1:2:299:LEU:HD23	1.81	0.41
1:4:156:VAL:O	1:4:160:LEU:HB2	2.21	0.41
1:4:173:THR:HG22	1:4:227:MET:O	2.20	0.41
1:4:159:VAL:HG11	1:4:258:MET:HG3	2.02	0.41
1:4:280:SER:HB3	2:4:358:HOH:O	2.20	0.41
1:4:81:ILE:HG22	1:4:83:TRP:NE1	2.35	0.41
1:3:102:GLU:HG3	1:3:103:LYS:N	2.35	0.41
1:3:242:THR:C	1:3:243:VAL:HG13	2.41	0.41
1:2:135:LYS:HZ3	1:2:140:MET:CE	2.34	0.41
1:1:227:MET:HB2	1:1:227:MET:HE3	1.82	0.41
1:1:285:ASP:O	1:1:286:ASN:C	2.60	0.40
1:1:28:ALA:HB3	1:1:83:TRP:HZ3	1.86	0.40
1:2:305:LYS:HD3	1:3:227:MET:SD	2.61	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:251:TYR:HE1	1:4:255:LYS:HE3	1.85	0.40
1:4:2:LYS:C	1:4:3:ILE:HG13	2.42	0.40
1:3:114:LYS:CA	1:3:114:LYS:HE3	2.50	0.40
1:3:129:CYS:C	1:3:132:ASN:ND2	2.75	0.40
1:4:138:LYS:HD3	1:4:330:VAL:CG1	2.49	0.40
1:4:329:LYS:HD2	1:4:329:LYS:C	2.38	0.40
1:2:208:GLY:CA	1:2:211:LYS:HG2	2.51	0.40
1:3:178:THR:OG1	1:3:178:THR:O	2.37	0.40
1:4:265:PRO:HG2	2:4:352:HOH:O	2.21	0.40
1:4:37:GLU:H	1:4:37:GLU:HG3	1.42	0.40
1:1:128:VAL:HG13	1:1:151:ASN:ND2	2.35	0.40
1:1:324:LEU:CD1	1:1:324:LEU:C	2.88	0.40
1:2:113:LYS:HE2	1:2:114:LYS:HZ2	1.76	0.40
1:2:1:SER:O	1:2:2:LYS:CG	2.45	0.40
1:2:217:ILE:HA	1:2:218:PRO:HD2	1.82	0.40
1:2:266:LEU:O	1:2:267:GLN:C	2.60	0.40
1:2:276:ASP:HB2	1:2:277:VAL:H	1.14	0.40
1:4:1:SER:O	1:4:2:LYS:HG2	2.22	0.40
1:4:49:HIS:NE2	1:4:313:GLU:OE1	2.53	0.40
1:3:299:LEU:CD2	1:3:303:PHE:O	2.69	0.40
1:3:32:PRO:C	1:3:33:PHE:CG	2.95	0.40
1:4:133:LEU:H	1:4:133:LEU:CD2	2.25	0.40
1:4:136:TYR:CZ	1:4:327:MET:HG2	2.56	0.40
1:4:126:MET:CB	1:4:215:LYS:HD3	2.49	0.40
1:1:185:ASP:OD2	1:1:196:ARG:HD2	2.20	0.40
1:2:134:GLU:C	1:2:136:TYR:N	2.71	0.40
1:2:274:GLU:C	1:2:276:ASP:H	2.23	0.40
1:2:26:VAL:CG2	1:2:27:VAL:N	2.83	0.40
1:3:188:SER:HB3	1:3:192:TRP:HA	2.02	0.40
1:4:177:VAL:HG22	1:4:233:THR:O	2.21	0.40
1:4:17:ARG:NH2	1:4:46:ASP:HB2	2.36	0.40
1:3:112:ALA:O	1:3:113:LYS:CB	2.69	0.40
1:3:17:ARG:NH2	2:3:369:HOH:O	2.52	0.40
1:3:127:PHE:HB3	1:3:323:LEU:HD21	2.02	0.40
1:2:52:PHE:O	1:2:53:LYS:HB3	2.21	0.40
1:4:323:LEU:HD13	1:4:327:MET:SD	2.62	0.40
1:2:215:LYS:O	1:2:215:LYS:CD	2.69	0.40
1:3:203:ILE:O	1:3:203:ILE:HG22	2.21	0.40
1:1:184:VAL:O	1:1:184:VAL:CG1	2.69	0.40
1:2:223:LYS:H	1:2:223:LYS:HG2	1.56	0.40
1:2:160:LEU:HD21	1:2:254:ILE:HD12	2.02	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:310:TYR:HB2	1:2:311:ASP:H	1.47	0.40
1:4:175:HIS:CG	1:4:230:ARG:NH2	2.88	0.40
1:4:54:GLY:HA3	1:4:66:ASP:CG	2.42	0.40
1:4:94:SER:O	1:4:96:GLY:N	2.54	0.40
1:3:250:SER:HA	1:3:299:LEU:HD11	2.02	0.40
1:2:227:MET:SD	1:3:296:GLY:CA	3.09	0.40
1:3:77:LYS:C	2:3:378:HOH:O	2.60	0.40
1:2:66:ASP:O	1:2:68:LYS:CE	2.67	0.40
1:4:285:ASP:OD2	1:4:287:ARG:HB2	2.21	0.40
1:2:145:ASN:C	1:2:145:ASN:ND2	2.60	0.40
1:3:212:ALA:O	1:3:215:LYS:C	2.60	0.40
1:4:145:ASN:ND2	1:4:145:ASN:C	2.73	0.40
1:1:161:HIS:O	1:1:164:PHE:N	2.54	0.40
1:1:178:THR:OG1	1:1:179:ALA:N	2.39	0.40
1:2:131:VAL:H	1:2:131:VAL:HG13	1.47	0.40
1:2:166:ILE:N	1:2:245:LEU:O	2.45	0.40
1:3:48:THR:HG22	1:4:200:GLN:OE1	2.21	0.40
1:4:314:PHE:CA	1:4:317:SER:OG	2.69	0.40
1:2:173:THR:HG23	1:2:228:ALA:HB2	1.85	0.40
1:3:127:PHE:CE1	1:3:140:MET:HE2	2.57	0.40
1:2:227:MET:SD	1:3:305:LYS:HD3	2.61	0.40
1:3:319:ARG:O	1:3:321:ILE:N	2.55	0.40
1:3:32:PRO:CB	1:3:74:ASN:OD1	2.69	0.40
1:4:125:PRO:CB	1:4:140:MET:HE1	2.51	0.40
1:4:5:ILE:HD12	1:4:16:LEU:HG	2.04	0.40
1:2:263:GLU:O	1:2:264:GLY:C	2.60	0.40

All (31) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:108:PHE:CE2	1:4:138:LYS:O[1_565]	0.55	1.65
1:2:102:GLU:CB	2:4:351:HOH:O[1_565]	0.85	1.35
1:2:123:ASP:CB	1:4:108:PHE:CE2[1_565]	0.92	1.28
1:2:80:ASN:OD1	1:3:139:ASP:OD2[1_665]	0.98	1.22
1:2:108:PHE:CZ	1:4:138:LYS:O[1_565]	1.03	1.17
1:2:123:ASP:CB	1:4:108:PHE:CZ[1_565]	1.11	1.09
1:2:108:PHE:CE2	1:4:138:LYS:C[1_565]	1.29	0.91
1:3:102:GLU:N	2:2:403:HOH:O[1_445]	1.37	0.83
1:3:102:GLU:CA	2:2:403:HOH:O[1_445]	1.48	0.72

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:80:ASN:OD1	1:3:139:ASP:CG[1_665]	1.60	0.60
1:2:123:ASP:CA	1:4:108:PHE:CE2[1_565]	1.70	0.50
1:2:85:LYS:CE	2:3:380:HOH:O[1_665]	1.72	0.48
1:2:80:ASN:CG	1:3:139:ASP:OD2[1_665]	1.73	0.47
1:2:108:PHE:CZ	1:4:138:LYS:C[1_565]	1.74	0.46
1:3:101:ILE:C	2:2:403:HOH:O[1_445]	1.78	0.42
1:2:102:GLU:CG	2:4:351:HOH:O[1_565]	1.79	0.41
1:2:80:ASN:CG	1:3:139:ASP:OD1[1_665]	1.81	0.39
1:2:108:PHE:CE1	1:4:139:ASP:CA[1_565]	1.91	0.29
1:2:108:PHE:CD2	1:4:138:LYS:O[1_565]	1.91	0.29
1:3:267:GLN:OE1	1:4:247:LYS:CE[1_455]	1.96	0.24
1:3:101:ILE:O	2:2:403:HOH:O[1_445]	2.03	0.17
1:2:80:ASN:CG	1:3:139:ASP:CG[1_665]	2.03	0.17
1:2:108:PHE:CZ	1:4:139:ASP:N[1_565]	2.05	0.15
1:2:80:ASN:ND2	1:3:139:ASP:OD1[1_665]	2.05	0.15
1:2:106:ALA:O	1:4:139:ASP:OD1[1_565]	2.06	0.14
1:2:108:PHE:CZ	1:4:139:ASP:CA[1_565]	2.06	0.14
1:2:80:ASN:OD1	1:3:139:ASP:OD1[1_665]	2.07	0.13
1:1:90:TYR:OH	2:4:343:HOH:O[1_566]	2.09	0.11
1:2:80:ASN:ND2	1:3:139:ASP:OD2[1_665]	2.15	0.05
1:2:85:LYS:NZ	2:3:380:HOH:O[1_665]	2.16	0.04
1:1:134:GLU:OE1	1:2:135:LYS:CB[1_556]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	1	331/333 (99%)	177 (54%)	70 (21%)	84 (25%)	0	0
1	2	331/333 (99%)	180 (54%)	75 (23%)	76 (23%)	0	0
1	3	331/333 (99%)	175 (53%)	70 (21%)	86 (26%)	0	0
1	4	331/333 (99%)	180 (54%)	73 (22%)	78 (24%)	0	0
All	All	1324/1332 (99%)	712 (54%)	288 (22%)	324 (24%)	0	0

All (324) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	8	PHE
1	1	10	ARG
1	1	27	VAL
1	1	50	GLY
1	1	51	VAL
1	1	52	PHE
1	1	53	LYS
1	1	77	LYS
1	1	83	TRP
1	1	84	SER
1	1	86	ALA
1	1	89	GLU
1	1	95	THR
1	1	98	PHE
1	1	113	LYS
1	1	125	PRO
1	1	133	LEU
1	1	138	LYS
1	1	146	ALA
1	1	147	SER
1	1	158	LYS
1	1	161	HIS
1	1	177	VAL
1	1	184	VAL
1	1	189	ALA
1	1	198	ALA
1	1	204	PRO
1	1	211	LYS
1	1	221	ASP
1	1	237	SER
1	1	252	ASP
1	1	264	GLY
1	1	267	GLN
1	1	276	ASP
1	1	277	VAL
1	1	278	VAL
1	1	280	SER
1	1	281	ASP
1	1	282	PHE
1	1	294	LYS
1	1	311	ASP
1	1	312	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	326	HIS
1	2	26	VAL
1	2	27	VAL
1	2	50	GLY
1	2	51	VAL
1	2	53	LYS
1	2	60	ASP
1	2	77	LYS
1	2	86	ALA
1	2	95	THR
1	2	98	PHE
1	2	106	ALA
1	2	107	HIS
1	2	132	ASN
1	2	133	LEU
1	2	146	ALA
1	2	147	SER
1	2	177	VAL
1	2	181	GLN
1	2	184	VAL
1	2	189	ALA
1	2	192	TRP
1	2	204	PRO
1	2	211	LYS
1	2	221	ASP
1	2	233	THR
1	2	237	SER
1	2	251	TYR
1	2	267	GLN
1	2	276	ASP
1	2	277	VAL
1	2	278	VAL
1	2	281	ASP
1	2	282	PHE
1	2	311	ASP
1	2	312	ASN
1	2	326	HIS
1	3	26	VAL
1	3	27	VAL
1	3	50	GLY
1	3	52	PHE
1	3	53	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	3	60	ASP
1	3	77	LYS
1	3	83	TRP
1	3	86	ALA
1	3	95	THR
1	3	98	PHE
1	3	106	ALA
1	3	109	LYS
1	3	133	LEU
1	3	135	LYS
1	3	146	ALA
1	3	154	ALA
1	3	161	HIS
1	3	165	GLU
1	3	181	GLN
1	3	184	VAL
1	3	211	LYS
1	3	221	ASP
1	3	233	THR
1	3	237	SER
1	3	251	TYR
1	3	252	ASP
1	3	255	LYS
1	3	267	GLN
1	3	276	ASP
1	3	277	VAL
1	3	278	VAL
1	3	279	SER
1	3	282	PHE
1	3	294	LYS
1	3	301	LYS
1	3	311	ASP
1	3	312	ASN
1	3	326	HIS
1	3	330	VAL
1	3	331	ASP
1	4	26	VAL
1	4	27	VAL
1	4	50	GLY
1	4	51	VAL
1	4	52	PHE
1	4	53	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	4	60	ASP
1	4	75	GLU
1	4	86	ALA
1	4	95	THR
1	4	98	PHE
1	4	106	ALA
1	4	107	HIS
1	4	112	ALA
1	4	132	ASN
1	4	133	LEU
1	4	147	SER
1	4	154	ALA
1	4	160	LEU
1	4	177	VAL
1	4	184	VAL
1	4	185	ASP
1	4	189	ALA
1	4	192	TRP
1	4	204	PRO
1	4	211	LYS
1	4	221	ASP
1	4	237	SER
1	4	265	PRO
1	4	267	GLN
1	4	276	ASP
1	4	277	VAL
1	4	278	VAL
1	4	280	SER
1	4	282	PHE
1	4	285	ASP
1	4	294	LYS
1	4	311	ASP
1	4	312	ASN
1	4	326	HIS
1	1	26	VAL
1	1	54	GLY
1	1	60	ASP
1	1	109	LYS
1	1	132	ASN
1	1	157	ALA
1	1	160	LEU
1	1	166	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	1	181	GLN
1	1	185	ASP
1	1	197	GLY
1	1	219	GLU
1	1	262	SER
1	1	272	TYR
1	1	283	ILE
1	1	330	VAL
1	2	17	ARG
1	2	54	GLY
1	2	83	TRP
1	2	84	SER
1	2	108	PHE
1	2	112	ALA
1	2	113	LYS
1	2	125	PRO
1	2	129	CYS
1	2	130	GLY
1	2	161	HIS
1	2	215	LYS
1	2	219	GLU
1	2	264	GLY
1	2	265	PRO
1	2	280	SER
1	2	284	GLY
1	2	288	SER
1	2	294	LYS
1	2	300	SER
1	2	302	THR
1	3	8	PHE
1	3	13	ARG
1	3	51	VAL
1	3	112	ALA
1	3	113	LYS
1	3	118	SER
1	3	130	GLY
1	3	138	LYS
1	3	147	SER
1	3	189	ALA
1	3	198	ALA
1	3	204	PRO
1	3	219	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	3	264	GLY
1	3	265	PRO
1	3	283	ILE
1	3	284	GLY
1	3	288	SER
1	3	300	SER
1	3	321	ILE
1	3	325	LYS
1	4	8	PHE
1	4	83	TRP
1	4	105	SER
1	4	108	PHE
1	4	113	LYS
1	4	118	SER
1	4	146	ALA
1	4	158	LYS
1	4	165	GLU
1	4	181	GLN
1	4	219	GLU
1	4	251	TYR
1	4	255	LYS
1	4	264	GLY
1	4	283	ILE
1	4	286	ASN
1	4	288	SER
1	1	108	PHE
1	1	162	GLU
1	1	165	GLU
1	1	233	THR
1	1	236	VAL
1	1	251	TYR
1	1	285	ASP
1	1	288	SER
1	1	301	LYS
1	1	310	TYR
1	2	138	LYS
1	2	279	SER
1	2	285	ASP
1	2	327	MET
1	3	162	GLU
1	3	232	PRO
1	3	249	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	3	329	LYS
1	4	10	ARG
1	4	84	SER
1	4	109	LYS
1	4	110	GLY
1	4	130	GLY
1	4	180	THR
1	4	284	GLY
1	1	12	GLY
1	1	71	THR
1	1	106	ALA
1	1	268	GLY
1	1	287	ARG
1	1	329	LYS
1	2	52	PHE
1	2	166	ILE
1	2	236	VAL
1	2	328	GLN
1	3	12	GLY
1	3	28	ALA
1	3	166	ILE
1	3	185	ASP
1	3	253	ASP
1	3	272	TYR
1	3	280	SER
1	4	143	VAL
1	4	198	ALA
1	4	233	THR
1	4	236	VAL
1	4	279	SER
1	4	329	LYS
1	1	13	ARG
1	1	19	ALA
1	1	22	CYS
1	1	105	SER
1	1	154	ALA
1	1	279	SER
1	2	35	ALA
1	2	105	SER
1	2	109	LYS
1	2	154	ALA
1	2	180	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	3	39	MET
1	3	75	GLU
1	3	108	PHE
1	3	188	SER
1	3	281	ASP
1	3	287	ARG
1	4	138	LYS
1	4	161	HIS
1	4	166	ILE
1	4	205	SER
1	4	272	TYR
1	1	107	HIS
1	1	232	PRO
1	2	158	LYS
1	2	283	ILE
1	2	289	SER
1	2	330	VAL
1	3	236	VAL
1	3	289	SER
1	4	281	ASP
1	4	330	VAL
1	4	125	PRO
1	1	284	GLY
1	2	218	PRO
1	3	177	VAL
1	3	320	VAL
1	2	87	GLY
1	3	218	PRO
1	3	101	ILE
1	3	125	PRO

### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	1	271/271 (100%)	169 (62%)	102 (38%)	<b>0</b> <b>0</b>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	271/271 (100%)	182 (67%)	89 (33%)	0	1
1	3	271/271 (100%)	171 (63%)	100 (37%)	0	0
1	4	271/271 (100%)	178 (66%)	93 (34%)	0	0
All	All	1084/1084 (100%)	700 (65%)	384 (35%)	0	0

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	8	PHE
1	1	11	ILE
1	1	14	LEU
1	1	16	LEU
1	1	17	ARG
1	1	26	VAL
1	1	30	ASN
1	1	31	ASP
1	1	33	PHE
1	1	34	ILE
1	1	37	GLU
1	1	38	TYR
1	1	41	TYR
1	1	44	LYS
1	1	46	ASP
1	1	47	SER
1	1	51	VAL
1	1	53	LYS
1	1	57	LYS
1	1	58	MET
1	1	60	ASP
1	1	64	VAL
1	1	65	VAL
1	1	68	LYS
1	1	70	ILE
1	1	73	PHE
1	1	76	MET
1	1	77	LYS
1	1	78	PRO
1	1	81	ILE
1	1	84	SER
1	1	85	LYS
1	1	90	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	91	ILE
1	1	97	VAL
1	1	99	THR
1	1	103	LYS
1	1	114	LYS
1	1	116	VAL
1	1	117	ILE
1	1	123	ASP
1	1	129	CYS
1	1	131	VAL
1	1	132	ASN
1	1	138	LYS
1	1	140	MET
1	1	142	VAL
1	1	143	VAL
1	1	144	SER
1	1	145	ASN
1	1	153	LEU
1	1	170	LEU
1	1	171	MET
1	1	178	THR
1	1	180	THR
1	1	183	THR
1	1	184	VAL
1	1	187	PRO
1	1	190	LYS
1	1	204	PRO
1	1	206	SER
1	1	211	LYS
1	1	215	LYS
1	1	220	LEU
1	1	223	LYS
1	1	224	LEU
1	1	227	MET
1	1	230	ARG
1	1	231	VAL
1	1	232	PRO
1	1	238	VAL
1	1	239	VAL
1	1	244	ARG
1	1	253	ASP
1	1	258	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	1	262	SER
1	1	263	GLU
1	1	266	LEU
1	1	273	THR
1	1	275	ASP
1	1	277	VAL
1	1	279	SER
1	1	286	ASN
1	1	290	ILE
1	1	292	ASP
1	1	297	ILE
1	1	298	GLN
1	1	299	LEU
1	1	302	THR
1	1	304	VAL
1	1	305	LYS
1	1	309	TRP
1	1	310	TYR
1	1	312	ASN
1	1	314	PHE
1	1	318	GLN
1	1	320	VAL
1	1	322	ASP
1	1	323	LEU
1	1	324	LEU
1	1	328	GLN
1	1	329	LYS
1	2	1	SER
1	2	2	LYS
1	2	8	PHE
1	2	11	ILE
1	2	14	LEU
1	2	16	LEU
1	2	30	ASN
1	2	34	ILE
1	2	44	LYS
1	2	46	ASP
1	2	47	SER
1	2	51	VAL
1	2	53	LYS
1	2	58	MET
1	2	60	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	2	68	LYS
1	2	70	ILE
1	2	73	PHE
1	2	77	LYS
1	2	79	GLU
1	2	80	ASN
1	2	81	ILE
1	2	89	GLU
1	2	91	ILE
1	2	99	THR
1	2	101	ILE
1	2	102	GLU
1	2	108	PHE
1	2	109	LYS
1	2	114	LYS
1	2	117	ILE
1	2	121	SER
1	2	123	ASP
1	2	132	ASN
1	2	138	LYS
1	2	139	ASP
1	2	140	MET
1	2	144	SER
1	2	145	ASN
1	2	153	LEU
1	2	155	PRO
1	2	156	VAL
1	2	165	GLU
1	2	170	LEU
1	2	171	MET
1	2	177	VAL
1	2	180	THR
1	2	183	THR
1	2	188	SER
1	2	190	LYS
1	2	205	SER
1	2	207	THR
1	2	211	LYS
1	2	215	LYS
1	2	220	LEU
1	2	223	LYS
1	2	225	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	2	230	ARG
1	2	237	SER
1	2	239	VAL
1	2	253	ASP
1	2	255	LYS
1	2	258	MET
1	2	262	SER
1	2	263	GLU
1	2	266	LEU
1	2	270	LEU
1	2	274	GLU
1	2	275	ASP
1	2	279	SER
1	2	288	SER
1	2	289	SER
1	2	290	ILE
1	2	292	ASP
1	2	297	ILE
1	2	298	GLN
1	2	299	LEU
1	2	300	SER
1	2	301	LYS
1	2	304	VAL
1	2	309	TRP
1	2	310	TYR
1	2	314	PHE
1	2	318	GLN
1	2	321	ILE
1	2	322	ASP
1	2	324	LEU
1	2	328	GLN
1	2	329	LYS
1	3	2	LYS
1	3	8	PHE
1	3	11	ILE
1	3	14	LEU
1	3	16	LEU
1	3	17	ARG
1	3	21	SER
1	3	27	VAL
1	3	30	ASN
1	3	34	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	3	37	GLU
1	3	40	VAL
1	3	44	LYS
1	3	46	ASP
1	3	51	VAL
1	3	53	LYS
1	3	55	GLU
1	3	58	MET
1	3	63	LEU
1	3	64	VAL
1	3	68	LYS
1	3	70	ILE
1	3	72	VAL
1	3	80	ASN
1	3	81	ILE
1	3	85	LYS
1	3	90	TYR
1	3	91	ILE
1	3	95	THR
1	3	101	ILE
1	3	103	LYS
1	3	105	SER
1	3	108	PHE
1	3	114	LYS
1	3	121	SER
1	3	123	ASP
1	3	125	PRO
1	3	126	MET
1	3	135	LYS
1	3	138	LYS
1	3	139	ASP
1	3	140	MET
1	3	145	ASN
1	3	150	THR
1	3	153	LEU
1	3	156	VAL
1	3	163	ASN
1	3	167	VAL
1	3	171	MET
1	3	174	VAL
1	3	180	THR
1	3	184	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	3	187	PRO
1	3	188	SER
1	3	190	LYS
1	3	196	ARG
1	3	204	PRO
1	3	211	LYS
1	3	215	LYS
1	3	216	VAL
1	3	220	LEU
1	3	223	LYS
1	3	227	MET
1	3	230	ARG
1	3	231	VAL
1	3	237	SER
1	3	238	VAL
1	3	239	VAL
1	3	253	ASP
1	3	255	LYS
1	3	258	MET
1	3	260	THR
1	3	263	GLU
1	3	266	LEU
1	3	274	GLU
1	3	275	ASP
1	3	286	ASN
1	3	288	SER
1	3	289	SER
1	3	290	ILE
1	3	292	ASP
1	3	294	LYS
1	3	297	ILE
1	3	298	GLN
1	3	299	LEU
1	3	301	LYS
1	3	302	THR
1	3	303	PHE
1	3	304	VAL
1	3	305	LYS
1	3	309	TRP
1	3	310	TYR
1	3	314	PHE
1	3	318	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	3	321	ILE
1	3	322	ASP
1	3	323	LEU
1	3	324	LEU
1	3	328	GLN
1	3	329	LYS
1	4	1	SER
1	4	2	LYS
1	4	8	PHE
1	4	11	ILE
1	4	16	LEU
1	4	20	LEU
1	4	21	SER
1	4	25	GLN
1	4	26	VAL
1	4	27	VAL
1	4	29	VAL
1	4	30	ASN
1	4	37	GLU
1	4	40	VAL
1	4	43	PHE
1	4	46	ASP
1	4	53	LYS
1	4	56	VAL
1	4	58	MET
1	4	63	LEU
1	4	64	VAL
1	4	65	VAL
1	4	68	LYS
1	4	70	ILE
1	4	72	VAL
1	4	76	MET
1	4	77	LYS
1	4	79	GLU
1	4	81	ILE
1	4	97	VAL
1	4	108	PHE
1	4	114	LYS
1	4	116	VAL
1	4	117	ILE
1	4	118	SER
1	4	120	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	4	126	MET
1	4	132	ASN
1	4	138	LYS
1	4	145	ASN
1	4	151	ASN
1	4	153	LEU
1	4	156	VAL
1	4	163	ASN
1	4	166	ILE
1	4	171	MET
1	4	172	THR
1	4	173	THR
1	4	180	THR
1	4	183	THR
1	4	191	ASP
1	4	196	ARG
1	4	201	ASN
1	4	204	PRO
1	4	205	SER
1	4	211	LYS
1	4	213	VAL
1	4	217	ILE
1	4	220	LEU
1	4	223	LYS
1	4	227	MET
1	4	230	ARG
1	4	231	VAL
1	4	232	PRO
1	4	253	ASP
1	4	258	MET
1	4	263	GLU
1	4	266	LEU
1	4	274	GLU
1	4	277	VAL
1	4	279	SER
1	4	283	ILE
1	4	286	ASN
1	4	289	SER
1	4	290	ILE
1	4	292	ASP
1	4	294	LYS
1	4	297	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	4	298	GLN
1	4	299	LEU
1	4	302	THR
1	4	305	LYS
1	4	310	TYR
1	4	312	ASN
1	4	314	PHE
1	4	317	SER
1	4	318	GLN
1	4	323	LEU
1	4	324	LEU
1	4	328	GLN
1	4	329	LYS
1	4	331	ASP
1	4	332	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	25	GLN
1	1	30	ASN
1	1	132	ASN
1	1	175	HIS
1	1	201	ASN
1	1	312	ASN
1	1	328	GLN
1	2	6	ASN
1	2	25	GLN
1	2	30	ASN
1	2	132	ASN
1	2	175	HIS
1	2	181	GLN
1	2	201	ASN
1	2	328	GLN
1	3	6	ASN
1	3	25	GLN
1	3	30	ASN
1	3	49	HIS
1	3	132	ASN
1	3	175	HIS
1	3	201	ASN
1	3	328	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	4	25	GLN
1	4	80	ASN
1	4	132	ASN
1	4	145	ASN
1	4	151	ASN
1	4	181	GLN
1	4	201	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	333/333 (100%)	-0.73	1 (0%) 94 92	2, 9, 28, 32	0
1	2	333/333 (100%)	-0.76	1 (0%) 94 92	2, 9, 28, 32	0
1	3	333/333 (100%)	-0.68	3 (0%) 85 79	2, 9, 28, 32	0
1	4	333/333 (100%)	-0.70	1 (0%) 94 92	2, 9, 28, 32	0
All	All	1332/1332 (100%)	-0.71	6 (0%) 91 88	2, 9, 28, 32	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	3	106	ALA	3.0
1	1	110	GLY	2.8
1	2	212	ALA	2.6
1	3	132	ASN	2.5
1	4	110	GLY	2.5
1	3	111	GLY	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.