



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:27 AM GMT

PDB ID : 2QQP  
Title : Crystal Structure of Authentic Providence Virus  
Authors : Speir, J.A.; Taylor, D.J.; Johnson, J.E.  
Deposited on : 2007-07-26  
Resolution : 3.80 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

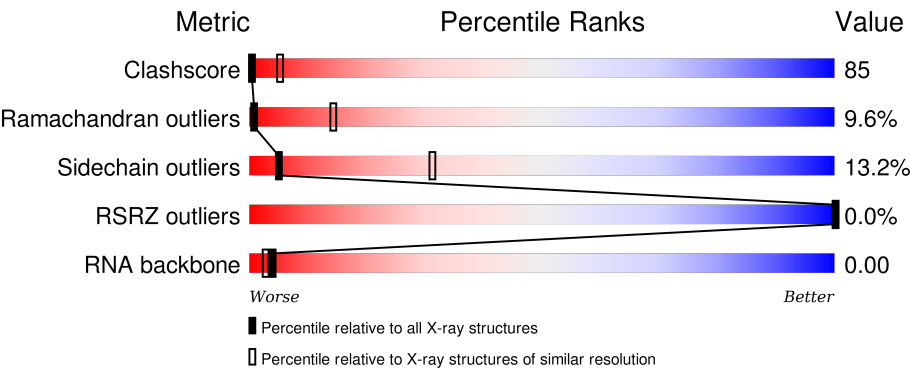
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)
RNA backbone	2183	1070 (4.76-2.80)

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	A	556	<div><div></div><div><div></div><div>17%</div><div>55%</div><div>14%</div><div>•</div><div>13%</div></div></div>
1	C	556	<div><div></div><div><div></div><div>15%</div><div>56%</div><div>15%</div><div>•</div><div>13%</div></div></div>
1	E	556	<div><div></div><div><div></div><div>18%</div><div>63%</div><div>12%</div><div>•</div><div>7%</div></div></div>
1	G	556	<div><div></div><div><div></div><div>18%</div><div>58%</div><div>15%</div><div>•</div><div>7%</div></div></div>
2	B	75	<div><div></div><div><div></div><div>20%</div><div>24%</div><div>8%</div><div>48%</div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	75	<div><div></div><div></div><div></div><div></div></div> <div>9%36%7%47%</div>
2	F	75	<div><div></div><div></div><div></div><div></div></div> <div>16%60%13%11%</div>
2	H	75	<div><div></div><div></div><div></div><div></div></div> <div>9%33%7%49%</div>
3	R	4	<div><div></div><div></div></div> <div>25%75%</div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16634 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 Large Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3714	2359	604	740	11			
1	C	484	Total	C	N	O	S	0	0	0
			3714	2359	604	740	11			
1	E	517	Total	C	N	O	S	0	0	0
			3948	2505	645	785	13			
1	G	518	Total	C	N	O	S	0	0	0
			3957	2510	646	788	13			

- Molecule 2 is a protein called Small capsid protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	0	0	0
			255	162	44	49			
2	D	40	Total	C	N	O	0	0	0
			263	166	46	51			
2	F	67	Total	C	N	O	0	0	0
			448	282	84	82			
2	H	38	Total	C	N	O	0	0	0
			250	159	43	48			

- Molecule 3 is a RNA chain called RNA (5'-R(\*UP\*UP\*UP\*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

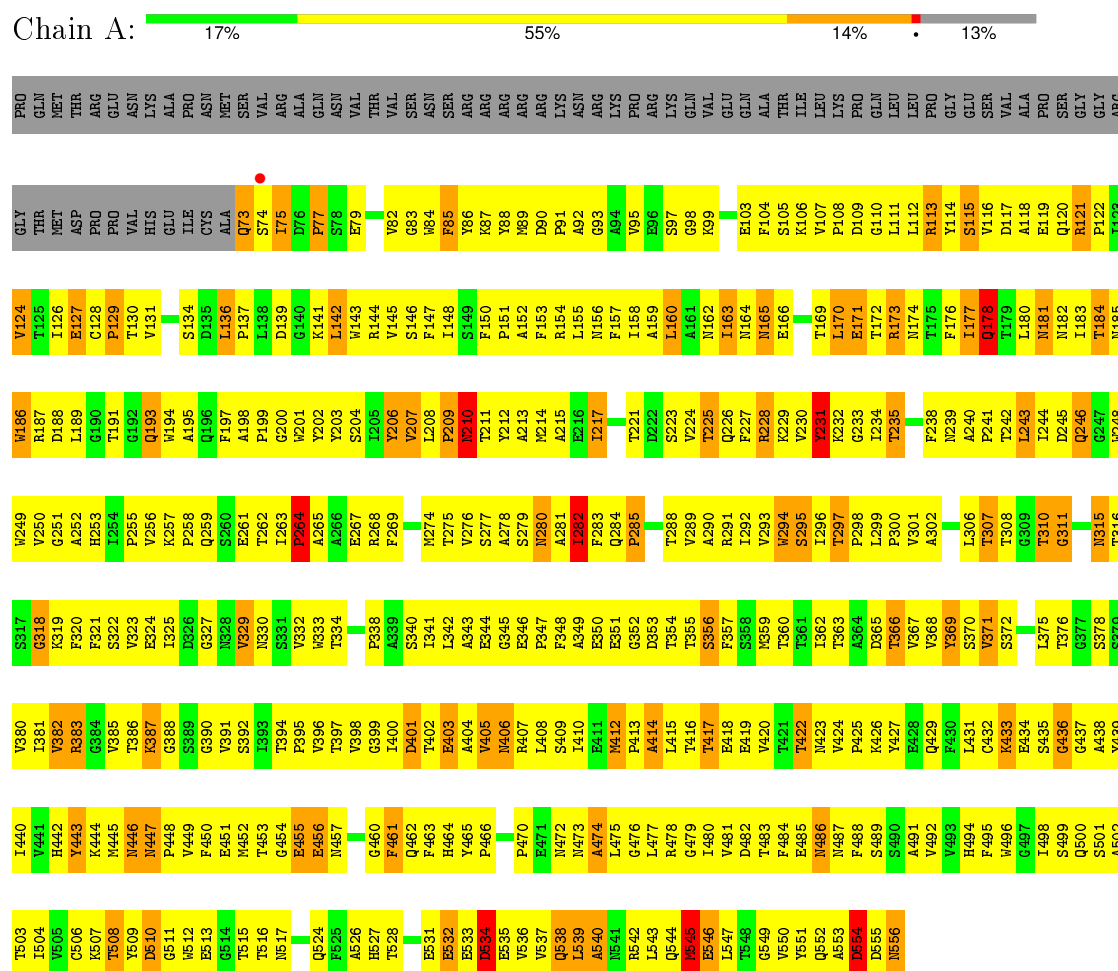
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	C	2	Total	O	0	0
			2	2		
5	E	2	Total	O	0	0
			2	2		
5	G	1	Total	O	0	0
			1	1		

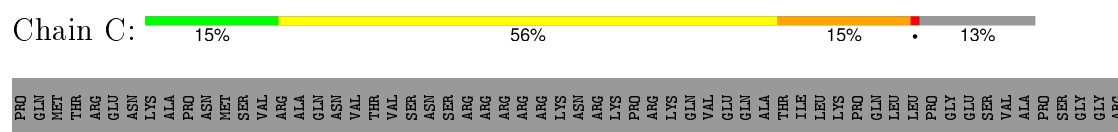
### 3 Residue-property plots

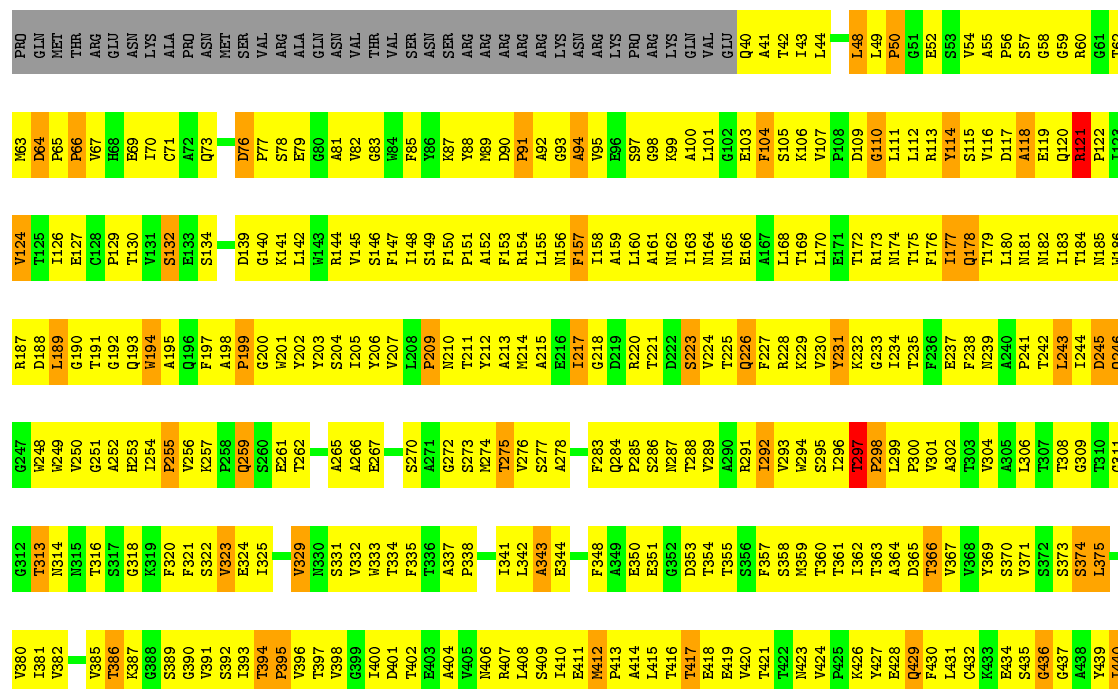
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

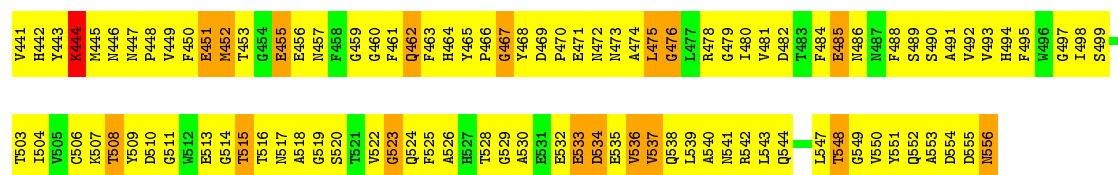
#### • Molecule 1: Large Capsid protein



#### • Molecule 1: Large Capsid protein

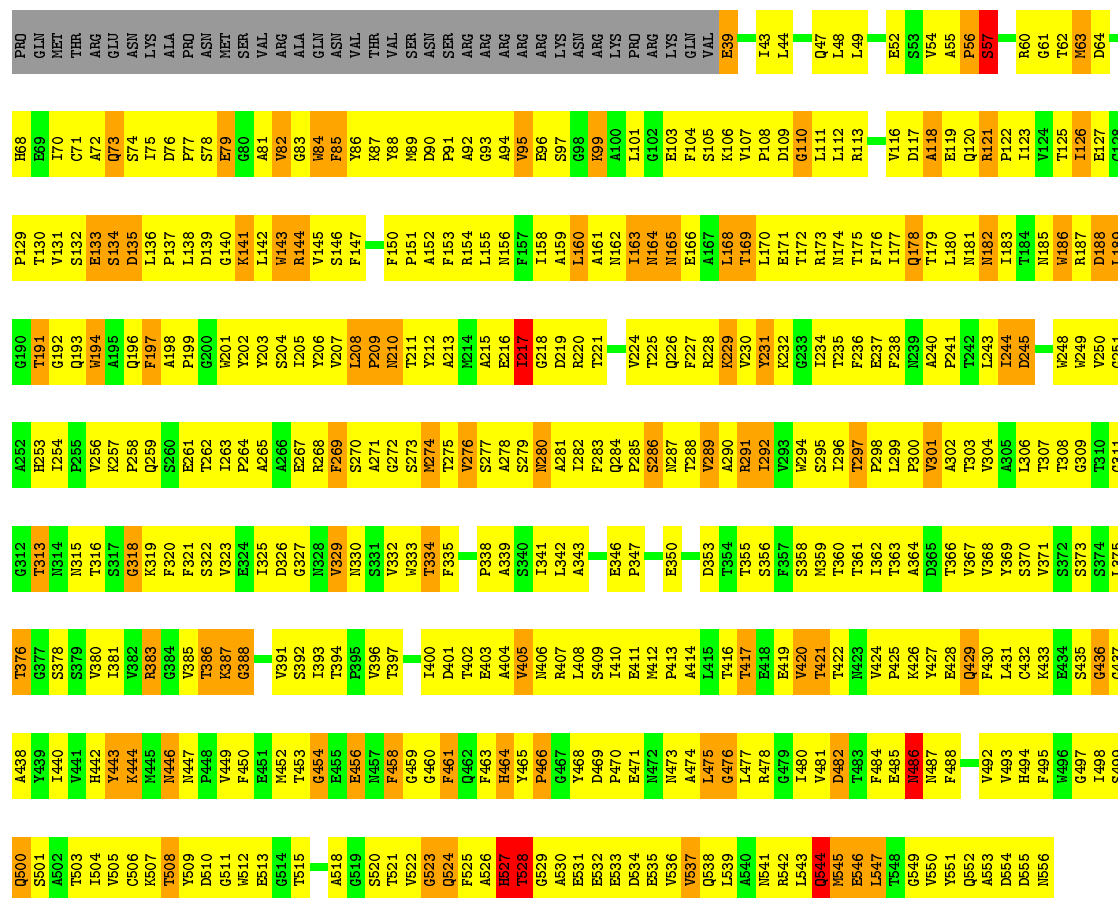






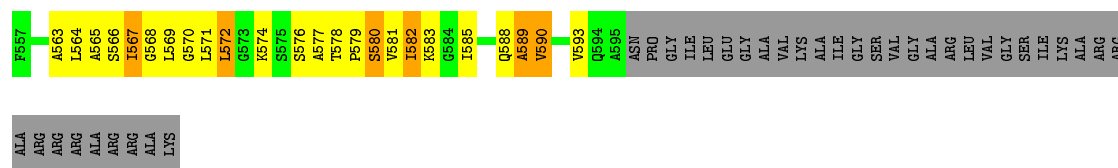
### • Molecule 1: Large Capsid protein

Chain G: 18% 58% 15% 7%



### • Molecule 2: Small capsid protein

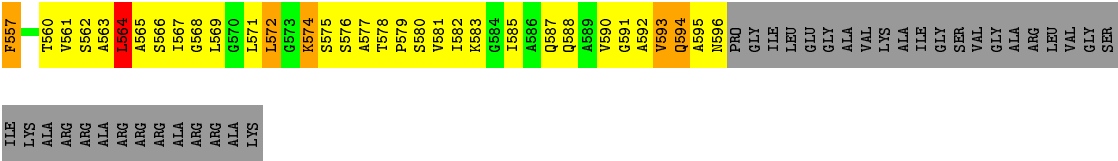
Chain B: 20% 24% 8% 48%



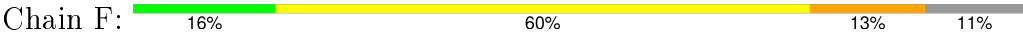
### • Molecule 2: Small capsid protein

Chain D: 9% 36% 7% 47%

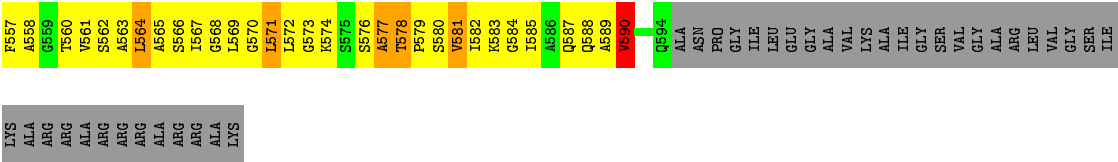




• Molecule 2: Small capsid protein



• Molecule 2: Small capsid protein



• Molecule 3: RNA (5'-R(\*UP\*UP\*UP\*U)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	659.79Å 434.07Å 415.85Å 90.00° 126.13° 90.00°	Depositor
Resolution (Å)	49.42 – 3.80 50.01 – 3.80	Depositor EDS
% Data completeness (in resolution range)	28.6 (49.42-3.80) 26.5 (50.01-3.80)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 3.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.285 , (Not available) 0.265 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.059 for -h-2*l,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 272211 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.74	EDS
Total number of atoms	16634	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% 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

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	A	0.54	0/3807	0.78	0/5203
1	C	0.53	0/3807	0.78	0/5203
1	E	0.55	0/4047	0.78	0/5532
1	G	0.52	0/4056	0.79	0/5544
2	B	0.60	0/256	0.72	0/346
2	D	0.55	0/264	0.83	0/357
2	F	0.58	0/450	0.85	0/606
2	H	0.51	0/251	0.74	0/339
3	R	1.57	0/84	0.91	0/128
All	All	0.55	0/17022	0.78	0/23258

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	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	TYR	Sidechain
1	C	206	TYR	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	A	3714	0	3548	661	0
1	C	3714	0	3548	689	0
1	E	3948	0	3786	744	0
1	G	3957	0	3792	703	0
2	B	255	0	275	40	0
2	D	263	0	281	66	0
2	F	448	0	491	90	0
2	H	250	0	270	47	0
3	R	77	0	42	4	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
5	G	1	0	0	0	0
All	All	16634	0	16033	2780	0

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 85.

All (2780) 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:C:475:LEU:HD11	1:E:267:GLU:CG	1.36	1.52
1:C:297:THR:HG23	1:C:476:GLY:CA	1.55	1.35
1:C:120:GLN:NE2	1:C:208:LEU:HB3	1.45	1.29
1:E:297:THR:HG22	1:E:298:PRO:CD	1.64	1.27
1:C:475:LEU:HD11	1:E:267:GLU:CB	1.68	1.21
1:E:220:ARG:NH1	1:G:215:ALA:HB1	1.56	1.21
1:C:297:THR:CG2	1:C:476:GLY:HA3	1.70	1.20
1:E:297:THR:CG2	1:E:298:PRO:HD3	1.71	1.20
1:G:416:THR:HB	1:G:419:GLU:HB2	1.23	1.14
1:A:475:LEU:HD22	1:C:267:GLU:HG2	1.28	1.14
1:E:220:ARG:HH11	1:G:215:ALA:CB	1.62	1.13
1:A:383:ARG:HH11	1:A:383:ARG:HB2	1.04	1.13

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:ALA:HB3	1:E:201:TRP:HB2	1.27	1.11
1:A:234:ILE:HG12	1:A:508:THR:HG23	1.30	1.11
1:C:297:THR:CG2	1:C:476:GLY:CA	2.26	1.10
1:A:383:ARG:NH1	1:A:383:ARG:HB2	1.64	1.10
1:E:220:ARG:HD2	1:G:215:ALA:HB2	1.22	1.09
1:A:549:GLY:HA2	1:C:113:ARG:HH21	1.16	1.09
1:C:475:LEU:CD1	1:E:267:GLU:CG	2.31	1.08
1:E:255:PRO:HB3	1:E:445:MET:HG2	1.30	1.08
1:A:262:THR:HA	1:A:406:ASN:HB3	1.35	1.08
1:G:168:LEU:HD22	1:G:173:ARG:HG3	1.34	1.08
1:C:273:SER:HB3	1:C:475:LEU:HD12	1.28	1.08
1:G:297:THR:CG2	1:G:476:GLY:HA3	1.83	1.08
1:C:475:LEU:CD1	1:E:267:GLU:HB2	1.84	1.07
1:G:297:THR:HG21	1:G:476:GLY:HA3	1.10	1.07
1:G:47:GLN:NE2	1:G:63:MET:HA	1.70	1.06
1:E:416:THR:HB	1:E:419:GLU:HB2	1.08	1.05
1:C:475:LEU:HD11	1:E:267:GLU:HG2	1.32	1.05
1:A:225:THR:HG23	1:A:517:ASN:HB2	1.40	1.03
1:C:105:SER:HB2	1:C:117:ASP:HB2	1.40	1.02
1:A:107:VAL:HG23	1:A:230:VAL:HG22	1.38	1.02
1:A:413:PRO:HA	1:C:517:ASN:OD1	1.59	1.02
1:A:129:PRO:HG2	1:A:163:ILE:HG23	1.41	1.02
1:C:184:THR:HG21	1:C:295:SER:HB2	1.41	1.01
1:C:363:THR:HG23	1:C:365:ASP:H	1.23	1.00
1:C:405:VAL:HG11	1:C:477:LEU:HD13	1.41	1.00
1:C:87:LYS:HD3	1:C:91:PRO:HA	1.39	1.00
1:G:297:THR:HG21	1:G:476:GLY:CA	1.91	0.99
1:C:475:LEU:CD1	1:E:267:GLU:CB	2.40	0.99
1:A:404:ALA:HB3	1:E:261:GLU:OE2	1.60	0.99
1:A:400:ILE:HG12	1:A:401:ASP:H	1.22	0.99
1:A:404:ALA:HB1	1:E:261:GLU:HB3	1.44	0.99
2:F:599:ILE:O	2:F:600:LEU:HG	1.61	0.99
1:C:275:THR:HG23	1:C:478:ARG:HH22	1.25	0.98
1:A:538:GLN:HG2	2:B:582:ILE:HD13	1.43	0.98
1:E:237:GLU:HG3	1:E:507:LYS:HE2	1.42	0.98
1:G:281:ALA:HB3	1:G:284:GLN:HG3	1.39	0.98
1:C:290:ALA:HB2	1:C:387:LYS:HZ1	1.27	0.97
1:C:475:LEU:HD11	1:E:267:GLU:CD	1.83	0.97
2:F:564:LEU:O	2:F:567:ILE:HG23	1.64	0.97
1:C:275:THR:HG23	1:C:478:ARG:NH2	1.79	0.97
1:A:363:THR:HG22	1:A:365:ASP:H	1.30	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:578:THR:HG22	2:H:581:VAL:H	1.27	0.97
1:A:73:GLN:HE22	2:F:578:THR:HG21	1.28	0.96
1:G:198:ALA:HB3	1:G:201:TRP:HB2	1.44	0.96
1:E:385:VAL:HG12	1:E:392:SER:HB3	1.48	0.96
1:C:302:ALA:HB2	1:C:338:PRO:HG3	1.48	0.96
1:A:549:GLY:CA	1:C:113:ARG:HH21	1.79	0.95
1:G:189:LEU:HD23	1:G:189:LEU:H	1.27	0.95
1:E:69:GLU:HA	1:E:78:SER:HA	1.47	0.95
1:E:297:THR:HG23	1:E:476:GLY:HA3	1.45	0.95
1:G:132:SER:C	1:G:134:SER:H	1.69	0.94
1:A:262:THR:HA	1:A:406:ASN:CB	1.96	0.94
1:E:273:SER:H	1:E:297:THR:HB	1.31	0.94
1:C:272:GLY:HA3	1:C:298:PRO:HD3	1.50	0.94
1:G:274:MET:HB3	1:G:296:ILE:HG13	1.49	0.94
1:E:253:HIS:CD2	1:E:549:GLY:HA3	2.01	0.94
1:E:266:ALA:HB3	1:E:402:THR:HB	1.50	0.94
1:A:127:GLU:HA	1:A:503:THR:HG22	1.50	0.94
1:C:246:GLN:HG3	1:G:241:PRO:HB3	1.50	0.93
1:A:531:GLU:HG3	2:F:583:LYS:HE3	1.48	0.93
1:A:255:PRO:O	1:C:225:THR:HG21	1.67	0.93
1:G:544:GLN:O	1:G:547:LEU:HD23	1.66	0.93
1:A:516:THR:HB	1:E:423:ASN:HB3	1.50	0.93
1:A:285:PRO:HB2	1:A:288:THR:HB	1.49	0.93
1:C:120:GLN:NE2	1:C:208:LEU:CB	2.31	0.93
1:G:106:LYS:HG3	1:G:117:ASP:HB3	1.50	0.92
1:A:480:ILE:H	1:A:480:ILE:HD12	1.30	0.92
1:A:276:VAL:HG21	1:A:369:TYR:HE1	1.33	0.92
1:E:416:THR:CB	1:E:419:GLU:HB2	1.99	0.92
1:A:198:ALA:HB3	1:A:201:TRP:HB2	1.52	0.91
2:D:581:VAL:O	2:D:585:ILE:HD12	1.70	0.91
1:G:225:THR:HG22	1:G:226:GLN:HG3	1.52	0.91
1:G:329:VAL:HG22	1:G:362:ILE:HG12	1.53	0.91
1:E:174:ASN:HA	1:E:177:ILE:HD12	1.53	0.91
1:C:234:ILE:HD11	1:C:236:PHE:CZ	2.06	0.90
2:D:581:VAL:HG12	2:D:585:ILE:HD11	1.51	0.90
1:E:309:GLY:HA3	1:E:331:SER:HA	1.52	0.90
1:C:425:PRO:HB2	1:E:62:THR:HG21	1.54	0.90
1:G:405:VAL:HG21	1:G:477:LEU:HD22	1.53	0.90
1:E:163:ILE:HD12	1:E:163:ILE:H	1.37	0.90
1:A:375:LEU:HB3	1:A:378:SER:HB3	1.51	0.90
1:C:396:VAL:HG12	1:C:397:THR:H	1.36	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:VAL:HG22	1:E:429:GLN:HG3	1.54	0.90
1:G:234:ILE:HG12	1:G:508:THR:HB	1.54	0.89
1:A:198:ALA:HB1	1:A:199:PRO:HD2	1.53	0.89
1:E:416:THR:HB	1:E:419:GLU:CB	2.01	0.89
1:C:371:VAL:HG23	1:C:381:ILE:HB	1.53	0.89
1:A:394:THR:O	1:A:396:VAL:HG23	1.72	0.89
1:C:154:ARG:HB3	1:C:211:THR:HG22	1.52	0.89
1:C:293:VAL:HG22	1:C:324:GLU:HG3	1.55	0.89
1:G:248:TRP:HE1	1:G:429:GLN:HG2	1.34	0.89
1:E:220:ARG:HD2	1:G:215:ALA:CB	2.03	0.88
1:C:103:GLU:HG3	1:C:117:ASP:OD1	1.74	0.88
1:A:242:THR:HA	1:A:245:ASP:HB2	1.55	0.88
1:A:446:ASN:HB2	1:A:487:ASN:HA	1.55	0.88
1:C:275:THR:HB	1:C:391:VAL:HG11	1.54	0.88
1:E:309:GLY:CA	1:E:331:SER:HA	2.03	0.88
1:A:385:VAL:HG22	1:A:392:SER:HB2	1.55	0.88
1:C:275:THR:HG21	1:C:478:ARG:NH1	1.88	0.88
1:E:187:ARG:HH12	1:E:215:ALA:HA	1.37	0.88
1:C:405:VAL:CG1	1:C:477:LEU:HD13	2.04	0.88
1:A:380:VAL:HG12	1:A:381:ILE:H	1.36	0.88
1:A:447:ASN:CB	1:C:451:GLU:HG3	2.03	0.87
1:A:405:VAL:HG11	1:A:477:LEU:HD22	1.53	0.87
1:C:164:ASN:OD1	1:C:166:GLU:HB3	1.74	0.87
1:A:297:THR:CG2	1:A:478:ARG:HE	1.86	0.87
1:G:47:GLN:HE22	1:G:63:MET:HA	1.31	0.87
1:C:120:GLN:HE22	1:C:208:LEU:HB3	1.39	0.87
1:G:122:PRO:HG2	1:G:508:THR:HG23	1.57	0.86
1:E:169:THR:HB	1:E:172:THR:OG1	1.75	0.86
1:C:215:ALA:HB3	1:C:218:GLY:HA2	1.54	0.86
1:A:371:VAL:HG22	1:A:381:ILE:HG21	1.56	0.86
1:A:154:ARG:HB3	1:A:211:THR:HG22	1.56	0.86
1:G:411:GLU:HA	1:G:464:HIS:HB3	1.55	0.86
1:E:297:THR:HG22	1:E:298:PRO:HD3	0.90	0.86
2:B:588:GLN:HG3	2:B:593:VAL:HA	1.57	0.86
1:G:481:VAL:O	1:G:482:ASP:HB2	1.75	0.86
1:C:457:ASN:O	1:C:457:ASN:ND2	2.07	0.86
1:E:465:TYR:CG	1:E:466:PRO:HD2	2.11	0.86
1:G:183:ILE:O	1:G:478:ARG:HB2	1.75	0.86
1:E:73:GLN:HB3	2:F:574:LYS:HA	1.57	0.86
1:E:220:ARG:HH11	1:G:215:ALA:HB1	0.72	0.86
1:E:198:ALA:HB1	1:E:199:PRO:HD2	1.56	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:ALA:HB3	1:G:387:LYS:HA	1.56	0.86
1:A:171:GLU:H	1:A:171:GLU:CD	1.79	0.85
1:G:207:VAL:CG1	1:G:212:TYR:HB2	2.05	0.85
1:C:313:THR:HA	1:C:325:ILE:HG22	1.55	0.85
1:G:362:ILE:HG22	1:G:367:VAL:HG13	1.58	0.85
1:G:127:GLU:HG2	1:G:503:THR:HG21	1.58	0.85
1:E:55:ALA:HB1	1:E:56:PRO:HD2	1.56	0.85
1:E:148:ILE:HG12	1:E:412:MET:HE1	1.56	0.85
1:G:111:LEU:HG	1:G:112:LEU:HD12	1.59	0.85
1:A:395:PRO:HB3	1:C:267:GLU:HB3	1.59	0.85
1:C:297:THR:HG23	1:C:476:GLY:HA3	0.85	0.85
1:A:461:PHE:HE1	1:A:480:ILE:HB	1.40	0.84
1:C:120:GLN:HE21	1:C:208:LEU:HB3	1.40	0.84
1:A:281:ALA:HB2	1:A:291:ARG:HB2	1.59	0.84
1:A:549:GLY:HA2	1:C:113:ARG:NH2	1.93	0.84
1:A:107:VAL:HG11	1:A:450:PHE:HD1	1.40	0.84
1:C:396:VAL:HG12	1:C:397:THR:N	1.90	0.84
1:G:131:VAL:O	1:G:282:ILE:HG23	1.78	0.83
1:G:154:ARG:HG2	1:G:211:THR:HG22	1.60	0.83
1:E:284:GLN:CB	1:E:289:VAL:HG11	2.07	0.83
1:E:457:ASN:HD21	1:E:486:ASN:HB3	1.43	0.83
1:A:252:ALA:HB2	1:A:427:TYR:HB2	1.60	0.83
1:C:332:VAL:HG22	1:C:358:SER:HB2	1.61	0.83
1:G:307:THR:HB	1:G:332:VAL:HG12	1.60	0.83
1:C:421:THR:HG21	1:G:123:ILE:HD12	1.60	0.83
1:C:405:VAL:HG11	1:C:477:LEU:CD1	2.09	0.83
1:A:366:THR:O	1:A:367:VAL:HG23	1.79	0.83
1:A:371:VAL:H	1:A:381:ILE:HG22	1.42	0.83
1:C:475:LEU:CD2	1:E:267:GLU:HB2	2.09	0.82
1:G:207:VAL:HG11	1:G:212:TYR:HB2	1.62	0.82
1:G:241:PRO:CG	1:G:244:ILE:HB	2.09	0.82
1:G:292:ILE:HD11	1:G:325:ILE:HG13	1.61	0.82
1:C:184:THR:HG21	1:C:295:SER:CB	2.09	0.82
1:E:220:ARG:CD	1:G:215:ALA:HB2	2.06	0.82
1:C:273:SER:H	1:C:297:THR:HB	1.44	0.82
1:E:265:ALA:HB2	1:E:404:ALA:HB2	1.61	0.82
1:A:342:LEU:HD22	1:A:347:PRO:HA	1.60	0.82
1:C:363:THR:CG2	1:C:366:THR:H	1.92	0.82
1:E:229:LYS:HB2	1:E:485:GLU:HG2	1.61	0.82
1:G:447:ASN:ND2	1:G:449:VAL:HG12	1.95	0.82
1:C:339:ALA:HB3	1:C:400:ILE:HD11	1.62	0.82

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:GLN:HB2	1:E:289:VAL:HG11	1.60	0.81
1:G:534:ASP:HA	1:G:537:VAL:HB	1.61	0.81
2:H:578:THR:HG22	2:H:581:VAL:N	1.93	0.81
1:C:545:MET:HE1	1:C:546:GLU:HA	1.61	0.81
2:D:578:THR:HG22	2:D:580:SER:H	1.44	0.81
1:G:408:LEU:HB2	1:G:461:PHE:HB3	1.61	0.81
1:G:248:TRP:HE1	1:G:429:GLN:CG	1.94	0.81
1:E:122:PRO:O	1:E:508:THR:HG23	1.81	0.81
1:C:229:LYS:H	1:C:485:GLU:HG3	1.45	0.81
1:E:274:MET:HE2	1:E:296:ILE:HD11	1.63	0.81
1:E:90:ASP:HB2	2:F:561:VAL:HB	1.62	0.81
1:A:405:VAL:HG11	1:A:477:LEU:CD2	2.10	0.81
1:A:383:ARG:CB	1:A:383:ARG:HH11	1.90	0.80
1:C:87:LYS:CE	1:C:95:VAL:HG23	2.11	0.80
1:G:363:THR:HG22	1:G:364:ALA:H	1.45	0.80
1:C:306:LEU:HD13	1:C:311:GLY:HA2	1.63	0.80
1:A:244:ILE:HD11	1:A:501:SER:HB2	1.64	0.80
1:A:414:ALA:HB2	1:C:517:ASN:O	1.81	0.80
1:G:258:PRO:HB3	1:G:410:ILE:HG12	1.63	0.80
1:E:299:LEU:HD12	1:E:300:PRO:HD2	1.62	0.80
1:G:130:THR:HB	1:G:282:ILE:HD13	1.62	0.80
1:C:302:ALA:HB2	1:C:338:PRO:CG	2.12	0.80
1:E:435:SER:O	1:E:437:GLY:N	2.14	0.80
1:G:447:ASN:HD21	1:G:449:VAL:HG12	1.47	0.80
1:C:475:LEU:CD1	1:E:267:GLU:HG2	2.03	0.79
1:G:444:LYS:HB3	1:G:450:PHE:CE2	2.16	0.79
1:E:43:ILE:HB	1:E:67:VAL:HB	1.61	0.79
1:A:249:TRP:O	1:A:429:GLN:HG2	1.82	0.79
1:A:447:ASN:HB3	1:C:451:GLU:HG3	1.65	0.79
1:G:241:PRO:HG3	1:G:244:ILE:HB	1.64	0.79
1:G:217:ILE:HD13	1:G:217:ILE:O	1.83	0.79
1:A:455:GLU:HG3	1:E:259:GLN:HB2	1.62	0.79
1:E:107:VAL:O	1:E:530:ALA:HB3	1.82	0.79
1:A:370:SER:HB2	1:A:381:ILE:O	1.83	0.79
1:E:116:VAL:HG21	1:E:522:VAL:CG1	2.13	0.79
1:C:435:SER:O	1:C:437:GLY:N	2.14	0.79
1:G:93:GLY:O	1:G:97:SER:HB3	1.82	0.79
1:A:435:SER:O	1:A:437:GLY:N	2.14	0.78
1:A:151:PRO:HB2	1:A:485:GLU:HB3	1.66	0.78
1:C:143:TRP:HE1	1:C:498:ILE:HG22	1.48	0.78
1:A:279:SER:HA	1:A:387:LYS:CG	2.14	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ALA:HB3	1:G:63:MET:HE2	1.65	0.78
1:G:396:VAL:HG12	1:G:397:THR:H	1.45	0.78
1:A:259:GLN:HB2	1:C:455:GLU:HG3	1.65	0.78
1:C:439:TYR:CE2	1:C:556:ASN:HA	2.19	0.78
1:E:107:VAL:HB	1:E:228:ARG:HH11	1.48	0.78
1:A:279:SER:HA	1:A:387:LYS:HG3	1.64	0.78
1:A:448:PRO:HD3	1:C:111:LEU:HD22	1.65	0.78
1:G:189:LEU:HD23	1:G:189:LEU:N	1.99	0.78
1:C:267:GLU:OE1	1:C:267:GLU:HA	1.83	0.78
1:C:154:ARG:HG2	1:C:482:ASP:OD1	1.83	0.78
1:E:237:GLU:HG3	1:E:507:LYS:CE	2.13	0.78
1:G:77:PRO:HA	1:G:533:GLU:OE2	1.82	0.77
1:A:329:VAL:HG23	1:A:362:ILE:HG13	1.65	0.77
1:E:284:GLN:HB3	1:E:285:PRO:HD2	1.65	0.77
1:E:457:ASN:ND2	1:E:486:ASN:HB3	1.98	0.77
1:C:398:VAL:HB	1:C:400:ILE:HD13	1.66	0.77
1:E:278:ALA:HB2	1:E:385:VAL:HG21	1.67	0.77
1:A:297:THR:OG1	1:A:298:PRO:HD3	1.85	0.77
1:A:262:THR:CA	1:A:406:ASN:HB3	2.13	0.77
1:A:517:ASN:O	1:E:414:ALA:HB2	1.85	0.77
1:G:168:LEU:HD23	1:G:172:THR:HB	1.65	0.77
1:G:174:ASN:ND2	1:G:468:TYR:HA	1.98	0.77
1:C:542:ARG:O	1:C:546:GLU:HB2	1.84	0.77
1:E:56:PRO:HB2	1:G:554:ASP:HA	1.67	0.77
1:A:453:THR:HG21	1:A:484:PHE:O	1.84	0.77
1:C:168:LEU:HD13	1:C:201:TRP:CZ3	2.19	0.77
1:C:87:LYS:O	1:C:91:PRO:HD3	1.84	0.77
1:A:400:ILE:HG12	1:A:401:ASP:N	2.00	0.77
1:A:341:ILE:O	1:A:342:LEU:HD23	1.84	0.77
1:E:185:ASN:CG	1:E:318:GLY:HA3	2.05	0.77
1:C:297:THR:CG2	1:C:476:GLY:HA2	2.13	0.76
1:A:444:LYS:HD3	1:A:450:PHE:CD2	2.20	0.76
1:A:105:SER:O	1:A:230:VAL:HG21	1.84	0.76
1:E:173:ARG:O	1:E:176:PHE:HB3	1.84	0.76
1:G:416:THR:HB	1:G:419:GLU:CB	2.09	0.76
1:C:290:ALA:N	1:C:362:ILE:HD11	1.99	0.76
1:C:164:ASN:ND2	1:C:200:GLY:HA3	2.00	0.76
1:E:278:ALA:HA	1:E:292:ILE:HG22	1.66	0.76
1:A:371:VAL:H	1:A:381:ILE:CG2	1.97	0.76
1:C:143:TRP:NE1	1:C:498:ILE:HG22	2.00	0.76
1:A:517:ASN:OD1	1:E:413:PRO:HA	1.86	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:THR:HG23	1:G:193:GLN:HG2	1.68	0.76
1:E:418:GLU:HA	1:E:421:THR:HG23	1.65	0.76
1:G:248:TRP:HD1	1:G:431:LEU:HD23	1.50	0.76
1:A:113:ARG:HG3	1:E:443:TYR:CE2	2.21	0.76
1:C:154:ARG:HB3	1:C:211:THR:CG2	2.16	0.76
1:A:371:VAL:HG22	1:A:381:ILE:CG2	2.14	0.76
1:A:189:LEU:HD12	1:A:189:LEU:N	2.00	0.76
1:A:103:GLU:HG3	1:A:117:ASP:OD2	1.85	0.76
1:A:485:GLU:HG3	1:A:488:PHE:H	1.50	0.76
1:A:297:THR:HG23	1:A:478:ARG:HE	1.50	0.76
1:E:418:GLU:HA	1:E:421:THR:CG2	2.16	0.76
1:C:304:VAL:HG12	1:C:305:ALA:H	1.50	0.76
1:G:188:ASP:OD1	1:G:316:THR:HG22	1.86	0.76
1:A:461:PHE:CE1	1:A:480:ILE:HB	2.21	0.76
1:C:458:PHE:HB2	1:C:483:THR:HG23	1.68	0.75
1:G:412:MET:SD	1:G:413:PRO:HD2	2.27	0.75
1:C:105:SER:CB	1:C:117:ASP:HB2	2.16	0.75
1:E:228:ARG:HB3	1:E:452:MET:CE	2.16	0.75
1:G:329:VAL:HG13	1:G:362:ILE:HG23	1.68	0.75
1:G:306:LEU:HD22	1:G:311:GLY:HA2	1.67	0.75
1:C:297:THR:HB	1:C:298:PRO:HD3	1.68	0.75
1:C:407:ARG:HH21	1:C:478:ARG:HB2	1.52	0.75
1:E:412:MET:SD	1:E:413:PRO:HD2	2.27	0.75
1:G:248:TRP:CD1	1:G:431:LEU:HD23	2.20	0.75
1:C:407:ARG:HD2	1:C:462:GLN:CB	2.16	0.75
1:A:239:ASN:HB3	1:A:503:THR:O	1.86	0.75
1:G:142:LEU:HA	1:G:500:GLN:H	1.52	0.75
1:A:178:GLN:NE2	1:A:390:GLY:HA2	2.02	0.75
1:G:56:PRO:HG2	1:G:57:SER:H	1.52	0.75
1:A:423:ASN:HA	1:C:523:GLY:HA3	1.69	0.75
1:A:447:ASN:HB2	1:C:451:GLU:HA	1.68	0.74
1:G:142:LEU:HD12	1:G:497:GLY:HA2	1.67	0.74
1:A:475:LEU:HD22	1:C:267:GLU:CG	2.15	0.74
1:A:276:VAL:HG21	1:A:369:TYR:CE1	2.19	0.74
1:C:304:VAL:HG12	1:C:305:ALA:N	2.00	0.74
1:G:132:SER:C	1:G:134:SER:N	2.33	0.74
1:E:210:ASN:ND2	1:G:524:GLN:HG3	2.01	0.74
1:G:199:PRO:HD3	1:G:388:GLY:HA3	1.69	0.74
1:C:87:LYS:C	1:C:89:MET:H	1.88	0.74
1:G:92:ALA:O	1:G:95:VAL:HG13	1.87	0.74
1:A:108:PRO:HB2	1:A:533:GLU:HB2	1.67	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:GLN:OE1	2:F:574:LYS:HB2	1.87	0.74
1:G:465:TYR:CG	1:G:466:PRO:HD2	2.22	0.74
1:G:460:GLY:HA2	1:G:481:VAL:HA	1.67	0.74
2:D:583:LYS:O	2:D:587:GLN:HG3	1.86	0.74
1:C:235:THR:HG22	1:C:439:TYR:CD1	2.22	0.74
1:C:180:LEU:HA	1:C:183:ILE:HD11	1.70	0.74
1:E:469:ASP:CG	1:E:471:GLU:HG2	2.08	0.74
1:E:107:VAL:HB	1:E:228:ARG:NH1	2.03	0.74
1:A:263:ILE:HB	1:A:405:VAL:O	1.87	0.74
1:E:262:THR:HA	1:E:406:ASN:HA	1.68	0.74
1:G:542:ARG:O	1:G:546:GLU:HG2	1.88	0.74
3:R:1:U:H2'	3:R:2:U:C6	2.22	0.74
1:C:375:LEU:HB3	1:C:378:SER:HB3	1.70	0.74
1:G:122:PRO:HG2	1:G:508:THR:CG2	2.18	0.74
1:G:444:LYS:HB3	1:G:450:PHE:HE2	1.50	0.74
1:G:405:VAL:CG2	1:G:477:LEU:HD22	2.18	0.74
1:A:447:ASN:HB2	1:C:451:GLU:HG3	1.68	0.74
1:E:139:ASP:O	1:E:141:LYS:N	2.19	0.74
1:G:205:ILE:HD13	1:G:480:ILE:HD11	1.70	0.73
1:C:475:LEU:CD1	1:E:267:GLU:CD	2.54	0.73
1:A:342:LEU:CD2	1:A:347:PRO:HA	2.17	0.73
1:E:79:GLU:HB3	1:E:101:LEU:HD12	1.68	0.73
1:E:416:THR:HG22	1:E:418:GLU:H	1.53	0.73
1:G:287:ASN:HA	1:G:364:ALA:HB2	1.68	0.73
1:A:276:VAL:HG13	1:A:294:TRP:HB2	1.70	0.73
1:A:380:VAL:HG12	1:A:381:ILE:N	2.03	0.73
1:A:124:VAL:HG23	1:A:506:CYS:HB2	1.71	0.73
1:E:204:SER:HB3	1:E:206:TYR:OH	1.88	0.73
1:G:274:MET:HE1	1:G:294:TRP:HE1	1.53	0.73
1:G:306:LEU:HD21	1:G:309:GLY:O	1.87	0.73
1:E:533:GLU:OE2	1:E:533:GLU:HA	1.87	0.73
1:G:346:GLU:OE1	1:G:347:PRO:HD2	1.88	0.73
1:A:124:VAL:HG11	1:A:206:TYR:CD2	2.24	0.73
1:E:445:MET:HB2	1:E:489:SER:HB2	1.71	0.73
2:D:579:PRO:HG2	1:E:535:GLU:OE1	1.89	0.73
1:E:248:TRP:HA	1:E:431:LEU:HA	1.71	0.73
1:E:314:ASN:O	1:E:324:GLU:HB3	1.89	0.73
2:F:596:ASN:HB2	2:F:597:PRO:CD	2.19	0.73
1:E:252:ALA:HB2	1:E:427:TYR:HB2	1.71	0.73
1:C:475:LEU:CD1	1:E:267:GLU:OE2	2.37	0.73
1:C:407:ARG:HD3	1:C:460:GLY:O	1.87	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:THR:HG22	1:C:366:THR:O	1.89	0.73
1:A:449:VAL:HG12	1:E:448:PRO:HG2	1.71	0.72
1:C:277:SER:HB3	1:C:391:VAL:HG22	1.71	0.72
1:G:132:SER:O	1:G:134:SER:N	2.21	0.72
1:G:176:PHE:O	1:G:179:THR:HB	1.89	0.72
1:C:400:ILE:HD12	1:C:400:ILE:N	2.04	0.72
1:A:480:ILE:N	1:A:480:ILE:HD12	2.02	0.72
1:C:181:ASN:O	1:C:407:ARG:NH2	2.22	0.72
1:G:546:GLU:HA	1:G:546:GLU:OE2	1.88	0.72
1:G:405:VAL:HG21	1:G:477:LEU:CD2	2.19	0.72
1:E:252:ALA:HB1	1:E:424:VAL:HG11	1.71	0.72
1:E:359:MET:SD	1:E:362:ILE:HD11	2.28	0.72
1:A:229:LYS:HD3	1:A:512:TRP:HB3	1.69	0.72
1:C:107:VAL:HG22	1:C:230:VAL:HG13	1.71	0.72
1:C:120:GLN:HE22	1:C:208:LEU:CB	2.00	0.72
1:C:428:GLU:HG2	1:C:430:PHE:HE1	1.52	0.72
1:E:348:PHE:CE1	1:E:373:SER:HB2	2.25	0.72
1:C:538:GLN:HG2	2:D:582:ILE:HD12	1.69	0.72
1:A:535:GLU:O	1:A:538:GLN:HB3	1.90	0.72
1:A:544:GLN:HB3	1:C:113:ARG:NH1	2.05	0.72
1:A:274:MET:HG3	1:A:296:ILE:HG12	1.72	0.72
1:G:181:ASN:O	1:G:407:ARG:NH2	2.22	0.71
1:A:357:PHE:HE1	1:A:369:TYR:HD1	1.37	0.71
1:G:230:VAL:HG23	1:G:512:TRP:HA	1.70	0.71
1:C:272:GLY:HA3	1:C:298:PRO:CD	2.19	0.71
1:E:435:SER:C	1:E:437:GLY:H	1.90	0.71
1:C:398:VAL:HB	1:C:400:ILE:CD1	2.20	0.71
1:C:266:ALA:HB3	1:C:270:SER:HB3	1.71	0.71
1:C:275:THR:CG2	1:C:478:ARG:NH1	2.53	0.71
1:E:163:ILE:N	1:E:163:ILE:HD12	2.05	0.71
1:A:495:PHE:HB3	1:A:498:ILE:HD11	1.73	0.71
1:C:245:ASP:HB2	1:C:433:LYS:HG2	1.72	0.71
1:C:407:ARG:NH2	1:C:478:ARG:HB2	2.03	0.71
1:G:375:LEU:HB3	1:G:378:SER:HB3	1.71	0.71
1:A:156:ASN:HB3	1:A:206:TYR:O	1.90	0.71
1:C:168:LEU:HG	1:C:173:ARG:HB3	1.72	0.71
1:G:75:ILE:HG21	1:G:535:GLU:HG2	1.71	0.71
1:C:265:ALA:HB2	1:C:404:ALA:N	2.06	0.71
1:C:154:ARG:O	1:C:207:VAL:HG13	1.90	0.71
1:A:144:ARG:HD2	1:A:496:TRP:CD1	2.25	0.71
1:G:49:LEU:HB2	1:G:52:GLU:HG3	1.70	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:THR:CG2	1:C:478:ARG:NH2	2.54	0.71
1:C:453:THR:HA	1:C:456:GLU:OE1	1.91	0.71
1:E:250:VAL:HG22	1:E:429:GLN:CG	2.20	0.71
1:G:151:PRO:HB2	1:G:485:GLU:HB3	1.71	0.71
2:B:564:LEU:HD11	2:B:590:VAL:HG22	1.73	0.71
1:C:106:LYS:HE3	1:C:115:SER:OG	1.90	0.71
1:C:229:LYS:H	1:C:485:GLU:CG	2.04	0.71
1:E:444:LYS:O	1:E:444:LYS:HD2	1.91	0.71
1:A:198:ALA:HA	1:A:388:GLY:O	1.90	0.71
1:A:88:TYR:CE2	1:A:544:GLN:HG3	2.26	0.70
2:D:581:VAL:HG12	2:D:585:ILE:CD1	2.21	0.70
1:G:363:THR:HG22	1:G:364:ALA:N	2.04	0.70
1:A:238:PHE:CG	1:A:432:CYS:HB3	2.26	0.70
1:G:105:SER:OG	1:G:117:ASP:HB2	1.92	0.70
2:H:583:LYS:O	2:H:587:GLN:HG3	1.90	0.70
2:B:563:ALA:O	2:B:567:ILE:HG22	1.91	0.70
1:G:166:GLU:HB3	1:G:201:TRP:CZ2	2.25	0.70
1:C:198:ALA:HB3	1:C:201:TRP:HB2	1.73	0.70
1:A:197:PHE:CZ	1:A:201:TRP:HB3	2.26	0.70
1:C:233:GLY:HA2	1:C:441:VAL:HA	1.74	0.70
1:G:543:LEU:O	1:G:546:GLU:HB2	1.91	0.70
1:G:75:ILE:CG2	1:G:535:GLU:HG2	2.20	0.70
1:E:474:ALA:CB	1:E:478:ARG:HD2	2.21	0.70
1:E:420:VAL:HG23	1:E:421:THR:H	1.54	0.70
1:A:444:LYS:HD3	1:A:450:PHE:HD2	1.56	0.70
1:A:363:THR:HB	1:A:366:THR:H	1.57	0.70
1:G:290:ALA:HB2	1:G:387:LYS:HE2	1.72	0.70
1:A:207:VAL:HG11	1:A:212:TYR:CD1	2.26	0.70
2:D:585:ILE:HD12	2:D:585:ILE:H	1.55	0.70
1:G:385:VAL:HG12	1:G:392:SER:HB3	1.74	0.70
1:A:124:VAL:HG11	1:A:206:TYR:HD2	1.57	0.70
1:C:160:LEU:HD22	1:C:161:ALA:H	1.57	0.70
1:A:160:LEU:HD12	1:A:160:LEU:H	1.57	0.70
1:C:139:ASP:CG	1:C:141:LYS:HG3	2.12	0.70
1:E:306:LEU:HA	1:E:333:TRP:HA	1.72	0.70
1:E:187:ARG:NH1	1:E:215:ALA:HA	2.06	0.70
1:A:424:VAL:O	1:A:427:TYR:HD2	1.75	0.69
1:C:371:VAL:CG2	1:C:381:ILE:HB	2.22	0.69
1:A:73:GLN:NE2	2:F:578:THR:HG21	2.06	0.69
1:G:143:TRP:CD1	1:G:500:GLN:HA	2.27	0.69
1:E:163:ILE:CD1	1:E:163:ILE:H	2.04	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:GLU:HB3	1:A:423:ASN:ND2	2.06	0.69
1:E:313:THR:HB	1:E:333:TRP:HE1	1.56	0.69
1:C:207:VAL:HG11	1:C:212:TYR:HB2	1.73	0.69
1:G:272:GLY:O	1:G:475:LEU:HD12	1.91	0.69
1:C:262:THR:HB	1:E:262:THR:HG21	1.73	0.69
1:A:252:ALA:HB1	1:A:424:VAL:HG11	1.73	0.69
1:G:60:ARG:HG2	1:G:62:THR:O	1.92	0.69
1:G:198:ALA:HB3	1:G:201:TRP:CB	2.22	0.69
2:B:578:THR:HB	2:B:581:VAL:HG23	1.74	0.69
1:E:446:ASN:ND2	1:E:486:ASN:O	2.22	0.69
1:G:263:ILE:HB	1:G:405:VAL:O	1.92	0.69
1:E:168:LEU:HD12	1:E:172:THR:HG22	1.75	0.69
1:G:360:THR:HB	1:G:368:VAL:HG12	1.74	0.69
1:E:107:VAL:HG23	1:E:230:VAL:HG22	1.73	0.69
1:C:407:ARG:HD2	1:C:462:GLN:HB2	1.75	0.69
1:G:204:SER:HB3	1:G:206:TYR:OH	1.93	0.69
1:A:297:THR:HG21	1:A:476:GLY:H	1.56	0.69
1:G:290:ALA:O	1:G:326:ASP:HA	1.92	0.69
1:A:329:VAL:CG1	1:A:330:ASN:N	2.56	0.69
1:E:225:THR:O	1:E:226:GLN:HB3	1.91	0.69
1:G:228:ARG:HD3	1:G:452:MET:SD	2.33	0.69
1:G:292:ILE:CD1	1:G:325:ILE:HG13	2.22	0.69
1:A:148:ILE:HG12	1:A:492:VAL:HG12	1.75	0.69
1:G:126:ILE:H	1:G:126:ILE:HD12	1.58	0.69
1:A:105:SER:HB3	1:A:117:ASP:OD2	1.93	0.69
1:E:335:PHE:CE2	1:E:355:THR:HB	2.26	0.69
1:A:186:TRP:CE3	1:A:480:ILE:HG23	2.28	0.69
1:E:130:THR:HG22	1:E:132:SER:N	2.08	0.69
2:F:606:ALA:O	2:F:610:VAL:HG23	1.93	0.69
1:E:294:TRP:O	1:E:323:VAL:HG23	1.93	0.68
1:A:357:PHE:HD1	1:A:371:VAL:HG12	1.58	0.68
1:C:290:ALA:H	1:C:362:ILE:HD11	1.58	0.68
2:B:564:LEU:O	2:B:567:ILE:HG23	1.94	0.68
1:C:363:THR:HG23	1:C:364:ALA:N	2.09	0.68
1:G:253:HIS:CD2	1:G:549:GLY:HA3	2.28	0.68
1:A:375:LEU:CB	1:A:378:SER:HB3	2.22	0.68
1:A:416:THR:O	1:A:420:VAL:HG23	1.93	0.68
1:C:445:MET:O	1:C:445:MET:HG2	1.92	0.68
1:E:249:TRP:O	1:E:429:GLN:HG2	1.94	0.68
1:C:543:LEU:O	1:C:547:LEU:HG	1.94	0.68
1:A:144:ARG:NH2	1:A:417:THR:OG1	2.26	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:THR:HG23	1:C:476:GLY:HA2	1.65	0.68
1:G:142:LEU:HG	1:G:165:ASN:ND2	2.07	0.68
1:E:199:PRO:HG2	1:E:200:GLY:H	1.59	0.68
1:G:251:GLY:C	1:G:550:VAL:HG21	2.14	0.68
1:E:207:VAL:HG21	1:E:212:TYR:CD2	2.28	0.68
1:C:127:GLU:HA	1:C:503:THR:HG22	1.76	0.68
2:D:571:LEU:HD12	2:D:585:ILE:HG23	1.75	0.68
1:E:407:ARG:HD2	1:E:460:GLY:HA3	1.76	0.68
1:A:297:THR:HG23	1:A:478:ARG:HH21	1.58	0.68
1:G:84:TRP:CD1	1:G:230:VAL:HG12	2.29	0.68
1:C:148:ILE:N	1:C:148:ILE:HD12	2.09	0.68
1:A:256:VAL:O	1:A:484:PHE:HE2	1.75	0.68
1:C:440:ILE:HG22	1:C:550:VAL:HG12	1.76	0.68
1:G:295:SER:HB3	1:G:322:SER:HA	1.75	0.68
1:E:155:LEU:HD12	1:E:156:ASN:H	1.59	0.68
1:E:90:ASP:OD2	1:E:93:GLY:HA3	1.94	0.68
1:A:435:SER:HB2	1:A:552:GLN:HG2	1.76	0.68
1:A:544:GLN:HB3	1:C:113:ARG:HH12	1.59	0.67
1:C:207:VAL:HG12	1:C:208:LEU:N	2.09	0.67
1:G:155:LEU:HA	1:G:207:VAL:HG13	1.75	0.67
1:A:371:VAL:O	1:A:381:ILE:HG22	1.94	0.67
1:A:353:ASP:OD2	1:A:375:LEU:HB2	1.95	0.67
1:C:504:ILE:HG22	1:C:506:CYS:SG	2.34	0.67
1:A:276:VAL:HG22	1:A:294:TRP:CD1	2.30	0.67
1:A:136:LEU:HD21	1:A:501:SER:HA	1.76	0.67
1:C:152:ALA:HB3	1:C:155:LEU:HB3	1.76	0.67
1:A:444:LYS:HD2	1:A:447:ASN:O	1.94	0.67
1:E:313:THR:HB	1:E:333:TRP:NE1	2.10	0.67
1:E:444:LYS:HB3	1:E:444:LYS:HZ2	1.59	0.67
1:A:277:SER:O	1:A:292:ILE:HB	1.94	0.67
1:C:457:ASN:HD22	1:C:457:ASN:C	1.97	0.67
1:E:239:ASN:HB3	1:E:503:THR:O	1.93	0.67
1:C:206:TYR:N	1:C:206:TYR:CD1	2.59	0.67
1:C:446:ASN:O	1:E:111:LEU:HD21	1.94	0.67
1:E:169:THR:HG22	1:E:170:LEU:N	2.10	0.67
1:E:241:PRO:O	1:E:243:LEU:N	2.25	0.67
1:C:467:GLY:N	1:E:218:GLY:O	2.27	0.67
1:C:297:THR:HG21	1:C:476:GLY:CA	2.22	0.67
1:G:198:ALA:HA	1:G:388:GLY:O	1.95	0.67
1:G:444:LYS:HG2	1:G:447:ASN:O	1.94	0.67
1:C:151:PRO:O	1:C:485:GLU:HB2	1.95	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:367:VAL:HB	1:E:385:VAL:CG2	2.25	0.67
1:G:408:LEU:HG	1:G:459:GLY:HA3	1.76	0.67
1:C:465:TYR:CD1	1:C:466:PRO:HD2	2.29	0.67
1:A:539:LEU:CD1	1:A:543:LEU:HG	2.25	0.67
1:C:106:LYS:HA	1:C:513:GLU:OE1	1.94	0.67
1:E:168:LEU:HD12	1:E:172:THR:CG2	2.25	0.67
1:A:253:HIS:ND1	1:A:491:ALA:HB2	2.10	0.67
1:G:89:MET:HE1	1:G:544:GLN:N	2.10	0.67
1:C:250:VAL:HB	1:C:429:GLN:HB3	1.75	0.67
1:G:73:GLN:HG2	1:G:73:GLN:O	1.94	0.67
1:C:106:LYS:HG3	1:C:117:ASP:HB3	1.77	0.66
1:C:234:ILE:HB	1:C:508:THR:HG22	1.77	0.66
1:G:258:PRO:HB2	1:G:408:LEU:HB3	1.77	0.66
1:C:341:ILE:HG12	1:C:398:VAL:HG12	1.77	0.66
1:C:292:ILE:HD11	1:C:325:ILE:HD11	1.77	0.66
1:C:319:LYS:HG3	1:C:320:PHE:CD1	2.30	0.66
1:C:163:ILE:HG13	1:C:164:ASN:H	1.61	0.66
1:A:230:VAL:HG12	1:A:231:TYR:CD2	2.30	0.66
1:A:480:ILE:CD1	1:A:480:ILE:H	2.05	0.66
1:G:369:TYR:CZ	1:G:383:ARG:HB3	2.30	0.66
1:C:176:PHE:CZ	1:C:180:LEU:HD11	2.30	0.66
1:A:448:PRO:HG3	1:C:449:VAL:HG22	1.77	0.66
1:E:474:ALA:HB3	1:E:478:ARG:HD2	1.75	0.66
1:G:332:VAL:HG22	1:G:358:SER:HB2	1.78	0.66
1:E:308:THR:HB	1:E:332:VAL:HB	1.78	0.66
2:D:567:ILE:HG23	2:D:568:GLY:N	2.09	0.66
1:E:119:GLU:HA	1:E:510:ASP:O	1.94	0.66
1:A:145:VAL:HG12	1:A:498:ILE:HD12	1.78	0.66
1:A:455:GLU:CG	1:E:259:GLN:HB2	2.25	0.66
1:G:381:ILE:HG23	1:G:383:ARG:HH21	1.61	0.66
1:C:137:PRO:O	1:C:501:SER:HB3	1.95	0.66
2:D:578:THR:HB	2:D:581:VAL:HG23	1.78	0.66
1:E:284:GLN:HB3	1:E:289:VAL:HG11	1.77	0.66
1:G:173:ARG:O	1:G:176:PHE:HB3	1.95	0.66
1:A:404:ALA:CB	1:E:261:GLU:HB3	2.24	0.66
2:F:563:ALA:O	2:F:567:ILE:HG22	1.95	0.66
2:H:564:LEU:HD23	2:H:564:LEU:H	1.59	0.66
1:G:304:VAL:HG11	1:G:323:VAL:HG21	1.76	0.66
1:C:159:ALA:O	1:C:203:TYR:HA	1.96	0.66
1:A:176:PHE:CZ	1:A:180:LEU:HD11	2.29	0.66
1:C:304:VAL:HG22	1:C:335:PHE:HB3	1.78	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ILE:HD13	1:E:506:CYS:SG	2.35	0.66
1:C:475:LEU:HG	1:E:267:GLU:OE2	1.94	0.66
1:G:106:LYS:HA	1:G:513:GLU:OE1	1.95	0.66
1:C:248:TRP:HB2	1:C:431:LEU:HD23	1.78	0.66
1:A:170:LEU:O	1:A:173:ARG:HB3	1.96	0.66
2:D:564:LEU:CD1	1:E:50:PRO:HG2	2.26	0.66
1:E:98:GLY:HA2	1:G:63:MET:HE1	1.77	0.66
1:A:253:HIS:CD2	1:A:549:GLY:HA3	2.31	0.65
1:C:357:PHE:CE1	1:C:369:TYR:HB2	2.31	0.65
1:C:421:THR:O	1:G:121:ARG:NH1	2.28	0.65
1:E:518:ALA:C	1:E:520:SER:H	1.97	0.65
1:A:243:LEU:HD12	1:A:243:LEU:C	2.17	0.65
1:E:155:LEU:HD12	1:E:156:ASN:N	2.11	0.65
1:E:297:THR:N	1:E:478:ARG:HH21	1.94	0.65
1:E:396:VAL:CG1	1:E:397:THR:N	2.58	0.65
1:C:275:THR:HG21	1:C:478:ARG:CZ	2.25	0.65
1:A:325:ILE:C	1:A:325:ILE:HD12	2.16	0.65
1:A:255:PRO:HG3	1:C:515:THR:HG21	1.78	0.65
1:C:447:ASN:HB3	1:C:449:VAL:O	1.96	0.65
1:E:173:ARG:HD3	1:E:465:TYR:CD2	2.31	0.65
1:E:256:VAL:HG11	1:E:410:ILE:CG2	2.26	0.65
1:G:84:TRP:O	1:G:85:PHE:C	2.35	0.65
1:C:400:ILE:HG22	1:C:401:ASP:N	2.12	0.65
1:C:292:ILE:CD1	1:C:325:ILE:HG13	2.27	0.65
1:A:244:ILE:HD11	1:A:501:SER:CB	2.27	0.65
1:E:465:TYR:CD1	1:E:466:PRO:HD2	2.32	0.65
1:A:297:THR:CB	1:A:298:PRO:HD3	2.26	0.65
1:G:291:ARG:HA	1:G:326:ASP:HA	1.79	0.65
1:G:313:THR:HB	1:G:333:TRP:HE1	1.61	0.65
2:D:569:LEU:O	2:D:569:LEU:HD13	1.96	0.65
1:C:79:GLU:HB3	1:C:101:LEU:HD13	1.78	0.65
2:D:560:THR:HG22	2:D:564:LEU:HD21	1.79	0.65
1:E:225:THR:HG23	1:E:517:ASN:HB2	1.77	0.65
2:D:594:GLN:OE1	1:E:41:ALA:HB1	1.96	0.65
1:C:120:GLN:HG2	1:C:210:ASN:OD1	1.97	0.65
1:E:210:ASN:O	1:E:213:ALA:N	2.30	0.65
1:G:241:PRO:HG2	1:G:244:ILE:HB	1.78	0.65
1:G:297:THR:HB	1:G:298:PRO:HD3	1.77	0.65
1:C:475:LEU:HD13	1:E:267:GLU:HB2	1.79	0.65
1:E:297:THR:N	1:E:478:ARG:NH2	2.45	0.65
1:G:174:ASN:HD22	1:G:468:TYR:HD1	1.44	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:THR:CG2	1:C:295:SER:HB2	2.22	0.65
1:A:142:LEU:HB3	1:A:498:ILE:O	1.95	0.65
1:C:238:PHE:CG	1:C:432:CYS:HB3	2.31	0.65
1:E:48:LEU:HD12	1:E:52:GLU:O	1.97	0.65
1:A:542:ARG:O	1:A:545:MET:HB3	1.96	0.65
1:C:356:SER:OG	1:C:372:SER:HB2	1.97	0.65
1:G:194:TRP:CE3	1:G:194:TRP:HA	2.32	0.65
1:A:408:LEU:HB2	1:A:461:PHE:HB3	1.78	0.65
1:E:130:THR:HB	1:E:163:ILE:HG12	1.78	0.65
1:C:396:VAL:CG1	1:C:397:THR:H	2.08	0.64
1:E:413:PRO:O	1:E:415:LEU:HG	1.97	0.64
1:G:474:ALA:HB1	1:G:478:ARG:HD3	1.78	0.64
1:A:185:ASN:HB2	1:A:188:ASP:OD2	1.97	0.64
2:F:605:LYS:CG	2:F:610:VAL:HG22	2.27	0.64
1:G:224:VAL:HG12	1:G:225:THR:N	2.12	0.64
2:F:597:PRO:O	2:F:599:ILE:N	2.28	0.64
1:A:114:TYR:O	1:A:115:SER:HB3	1.96	0.64
2:B:570:GLY:O	2:B:574:LYS:HG2	1.98	0.64
1:A:129:PRO:CG	1:A:163:ILE:HG23	2.21	0.64
1:G:75:ILE:HG21	1:G:535:GLU:CG	2.27	0.64
1:C:275:THR:CG2	1:C:478:ARG:CZ	2.75	0.64
1:E:285:PRO:HG2	1:E:288:THR:HB	1.80	0.64
1:C:259:GLN:HG3	1:E:456:GLU:O	1.97	0.64
1:G:286:SER:O	1:G:364:ALA:HA	1.98	0.64
1:G:547:LEU:H	1:G:547:LEU:HD23	1.62	0.64
1:E:278:ALA:O	1:E:387:LYS:HA	1.98	0.64
1:E:183:ILE:O	1:E:479:GLY:N	2.31	0.64
1:E:469:ASP:OD1	1:E:471:GLU:HG2	1.98	0.64
1:C:246:GLN:OE1	1:C:499:SER:HB2	1.98	0.64
1:C:543:LEU:O	1:C:546:GLU:HB3	1.97	0.64
1:A:342:LEU:HB2	1:A:397:THR:HB	1.80	0.64
1:G:403:GLU:O	1:G:405:VAL:HG22	1.98	0.64
1:A:152:ALA:HB3	1:A:155:LEU:HB3	1.78	0.64
1:C:84:TRP:HE1	1:C:230:VAL:CG1	2.10	0.64
1:E:449:VAL:HG12	1:E:450:PHE:H	1.62	0.64
1:G:142:LEU:HA	1:G:500:GLN:N	2.11	0.64
1:G:235:THR:HG23	1:G:507:LYS:HB2	1.80	0.64
1:A:232:LYS:HB3	1:A:442:HIS:HB2	1.80	0.64
1:A:452:MET:HB2	1:E:446:ASN:O	1.98	0.64
2:D:581:VAL:CG1	2:D:585:ILE:HD11	2.24	0.64
1:E:176:PHE:CE1	1:E:180:LEU:HD11	2.33	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:GLU:HG2	1:E:517:ASN:HD22	1.62	0.64
1:A:396:VAL:HG12	1:A:397:THR:N	2.12	0.64
1:E:237:GLU:CG	1:E:507:LYS:HE2	2.24	0.64
1:E:436:GLY:N	1:E:554:ASP:OD2	2.31	0.64
1:A:169:THR:HG22	1:A:172:THR:HG23	1.80	0.64
1:A:77:PRO:HA	1:A:533:GLU:OE1	1.97	0.64
1:E:88:TYR:HA	1:E:231:TYR:HB2	1.80	0.64
1:E:144:ARG:HH11	1:E:144:ARG:HG2	1.62	0.64
1:G:249:TRP:HB3	1:G:495:PHE:CD2	2.33	0.63
1:E:244:ILE:O	1:E:244:ILE:HG13	1.98	0.63
1:E:148:ILE:N	1:E:148:ILE:HD12	2.12	0.63
1:E:176:PHE:O	1:E:179:THR:HB	1.97	0.63
1:E:181:ASN:O	1:E:407:ARG:NH2	2.31	0.63
1:G:129:PRO:HB2	1:G:163:ILE:HD11	1.80	0.63
1:G:88:TYR:HA	1:G:231:TYR:CB	2.29	0.63
2:D:594:GLN:CD	1:E:41:ALA:HB1	2.17	0.63
1:E:165:ASN:ND2	1:E:497:GLY:HA2	2.12	0.63
1:C:142:LEU:O	1:C:143:TRP:HB3	1.99	0.63
1:C:443:TYR:HE2	1:E:113:ARG:HD2	1.64	0.63
1:G:145:VAL:HG23	1:G:161:ALA:HB2	1.81	0.63
1:G:224:VAL:HG12	1:G:225:THR:H	1.62	0.63
1:E:63:MET:O	1:E:64:ASP:C	2.36	0.63
1:G:542:ARG:HD2	2:H:582:ILE:HG22	1.81	0.63
1:E:262:THR:HB	1:E:406:ASN:OD1	1.98	0.63
1:E:87:LYS:O	1:E:91:PRO:HD3	1.98	0.63
1:C:287:ASN:O	1:C:362:ILE:HG23	1.99	0.63
1:C:363:THR:HG22	1:C:366:THR:H	1.63	0.63
1:E:274:MET:HG3	1:E:296:ILE:HG12	1.80	0.63
1:G:366:THR:HG22	1:G:386:THR:HG22	1.81	0.63
1:A:186:TRP:CZ3	1:A:480:ILE:HG23	2.34	0.63
1:C:297:THR:HG22	1:C:298:PRO:CD	2.29	0.63
1:E:228:ARG:HD2	1:E:513:GLU:OE1	1.99	0.63
1:G:121:ARG:HG3	1:G:121:ARG:HH11	1.63	0.63
1:E:94:ALA:HA	1:E:97:SER:HB3	1.79	0.63
1:C:363:THR:HG23	1:C:365:ASP:N	2.05	0.63
1:C:400:ILE:HD12	1:C:400:ILE:H	1.62	0.63
1:G:301:VAL:HA	1:G:321:PHE:HA	1.81	0.63
1:C:475:LEU:HD21	1:E:267:GLU:HB2	1.77	0.63
1:A:553:ALA:O	1:A:555:ASP:N	2.32	0.63
1:G:370:SER:HA	1:G:381:ILE:O	1.99	0.63
1:C:146:SER:HB3	1:C:494:HIS:ND1	2.14	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:HD12	1:A:539:LEU:O	1.99	0.63
1:C:105:SER:O	1:C:230:VAL:HG21	1.98	0.63
1:C:407:ARG:HD2	1:C:462:GLN:HB3	1.79	0.63
1:C:446:ASN:OD1	1:C:487:ASN:HA	1.99	0.63
1:G:121:ARG:HG3	1:G:121:ARG:NH1	2.13	0.63
1:A:182:ASN:HA	1:A:478:ARG:HD2	1.80	0.63
1:C:114:TYR:HA	1:C:527:HIS:O	1.98	0.63
1:C:76:ASP:CG	1:C:76:ASP:O	2.37	0.63
1:C:151:PRO:HD2	1:C:490:SER:HB3	1.80	0.63
1:C:177:ILE:CG2	1:C:181:ASN:HD21	2.11	0.63
1:E:129:PRO:HB3	1:E:194:TRP:CD1	2.34	0.63
1:G:123:ILE:HG12	1:G:507:LYS:HA	1.80	0.63
1:G:279:SER:HB3	1:G:291:ARG:HE	1.64	0.63
1:C:382:VAL:O	1:C:383:ARG:HD2	1.99	0.62
1:E:230:VAL:HG12	1:E:231:TYR:HD2	1.64	0.62
1:A:169:THR:HG22	1:A:172:THR:CG2	2.29	0.62
1:G:243:LEU:C	1:G:245:ASP:H	2.01	0.62
1:A:251:GLY:C	1:A:550:VAL:HG21	2.19	0.62
1:C:442:HIS:ND1	1:C:489:SER:O	2.32	0.62
1:E:309:GLY:HA3	1:E:331:SER:CA	2.25	0.62
1:G:156:ASN:HB2	1:G:208:LEU:HD23	1.81	0.62
1:E:93:GLY:O	1:E:97:SER:HB2	1.99	0.62
1:A:455:GLU:O	1:E:259:GLN:HG2	1.99	0.62
1:E:160:LEU:HD23	1:E:160:LEU:H	1.64	0.62
1:C:471:GLU:HA	1:C:471:GLU:OE1	1.99	0.62
1:C:185:ASN:ND2	1:C:318:GLY:HA3	2.14	0.62
1:C:252:ALA:HB1	1:C:424:VAL:HG11	1.80	0.62
1:C:369:TYR:CE1	1:C:383:ARG:HB2	2.35	0.62
1:G:106:LYS:HB3	1:G:530:ALA:HB2	1.80	0.62
1:A:232:LYS:HE2	1:A:510:ASP:OD2	1.99	0.62
1:C:411:GLU:CG	1:E:517:ASN:HD22	2.12	0.62
1:A:292:ILE:C	1:A:292:ILE:HD12	2.18	0.62
1:A:297:THR:HG23	1:A:478:ARG:NE	2.14	0.62
1:G:443:TYR:CB	1:G:544:GLN:HG2	2.30	0.62
1:E:169:THR:H	1:E:172:THR:HB	1.64	0.62
1:A:250:VAL:HG22	1:A:429:GLN:CG	2.29	0.62
1:E:371:VAL:HB	1:E:381:ILE:HD12	1.80	0.62
2:F:607:ILE:HA	2:F:610:VAL:CG2	2.30	0.62
1:C:79:GLU:OE2	1:C:79:GLU:N	2.32	0.62
1:E:106:LYS:HG3	1:E:117:ASP:OD2	2.00	0.62
2:D:592:ALA:O	2:D:593:VAL:HG13	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ARG:HD3	1:C:212:TYR:CE1	2.34	0.62
1:C:230:VAL:HG12	1:C:231:TYR:HD2	1.65	0.62
1:C:495:PHE:HB3	1:C:498:ILE:CD1	2.30	0.62
1:E:184:THR:HG21	1:E:295:SER:HB2	1.80	0.62
1:A:285:PRO:HB2	1:A:288:THR:CB	2.27	0.62
1:A:171:GLU:CD	1:A:171:GLU:N	2.50	0.62
1:C:428:GLU:HG2	1:C:430:PHE:CE1	2.34	0.62
2:H:564:LEU:HD23	2:H:564:LEU:N	2.14	0.62
1:C:354:THR:N	1:C:374:SER:HB3	2.13	0.62
1:A:228:ARG:HG2	1:A:452:MET:SD	2.39	0.62
1:C:538:GLN:HG3	1:C:542:ARG:HH11	1.65	0.62
1:C:542:ARG:NH2	1:E:532:GLU:O	2.33	0.62
1:E:169:THR:HB	1:E:172:THR:HG1	1.63	0.62
1:E:224:VAL:HB	1:E:515:THR:O	2.00	0.62
1:E:184:THR:HG21	1:E:295:SER:CB	2.29	0.62
1:G:116:VAL:HG11	1:G:522:VAL:HG11	1.81	0.62
1:A:128:CYS:HA	1:A:143:TRP:CZ3	2.34	0.62
1:E:297:THR:CG2	1:E:298:PRO:CD	2.53	0.62
1:G:127:GLU:O	1:G:194:TRP:NE1	2.32	0.62
1:A:129:PRO:HG2	1:A:163:ILE:CG2	2.24	0.62
1:E:160:LEU:HD23	1:E:160:LEU:N	2.15	0.62
1:G:435:SER:O	1:G:437:GLY:N	2.33	0.62
1:A:535:GLU:OE2	2:F:579:PRO:HG2	2.00	0.62
1:G:170:LEU:HD23	1:G:171:GLU:N	2.15	0.62
1:G:342:LEU:CD2	1:G:347:PRO:HA	2.29	0.62
1:C:297:THR:CB	1:C:298:PRO:HD3	2.30	0.61
1:A:444:LYS:HB2	1:A:450:PHE:HE2	1.65	0.61
1:E:274:MET:HE2	1:E:294:TRP:HE1	1.63	0.61
1:G:127:GLU:HG2	1:G:503:THR:CG2	2.29	0.61
1:G:210:ASN:O	1:G:213:ALA:HB3	1.99	0.61
1:G:465:TYR:CD1	1:G:466:PRO:HD2	2.35	0.61
1:C:425:PRO:CB	1:E:62:THR:HG21	2.28	0.61
1:G:90:ASP:OD2	2:H:561:VAL:HB	2.00	0.61
1:G:469:ASP:C	1:G:471:GLU:H	2.03	0.61
1:E:444:LYS:HE3	1:E:450:PHE:HE2	1.65	0.61
1:A:495:PHE:CB	1:A:498:ILE:HD11	2.30	0.61
1:E:126:ILE:HG12	1:E:147:PHE:HE2	1.64	0.61
1:E:295:SER:HA	1:E:322:SER:HA	1.83	0.61
1:E:420:VAL:HG23	1:E:421:THR:N	2.14	0.61
1:E:435:SER:HA	1:E:554:ASP:OD2	1.99	0.61
1:G:299:LEU:HD11	1:G:338:PRO:HG2	1.82	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:VAL:HG12	1:G:397:THR:N	2.15	0.61
1:C:465:TYR:CG	1:C:466:PRO:HD2	2.36	0.61
2:H:569:LEU:O	2:H:572:LEU:HB3	2.00	0.61
1:A:154:ARG:HB3	1:A:211:THR:CG2	2.27	0.61
1:C:128:CYS:SG	1:C:129:PRO:HD2	2.41	0.61
2:F:574:LYS:HG2	2:F:575:SER:H	1.64	0.61
1:G:280:ASN:N	1:G:280:ASN:ND2	2.49	0.61
1:G:116:VAL:O	1:G:513:GLU:HA	1.99	0.61
1:E:207:VAL:HB	1:E:212:TYR:HB2	1.81	0.61
1:E:177:ILE:HG22	1:E:181:ASN:HD21	1.65	0.61
1:E:253:HIS:ND1	1:E:491:ALA:HB2	2.16	0.61
1:G:107:VAL:HG11	1:G:450:PHE:CD1	2.36	0.61
1:C:299:LEU:HD23	1:C:321:PHE:CB	2.30	0.61
2:B:578:THR:HB	2:B:581:VAL:CG2	2.30	0.61
1:E:297:THR:H	1:E:478:ARG:NH2	1.99	0.61
1:C:421:THR:HG21	1:G:123:ILE:CD1	2.29	0.61
1:A:282:ILE:HD13	1:A:282:ILE:H	1.65	0.61
1:C:334:THR:HG22	1:C:356:SER:HA	1.83	0.61
1:G:411:GLU:HG3	1:G:464:HIS:ND1	2.15	0.61
2:D:595:ALA:O	2:D:596:ASN:HB2	2.00	0.61
1:A:556:ASN:C	1:A:556:ASN:ND2	2.52	0.61
1:A:276:VAL:HG22	1:A:294:TRP:HB2	1.81	0.61
1:C:185:ASN:CG	1:C:318:GLY:HA3	2.20	0.61
1:A:162:ASN:ND2	1:A:166:GLU:HB2	2.16	0.61
1:C:273:SER:CB	1:C:475:LEU:HD12	2.18	0.61
2:B:581:VAL:HG12	2:B:582:ILE:N	2.16	0.61
1:E:220:ARG:HH12	1:G:218:GLY:HA3	1.65	0.61
1:A:357:PHE:HE1	1:A:369:TYR:CD1	2.19	0.61
1:C:177:ILE:HG22	1:C:181:ASN:ND2	2.16	0.60
1:C:444:LYS:HD2	1:C:447:ASN:O	2.01	0.60
1:E:507:LYS:HE3	1:G:57:SER:HB2	1.82	0.60
1:G:284:GLN:OE1	1:G:289:VAL:HG11	2.00	0.60
1:E:299:LEU:HD12	1:E:300:PRO:CD	2.30	0.60
1:E:158:ILE:HG22	1:E:159:ALA:N	2.15	0.60
1:C:205:ILE:HD13	1:C:480:ILE:CD1	2.30	0.60
1:E:178:GLN:HA	1:E:181:ASN:HD22	1.66	0.60
1:G:136:LEU:HD12	1:G:141:LYS:HD3	1.83	0.60
1:E:90:ASP:CB	2:F:561:VAL:HB	2.31	0.60
1:C:87:LYS:C	1:C:89:MET:N	2.55	0.60
2:H:578:THR:CG2	2:H:581:VAL:H	2.09	0.60
1:C:535:GLU:CD	1:C:535:GLU:H	2.03	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:SER:CB	1:A:552:GLN:HG2	2.30	0.60
1:A:180:LEU:HA	1:A:183:ILE:HD11	1.83	0.60
1:A:424:VAL:HG12	1:A:427:TYR:HB3	1.83	0.60
1:A:243:LEU:CD1	1:A:244:ILE:HG23	2.31	0.60
2:D:560:THR:HG22	2:D:564:LEU:CD2	2.31	0.60
1:G:159:ALA:HB2	1:G:206:TYR:HE1	1.66	0.60
1:E:100:ALA:O	1:E:101:LEU:HB3	2.01	0.60
1:G:287:ASN:CA	1:G:364:ALA:HB2	2.30	0.60
1:G:217:ILE:HG23	1:G:319:LYS:NZ	2.15	0.60
1:E:154:ARG:HG3	1:E:154:ARG:HH11	1.67	0.60
1:A:329:VAL:HG12	1:A:330:ASN:H	1.66	0.60
1:C:273:SER:H	1:C:297:THR:CB	2.14	0.60
1:E:267:GLU:O	1:E:401:ASP:HA	2.02	0.60
1:E:210:ASN:HD22	1:G:524:GLN:HG3	1.64	0.60
1:E:386:THR:O	1:E:389:SER:HB3	2.00	0.60
1:C:448:PRO:HG3	1:E:449:VAL:CG1	2.31	0.60
1:G:290:ALA:CB	1:G:387:LYS:HE2	2.32	0.60
1:E:189:LEU:HD12	1:E:205:ILE:HG12	1.82	0.60
1:C:105:SER:HB2	1:C:117:ASP:CB	2.25	0.60
1:C:256:VAL:CG1	1:C:410:ILE:HG23	2.32	0.60
1:G:277:SER:N	1:G:391:VAL:HG13	2.17	0.60
1:A:455:GLU:HG3	1:E:259:GLN:CB	2.32	0.60
1:C:385:VAL:HG22	1:C:392:SER:OG	2.01	0.60
2:F:611:GLY:O	2:F:615:VAL:HG23	2.00	0.60
1:E:88:TYR:HA	1:E:231:TYR:CB	2.31	0.60
1:G:194:TRP:CE3	1:G:204:SER:HB2	2.37	0.60
1:A:180:LEU:HA	1:A:183:ILE:CD1	2.32	0.60
1:G:411:GLU:HG3	1:G:464:HIS:CE1	2.36	0.60
1:E:367:VAL:O	1:E:385:VAL:HG22	2.02	0.60
1:C:177:ILE:O	1:C:180:LEU:N	2.34	0.59
1:C:297:THR:HG22	1:C:298:PRO:N	2.18	0.59
1:E:295:SER:HB3	1:E:322:SER:CB	2.31	0.59
1:G:121:ARG:HA	1:G:508:THR:O	2.01	0.59
1:G:159:ALA:HB2	1:G:206:TYR:CE1	2.36	0.59
1:E:431:LEU:H	1:E:431:LEU:HD12	1.66	0.59
1:G:126:ILE:HG12	1:G:147:PHE:HE1	1.66	0.59
1:G:254:ILE:CG1	1:G:424:VAL:HG21	2.32	0.59
1:C:542:ARG:HD3	2:D:582:ILE:CG2	2.32	0.59
1:E:297:THR:CB	1:E:298:PRO:HD3	2.32	0.59
1:G:485:GLU:HG3	1:G:488:PHE:H	1.67	0.59
1:E:241:PRO:C	1:E:243:LEU:H	2.04	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LYS:HD3	1:C:456:GLU:HB2	1.83	0.59
1:E:297:THR:HG23	1:E:476:GLY:CA	2.27	0.59
1:G:280:ASN:N	1:G:280:ASN:HD22	1.99	0.59
1:G:257:LYS:HE2	1:G:446:ASN:HB3	1.84	0.59
2:D:561:VAL:HA	2:D:564:LEU:HD22	1.83	0.59
1:E:110:GLY:HA2	1:E:530:ALA:O	2.02	0.59
1:A:306:LEU:CD1	1:A:311:GLY:HA2	2.32	0.59
1:A:366:THR:O	1:A:367:VAL:CG2	2.50	0.59
1:E:90:ASP:HB3	2:F:562:SER:HB3	1.83	0.59
1:A:128:CYS:HB3	1:A:131:VAL:CG2	2.32	0.59
1:C:205:ILE:HD13	1:C:480:ILE:HD11	1.85	0.59
1:G:342:LEU:HD22	1:G:347:PRO:HA	1.84	0.59
1:E:342:LEU:O	1:E:343:ALA:HB2	2.02	0.59
1:A:542:ARG:HE	2:B:583:LYS:HA	1.67	0.59
1:E:229:LYS:HE3	1:E:510:ASP:OD2	2.01	0.59
1:E:297:THR:HG21	1:E:476:GLY:H	1.68	0.59
1:E:228:ARG:HB3	1:E:452:MET:HE3	1.85	0.59
1:A:445:MET:CE	1:C:113:ARG:HB2	2.32	0.59
1:E:153:PHE:HB3	1:E:482:ASP:OD2	2.03	0.59
1:E:116:VAL:HG12	1:E:514:GLY:O	2.03	0.59
1:G:329:VAL:HG12	1:G:359:MET:O	2.03	0.59
1:G:538:GLN:HG2	2:H:582:ILE:HG21	1.84	0.59
1:G:274:MET:CB	1:G:296:ILE:HG13	2.28	0.59
1:A:495:PHE:HB3	1:A:498:ILE:CD1	2.32	0.59
1:G:435:SER:C	1:G:437:GLY:H	2.06	0.59
1:A:315:ASN:HD22	1:A:316:THR:H	1.50	0.59
1:E:148:ILE:HA	1:E:492:VAL:HG12	1.85	0.59
1:E:306:LEU:HD13	1:E:311:GLY:HA2	1.84	0.59
1:G:191:THR:HG21	1:G:193:GLN:OE1	2.03	0.59
1:G:325:ILE:HD12	1:G:333:TRP:CE3	2.37	0.59
1:C:375:LEU:HD12	1:C:376:THR:H	1.66	0.59
1:C:108:PRO:HA	1:C:530:ALA:CB	2.32	0.59
1:C:160:LEU:HD22	1:C:161:ALA:N	2.17	0.59
1:C:129:PRO:HA	1:C:194:TRP:CD1	2.38	0.59
1:E:301:VAL:HA	1:E:321:PHE:HA	1.84	0.59
1:E:313:THR:CB	1:E:325:ILE:HG22	2.33	0.59
1:A:395:PRO:CB	1:C:267:GLU:HB3	2.32	0.59
1:A:265:ALA:HB2	1:A:404:ALA:N	2.18	0.59
1:C:262:THR:H	1:E:262:THR:HG21	1.68	0.59
1:G:291:ARG:C	1:G:291:ARG:HD2	2.22	0.59
1:A:422:THR:O	1:C:523:GLY:HA3	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:THR:HG22	1:G:361:THR:OG1	2.02	0.59
1:A:451:GLU:HA	1:E:448:PRO:HD3	1.85	0.58
1:C:244:ILE:HD12	1:C:501:SER:OG	2.03	0.58
1:G:460:GLY:HA2	1:G:480:ILE:O	2.03	0.58
1:A:278:ALA:HA	1:A:292:ILE:HG22	1.85	0.58
1:A:408:LEU:H	1:A:461:PHE:HA	1.67	0.58
1:G:313:THR:HB	1:G:325:ILE:HG22	1.85	0.58
1:E:265:ALA:CB	1:E:404:ALA:HB2	2.33	0.58
1:C:239:ASN:OD1	1:C:503:THR:OG1	2.21	0.58
1:E:220:ARG:NH1	1:G:215:ALA:CB	2.40	0.58
1:A:297:THR:HG23	1:A:478:ARG:NH2	2.18	0.58
1:E:207:VAL:HG11	1:E:212:TYR:CD1	2.38	0.58
1:C:244:ILE:HD12	1:C:501:SER:HG	1.68	0.58
1:E:153:PHE:HD2	1:E:154:ARG:NH1	2.00	0.58
1:E:153:PHE:HB2	1:E:227:PHE:CE2	2.38	0.58
2:F:577:ALA:HB1	2:F:582:ILE:HD11	1.85	0.58
1:A:424:VAL:O	1:A:427:TYR:CD2	2.57	0.58
1:C:84:TRP:HE1	1:C:230:VAL:HG13	1.68	0.58
2:F:578:THR:HB	2:F:581:VAL:HG23	1.85	0.58
1:G:333:TRP:O	1:G:334:THR:HB	2.04	0.58
1:C:304:VAL:CG1	1:C:305:ALA:H	2.16	0.58
1:A:422:THR:HG22	1:A:422:THR:O	2.02	0.58
1:G:485:GLU:C	1:G:487:ASN:H	2.06	0.58
1:A:226:GLN:NE2	1:A:452:MET:HG2	2.18	0.58
1:A:234:ILE:CG1	1:A:508:THR:HG23	2.19	0.58
1:C:443:TYR:CE2	1:E:113:ARG:HD2	2.38	0.58
1:E:452:MET:HE2	1:E:452:MET:HA	1.83	0.58
1:E:89:MET:HE1	1:E:540:ALA:HB1	1.85	0.58
2:F:577:ALA:CB	2:F:582:ILE:HD11	2.34	0.58
1:G:181:ASN:C	1:G:407:ARG:HH22	2.06	0.58
1:A:306:LEU:HD13	1:A:311:GLY:HA2	1.86	0.58
1:G:443:TYR:CG	1:G:544:GLN:HG2	2.38	0.58
1:A:136:LEU:HD21	1:A:501:SER:CA	2.33	0.58
1:A:112:LEU:HB3	1:A:114:TYR:O	2.03	0.58
1:A:106:LYS:HG2	1:A:117:ASP:HB3	1.84	0.58
1:C:542:ARG:HD3	2:D:582:ILE:HG22	1.85	0.58
1:E:309:GLY:HA2	1:E:331:SER:HA	1.81	0.58
1:E:168:LEU:CD1	1:E:172:THR:HG22	2.33	0.58
1:A:74:SER:O	1:A:75:ILE:HB	2.04	0.58
1:C:275:THR:CG2	1:C:478:ARG:HH12	2.13	0.58
1:E:178:GLN:NE2	1:E:390:GLY:HA2	2.19	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:160:LEU:HD12	1:G:161:ALA:N	2.19	0.58
1:G:162:ASN:OD1	1:G:166:GLU:N	2.37	0.58
1:G:475:LEU:O	1:G:476:GLY:O	2.21	0.58
1:A:144:ARG:HD2	1:A:496:TRP:HD1	1.66	0.58
1:C:246:GLN:HG3	1:G:241:PRO:CB	2.29	0.58
1:C:81:ALA:O	1:C:84:TRP:HB3	2.03	0.58
1:E:57:SER:HB3	1:G:237:GLU:OE2	2.04	0.58
1:G:297:THR:HG22	1:G:298:PRO:N	2.17	0.58
1:A:357:PHE:CE1	1:A:369:TYR:HD1	2.19	0.58
1:A:279:SER:HB3	1:A:388:GLY:HA2	1.85	0.58
1:C:360:THR:HB	1:C:368:VAL:CG1	2.34	0.58
1:E:194:TRP:CE3	1:E:194:TRP:HA	2.39	0.58
1:E:275:THR:CG2	1:E:478:ARG:HH12	2.17	0.58
1:E:470:PRO:O	1:E:473:ASN:HB2	2.04	0.58
1:E:255:PRO:HB3	1:E:445:MET:CG	2.20	0.57
1:E:389:SER:OG	1:E:390:GLY:N	2.36	0.57
1:E:304:VAL:HG21	1:E:323:VAL:CG2	2.34	0.57
1:E:313:THR:HA	1:E:325:ILE:HG22	1.86	0.57
1:E:227:PHE:C	1:E:452:MET:HE2	2.24	0.57
1:A:292:ILE:HG13	1:A:325:ILE:HD11	1.85	0.57
2:F:562:SER:O	2:F:566:SER:N	2.31	0.57
1:C:300:PRO:CG	1:C:400:ILE:HG12	2.33	0.57
1:A:164:ASN:HB2	1:A:166:GLU:HG3	1.85	0.57
1:G:257:LYS:HB3	1:G:257:LYS:NZ	2.18	0.57
1:A:456:GLU:OE1	1:E:257:LYS:HD3	2.04	0.57
1:C:149:SER:OG	1:C:232:LYS:HE2	2.03	0.57
1:A:197:PHE:CE2	1:A:201:TRP:HB3	2.39	0.57
1:A:297:THR:HB	1:A:476:GLY:HA3	1.87	0.57
1:E:238:PHE:CG	1:E:432:CYS:HB3	2.39	0.57
1:C:122:PRO:HD2	1:C:508:THR:OG1	2.03	0.57
1:G:226:GLN:HA	1:G:454:GLY:HA2	1.86	0.57
1:C:363:THR:CG2	1:C:366:THR:N	2.66	0.57
1:G:287:ASN:HA	1:G:364:ALA:CB	2.34	0.57
1:G:261:GLU:O	1:G:406:ASN:HB2	2.05	0.57
1:G:268:ARG:HG2	1:G:268:ARG:HH11	1.69	0.57
1:E:246:GLN:HE22	1:E:499:SER:HB2	1.70	0.57
1:A:206:TYR:N	1:A:206:TYR:CD1	2.72	0.57
1:E:253:HIS:HD2	1:E:549:GLY:HA3	1.59	0.57
1:G:196:GLN:HB2	1:G:202:TYR:CE2	2.40	0.57
1:A:363:THR:HB	1:A:366:THR:HG22	1.87	0.57
1:G:279:SER:HB3	1:G:291:ARG:NE	2.19	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD13	1:C:341:ILE:HD11	1.86	0.57
1:E:306:LEU:HD12	1:E:333:TRP:CE2	2.38	0.57
1:G:156:ASN:HB3	1:G:206:TYR:O	2.04	0.57
1:G:272:GLY:HA3	1:G:298:PRO:HD3	1.86	0.57
1:A:262:THR:O	1:A:264:PRO:HD3	2.05	0.57
1:E:417:THR:HG22	1:E:418:GLU:OE1	2.05	0.57
1:G:271:ALA:HA	1:G:397:THR:HA	1.86	0.57
1:G:313:THR:HB	1:G:333:TRP:NE1	2.19	0.57
1:A:185:ASN:CG	1:A:318:GLY:HA3	2.25	0.57
1:A:346:GLU:OE1	1:A:346:GLU:HA	2.04	0.57
1:A:217:ILE:HG23	1:E:467:GLY:H	1.68	0.57
1:C:136:LEU:HD12	1:C:137:PRO:O	2.05	0.57
1:C:180:LEU:HA	1:C:183:ILE:CD1	2.35	0.57
1:E:210:ASN:O	1:E:213:ALA:HB3	2.05	0.57
1:E:184:THR:HA	1:E:478:ARG:HB2	1.87	0.57
1:E:538:GLN:HA	1:E:541:ASN:HD22	1.69	0.57
1:G:235:THR:CG2	1:G:507:LYS:HB2	2.35	0.57
1:A:366:THR:HG23	1:A:367:VAL:N	2.19	0.57
1:G:443:TYR:HB3	1:G:544:GLN:HG2	1.86	0.57
1:C:238:PHE:CD2	1:C:432:CYS:HB3	2.39	0.57
1:E:238:PHE:CD1	1:E:432:CYS:HB3	2.39	0.57
1:E:475:LEU:O	1:E:476:GLY:O	2.23	0.57
2:F:575:SER:OG	2:F:581:VAL:HG11	2.04	0.57
1:G:199:PRO:HD3	1:G:388:GLY:CA	2.35	0.57
1:E:145:VAL:HG23	1:E:161:ALA:HB2	1.86	0.57
1:C:110:GLY:HA2	1:C:530:ALA:O	2.04	0.57
2:F:578:THR:O	2:F:582:ILE:HG12	2.05	0.57
1:A:306:LEU:HD23	1:A:332:VAL:O	2.05	0.57
1:G:63:MET:HG3	1:G:64:ASP:N	2.19	0.57
1:G:296:ILE:HD13	1:G:321:PHE:CD2	2.40	0.57
1:G:292:ILE:N	1:G:292:ILE:HD13	2.20	0.57
2:D:557:PHE:CD2	2:D:557:PHE:N	2.73	0.57
1:A:531:GLU:CG	2:F:583:LYS:HE3	2.30	0.57
1:A:299:LEU:HD12	1:A:300:PRO:HD2	1.87	0.57
2:F:596:ASN:HB2	2:F:597:PRO:HD2	1.86	0.57
1:G:88:TYR:HA	1:G:231:TYR:HB2	1.87	0.57
1:E:130:THR:CB	1:E:163:ILE:HG12	2.34	0.57
1:E:185:ASN:OD1	1:E:318:GLY:HA3	2.05	0.57
1:A:253:HIS:CE1	1:A:442:HIS:HA	2.40	0.56
1:C:128:CYS:HA	1:C:143:TRP:CZ3	2.40	0.56
1:C:151:PRO:CD	1:C:490:SER:HB3	2.34	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:HIS:NE2	1:E:549:GLY:HA3	2.19	0.56
1:G:162:ASN:CG	1:G:166:GLU:HB2	2.25	0.56
1:G:174:ASN:HD21	1:G:468:TYR:HA	1.66	0.56
2:F:607:ILE:HA	2:F:610:VAL:HG23	1.86	0.56
2:B:578:THR:HB	2:B:581:VAL:CB	2.34	0.56
1:E:119:GLU:OE2	1:E:509:TYR:HD2	1.87	0.56
1:G:205:ILE:CD1	1:G:480:ILE:HD11	2.35	0.56
1:A:412:MET:HG2	1:A:463:PHE:HB3	1.88	0.56
1:E:162:ASN:HA	1:E:200:GLY:O	2.04	0.56
1:A:173:ARG:O	1:A:176:PHE:HB3	2.05	0.56
1:A:242:THR:CA	1:A:245:ASP:HB2	2.29	0.56
1:C:312:GLY:HA3	1:C:326:ASP:OD1	2.05	0.56
1:C:97:SER:C	1:C:99:LYS:H	2.07	0.56
1:A:257:LYS:HD2	1:C:452:MET:O	2.05	0.56
1:E:538:GLN:HE22	2:F:582:ILE:HG13	1.71	0.56
1:A:281:ALA:O	1:A:282:ILE:C	2.43	0.56
1:A:177:ILE:O	1:A:181:ASN:ND2	2.39	0.56
1:A:299:LEU:HD22	1:A:341:ILE:HD11	1.88	0.56
1:C:363:THR:HG21	1:C:366:THR:OG1	2.05	0.56
1:G:185:ASN:HB3	1:G:318:GLY:HA3	1.86	0.56
1:G:276:VAL:HG13	1:G:294:TRP:HB2	1.86	0.56
1:G:299:LEU:HD12	1:G:300:PRO:HD2	1.87	0.56
1:A:170:LEU:O	1:A:173:ARG:N	2.39	0.56
1:E:121:ARG:HH11	1:E:121:ARG:HG3	1.70	0.56
1:A:146:SER:HB2	1:A:160:LEU:HD11	1.86	0.56
1:C:342:LEU:CD2	1:C:347:PRO:HA	2.36	0.56
1:C:282:ILE:HG13	1:C:282:ILE:O	2.04	0.56
1:C:475:LEU:HD21	1:E:267:GLU:CB	2.35	0.56
1:E:206:TYR:N	1:E:206:TYR:CD1	2.73	0.56
2:F:599:ILE:C	2:F:600:LEU:HG	2.26	0.56
1:G:534:ASP:HA	1:G:537:VAL:CB	2.34	0.56
1:E:40:GLN:OE1	1:E:70:ILE:HA	2.05	0.56
1:A:250:VAL:HG22	1:A:429:GLN:HG3	1.88	0.56
1:A:235:THR:HG23	1:A:507:LYS:HB3	1.88	0.56
1:A:107:VAL:CG1	1:A:450:PHE:HD1	2.13	0.56
1:C:407:ARG:CD	1:C:462:GLN:HB2	2.36	0.56
1:E:253:HIS:CD2	1:E:549:GLY:CA	2.84	0.56
1:E:107:VAL:HG11	1:E:450:PHE:CD1	2.40	0.56
1:A:274:MET:HB3	1:A:394:THR:HB	1.87	0.56
1:E:163:ILE:HD11	1:E:202:TYR:CE1	2.40	0.56
1:E:163:ILE:HD11	1:E:202:TYR:CD1	2.41	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:LEU:HD12	1:A:543:LEU:HG	1.87	0.56
1:C:145:VAL:HG13	1:C:145:VAL:O	2.06	0.56
1:G:258:PRO:HB3	1:G:410:ILE:CG1	2.36	0.56
1:C:292:ILE:H	1:C:292:ILE:HD13	1.71	0.56
1:E:302:ALA:HB2	1:E:338:PRO:CG	2.35	0.56
1:A:165:ASN:O	1:A:165:ASN:ND2	2.38	0.56
1:A:217:ILE:HG12	1:E:466:PRO:HA	1.88	0.56
2:D:567:ILE:HG23	2:D:568:GLY:H	1.71	0.56
1:C:349:ALA:HB2	1:C:373:SER:OG	2.06	0.56
1:C:273:SER:HA	1:C:396:VAL:HG23	1.88	0.56
1:A:444:LYS:CB	1:A:450:PHE:HE2	2.18	0.56
1:A:535:GLU:CD	2:F:579:PRO:HG2	2.26	0.56
1:E:518:ALA:C	1:E:520:SER:N	2.59	0.56
1:G:131:VAL:O	1:G:132:SER:OG	2.23	0.56
1:G:244:ILE:O	1:G:244:ILE:HG22	2.05	0.56
1:A:380:VAL:CG1	1:A:381:ILE:H	2.15	0.56
1:E:126:ILE:HD12	1:E:126:ILE:N	2.21	0.56
1:A:91:PRO:CG	1:A:233:GLY:HA3	2.36	0.56
1:C:122:PRO:HG3	1:C:209:PRO:HD2	1.87	0.56
1:G:169:THR:HG22	1:G:172:THR:H	1.71	0.56
1:A:126:ILE:O	1:A:126:ILE:HG22	2.06	0.56
1:G:369:TYR:CE1	1:G:383:ARG:HB3	2.41	0.56
1:G:425:PRO:HG2	1:G:426:LYS:H	1.71	0.56
1:C:453:THR:HG21	1:C:485:GLU:HA	1.88	0.56
1:C:142:LEU:O	1:C:500:GLN:OE1	2.23	0.56
1:C:547:LEU:O	1:E:113:ARG:HG2	2.06	0.56
1:A:449:VAL:HG11	1:E:448:PRO:HB2	1.88	0.56
1:E:154:ARG:N	1:E:482:ASP:OD1	2.37	0.56
2:F:567:ILE:HD11	2:F:571:LEU:HD21	1.86	0.56
1:C:250:VAL:O	1:C:250:VAL:HG13	2.04	0.56
1:A:75:ILE:HD12	2:B:577:ALA:HB2	1.88	0.55
1:E:272:GLY:O	1:E:475:LEU:HD12	2.06	0.55
1:G:207:VAL:HG12	1:G:208:LEU:H	1.70	0.55
1:G:122:PRO:HB3	1:G:209:PRO:HG3	1.87	0.55
1:A:289:VAL:HG12	1:A:290:ALA:H	1.70	0.55
1:A:342:LEU:O	1:A:396:VAL:HG13	2.06	0.55
1:E:93:GLY:O	1:E:97:SER:N	2.38	0.55
1:G:262:THR:O	1:G:264:PRO:HD3	2.06	0.55
1:G:257:LYS:HZ2	1:G:257:LYS:HB3	1.71	0.55
1:E:152:ALA:O	1:E:229:LYS:NZ	2.35	0.55
1:E:295:SER:HB3	1:E:322:SER:HB2	1.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ASP:N	1:G:117:ASP:OD2	2.39	0.55
1:A:279:SER:HA	1:A:387:LYS:HG2	1.88	0.55
1:E:435:SER:C	1:E:437:GLY:N	2.59	0.55
1:G:373:SER:C	1:G:375:LEU:H	2.08	0.55
1:A:537:VAL:HG23	1:A:538:GLN:N	2.20	0.55
1:C:121:ARG:HA	1:C:508:THR:O	2.06	0.55
1:C:495:PHE:HB3	1:C:498:ILE:HD11	1.88	0.55
1:C:440:ILE:HA	1:C:549:GLY:O	2.05	0.55
1:G:142:LEU:N	1:G:142:LEU:HD23	2.21	0.55
1:E:220:ARG:CD	1:G:215:ALA:CB	2.77	0.55
1:G:313:THR:CB	1:G:325:ILE:HG22	2.36	0.55
1:A:465:TYR:CD1	1:A:466:PRO:HD2	2.41	0.55
1:E:410:ILE:O	1:E:463:PHE:HA	2.07	0.55
1:A:451:GLU:OE1	1:E:451:GLU:OE1	2.24	0.55
1:G:189:LEU:CD2	1:G:189:LEU:N	2.70	0.55
1:G:206:TYR:N	1:G:206:TYR:CD1	2.74	0.55
1:A:292:ILE:HG13	1:A:325:ILE:CD1	2.35	0.55
1:C:329:VAL:HG12	1:C:362:ILE:HB	1.88	0.55
1:G:288:THR:C	1:G:362:ILE:HD11	2.27	0.55
1:G:301:VAL:HG12	1:G:319:LYS:O	2.07	0.55
1:C:304:VAL:CG1	1:C:305:ALA:N	2.69	0.55
1:C:475:LEU:CG	1:E:267:GLU:OE2	2.54	0.55
1:C:136:LEU:HD11	1:C:138:LEU:HD23	1.87	0.55
1:C:485:GLU:O	1:C:486:ASN:C	2.44	0.55
1:C:546:GLU:CG	2:D:590:VAL:HG21	2.37	0.55
1:E:210:ASN:HD22	1:G:524:GLN:CD	2.10	0.55
1:C:435:SER:HB2	1:C:552:GLN:HG2	1.87	0.55
1:A:444:LYS:HB2	1:A:450:PHE:CE2	2.42	0.55
1:A:87:LYS:HZ3	1:A:95:VAL:CG2	2.20	0.55
1:E:452:MET:CE	1:E:452:MET:HA	2.36	0.55
1:E:183:ILE:O	1:E:478:ARG:HB2	2.07	0.55
2:F:572:LEU:HD11	2:F:577:ALA:HB2	1.89	0.55
1:C:319:LYS:HG3	1:C:320:PHE:CE1	2.42	0.55
1:A:302:ALA:HB3	1:A:321:PHE:CD1	2.41	0.55
2:B:567:ILE:O	2:B:571:LEU:HG	2.07	0.55
1:G:230:VAL:HG23	1:G:512:TRP:CA	2.37	0.55
1:E:130:THR:HG22	1:E:132:SER:H	1.72	0.55
1:C:313:THR:CA	1:C:325:ILE:HG22	2.31	0.55
2:H:562:SER:HA	2:H:565:ALA:HB3	1.87	0.55
1:G:259:GLN:O	1:G:409:SER:HB3	2.07	0.55
1:E:149:SER:HG	1:E:442:HIS:CE1	2.25	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ILE:HG22	1:C:181:ASN:HD21	1.71	0.55
1:E:228:ARG:HG2	1:E:452:MET:HE1	1.89	0.55
1:E:273:SER:OG	1:E:475:LEU:HG	2.05	0.55
1:G:248:TRP:NE1	1:G:429:GLN:HG2	2.13	0.55
1:A:107:VAL:HG12	1:A:109:ASP:OD1	2.07	0.55
1:A:297:THR:HG21	1:A:476:GLY:N	2.21	0.55
1:G:533:GLU:OE1	1:G:533:GLU:HA	2.07	0.55
1:A:139:ASP:HB3	1:A:141:LYS:HG3	1.89	0.55
1:E:337:ALA:O	1:E:351:GLU:O	2.25	0.55
1:G:228:ARG:HG3	1:G:228:ARG:O	2.06	0.55
1:C:290:ALA:HB2	1:C:387:LYS:NZ	2.12	0.55
1:A:95:VAL:HG21	1:A:509:TYR:CE2	2.42	0.54
1:A:400:ILE:CG1	1:A:401:ASP:H	2.08	0.54
1:C:385:VAL:HG22	1:C:392:SER:CB	2.37	0.54
1:C:86:TYR:OH	2:D:566:SER:HA	2.07	0.54
1:C:207:VAL:CG1	1:C:208:LEU:N	2.69	0.54
1:A:111:LEU:HD22	1:E:448:PRO:HG3	1.89	0.54
1:C:279:SER:HA	1:C:387:LYS:HB2	1.89	0.54
1:A:137:PRO:O	1:A:137:PRO:HG2	2.07	0.54
1:C:423:ASN:OD1	1:E:520:SER:HB2	2.08	0.54
1:C:443:TYR:HD2	1:E:113:ARG:NH1	2.06	0.54
1:E:227:PHE:HD1	1:E:228:ARG:N	2.06	0.54
1:G:205:ILE:HD13	1:G:480:ILE:CD1	2.38	0.54
1:E:552:GLN:C	1:E:554:ASP:H	2.10	0.54
1:G:109:ASP:HA	1:G:532:GLU:HA	1.89	0.54
1:G:125:THR:O	1:G:126:ILE:C	2.46	0.54
1:A:451:GLU:OE1	1:C:451:GLU:OE2	2.26	0.54
1:E:186:TRP:CD1	1:E:481:VAL:HG23	2.42	0.54
1:A:363:THR:HG22	1:A:365:ASP:N	2.13	0.54
1:G:82:VAL:O	1:G:83:GLY:C	2.44	0.54
1:C:131:VAL:CG1	1:C:132:SER:N	2.71	0.54
1:C:495:PHE:CD2	1:C:498:ILE:HD11	2.42	0.54
1:C:546:GLU:HG3	2:D:590:VAL:HG21	1.89	0.54
1:A:385:VAL:CG2	1:A:392:SER:HB2	2.34	0.54
1:G:107:VAL:HG23	1:G:230:VAL:HG13	1.88	0.54
1:G:88:TYR:HA	1:G:231:TYR:HB3	1.89	0.54
1:G:86:TYR:HB3	1:G:94:ALA:HB1	1.89	0.54
1:E:169:THR:N	1:E:172:THR:HB	2.22	0.54
1:G:125:THR:HG23	1:G:505:VAL:HG22	1.89	0.54
1:C:250:VAL:HA	1:C:429:GLN:HA	1.89	0.54
2:H:560:THR:O	2:H:563:ALA:HB3	2.07	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:VAL:HG11	1:C:494:HIS:NE2	2.21	0.54
1:A:86:TYR:O	1:A:90:ASP:N	2.27	0.54
1:C:499:SER:O	1:C:500:GLN:C	2.45	0.54
1:E:443:TYR:O	1:E:445:MET:N	2.41	0.54
2:F:575:SER:OG	2:F:585:ILE:HD11	2.07	0.54
1:A:325:ILE:O	1:A:325:ILE:HD12	2.07	0.54
1:E:261:GLU:OE1	1:E:409:SER:HB2	2.08	0.54
1:E:214:MET:HA	1:E:221:THR:HG21	1.88	0.54
1:A:329:VAL:HG12	1:A:330:ASN:N	2.22	0.54
1:C:97:SER:O	1:C:99:LYS:N	2.41	0.54
1:E:225:THR:CG2	1:E:517:ASN:HB2	2.36	0.54
1:E:297:THR:CA	1:E:478:ARG:HH21	2.21	0.54
1:G:458:PHE:CD1	1:G:458:PHE:C	2.81	0.54
1:G:550:VAL:O	1:G:551:TYR:CD2	2.61	0.54
1:G:68:HIS:O	1:G:78:SER:HA	2.08	0.54
1:G:267:GLU:O	1:G:268:ARG:C	2.44	0.54
1:A:293:VAL:HG22	1:A:324:GLU:CB	2.38	0.54
1:E:354:THR:N	1:E:374:SER:OG	2.27	0.54
1:A:75:ILE:O	1:A:75:ILE:HG22	2.06	0.54
1:C:189:LEU:HD11	1:C:203:TYR:OH	2.08	0.54
1:C:236:PHE:HD2	1:C:506:CYS:HG	1.53	0.54
1:E:175:THR:O	1:E:178:GLN:HG3	2.08	0.54
1:A:363:THR:HB	1:A:366:THR:N	2.22	0.54
1:E:121:ARG:NH1	1:E:121:ARG:HG3	2.23	0.54
1:E:190:GLY:C	1:E:192:GLY:H	2.10	0.54
1:A:426:LYS:HD2	1:C:113:ARG:O	2.08	0.54
1:C:256:VAL:HG11	1:C:410:ILE:HG23	1.90	0.54
1:E:295:SER:O	1:E:296:ILE:HG13	2.08	0.54
1:E:518:ALA:O	1:E:520:SER:N	2.41	0.54
1:E:536:VAL:O	1:E:539:LEU:N	2.40	0.54
1:E:210:ASN:HD22	1:G:524:GLN:CG	2.20	0.54
1:A:295:SER:HB3	1:A:322:SER:CB	2.38	0.54
1:G:296:ILE:H	1:G:321:PHE:HD2	1.54	0.54
1:E:181:ASN:OD1	1:E:463:PHE:N	2.40	0.54
2:F:577:ALA:CA	2:F:582:ILE:HD11	2.38	0.54
1:G:168:LEU:HD22	1:G:173:ARG:CG	2.23	0.54
1:G:238:PHE:CD2	1:G:432:CYS:HB3	2.43	0.54
1:A:306:LEU:HD11	1:A:310:THR:O	2.09	0.54
1:G:444:LYS:CG	1:G:447:ASN:O	2.56	0.54
2:D:594:GLN:HA	1:E:42:THR:O	2.08	0.54
1:A:92:ALA:HB3	1:A:556:ASN:HB2	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLN:C	1:C:122:PRO:HD3	2.28	0.53
1:C:145:VAL:HG13	1:C:495:PHE:HB2	1.90	0.53
1:G:272:GLY:HA3	1:G:298:PRO:CD	2.38	0.53
1:A:404:ALA:CB	1:E:261:GLU:OE2	2.47	0.53
1:A:169:THR:N	1:A:172:THR:OG1	2.41	0.53
1:E:187:ARG:HG3	1:E:212:TYR:CE1	2.43	0.53
1:C:336:THR:HG22	1:C:352:GLY:O	2.09	0.53
1:A:84:TRP:CD1	1:A:230:VAL:HG13	2.43	0.53
1:C:128:CYS:HB3	1:C:131:VAL:CG2	2.37	0.53
1:G:207:VAL:HG12	1:G:208:LEU:N	2.23	0.53
1:A:403:GLU:HB3	1:A:405:VAL:HG23	1.90	0.53
1:C:295:SER:HB3	1:C:322:SER:CB	2.37	0.53
1:A:401:ASP:N	1:A:401:ASP:OD2	2.40	0.53
1:G:83:GLY:HA2	1:G:101:LEU:H	1.73	0.53
1:A:259:GLN:OE1	1:C:456:GLU:O	2.27	0.53
1:C:108:PRO:HA	1:C:530:ALA:HB1	1.90	0.53
1:C:128:CYS:HB3	1:C:131:VAL:HG21	1.88	0.53
2:D:580:SER:HB2	1:E:535:GLU:OE1	2.08	0.53
1:E:296:ILE:HD12	1:E:321:PHE:CE2	2.43	0.53
2:D:580:SER:N	1:E:535:GLU:OE1	2.41	0.53
1:E:537:VAL:O	1:E:540:ALA:HB3	2.09	0.53
1:A:178:GLN:HE22	1:A:391:VAL:N	2.06	0.53
1:A:363:THR:CB	1:A:366:THR:HG22	2.38	0.53
1:G:109:ASP:O	1:G:111:LEU:N	2.41	0.53
2:F:605:LYS:HG3	2:F:610:VAL:HG22	1.89	0.53
1:C:139:ASP:OD1	1:C:141:LYS:HG3	2.09	0.53
1:C:144:ARG:CZ	1:C:496:TRP:HZ2	2.22	0.53
1:E:116:VAL:HG21	1:E:522:VAL:HG12	1.88	0.53
1:E:394:THR:O	1:E:395:PRO:C	2.46	0.53
1:E:228:ARG:HE	1:E:452:MET:HE3	1.72	0.53
1:G:160:LEU:HD11	1:G:201:TRP:CE3	2.43	0.53
1:G:461:PHE:HE1	1:G:480:ILE:HB	1.73	0.53
1:A:281:ALA:CB	1:A:291:ARG:HB2	2.33	0.53
1:G:442:HIS:O	1:G:443:TYR:HB3	2.06	0.53
1:E:69:GLU:CA	1:E:78:SER:HA	2.31	0.53
1:G:296:ILE:HD13	1:G:321:PHE:CE2	2.43	0.53
1:E:139:ASP:C	1:E:141:LYS:H	2.08	0.53
1:E:348:PHE:CD1	1:E:373:SER:HB2	2.42	0.53
1:E:428:GLU:OE1	1:E:548:THR:HG21	2.08	0.53
1:C:276:VAL:HG11	1:C:369:TYR:CD2	2.44	0.53
1:E:256:VAL:CG1	1:E:410:ILE:HG23	2.37	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:GLN:NE2	2:F:582:ILE:HG13	2.23	0.53
1:E:220:ARG:NH1	1:G:221:THR:OG1	2.41	0.53
1:A:371:VAL:N	1:A:381:ILE:HG22	2.17	0.53
1:G:93:GLY:O	1:G:97:SER:CB	2.56	0.53
1:E:370:SER:HA	1:E:381:ILE:O	2.08	0.53
1:C:97:SER:C	1:C:99:LYS:N	2.61	0.53
1:C:284:GLN:OE1	1:C:289:VAL:HG11	2.09	0.53
2:F:593:VAL:HG12	2:F:594:GLN:N	2.23	0.53
1:E:304:VAL:HG12	1:E:333:TRP:HB3	1.90	0.53
1:G:176:PHE:HB2	1:G:197:PHE:CE1	2.44	0.53
1:A:369:TYR:HE2	1:A:383:ARG:HB3	1.73	0.53
1:C:295:SER:HB3	1:C:322:SER:HB2	1.89	0.53
2:F:599:ILE:O	2:F:600:LEU:CG	2.47	0.53
1:E:54:VAL:HG12	1:E:55:ALA:O	2.09	0.53
1:A:556:ASN:C	1:A:556:ASN:HD22	2.10	0.53
1:C:297:THR:HG22	1:C:298:PRO:HG3	1.90	0.53
1:C:215:ALA:CB	1:C:218:GLY:HA2	2.33	0.53
1:A:460:GLY:HA2	1:A:481:VAL:HA	1.90	0.53
1:E:252:ALA:HB2	1:E:427:TYR:CB	2.38	0.53
1:C:292:ILE:HD11	1:C:325:ILE:CD1	2.37	0.53
1:C:265:ALA:HB2	1:C:404:ALA:H	1.74	0.53
1:G:90:ASP:HB3	2:H:562:SER:OG	2.08	0.53
1:C:413:PRO:O	1:C:414:ALA:C	2.47	0.53
1:G:254:ILE:HD11	1:G:424:VAL:HG21	1.90	0.53
1:E:353:ASP:OD1	1:E:375:LEU:HB2	2.09	0.53
1:E:556:ASN:O	1:E:556:ASN:CG	2.46	0.53
1:C:195:ALA:HB3	1:C:203:TYR:CE2	2.43	0.53
1:C:363:THR:HG23	1:C:366:THR:H	1.72	0.53
1:G:81:ALA:O	1:G:84:TRP:HB3	2.09	0.53
1:A:169:THR:HG22	1:A:172:THR:OG1	2.09	0.53
1:G:477:LEU:HG	1:G:477:LEU:O	2.09	0.53
1:E:130:THR:HB	1:E:163:ILE:CG1	2.38	0.53
1:A:249:TRP:CD2	1:A:438:ALA:HB2	2.44	0.53
1:E:348:PHE:CD2	1:E:381:ILE:HD11	2.43	0.53
1:E:235:THR:HG1	1:E:439:TYR:HD1	1.56	0.53
1:A:350:GLU:C	1:A:352:GLY:H	2.12	0.53
1:C:162:ASN:HA	1:C:200:GLY:O	2.09	0.53
1:E:194:TRP:HZ3	1:E:204:SER:N	2.06	0.53
1:A:269:PHE:CD1	1:A:399:GLY:HA2	2.44	0.53
1:G:262:THR:HA	1:G:406:ASN:HA	1.91	0.53
2:H:576:SER:O	2:H:577:ALA:C	2.46	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLN:HE22	1:A:211:THR:H	1.55	0.53
1:A:464:HIS:CE1	1:C:455:GLU:OE2	2.62	0.53
1:A:539:LEU:HD12	1:A:539:LEU:C	2.29	0.53
1:E:256:VAL:HG11	1:E:410:ILE:HG23	1.90	0.53
1:G:170:LEU:HA	1:G:173:ARG:HD3	1.91	0.53
1:G:194:TRP:HE3	1:G:194:TRP:HA	1.73	0.53
1:A:297:THR:OG1	1:A:298:PRO:CD	2.56	0.53
1:C:87:LYS:NZ	1:C:95:VAL:HG23	2.23	0.53
2:D:574:LYS:HD2	2:D:574:LYS:N	2.23	0.53
1:A:267:GLU:HA	1:A:267:GLU:OE1	2.08	0.52
1:A:542:ARG:HH21	2:B:583:LYS:HB2	1.73	0.52
1:A:83:GLY:O	1:A:87:LYS:HG2	2.09	0.52
1:C:424:VAL:O	1:C:427:TYR:HD2	1.91	0.52
1:C:443:TYR:O	1:C:445:MET:N	2.42	0.52
1:C:461:PHE:HB2	1:C:480:ILE:HB	1.90	0.52
2:F:578:THR:O	2:F:579:PRO:C	2.44	0.52
1:G:254:ILE:HG12	1:G:424:VAL:HG21	1.90	0.52
1:G:142:LEU:HG	1:G:165:ASN:HD21	1.73	0.52
1:A:470:PRO:HA	1:A:473:ASN:OD1	2.09	0.52
1:G:286:SER:O	1:G:387:LYS:NZ	2.42	0.52
1:C:93:GLY:O	1:C:97:SER:N	2.37	0.52
1:A:91:PRO:HG2	1:A:233:GLY:HA3	1.92	0.52
1:E:253:HIS:HA	1:E:491:ALA:CB	2.40	0.52
1:G:92:ALA:HB3	1:G:556:ASN:HB2	1.91	0.52
1:E:169:THR:CG2	1:E:170:LEU:N	2.72	0.52
1:C:93:GLY:O	1:C:97:SER:HB3	2.09	0.52
1:A:97:SER:HB3	1:A:99:LYS:HE2	1.91	0.52
1:A:152:ALA:CB	1:A:155:LEU:HB3	2.39	0.52
1:C:144:ARG:HH12	1:C:168:LEU:HB2	1.74	0.52
1:G:154:ARG:HA	1:G:211:THR:CG2	2.39	0.52
1:A:282:ILE:O	1:A:283:PHE:HB2	2.09	0.52
1:E:44:LEU:HD11	1:E:63:MET:HE3	1.90	0.52
1:E:40:GLN:O	1:E:41:ALA:HB2	2.09	0.52
1:G:216:GLU:O	1:G:217:ILE:HG22	2.09	0.52
1:E:147:PHE:CD2	1:E:159:ALA:HB2	2.44	0.52
1:C:342:LEU:HD22	1:C:347:PRO:HA	1.91	0.52
1:A:153:PHE:CE2	1:A:211:THR:HG23	2.45	0.52
1:C:461:PHE:HB3	1:C:463:PHE:CZ	2.45	0.52
1:G:162:ASN:OD1	1:G:165:ASN:N	2.43	0.52
1:G:334:THR:OG1	1:G:335:PHE:N	2.43	0.52
1:C:412:MET:CE	1:C:415:LEU:HD21	2.39	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:VAL:HG22	1:E:358:SER:HB2	1.91	0.52
1:C:92:ALA:O	1:C:96:GLU:HB2	2.10	0.52
1:C:175:THR:O	1:C:178:GLN:HG3	2.08	0.52
1:C:236:PHE:CE1	1:C:493:VAL:HG21	2.44	0.52
1:C:276:VAL:H	1:C:391:VAL:HG13	1.74	0.52
1:G:287:ASN:HA	1:G:364:ALA:CA	2.39	0.52
1:G:366:THR:HG22	1:G:386:THR:CG2	2.39	0.52
1:G:430:PHE:CE2	1:G:552:GLN:HG2	2.45	0.52
1:G:89:MET:SD	1:G:543:LEU:HD23	2.50	0.52
1:A:144:ARG:N	1:A:165:ASN:HA	2.25	0.52
1:A:553:ALA:C	1:A:555:ASP:H	2.13	0.52
1:C:375:LEU:HB3	1:C:378:SER:CB	2.39	0.52
2:H:563:ALA:O	2:H:566:SER:HB2	2.10	0.52
1:C:522:VAL:O	1:C:524:GLN:N	2.42	0.52
1:G:504:ILE:HG22	1:G:506:CYS:SG	2.49	0.52
1:A:433:LYS:HG3	1:A:434:GLU:N	2.25	0.52
1:A:537:VAL:O	1:A:540:ALA:HB3	2.10	0.52
1:C:163:ILE:HG13	1:C:164:ASN:N	2.25	0.52
1:C:538:GLN:HE21	2:D:579:PRO:HB3	1.75	0.52
1:E:194:TRP:CE3	1:E:204:SER:HB2	2.44	0.52
1:E:359:MET:HA	1:E:369:TYR:HA	1.90	0.52
1:A:113:ARG:N	1:E:443:TYR:OH	2.42	0.52
1:G:280:ASN:OD1	1:G:286:SER:HB2	2.09	0.52
1:G:86:TYR:CD1	1:G:99:LYS:HB3	2.45	0.52
1:C:292:ILE:HD13	1:C:325:ILE:HG13	1.91	0.52
1:E:297:THR:HG22	1:E:298:PRO:N	2.15	0.52
1:E:272:GLY:HA3	1:E:298:PRO:CD	2.39	0.52
1:G:301:VAL:HG12	1:G:319:LYS:C	2.30	0.52
1:A:419:GLU:HB3	1:A:423:ASN:HD22	1.71	0.52
2:F:605:LYS:HG2	2:F:610:VAL:CG2	2.40	0.52
2:F:613:ARG:HD2	3:R:3:U:O2	2.09	0.52
1:E:363:THR:HB	1:E:366:THR:H	1.75	0.52
1:E:278:ALA:C	1:E:387:LYS:HA	2.30	0.52
1:E:485:GLU:O	1:E:485:GLU:HG3	2.10	0.52
1:G:179:THR:O	1:G:180:LEU:C	2.48	0.52
1:G:297:THR:CB	1:G:298:PRO:HD3	2.40	0.52
2:F:564:LEU:C	2:F:564:LEU:CD2	2.78	0.52
1:A:340:SER:HA	1:A:349:ALA:O	2.09	0.52
1:A:552:GLN:HB2	1:A:555:ASP:OD2	2.10	0.52
1:G:485:GLU:CD	1:G:487:ASN:HB2	2.30	0.52
1:A:146:SER:O	1:A:160:LEU:HD12	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:360:THR:HG22	1:G:361:THR:N	2.25	0.52
1:C:93:GLY:O	1:C:97:SER:CB	2.57	0.52
1:C:144:ARG:NH1	1:C:168:LEU:HB2	2.25	0.52
1:C:545:MET:HE1	1:C:546:GLU:CA	2.37	0.52
1:E:313:THR:HB	1:E:333:TRP:CD1	2.45	0.52
1:A:297:THR:CB	1:A:298:PRO:CD	2.88	0.52
1:C:285:PRO:HB2	1:C:288:THR:HB	1.91	0.52
1:G:278:ALA:CB	1:G:387:LYS:HA	2.35	0.52
1:A:188:ASP:C	1:A:189:LEU:HD12	2.31	0.52
1:G:373:SER:HB2	1:G:378:SER:OG	2.10	0.52
1:G:74:SER:O	1:G:75:ILE:CG2	2.58	0.52
2:F:618:ILE:HG23	2:F:619:LYS:HG3	1.92	0.52
1:C:440:ILE:HD12	1:C:491:ALA:HB3	1.92	0.51
1:E:444:LYS:HD3	1:E:448:PRO:O	2.10	0.51
1:A:181:ASN:H	1:A:181:ASN:HD22	1.58	0.51
1:A:295:SER:HB3	1:A:322:SER:HB2	1.91	0.51
1:A:365:ASP:O	1:A:387:LYS:HB3	2.10	0.51
1:E:98:GLY:O	1:G:63:MET:HE3	2.10	0.51
2:H:584:GLY:O	2:H:588:GLN:HG3	2.10	0.51
1:G:76:ASP:OD1	1:G:76:ASP:N	2.43	0.51
1:C:126:ILE:HG22	1:C:126:ILE:O	2.09	0.51
1:A:257:LYS:HG3	1:C:226:GLN:NE2	2.25	0.51
1:C:291:ARG:HG2	1:C:291:ARG:HH11	1.75	0.51
1:E:106:LYS:HG3	1:E:117:ASP:CG	2.31	0.51
1:C:339:ALA:HB3	1:C:400:ILE:CD1	2.38	0.51
1:C:332:VAL:HG22	1:C:358:SER:CB	2.37	0.51
1:G:453:THR:HG22	1:G:486:ASN:HD22	1.75	0.51
2:H:561:VAL:O	2:H:564:LEU:HG	2.10	0.51
1:C:146:SER:HB3	1:C:494:HIS:CE1	2.44	0.51
1:A:293:VAL:HG22	1:A:324:GLU:HB2	1.91	0.51
1:A:87:LYS:NZ	1:A:95:VAL:HG23	2.26	0.51
1:C:145:VAL:HA	1:C:160:LEU:O	2.10	0.51
1:C:181:ASN:OD1	1:C:463:PHE:O	2.27	0.51
1:C:255:PRO:HB3	1:C:445:MET:SD	2.50	0.51
1:E:544:GLN:HA	1:E:544:GLN:OE1	2.09	0.51
1:A:276:VAL:HG22	1:A:294:TRP:CG	2.44	0.51
1:G:284:GLN:O	1:G:286:SER:N	2.43	0.51
1:G:87:LYS:NZ	1:G:95:VAL:CG1	2.74	0.51
1:A:144:ARG:H	1:A:165:ASN:HA	1.75	0.51
1:G:412:MET:HB2	1:G:463:PHE:HB3	1.91	0.51
1:C:475:LEU:CG	1:E:267:GLU:HB2	2.37	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:PRO:C	1:C:139:ASP:H	2.14	0.51
1:E:150:PHE:O	1:E:152:ALA:N	2.40	0.51
1:E:95:VAL:HG13	1:G:63:MET:HB3	1.92	0.51
1:E:554:ASP:HA	1:G:56:PRO:HG3	1.92	0.51
1:G:542:ARG:NH1	2:H:583:LYS:HB2	2.26	0.51
1:A:461:PHE:CD1	1:A:480:ILE:O	2.64	0.51
1:G:270:SER:CB	1:G:402:THR:HG1	2.23	0.51
1:G:126:ILE:CD1	1:G:126:ILE:H	2.22	0.51
1:E:158:ILE:CG2	1:E:159:ALA:N	2.72	0.51
1:E:396:VAL:HG13	1:E:397:THR:N	2.25	0.51
2:F:617:SER:O	2:F:618:ILE:C	2.49	0.51
1:C:141:LYS:HG2	1:G:136:LEU:HB3	1.93	0.51
1:E:173:ARG:O	1:E:177:ILE:HG13	2.10	0.51
1:E:210:ASN:HA	1:E:213:ALA:HB3	1.92	0.51
1:G:192:GLY:HA2	1:G:205:ILE:O	2.11	0.51
1:A:289:VAL:HG12	1:A:290:ALA:N	2.26	0.51
1:G:250:VAL:O	1:G:493:VAL:HA	2.11	0.51
1:A:422:THR:HG21	1:C:520:SER:HA	1.93	0.51
2:F:605:LYS:NZ	2:F:610:VAL:HG13	2.26	0.51
1:A:121:ARG:HA	1:A:508:THR:O	2.11	0.51
1:A:268:ARG:H	1:E:395:PRO:HB3	1.74	0.51
1:E:107:VAL:CG2	1:E:230:VAL:HG13	2.41	0.51
1:G:272:GLY:C	1:G:475:LEU:HD12	2.30	0.51
1:A:375:LEU:HB3	1:A:378:SER:CB	2.34	0.51
1:E:555:ASP:O	1:E:556:ASN:C	2.48	0.51
1:E:154:ARG:NH1	1:E:154:ARG:HG3	2.26	0.51
1:E:369:TYR:O	1:E:382:VAL:HA	2.11	0.51
1:C:447:ASN:CG	1:E:451:GLU:HG2	2.31	0.51
1:G:523:GLY:O	1:G:526:ALA:HB3	2.10	0.51
1:A:277:SER:HB3	1:A:391:VAL:HG12	1.93	0.51
1:A:263:ILE:HG22	1:A:263:ILE:O	2.11	0.51
1:A:262:THR:OG1	1:E:262:THR:HG22	2.11	0.51
1:E:132:SER:HB2	1:E:141:LYS:NZ	2.25	0.51
1:E:169:THR:H	1:E:172:THR:CB	2.24	0.51
1:G:72:ALA:HB3	1:G:75:ILE:O	2.10	0.51
1:G:330:ASN:OD1	1:G:330:ASN:N	2.43	0.51
1:A:113:ARG:HG2	1:E:547:LEU:O	2.11	0.51
2:B:578:THR:CB	2:B:581:VAL:HG23	2.40	0.51
1:G:191:THR:CG2	1:G:193:GLN:OE1	2.59	0.51
1:C:395:PRO:HB3	1:E:267:GLU:CG	2.40	0.51
2:B:578:THR:HB	2:B:581:VAL:HB	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:PHE:O	1:C:179:THR:HB	2.11	0.51
1:E:256:VAL:HG11	1:E:410:ILE:HG22	1.92	0.51
1:E:466:PRO:C	1:E:468:TYR:H	2.14	0.51
1:G:258:PRO:CB	1:G:410:ILE:HG12	2.39	0.51
1:C:365:ASP:O	1:C:386:THR:HG23	2.11	0.51
1:G:281:ALA:CB	1:G:284:GLN:HG3	2.27	0.51
1:C:149:SER:HA	1:C:157:PHE:HB3	1.91	0.51
2:D:572:LEU:HA	2:D:575:SER:OG	2.11	0.51
1:E:286:SER:HB3	1:E:364:ALA:O	2.11	0.51
1:E:416:THR:O	1:E:418:GLU:N	2.44	0.51
1:E:418:GLU:HA	1:E:421:THR:HG21	1.92	0.51
1:E:55:ALA:HB1	1:E:56:PRO:CD	2.35	0.51
1:E:314:ASN:N	1:E:324:GLU:O	2.43	0.51
1:E:380:VAL:HG12	1:E:381:ILE:N	2.26	0.51
1:C:354:THR:H	1:C:374:SER:CB	2.24	0.51
1:G:417:THR:O	1:G:421:THR:HG23	2.10	0.51
1:A:485:GLU:C	1:A:487:ASN:H	2.14	0.50
1:A:537:VAL:CG2	1:A:538:GLN:N	2.75	0.50
1:C:241:PRO:HG2	1:C:244:ILE:HG13	1.93	0.50
1:G:117:ASP:O	1:G:118:ALA:HB2	2.10	0.50
1:G:122:PRO:O	1:G:508:THR:HG23	2.10	0.50
1:G:203:TYR:C	1:G:203:TYR:CD1	2.83	0.50
1:G:226:GLN:O	1:G:227:PHE:HB3	2.10	0.50
2:F:567:ILE:CD1	2:F:571:LEU:HD21	2.41	0.50
1:G:151:PRO:CB	1:G:488:PHE:HB2	2.41	0.50
1:E:156:ASN:HB3	1:E:206:TYR:O	2.11	0.50
1:E:542:ARG:HD2	2:F:582:ILE:HG22	1.93	0.50
1:G:166:GLU:HB3	1:G:201:TRP:HZ2	1.75	0.50
1:G:232:LYS:O	1:G:442:HIS:HD2	1.95	0.50
2:H:578:THR:O	2:H:579:PRO:C	2.50	0.50
1:G:302:ALA:HB2	1:G:338:PRO:HD3	1.94	0.50
1:A:462:GLN:HG3	1:A:462:GLN:O	2.10	0.50
1:C:292:ILE:HD11	1:C:325:ILE:CG1	2.40	0.50
1:E:528:THR:HG22	1:E:529:GLY:O	2.11	0.50
1:C:122:PRO:HG3	1:C:209:PRO:CD	2.41	0.50
1:C:182:ASN:OD1	1:C:474:ALA:N	2.33	0.50
1:A:113:ARG:HD3	1:E:547:LEU:O	2.11	0.50
1:A:280:ASN:N	1:A:387:LYS:HD3	2.26	0.50
1:C:405:VAL:HG11	1:C:477:LEU:HD22	1.93	0.50
1:G:87:LYS:NZ	1:G:95:VAL:HG11	2.26	0.50
1:C:299:LEU:HD12	1:C:300:PRO:HD2	1.92	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:CYS:HB2	1:A:143:TRP:CE2	2.46	0.50
1:G:71:CYS:HA	1:G:76:ASP:HB3	1.93	0.50
1:G:414:ALA:CB	1:G:420:VAL:HG22	2.40	0.50
1:A:268:ARG:HH11	1:A:268:ARG:HG3	1.75	0.50
1:C:239:ASN:HB3	1:C:503:THR:O	2.11	0.50
1:C:498:ILE:HD13	1:C:504:ILE:HD11	1.93	0.50
1:E:287:ASN:HB3	1:E:364:ALA:HB2	1.93	0.50
2:F:572:LEU:HD12	2:F:572:LEU:O	2.11	0.50
1:G:248:TRP:HB2	1:G:431:LEU:CD2	2.41	0.50
1:G:82:VAL:O	1:G:85:PHE:HB3	2.11	0.50
1:A:439:TYR:HB2	1:A:553:ALA:HA	1.94	0.50
3:R:3:U:C5	3:R:4:U:C5	2.99	0.50
1:A:154:ARG:HG2	1:A:482:ASP:OD1	2.11	0.50
1:E:276:VAL:HG22	1:E:294:TRP:CD1	2.46	0.50
1:E:306:LEU:HD13	1:E:311:GLY:CA	2.41	0.50
1:G:207:VAL:HG21	1:G:212:TYR:CD1	2.47	0.50
1:G:547:LEU:N	1:G:547:LEU:HD23	2.26	0.50
1:A:170:LEU:HG	1:A:174:ASN:OD1	2.11	0.50
1:A:449:VAL:CG2	1:C:449:VAL:HG11	2.41	0.50
2:D:564:LEU:N	2:D:564:LEU:HD13	2.27	0.50
1:E:119:GLU:OE2	1:E:509:TYR:CD2	2.64	0.50
1:G:133:GLU:N	1:G:283:PHE:CZ	2.75	0.50
1:A:319:LYS:HE3	1:A:320:PHE:CE1	2.47	0.50
1:G:232:LYS:HD2	1:G:510:ASP:OD2	2.12	0.50
1:C:400:ILE:HG22	1:C:401:ASP:H	1.77	0.50
1:A:248:TRP:CZ3	1:A:250:VAL:HG23	2.46	0.50
2:F:601:GLU:CD	2:F:601:GLU:N	2.65	0.50
1:A:545:MET:C	1:A:547:LEU:H	2.15	0.50
1:C:207:VAL:CG1	1:C:212:TYR:HB2	2.39	0.50
1:G:162:ASN:ND2	1:G:166:GLU:HB2	2.26	0.50
1:A:298:PRO:HB2	1:A:398:VAL:HG21	1.94	0.50
1:G:185:ASN:O	1:G:188:ASP:HB2	2.11	0.50
1:E:214:MET:HE3	1:G:521:THR:HG22	1.93	0.50
1:A:189:LEU:CD1	1:A:189:LEU:N	2.72	0.50
1:C:297:THR:HG22	1:C:298:PRO:CG	2.41	0.50
1:A:120:GLN:OE1	1:A:208:LEU:HB3	2.12	0.50
2:B:579:PRO:HG2	1:C:535:GLU:OE2	2.11	0.50
2:D:564:LEU:C	2:D:567:ILE:HG22	2.32	0.50
1:E:226:GLN:NE2	1:E:452:MET:HB3	2.27	0.50
1:E:274:MET:CE	1:E:294:TRP:HE1	2.24	0.50
1:E:229:LYS:CB	1:E:485:GLU:HG2	2.35	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:VAL:O	1:E:537:VAL:C	2.49	0.50
1:G:116:VAL:HG11	1:G:522:VAL:CG1	2.41	0.50
1:A:278:ALA:O	1:A:388:GLY:N	2.36	0.50
1:G:274:MET:CE	1:G:296:ILE:HD11	2.41	0.50
1:E:134:SER:HB2	1:E:139:ASP:OD2	2.12	0.50
1:E:504:ILE:HG22	1:E:506:CYS:SG	2.51	0.50
1:G:257:LYS:HE2	1:G:446:ASN:CB	2.41	0.50
1:C:191:THR:C	1:C:193:GLN:H	2.14	0.50
1:C:209:PRO:O	1:C:212:TYR:N	2.45	0.50
2:D:567:ILE:CG2	2:D:568:GLY:N	2.75	0.50
2:D:581:VAL:O	2:D:585:ILE:CD1	2.54	0.50
1:E:275:THR:CG2	1:E:478:ARG:NH1	2.74	0.50
1:G:163:ILE:C	1:G:165:ASN:H	2.14	0.50
1:A:307:THR:HG23	1:A:308:THR:HG23	1.94	0.50
1:G:248:TRP:CZ2	1:G:429:GLN:HB2	2.47	0.50
1:G:552:GLN:C	1:G:554:ASP:H	2.14	0.50
1:G:84:TRP:CE3	1:G:108:PRO:HD2	2.47	0.50
1:G:185:ASN:CG	1:G:318:GLY:HA3	2.32	0.50
1:E:248:TRP:CA	1:E:431:LEU:HA	2.40	0.50
1:A:90:ASP:OD1	1:A:93:GLY:N	2.40	0.50
1:E:190:GLY:C	1:E:192:GLY:N	2.64	0.50
1:C:553:ALA:O	1:C:555:ASP:N	2.45	0.50
1:G:54:VAL:HG12	1:G:55:ALA:O	2.12	0.50
1:C:77:PRO:HA	1:C:533:GLU:OE2	2.12	0.50
1:A:447:ASN:HD21	1:A:451:GLU:HB2	1.77	0.49
1:C:545:MET:HE2	1:C:545:MET:O	2.12	0.49
1:G:177:ILE:O	1:G:178:GLN:C	2.50	0.49
1:A:274:MET:HG3	1:A:294:TRP:HE1	1.77	0.49
1:G:231:TYR:CE2	1:G:511:GLY:HA3	2.47	0.49
1:A:498:ILE:HG22	1:A:499:SER:N	2.27	0.49
1:A:131:VAL:HG21	1:A:500:GLN:HB3	1.94	0.49
1:C:522:VAL:C	1:C:524:GLN:H	2.15	0.49
1:G:48:LEU:CD2	1:G:54:VAL:HG21	2.42	0.49
2:D:571:LEU:N	2:D:571:LEU:HD23	2.27	0.49
1:E:227:PHE:CD1	1:E:227:PHE:C	2.85	0.49
1:E:227:PHE:CD1	1:E:228:ARG:N	2.80	0.49
1:G:218:GLY:HA3	1:G:221:THR:OG1	2.11	0.49
1:G:362:ILE:O	1:G:362:ILE:HG13	2.11	0.49
1:C:299:LEU:HD11	1:C:338:PRO:HD2	1.94	0.49
1:G:276:VAL:C	1:G:391:VAL:HG13	2.33	0.49
1:G:217:ILE:HG23	1:G:319:LYS:HZ1	1.76	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:THR:HG21	1:G:322:SER:HB3	1.94	0.49
1:A:553:ALA:C	1:A:555:ASP:N	2.65	0.49
1:E:516:THR:HG21	1:E:523:GLY:HA2	1.94	0.49
1:A:230:VAL:O	1:A:231:TYR:HB3	2.12	0.49
1:C:129:PRO:HG2	1:C:163:ILE:HG23	1.94	0.49
1:C:182:ASN:HA	1:C:478:ARG:HD2	1.94	0.49
2:D:582:ILE:HA	2:D:585:ILE:HD13	1.95	0.49
1:G:186:TRP:CE3	1:G:480:ILE:HG23	2.47	0.49
1:E:144:ARG:HG2	1:E:144:ARG:NH1	2.25	0.49
1:A:406:ASN:N	1:A:406:ASN:OD1	2.45	0.49
1:G:447:ASN:HD21	1:G:449:VAL:CG1	2.19	0.49
1:A:248:TRP:HZ3	1:A:250:VAL:CG2	2.25	0.49
1:E:185:ASN:ND2	1:E:320:PHE:O	2.36	0.49
1:A:146:SER:HB2	1:A:160:LEU:CD1	2.41	0.49
1:G:147:PHE:O	1:G:492:VAL:HA	2.12	0.49
2:D:569:LEU:C	2:D:569:LEU:HD13	2.31	0.49
1:G:39:GLU:O	1:G:71:CYS:N	2.46	0.49
1:A:119:GLU:HA	1:A:511:GLY:HA2	1.94	0.49
1:E:152:ALA:HB3	1:E:155:LEU:HB3	1.94	0.49
1:E:459:GLY:O	1:E:481:VAL:HA	2.13	0.49
1:G:493:VAL:HG12	1:G:495:PHE:CE1	2.47	0.49
1:E:215:ALA:HB3	1:E:221:THR:HB	1.93	0.49
1:A:136:LEU:HD23	1:A:137:PRO:HD2	1.93	0.49
1:E:470:PRO:O	1:E:473:ASN:N	2.38	0.49
1:C:428:GLU:HG3	1:E:59:GLY:O	2.12	0.49
1:G:125:THR:HG22	1:G:125:THR:O	2.13	0.49
1:E:165:ASN:HD21	1:E:497:GLY:HA2	1.74	0.49
1:E:142:LEU:HA	1:E:498:ILE:O	2.13	0.49
1:C:369:TYR:C	1:C:369:TYR:CD1	2.85	0.49
1:E:151:PRO:O	1:E:485:GLU:HB3	2.12	0.49
1:E:230:VAL:HG12	1:E:231:TYR:CD2	2.44	0.49
1:G:89:MET:HE1	1:G:544:GLN:H	1.76	0.49
1:E:78:SER:O	1:E:81:ALA:N	2.46	0.49
1:A:516:THR:CB	1:E:423:ASN:HB3	2.33	0.49
2:H:564:LEU:CD2	2:H:564:LEU:H	2.14	0.49
1:A:97:SER:C	1:A:99:LYS:H	2.16	0.49
1:C:396:VAL:CG1	1:C:397:THR:N	2.62	0.49
1:A:87:LYS:HB3	1:A:231:TYR:CE2	2.48	0.49
1:A:443:TYR:CE2	1:C:113:ARG:HD3	2.48	0.49
1:C:106:LYS:HE2	1:C:528:THR:O	2.13	0.49
2:D:563:ALA:C	2:D:565:ALA:H	2.16	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:225:THR:HB	1:G:515:THR:O	2.13	0.49
1:C:287:ASN:HA	1:C:363:THR:O	2.12	0.49
1:G:281:ALA:O	1:G:284:GLN:HB2	2.13	0.49
1:E:54:VAL:CG1	1:E:55:ALA:N	2.75	0.49
1:G:87:LYS:HZ1	1:G:95:VAL:CG1	2.26	0.49
1:G:74:SER:C	1:G:75:ILE:HG23	2.33	0.49
1:E:241:PRO:C	1:E:243:LEU:N	2.64	0.49
1:E:485:GLU:HG3	1:E:488:PHE:H	1.78	0.49
1:E:231:TYR:HA	1:E:488:PHE:CZ	2.48	0.49
1:G:153:PHE:O	1:G:208:LEU:HD12	2.13	0.49
1:A:298:PRO:HB2	1:A:398:VAL:CG2	2.43	0.49
1:E:214:MET:HG3	1:G:521:THR:HG22	1.94	0.49
1:C:306:LEU:HD13	1:C:311:GLY:CA	2.39	0.49
1:A:160:LEU:HD12	1:A:160:LEU:N	2.26	0.49
1:A:157:PHE:CD1	1:A:157:PHE:C	2.86	0.49
1:C:75:ILE:HD11	2:D:572:LEU:HG	1.94	0.49
2:D:561:VAL:HA	2:D:564:LEU:CD2	2.42	0.49
1:C:259:GLN:HB2	1:E:455:GLU:HG2	1.95	0.49
1:G:363:THR:CG2	1:G:364:ALA:H	2.21	0.49
1:G:276:VAL:HG22	1:G:294:TRP:HD1	1.78	0.49
1:A:169:THR:CG2	1:A:172:THR:HG23	2.42	0.49
1:E:248:TRP:HZ3	1:E:250:VAL:CG2	2.25	0.49
1:C:312:GLY:CA	1:C:326:ASP:OD1	2.61	0.49
1:A:128:CYS:SG	1:A:131:VAL:HG23	2.52	0.49
1:C:227:PHE:HA	1:C:514:GLY:HA2	1.95	0.49
1:E:107:VAL:HG22	1:E:230:VAL:HG13	1.95	0.49
1:E:253:HIS:ND1	1:E:491:ALA:CB	2.76	0.49
1:G:138:LEU:C	1:G:140:GLY:H	2.17	0.49
1:G:154:ARG:HA	1:G:211:THR:HG22	1.95	0.49
1:E:90:ASP:HB2	2:F:561:VAL:CB	2.37	0.49
1:G:88:TYR:CE1	1:G:544:GLN:NE2	2.80	0.49
1:G:262:THR:CG2	1:G:263:ILE:N	2.75	0.49
1:A:148:ILE:HA	1:A:492:VAL:HG12	1.95	0.49
2:F:607:ILE:O	2:F:608:GLY:C	2.50	0.49
2:B:572:LEU:C	2:B:572:LEU:HD12	2.33	0.49
1:A:485:GLU:CG	1:A:488:PHE:H	2.20	0.49
2:B:565:ALA:O	2:B:568:GLY:N	2.46	0.49
1:C:443:TYR:CD2	1:E:113:ARG:NH1	2.80	0.49
1:E:297:THR:HA	1:E:478:ARG:HH21	1.77	0.49
1:E:449:VAL:HG12	1:E:450:PHE:N	2.27	0.49
1:E:452:MET:O	1:E:453:THR:C	2.50	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:SER:HB3	1:A:382:VAL:HG13	1.95	0.49
1:A:396:VAL:CG1	1:A:397:THR:N	2.75	0.49
2:H:588:GLN:C	2:H:590:VAL:H	2.15	0.49
1:G:273:SER:HB2	1:G:393:ILE:HG22	1.93	0.49
1:G:296:ILE:HD12	1:G:296:ILE:N	2.27	0.49
1:E:265:ALA:HB2	1:E:404:ALA:CB	2.37	0.49
1:A:120:GLN:NE2	1:A:211:THR:H	2.11	0.48
1:A:536:VAL:O	1:A:537:VAL:C	2.50	0.48
1:A:545:MET:HE1	1:A:546:GLU:HB3	1.95	0.48
1:C:427:TYR:OH	1:G:121:ARG:HD2	2.13	0.48
1:E:194:TRP:HE3	1:E:194:TRP:HA	1.77	0.48
1:E:229:LYS:HB2	1:E:485:GLU:CG	2.38	0.48
1:G:113:ARG:O	1:G:528:THR:HA	2.12	0.48
1:E:195:ALA:HB3	1:E:203:TYR:CE2	2.47	0.48
1:C:87:LYS:O	1:C:89:MET:N	2.46	0.48
1:G:248:TRP:NE1	1:G:429:GLN:CG	2.72	0.48
1:E:380:VAL:CG1	1:E:381:ILE:N	2.76	0.48
1:G:486:ASN:CG	1:G:486:ASN:O	2.50	0.48
1:C:146:SER:CB	1:C:494:HIS:ND1	2.76	0.48
1:C:193:GLN:O	1:C:204:SER:HB3	2.13	0.48
1:C:241:PRO:O	1:C:244:ILE:N	2.47	0.48
2:D:560:THR:O	2:D:564:LEU:HD22	2.13	0.48
1:E:178:GLN:HE22	1:E:391:VAL:H	1.60	0.48
1:E:253:HIS:NE2	1:E:441:VAL:O	2.46	0.48
1:A:363:THR:OG1	1:A:366:THR:HG22	2.13	0.48
1:G:279:SER:OG	1:G:280:ASN:N	2.46	0.48
1:G:442:HIS:N	1:G:442:HIS:CD2	2.81	0.48
1:A:148:ILE:HG12	1:A:492:VAL:CG1	2.43	0.48
1:C:385:VAL:HG22	1:C:392:SER:HB3	1.95	0.48
1:A:454:GLY:O	1:A:456:GLU:N	2.46	0.48
1:A:257:LYS:O	1:C:455:GLU:HB3	2.12	0.48
2:B:566:SER:O	2:B:570:GLY:N	2.42	0.48
1:E:111:LEU:O	1:E:111:LEU:HD12	2.13	0.48
1:C:262:THR:HB	1:E:262:THR:CG2	2.42	0.48
1:G:107:VAL:CG2	1:G:230:VAL:HG13	2.44	0.48
1:G:343:ALA:HB2	1:G:396:VAL:HG13	1.94	0.48
1:E:214:MET:HG3	1:G:521:THR:CG2	2.43	0.48
1:E:234:ILE:HG12	1:E:508:THR:HB	1.95	0.48
1:E:341:ILE:HA	1:E:397:THR:O	2.13	0.48
1:G:143:TRP:N	1:G:143:TRP:CD1	2.79	0.48
1:A:289:VAL:HG13	1:A:327:GLY:C	2.34	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:HB	1:A:298:PRO:HD3	1.94	0.48
1:E:416:THR:O	1:E:417:THR:C	2.51	0.48
1:C:299:LEU:HD23	1:C:321:PHE:HB3	1.94	0.48
1:A:424:VAL:HG22	1:C:114:TYR:CZ	2.48	0.48
1:C:90:ASP:OD1	1:C:93:GLY:N	2.37	0.48
1:A:415:LEU:HD12	1:A:415:LEU:N	2.29	0.48
1:C:436:GLY:N	1:C:554:ASP:OD1	2.46	0.48
1:E:329:VAL:HG13	1:E:359:MET:O	2.13	0.48
1:G:193:GLN:O	1:G:193:GLN:HG3	2.13	0.48
1:E:98:GLY:C	1:G:63:MET:HE3	2.34	0.48
1:G:277:SER:CA	1:G:391:VAL:HG13	2.44	0.48
2:D:561:VAL:CA	2:D:564:LEU:HD22	2.43	0.48
1:E:274:MET:HG3	1:E:296:ILE:CG1	2.43	0.48
1:E:474:ALA:HB1	1:E:478:ARG:HD2	1.94	0.48
2:F:577:ALA:HA	2:F:582:ILE:HD11	1.94	0.48
1:G:178:GLN:HG3	1:G:179:THR:N	2.29	0.48
1:A:470:PRO:HB2	1:C:403:GLU:CB	2.44	0.48
1:G:230:VAL:O	1:G:231:TYR:HB3	2.13	0.48
1:G:253:HIS:CE1	1:G:442:HIS:HA	2.49	0.48
1:G:78:SER:O	1:G:81:ALA:HB3	2.13	0.48
1:A:122:PRO:HB3	1:A:209:PRO:HG3	1.96	0.48
1:E:182:ASN:O	1:E:183:ILE:C	2.50	0.48
1:C:448:PRO:HG3	1:E:449:VAL:HG12	1.94	0.48
1:E:538:GLN:O	1:E:539:LEU:C	2.52	0.48
1:C:285:PRO:O	1:C:287:ASN:N	2.43	0.48
1:G:81:ALA:O	1:G:84:TRP:N	2.46	0.48
1:G:316:THR:HG21	1:G:322:SER:CB	2.44	0.48
1:A:213:ALA:O	1:A:215:ALA:N	2.47	0.48
1:A:510:ASP:C	1:A:510:ASP:OD1	2.52	0.48
1:C:233:GLY:HA2	1:C:440:ILE:O	2.13	0.48
1:G:181:ASN:N	1:G:181:ASN:OD1	2.47	0.48
1:E:87:LYS:HG3	1:E:104:PHE:HB2	1.95	0.48
1:G:108:PRO:HB2	1:G:533:GLU:HB2	1.96	0.48
1:A:180:LEU:O	1:A:479:GLY:HA2	2.13	0.48
1:A:375:LEU:HD12	1:A:376:THR:N	2.29	0.48
2:H:566:SER:O	2:H:567:ILE:C	2.52	0.48
1:G:146:SER:HB3	1:G:494:HIS:ND1	2.28	0.48
1:A:232:LYS:HG3	1:A:510:ASP:HB2	1.96	0.48
1:A:267:GLU:HG2	1:E:475:LEU:CG	2.44	0.48
1:E:534:ASP:O	1:E:535:GLU:C	2.51	0.48
2:F:564:LEU:O	2:F:567:ILE:CG2	2.51	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:ARG:HG3	1:E:212:TYR:HE1	1.79	0.48
1:A:238:PHE:CD1	1:A:432:CYS:HB3	2.47	0.48
1:C:352:GLY:O	1:C:353:ASP:C	2.52	0.48
1:A:533:GLU:OE2	1:A:533:GLU:HA	2.14	0.48
1:C:142:LEU:HD21	1:G:501:SER:O	2.14	0.48
1:C:172:THR:HG21	1:C:201:TRP:CE2	2.49	0.48
1:C:427:TYR:C	1:C:427:TYR:CD1	2.87	0.48
1:E:157:PHE:CE2	1:E:206:TYR:CD1	3.02	0.48
1:E:298:PRO:HG2	1:E:398:VAL:CG2	2.44	0.48
2:F:561:VAL:O	2:F:564:LEU:HB3	2.12	0.48
1:G:251:GLY:O	1:G:550:VAL:HG21	2.13	0.48
1:G:543:LEU:O	1:G:547:LEU:CD2	2.62	0.48
1:G:341:ILE:HG23	1:G:396:VAL:HG11	1.96	0.48
1:C:412:MET:HE2	1:C:415:LEU:HD21	1.94	0.48
1:E:396:VAL:HG13	1:E:397:THR:H	1.79	0.48
1:A:113:ARG:CZ	1:E:443:TYR:CD2	2.97	0.47
1:A:543:LEU:O	1:A:544:GLN:C	2.50	0.47
1:C:131:VAL:HG12	1:C:132:SER:N	2.29	0.47
1:E:157:PHE:N	1:E:157:PHE:CD2	2.82	0.47
1:E:447:ASN:ND2	1:E:449:VAL:H	2.12	0.47
1:G:142:LEU:HB2	1:G:498:ILE:O	2.14	0.47
1:A:473:ASN:O	1:A:474:ALA:O	2.31	0.47
1:C:87:LYS:HE2	1:C:95:VAL:HG23	1.95	0.47
2:F:596:ASN:CB	2:F:597:PRO:CD	2.92	0.47
1:G:289:VAL:HA	1:G:327:GLY:O	2.14	0.47
1:G:249:TRP:CD2	1:G:438:ALA:HB2	2.49	0.47
2:H:578:THR:CG2	2:H:581:VAL:HG23	2.44	0.47
1:E:120:GLN:O	1:E:122:PRO:HD2	2.13	0.47
1:A:126:ILE:HB	1:A:504:ILE:O	2.14	0.47
1:C:238:PHE:HB2	1:C:437:GLY:HA2	1.95	0.47
1:G:381:ILE:HG23	1:G:383:ARG:NH2	2.27	0.47
1:E:92:ALA:HB3	1:E:439:TYR:CE1	2.48	0.47
1:A:128:CYS:O	1:A:130:THR:N	2.47	0.47
1:E:350:GLU:O	1:E:351:GLU:C	2.52	0.47
1:A:449:VAL:HG23	1:C:449:VAL:HG11	1.96	0.47
1:E:313:THR:HB	1:E:325:ILE:HG22	1.96	0.47
1:E:522:VAL:O	1:E:524:GLN:N	2.47	0.47
1:G:290:ALA:HB2	1:G:387:LYS:CE	2.43	0.47
1:G:291:ARG:O	1:G:291:ARG:HD2	2.14	0.47
1:G:536:VAL:O	1:G:537:VAL:C	2.52	0.47
1:A:251:GLY:O	1:A:550:VAL:HG21	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ASN:CG	1:A:166:GLU:HB2	2.34	0.47
1:E:251:GLY:C	1:E:550:VAL:HG21	2.33	0.47
1:C:177:ILE:O	1:C:178:GLN:C	2.51	0.47
1:E:194:TRP:CZ3	1:E:204:SER:N	2.82	0.47
1:E:297:THR:CG2	1:E:476:GLY:H	2.25	0.47
1:A:363:THR:CB	1:A:366:THR:H	2.26	0.47
1:A:413:PRO:O	1:A:414:ALA:C	2.52	0.47
1:G:56:PRO:HG2	1:G:57:SER:N	2.27	0.47
1:E:270:SER:OG	1:E:402:THR:OG1	2.30	0.47
1:E:266:ALA:CB	1:E:402:THR:HB	2.35	0.47
1:A:244:ILE:CD1	1:A:501:SER:HB2	2.38	0.47
1:E:302:ALA:HB2	1:E:338:PRO:HG3	1.95	0.47
1:G:485:GLU:HG3	1:G:487:ASN:H	1.80	0.47
2:F:613:ARG:O	2:F:616:GLY:N	2.47	0.47
1:A:230:VAL:HB	1:A:511:GLY:O	2.14	0.47
1:C:255:PRO:HB2	1:E:226:GLN:OE1	2.14	0.47
1:E:230:VAL:O	1:E:231:TYR:HB3	2.15	0.47
1:G:153:PHE:HB2	1:G:227:PHE:CZ	2.50	0.47
1:G:116:VAL:HG22	1:G:526:ALA:HB2	1.97	0.47
1:A:301:VAL:HA	1:A:320:PHE:O	2.15	0.47
1:G:533:GLU:O	1:G:537:VAL:HG23	2.14	0.47
1:A:252:ALA:HB2	1:A:427:TYR:CB	2.39	0.47
1:A:235:THR:HG21	1:A:507:LYS:HE2	1.95	0.47
1:E:185:ASN:O	1:E:188:ASP:OD1	2.32	0.47
1:G:75:ILE:HG22	1:G:535:GLU:HG2	1.96	0.47
1:A:344:GLU:C	1:A:346:GLU:H	2.16	0.47
1:A:443:TYR:OH	1:C:112:LEU:HA	2.14	0.47
1:C:162:ASN:OD1	1:C:166:GLU:O	2.32	0.47
1:E:112:LEU:HD21	1:E:452:MET:SD	2.54	0.47
1:E:278:ALA:HA	1:E:292:ILE:CG2	2.40	0.47
1:E:313:THR:CA	1:E:325:ILE:HG22	2.43	0.47
1:G:142:LEU:CD1	1:G:497:GLY:HA2	2.42	0.47
1:C:365:ASP:O	1:C:386:THR:HA	2.15	0.47
1:G:262:THR:HG22	1:G:263:ILE:N	2.28	0.47
1:A:495:PHE:CE1	1:A:504:ILE:HD13	2.49	0.47
1:A:121:ARG:N	1:A:122:PRO:CD	2.77	0.47
2:B:564:LEU:O	2:B:567:ILE:CG2	2.61	0.47
1:C:241:PRO:O	1:C:243:LEU:N	2.48	0.47
1:C:357:PHE:HD1	1:C:371:VAL:HG13	1.80	0.47
1:E:105:SER:OG	1:E:117:ASP:OD2	2.28	0.47
1:E:450:PHE:N	1:E:450:PHE:CD2	2.82	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:453:THR:HG21	1:E:484:PHE:O	2.13	0.47
1:E:198:ALA:HB1	1:E:199:PRO:CD	2.37	0.47
1:G:440:ILE:HG22	1:G:550:VAL:HG22	1.96	0.47
1:G:109:ASP:CA	1:G:532:GLU:HA	2.44	0.47
1:E:239:ASN:HB3	1:E:503:THR:HG23	1.95	0.47
2:F:614:LEU:HA	2:F:614:LEU:HD23	1.80	0.47
1:C:553:ALA:C	1:C:555:ASP:H	2.16	0.47
1:A:210:ASN:O	1:A:213:ALA:HB3	2.14	0.47
1:A:231:TYR:C	1:A:231:TYR:CD1	2.88	0.47
1:A:89:MET:HE1	1:A:543:LEU:CB	2.45	0.47
1:C:108:PRO:HA	1:C:530:ALA:HB3	1.97	0.47
1:C:227:PHE:HA	1:C:513:GLU:O	2.14	0.47
1:C:232:LYS:HG2	1:C:442:HIS:CE1	2.50	0.47
1:E:116:VAL:HB	1:E:526:ALA:HB2	1.97	0.47
1:E:210:ASN:CG	1:G:520:SER:O	2.53	0.47
1:G:297:THR:HG21	1:G:476:GLY:N	2.29	0.47
1:A:87:LYS:NZ	1:A:95:VAL:CG2	2.77	0.47
1:C:202:TYR:N	1:C:202:TYR:CD1	2.82	0.47
1:E:412:MET:HG2	1:E:463:PHE:HB3	1.97	0.47
1:E:534:ASP:HA	1:E:537:VAL:CG2	2.45	0.47
1:A:280:ASN:H	1:A:387:LYS:HD3	1.78	0.47
1:C:403:GLU:HG3	1:C:403:GLU:O	2.13	0.47
1:E:162:ASN:OD1	1:E:166:GLU:HB2	2.15	0.47
1:E:162:ASN:HB2	1:E:201:TRP:CE2	2.50	0.47
2:F:598:GLY:O	2:F:599:ILE:HG13	2.14	0.47
1:G:232:LYS:HA	1:G:509:TYR:O	2.15	0.47
1:G:265:ALA:HB2	1:G:404:ALA:N	2.29	0.47
1:E:134:SER:CB	1:E:139:ASP:HB2	2.44	0.47
1:C:292:ILE:HD11	1:C:325:ILE:HG13	1.97	0.47
1:A:424:VAL:CG1	1:A:427:TYR:HB3	2.44	0.47
1:G:306:LEU:HD12	1:G:332:VAL:O	2.15	0.47
1:A:244:ILE:C	1:A:246:GLN:HG3	2.34	0.47
1:A:235:THR:CG2	1:A:507:LYS:HB3	2.44	0.47
1:C:303:THR:O	1:C:335:PHE:HB2	2.15	0.47
1:G:126:ILE:HG12	1:G:147:PHE:CE1	2.49	0.47
1:C:359:MET:HA	1:C:368:VAL:O	2.14	0.47
1:C:346:GLU:OE1	1:C:347:PRO:HD2	2.15	0.47
1:C:222:ASP:CG	1:C:522:VAL:HG23	2.35	0.47
1:C:418:GLU:HG2	1:C:419:GLU:N	2.30	0.47
1:E:365:ASP:OD1	1:E:365:ASP:N	2.47	0.47
1:C:544:GLN:C	1:C:546:GLU:N	2.65	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:THR:HG22	1:G:298:PRO:CD	2.45	0.47
1:A:307:THR:N	1:A:332:VAL:O	2.40	0.47
1:G:539:LEU:O	1:G:543:LEU:HB2	2.14	0.47
1:C:435:SER:C	1:C:437:GLY:H	2.11	0.47
1:G:350:GLU:HG3	1:G:353:ASP:OD2	2.15	0.47
1:A:360:THR:HB	1:A:368:VAL:HB	1.95	0.47
1:C:350:GLU:O	1:C:351:GLU:C	2.53	0.47
1:C:273:SER:N	1:C:297:THR:HB	2.23	0.47
1:E:180:LEU:HD12	1:E:180:LEU:H	1.80	0.47
1:E:181:ASN:OD1	1:E:462:GLN:HA	2.14	0.47
1:E:304:VAL:HG21	1:E:323:VAL:HG22	1.97	0.47
1:E:95:VAL:O	1:G:47:GLN:HG3	2.15	0.47
1:G:284:GLN:CD	1:G:289:VAL:HG11	2.35	0.47
1:G:81:ALA:O	1:G:82:VAL:C	2.51	0.47
1:G:95:VAL:HG22	1:G:96:GLU:N	2.30	0.47
2:H:578:THR:O	2:H:582:ILE:HG13	2.15	0.47
1:A:223:SER:O	1:A:516:THR:HG23	2.15	0.47
1:A:461:PHE:CE1	1:A:480:ILE:O	2.68	0.47
1:A:243:LEU:HD11	1:A:244:ILE:HG23	1.96	0.47
1:A:187:ARG:HD3	1:A:212:TYR:CE1	2.50	0.47
1:C:475:LEU:HD21	1:E:267:GLU:CA	2.45	0.47
1:E:444:LYS:HD3	1:E:447:ASN:O	2.15	0.47
2:D:564:LEU:HD12	1:E:50:PRO:HG2	1.96	0.47
1:E:100:ALA:C	1:E:101:LEU:HD23	2.35	0.47
1:E:95:VAL:HG11	1:G:61:GLY:O	2.15	0.47
1:G:288:THR:O	1:G:288:THR:HG22	2.15	0.47
1:G:538:GLN:OE1	2:H:579:PRO:HA	2.15	0.47
1:G:245:ASP:OD2	1:G:433:LYS:HG2	2.15	0.47
2:B:588:GLN:C	2:B:590:VAL:N	2.68	0.46
1:E:154:ARG:NH1	1:E:482:ASP:OD2	2.48	0.46
2:D:593:VAL:O	1:E:43:ILE:HA	2.15	0.46
1:A:329:VAL:HA	1:A:362:ILE:HD11	1.97	0.46
1:C:265:ALA:HB2	1:C:404:ALA:HB2	1.97	0.46
1:G:424:VAL:O	1:G:427:TYR:HD2	1.97	0.46
1:G:43:ILE:O	1:G:44:LEU:HD23	2.15	0.46
1:C:178:GLN:CB	1:C:472:ASN:ND2	2.78	0.46
1:C:534:ASP:O	1:C:535:GLU:C	2.53	0.46
1:A:113:ARG:NH1	1:E:544:GLN:O	2.48	0.46
1:G:133:GLU:H	1:G:283:PHE:HE2	1.52	0.46
1:G:135:ASP:CG	1:G:136:LEU:N	2.69	0.46
1:A:181:ASN:OD1	1:A:463:PHE:N	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:VAL:CG1	1:A:477:LEU:HD13	2.45	0.46
1:A:403:GLU:OE1	1:A:405:VAL:HG23	2.15	0.46
1:C:285:PRO:C	1:C:287:ASN:H	2.19	0.46
1:G:428:GLU:HB3	1:G:430:PHE:HE1	1.81	0.46
1:C:400:ILE:CG2	1:C:401:ASP:N	2.78	0.46
1:A:455:GLU:HG3	1:E:259:GLN:CG	2.45	0.46
1:A:85:PHE:CD2	2:B:569:LEU:HD22	2.50	0.46
1:C:127:GLU:HA	1:C:503:THR:CG2	2.45	0.46
1:C:168:LEU:HD13	1:C:201:TRP:CH2	2.49	0.46
1:E:447:ASN:ND2	1:E:449:VAL:O	2.41	0.46
1:E:261:GLU:OE1	1:E:409:SER:CB	2.63	0.46
1:C:278:ALA:O	1:C:387:LYS:HA	2.16	0.46
1:G:447:ASN:CG	1:G:449:VAL:HG12	2.36	0.46
1:E:70:ILE:HG22	1:E:71:CYS:N	2.29	0.46
1:G:313:THR:HA	1:G:325:ILE:HA	1.97	0.46
1:G:292:ILE:N	1:G:325:ILE:O	2.39	0.46
1:C:418:GLU:HG2	1:C:419:GLU:H	1.79	0.46
1:C:84:TRP:NE1	1:C:230:VAL:CG1	2.77	0.46
1:E:154:ARG:H	1:E:482:ASP:CG	2.16	0.46
1:E:323:VAL:HG12	1:E:325:ILE:HG23	1.98	0.46
1:E:369:TYR:O	1:E:382:VAL:HG13	2.15	0.46
1:E:391:VAL:HG12	1:E:392:SER:N	2.30	0.46
1:E:99:LYS:O	1:E:101:LEU:CD2	2.63	0.46
1:A:180:LEU:HD23	1:A:183:ILE:HD11	1.97	0.46
1:A:195:ALA:HB3	1:A:203:TYR:CE2	2.50	0.46
1:E:276:VAL:HG11	1:E:369:TYR:CD2	2.51	0.46
1:E:474:ALA:HB1	1:E:478:ARG:NH1	2.31	0.46
1:A:369:TYR:HD2	1:A:369:TYR:H	1.63	0.46
1:E:99:LYS:O	1:E:101:LEU:HD23	2.15	0.46
1:E:90:ASP:O	1:E:91:PRO:C	2.52	0.46
1:G:248:TRP:HB2	1:G:431:LEU:HD23	1.97	0.46
1:G:84:TRP:O	1:G:87:LYS:N	2.49	0.46
1:E:402:THR:HG22	1:E:402:THR:O	2.13	0.46
1:A:249:TRP:CE2	1:A:438:ALA:HB2	2.50	0.46
2:F:605:LYS:CG	2:F:610:VAL:CG2	2.94	0.46
1:E:233:GLY:HA2	1:E:440:ILE:O	2.15	0.46
2:D:576:SER:O	2:D:577:ALA:HB3	2.16	0.46
1:E:453:THR:HB	1:E:485:GLU:OE1	2.16	0.46
1:E:69:GLU:HB2	1:E:76:ASP:O	2.14	0.46
1:E:265:ALA:CA	1:E:404:ALA:HB2	2.46	0.46
1:G:380:VAL:CG1	1:G:381:ILE:N	2.78	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:CYS:HB3	1:A:131:VAL:HG23	1.98	0.46
1:G:254:ILE:CD1	1:G:424:VAL:HG21	2.45	0.46
1:G:257:LYS:CE	1:G:446:ASN:HB3	2.46	0.46
2:D:588:GLN:O	2:D:591:GLY:N	2.49	0.46
1:A:539:LEU:HA	1:A:542:ARG:HB2	1.97	0.46
1:C:79:GLU:CB	1:C:101:LEU:HD13	2.46	0.46
1:C:191:THR:C	1:C:193:GLN:N	2.69	0.46
1:A:257:LYS:HG3	1:C:226:GLN:HE21	1.81	0.46
1:C:275:THR:HB	1:C:391:VAL:CG1	2.35	0.46
1:C:537:VAL:O	1:C:538:GLN:C	2.54	0.46
1:E:124:VAL:HG11	1:E:206:TYR:CD2	2.51	0.46
1:E:393:ILE:HG22	1:E:394:THR:N	2.30	0.46
1:G:142:LEU:O	1:G:165:ASN:ND2	2.48	0.46
1:G:461:PHE:CE1	1:G:480:ILE:HB	2.50	0.46
1:E:43:ILE:HB	1:E:67:VAL:CB	2.41	0.46
1:E:54:VAL:HG12	1:E:55:ALA:N	2.31	0.46
1:G:534:ASP:HA	1:G:537:VAL:CG2	2.46	0.46
1:G:89:MET:CE	1:G:543:LEU:HB3	2.45	0.46
2:H:589:ALA:C	2:H:590:VAL:HG22	2.36	0.46
1:G:273:SER:HA	1:G:396:VAL:HG23	1.96	0.46
2:H:564:LEU:O	2:H:568:GLY:N	2.42	0.46
1:E:145:VAL:HA	1:E:161:ALA:HA	1.97	0.46
1:C:195:ALA:O	1:C:202:TYR:HA	2.16	0.46
1:C:205:ILE:CD1	1:C:480:ILE:HD11	2.46	0.46
1:A:262:THR:H	1:C:262:THR:HG21	1.81	0.46
1:C:257:LYS:HB2	1:E:456:GLU:OE2	2.16	0.46
1:C:87:LYS:HE3	1:C:95:VAL:HG23	1.93	0.46
1:G:288:THR:O	1:G:289:VAL:HG23	2.15	0.46
1:E:70:ILE:O	1:E:76:ASP:HA	2.15	0.46
1:G:277:SER:HB3	1:G:391:VAL:HG22	1.97	0.46
1:E:266:ALA:HB3	1:E:270:SER:OG	2.16	0.46
1:G:325:ILE:HD12	1:G:333:TRP:CD2	2.51	0.46
2:F:617:SER:O	2:F:619:LYS:N	2.49	0.46
1:C:75:ILE:HG21	1:C:535:GLU:HG3	1.96	0.46
1:E:274:MET:HB3	1:E:394:THR:HB	1.98	0.46
1:E:49:LEU:O	1:E:50:PRO:C	2.54	0.46
1:G:142:LEU:HD12	1:G:497:GLY:CA	2.43	0.46
1:G:159:ALA:CB	1:G:206:TYR:HE1	2.28	0.46
1:A:177:ILE:O	1:A:178:GLN:C	2.53	0.46
1:A:275:THR:HG23	1:A:478:ARG:NH2	2.31	0.46
1:A:341:ILE:CG2	1:A:342:LEU:N	2.79	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:THR:C	1:A:365:ASP:N	2.67	0.46
1:A:264:PRO:HG2	1:C:264:PRO:CG	2.46	0.46
1:G:291:ARG:HA	1:G:326:ASP:CA	2.46	0.46
1:G:449:VAL:HG13	1:G:450:PHE:N	2.30	0.46
1:G:360:THR:HB	1:G:368:VAL:CG1	2.45	0.46
2:H:566:SER:O	2:H:570:GLY:N	2.48	0.46
1:A:111:LEU:HD23	1:A:228:ARG:HH12	1.81	0.46
1:C:127:GLU:HB2	1:C:503:THR:HG21	1.98	0.46
1:C:229:LYS:HB2	1:C:485:GLU:HG3	1.98	0.46
1:C:500:GLN:HA	1:C:500:GLN:OE1	2.15	0.46
1:C:251:GLY:C	1:C:550:VAL:HG11	2.36	0.46
1:G:136:LEU:HD11	1:G:141:LYS:HB2	1.98	0.46
1:A:325:ILE:CD1	1:A:325:ILE:C	2.84	0.46
1:E:456:GLU:H	1:E:456:GLU:CD	2.19	0.46
1:G:428:GLU:HB2	1:G:550:VAL:HG12	1.97	0.46
1:G:274:MET:HE2	1:G:296:ILE:HD11	1.97	0.46
1:G:411:GLU:HG3	1:G:464:HIS:CG	2.51	0.46
1:A:234:ILE:HG12	1:A:508:THR:CG2	2.22	0.45
1:A:485:GLU:OE1	1:A:487:ASN:HB2	2.16	0.45
1:E:148:ILE:HG23	1:E:413:PRO:HG3	1.98	0.45
1:E:89:MET:HE1	1:E:540:ALA:CB	2.46	0.45
1:G:145:VAL:HG13	1:G:145:VAL:O	2.15	0.45
1:G:173:ARG:NH2	1:G:466:PRO:O	2.49	0.45
1:G:518:ALA:C	1:G:520:SER:H	2.18	0.45
1:A:181:ASN:ND2	1:A:181:ASN:H	2.14	0.45
1:A:306:LEU:HA	1:A:333:TRP:HA	1.97	0.45
1:E:197:PHE:CE1	1:E:198:ALA:HB2	2.51	0.45
1:G:428:GLU:HB2	1:G:550:VAL:CG1	2.46	0.45
1:G:229:LYS:HE3	1:G:510:ASP:OD2	2.16	0.45
1:G:342:LEU:HD23	1:G:347:PRO:HA	1.97	0.45
2:H:564:LEU:CD2	2:H:564:LEU:N	2.78	0.45
1:A:114:TYR:HA	1:A:527:HIS:O	2.16	0.45
1:G:243:LEU:C	1:G:245:ASP:N	2.69	0.45
1:E:85:PHE:CE2	2:F:565:ALA:HB1	2.51	0.45
2:B:588:GLN:O	2:B:590:VAL:N	2.49	0.45
1:C:182:ASN:OD1	1:C:474:ALA:CB	2.64	0.45
1:C:88:TYR:O	1:C:88:TYR:CG	2.69	0.45
1:E:157:PHE:N	1:E:157:PHE:HD2	2.13	0.45
1:E:357:PHE:CE1	1:E:369:TYR:HB2	2.51	0.45
1:G:131:VAL:HG23	1:G:163:ILE:CD1	2.47	0.45
1:G:186:TRP:O	1:G:189:LEU:HD23	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:N	1:A:282:ILE:HD13	2.29	0.45
1:A:262:THR:HA	1:A:406:ASN:HB2	1.93	0.45
1:A:407:ARG:NE	1:A:460:GLY:O	2.49	0.45
1:C:155:LEU:HD22	1:C:156:ASN:N	2.31	0.45
1:G:470:PRO:HA	1:G:473:ASN:OD1	2.15	0.45
2:H:571:LEU:HD23	2:H:571:LEU:N	2.32	0.45
1:C:246:GLN:OE1	1:C:246:GLN:N	2.50	0.45
1:C:407:ARG:NE	1:C:462:GLN:HB2	2.32	0.45
1:C:544:GLN:O	1:C:546:GLU:N	2.50	0.45
2:D:560:THR:C	2:D:564:LEU:HD22	2.37	0.45
1:E:148:ILE:N	1:E:148:ILE:CD1	2.80	0.45
1:E:286:SER:C	1:E:288:THR:H	2.19	0.45
1:E:543:LEU:O	1:E:547:LEU:N	2.47	0.45
1:C:405:VAL:HG11	1:C:477:LEU:CD2	2.47	0.45
1:G:185:ASN:CB	1:G:318:GLY:HA3	2.45	0.45
1:A:145:VAL:CG1	1:A:498:ILE:HD12	2.45	0.45
1:A:238:PHE:CD2	1:A:432:CYS:HB3	2.50	0.45
1:E:147:PHE:N	1:E:147:PHE:CD1	2.83	0.45
1:C:228:ARG:HG3	1:C:228:ARG:O	2.17	0.45
1:A:267:GLU:HB3	1:E:395:PRO:HB3	1.99	0.45
1:A:446:ASN:O	1:C:452:MET:HG3	2.16	0.45
1:C:461:PHE:HD2	1:C:463:PHE:CZ	2.35	0.45
1:C:544:GLN:O	1:C:547:LEU:N	2.47	0.45
2:D:571:LEU:O	2:D:572:LEU:C	2.54	0.45
2:D:578:THR:HB	2:D:581:VAL:H	1.80	0.45
1:A:307:THR:HG22	1:A:308:THR:OG1	2.17	0.45
1:G:109:ASP:O	1:G:110:GLY:C	2.54	0.45
1:G:110:GLY:H	1:G:532:GLU:N	2.15	0.45
1:A:147:PHE:HE1	1:A:495:PHE:CD1	2.35	0.45
1:E:146:SER:O	1:E:159:ALA:HA	2.17	0.45
1:A:350:GLU:O	1:A:352:GLY:N	2.48	0.45
1:E:254:ILE:O	1:E:490:SER:HB3	2.16	0.45
1:A:109:ASP:N	1:A:109:ASP:OD1	2.42	0.45
1:E:148:ILE:HG21	1:E:150:PHE:CZ	2.51	0.45
1:G:191:THR:HG23	1:G:193:GLN:CG	2.43	0.45
1:A:356:SER:O	1:A:371:VAL:HA	2.16	0.45
1:A:443:TYR:CE2	1:A:445:MET:HB2	2.52	0.45
1:A:255:PRO:HA	1:A:489:SER:HA	1.99	0.45
1:A:549:GLY:HA3	1:C:113:ARG:HH21	1.74	0.45
1:C:197:PHE:CZ	1:C:201:TRP:HB3	2.51	0.45
1:C:225:THR:HB	1:C:515:THR:OG1	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:PHE:O	1:C:486:ASN:N	2.50	0.45
1:E:173:ARG:HD3	1:E:465:TYR:CE2	2.51	0.45
1:E:275:THR:HG21	1:E:478:ARG:NH1	2.31	0.45
1:E:534:ASP:N	1:E:534:ASP:OD1	2.48	0.45
1:G:176:PHE:CZ	1:G:180:LEU:HD11	2.52	0.45
1:G:297:THR:OG1	1:G:478:ARG:NH1	2.49	0.45
1:G:227:PHE:N	1:G:452:MET:HE3	2.31	0.45
1:A:181:ASN:ND2	1:A:181:ASN:N	2.64	0.45
1:A:307:THR:HG22	1:A:308:THR:N	2.31	0.45
1:C:259:GLN:HG2	1:E:406:ASN:ND2	2.32	0.45
2:D:574:LYS:HD2	2:D:574:LYS:H	1.80	0.45
2:H:571:LEU:HD23	2:H:571:LEU:H	1.81	0.45
1:E:277:SER:OG	1:E:293:VAL:HB	2.16	0.45
1:A:225:THR:CG2	1:A:517:ASN:HB2	2.29	0.45
1:A:448:PRO:HA	1:C:111:LEU:HD13	1.98	0.45
1:C:140:GLY:O	1:G:136:LEU:HD23	2.16	0.45
1:C:235:THR:HA	1:C:439:TYR:HA	1.99	0.45
1:E:286:SER:O	1:E:387:LYS:NZ	2.50	0.45
1:E:436:GLY:H	1:E:554:ASP:CG	2.20	0.45
1:A:407:ARG:NH2	1:A:462:GLN:HB3	2.31	0.45
1:G:151:PRO:HB3	1:G:488:PHE:HB2	1.99	0.45
2:F:609:SER:O	2:F:610:VAL:C	2.55	0.45
1:G:90:ASP:HB2	2:H:561:VAL:HB	1.99	0.45
1:A:456:GLU:HG2	1:A:457:ASN:N	2.32	0.45
2:H:557:PHE:CD1	2:H:558:ALA:N	2.84	0.45
1:C:475:LEU:CG	1:E:267:GLU:CD	2.85	0.45
1:A:107:VAL:HG12	1:A:109:ASP:CG	2.37	0.45
1:A:89:MET:HE1	1:A:543:LEU:HB3	1.99	0.45
1:C:410:ILE:HG22	1:C:411:GLU:O	2.17	0.45
1:C:537:VAL:HG12	1:C:541:ASN:OD1	2.17	0.45
1:E:105:SER:HA	1:E:231:TYR:HE2	1.82	0.45
1:E:463:PHE:N	1:E:463:PHE:CD1	2.85	0.45
1:A:403:GLU:OE1	1:E:261:GLU:OE2	2.34	0.45
2:H:578:THR:HG23	2:H:580:SER:H	1.82	0.45
1:A:143:TRP:NE1	1:A:500:GLN:HA	2.31	0.45
1:C:150:PHE:HE1	1:C:158:ILE:HD12	1.82	0.45
1:A:117:ASP:HA	1:A:513:GLU:HA	1.98	0.45
1:A:464:HIS:CD2	1:A:464:HIS:C	2.90	0.45
1:C:122:PRO:CG	1:C:209:PRO:HD2	2.47	0.45
1:C:210:ASN:O	1:C:213:ALA:HB3	2.16	0.45
1:C:334:THR:HG22	1:C:356:SER:CB	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:TYR:CE1	1:C:441:VAL:HG22	2.52	0.45
1:E:227:PHE:O	1:E:452:MET:HE2	2.17	0.45
1:E:272:GLY:HA2	1:E:297:THR:HG21	1.98	0.45
1:E:334:THR:O	1:E:335:PHE:HB3	2.16	0.45
2:F:576:SER:O	2:F:578:THR:N	2.50	0.45
1:G:133:GLU:O	1:G:134:SER:C	2.56	0.45
1:G:144:ARG:NH1	1:G:201:TRP:HH2	2.15	0.45
1:G:202:TYR:N	1:G:202:TYR:CD1	2.85	0.45
1:G:458:PHE:CD1	1:G:459:GLY:N	2.85	0.45
1:A:197:PHE:CD1	1:A:197:PHE:C	2.90	0.45
1:A:322:SER:O	1:A:323:VAL:HG23	2.16	0.45
1:A:323:VAL:HG12	1:A:325:ILE:HG23	1.99	0.45
1:A:320:PHE:CE2	1:A:477:LEU:HB3	2.52	0.45
1:A:404:ALA:O	1:A:405:VAL:C	2.55	0.45
1:C:285:PRO:CB	1:C:288:THR:HB	2.47	0.45
1:C:400:ILE:CD1	1:C:400:ILE:N	2.75	0.45
1:G:109:ASP:HA	1:G:532:GLU:HG3	1.97	0.45
1:A:248:TRP:HB3	1:A:431:LEU:HD22	1.98	0.45
1:G:72:ALA:C	1:G:74:SER:H	2.21	0.45
1:C:118:ALA:O	1:C:511:GLY:HA2	2.16	0.45
1:E:77:PRO:HB2	1:E:82:VAL:HG22	1.99	0.45
1:E:411:GLU:HB2	1:E:464:HIS:NE2	2.31	0.45
1:A:531:GLU:OE2	1:A:533:GLU:HG2	2.17	0.45
2:B:578:THR:HB	2:B:581:VAL:H	1.82	0.45
1:C:177:ILE:HG23	1:C:181:ASN:HD21	1.78	0.45
1:C:235:THR:HG21	1:C:556:ASN:CB	2.46	0.45
1:C:241:PRO:C	1:C:243:LEU:N	2.70	0.45
2:D:572:LEU:CA	2:D:575:SER:OG	2.65	0.45
1:A:268:ARG:HB2	1:E:395:PRO:HB2	1.99	0.45
1:G:113:ARG:O	1:G:529:GLY:N	2.49	0.45
1:G:436:GLY:N	1:G:554:ASP:OD2	2.50	0.45
1:G:88:TYR:OH	1:G:443:TYR:HB2	2.17	0.45
1:C:400:ILE:HG22	1:C:401:ASP:O	2.16	0.45
1:A:235:THR:HB	1:A:439:TYR:CD1	2.52	0.45
1:E:127:GLU:HB3	1:E:503:THR:OG1	2.17	0.45
1:E:493:VAL:HG13	1:E:493:VAL:O	2.15	0.45
1:C:316:THR:OG1	1:C:317:SER:N	2.49	0.45
1:E:153:PHE:HB2	1:E:227:PHE:CZ	2.52	0.44
1:G:181:ASN:C	1:G:407:ARG:NH2	2.69	0.44
1:G:189:LEU:C	1:G:191:THR:H	2.20	0.44
1:G:196:GLN:CG	1:G:197:PHE:N	2.80	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:VAL:O	1:G:209:PRO:HD3	2.16	0.44
1:A:202:TYR:N	1:A:202:TYR:CD1	2.85	0.44
1:E:87:LYS:O	1:E:91:PRO:CD	2.63	0.44
1:E:98:GLY:CA	1:G:63:MET:HE1	2.45	0.44
1:G:274:MET:HA	1:G:295:SER:O	2.17	0.44
1:A:235:THR:HA	1:A:439:TYR:HA	1.98	0.44
1:C:250:VAL:CB	1:C:429:GLN:HB3	2.44	0.44
2:H:564:LEU:O	2:H:565:ALA:C	2.55	0.44
1:E:189:LEU:HB3	1:E:205:ILE:HD11	1.99	0.44
1:A:538:GLN:HE21	1:A:538:GLN:HA	1.83	0.44
1:A:409:SER:OG	1:C:455:GLU:OE2	2.26	0.44
1:E:412:MET:CE	1:E:415:LEU:HD21	2.47	0.44
1:A:276:VAL:CG1	1:A:294:TRP:HB2	2.46	0.44
1:A:499:SER:O	1:A:502:ALA:N	2.46	0.44
1:C:359:MET:HE1	1:C:367:VAL:HG11	1.99	0.44
1:A:544:GLN:O	1:C:113:ARG:HD2	2.16	0.44
1:C:243:LEU:HG	1:C:244:ILE:HG23	2.00	0.44
1:A:426:LYS:HE2	1:C:528:THR:OG1	2.16	0.44
1:E:106:LYS:NZ	1:E:117:ASP:OD1	2.44	0.44
1:E:413:PRO:O	1:E:414:ALA:C	2.54	0.44
1:E:450:PHE:HD2	1:E:450:PHE:N	2.14	0.44
1:G:134:SER:O	1:G:135:ASP:O	2.35	0.44
1:G:162:ASN:HB2	1:G:201:TRP:CE3	2.51	0.44
1:G:186:TRP:CD1	1:G:481:VAL:HG23	2.52	0.44
1:E:210:ASN:OD1	1:G:520:SER:O	2.35	0.44
1:G:527:HIS:O	1:G:528:THR:O	2.35	0.44
1:G:381:ILE:HD13	1:G:394:THR:HG21	1.98	0.44
1:A:550:VAL:O	1:A:551:TYR:CG	2.70	0.44
1:C:88:TYR:HE1	1:C:443:TYR:HA	1.82	0.44
1:G:103:GLU:HB3	1:G:117:ASP:OD1	2.18	0.44
1:G:105:SER:O	1:G:117:ASP:CB	2.66	0.44
1:G:203:TYR:CD1	1:G:204:SER:N	2.86	0.44
1:G:481:VAL:O	1:G:482:ASP:CB	2.54	0.44
1:G:498:ILE:HG22	1:G:498:ILE:O	2.17	0.44
1:G:499:SER:O	1:G:500:GLN:C	2.56	0.44
1:A:178:GLN:HG3	1:A:472:ASN:HB3	1.99	0.44
1:G:363:THR:CG2	1:G:364:ALA:N	2.75	0.44
1:E:44:LEU:HD11	1:E:63:MET:CE	2.47	0.44
1:G:86:TYR:O	1:G:87:LYS:C	2.55	0.44
2:H:585:ILE:O	2:H:588:GLN:N	2.51	0.44
1:A:164:ASN:C	1:A:166:GLU:H	2.21	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ALA:HB3	1:A:321:PHE:CE1	2.53	0.44
1:C:125:THR:CG2	1:C:505:VAL:HG13	2.48	0.44
1:E:109:ASP:O	1:E:111:LEU:N	2.50	0.44
1:E:175:THR:O	1:E:176:PHE:C	2.56	0.44
1:E:295:SER:C	1:E:296:ILE:HG13	2.37	0.44
1:G:527:HIS:N	1:G:527:HIS:ND1	2.66	0.44
1:A:170:LEU:O	1:A:171:GLU:C	2.56	0.44
1:C:313:THR:HG22	1:C:314:ASN:N	2.32	0.44
1:E:160:LEU:HG	1:E:160:LEU:O	2.17	0.44
1:A:334:THR:HG21	1:A:354:THR:HG22	1.99	0.44
1:C:191:THR:HG22	1:C:191:THR:O	2.17	0.44
1:E:230:VAL:N	1:E:511:GLY:O	2.50	0.44
1:E:304:VAL:HG21	1:E:323:VAL:HG21	2.00	0.44
1:C:421:THR:CG2	1:G:123:ILE:HD12	2.39	0.44
1:G:138:LEU:HD22	1:G:244:ILE:CD1	2.47	0.44
1:A:198:ALA:HB1	1:A:199:PRO:CD	2.36	0.44
1:E:90:ASP:CG	2:F:561:VAL:HB	2.38	0.44
2:F:597:PRO:C	2:F:599:ILE:N	2.70	0.44
1:C:299:LEU:HD12	1:C:300:PRO:CD	2.47	0.44
1:C:300:PRO:HG3	1:C:400:ILE:HG12	1.99	0.44
1:G:265:ALA:HB1	1:G:402:THR:O	2.17	0.44
2:F:588:GLN:HG3	2:F:593:VAL:O	2.18	0.44
1:G:119:GLU:HG2	1:G:120:GLN:N	2.33	0.44
1:A:106:LYS:HG3	1:A:117:ASP:CG	2.38	0.44
1:A:538:GLN:HG2	2:B:582:ILE:CD1	2.30	0.44
1:C:407:ARG:HH11	1:C:407:ARG:HG3	1.83	0.44
1:G:189:LEU:C	1:G:191:THR:N	2.70	0.44
1:G:522:VAL:O	1:G:524:GLN:N	2.50	0.44
1:A:341:ILE:C	1:A:342:LEU:HD23	2.38	0.44
1:E:164:ASN:C	1:E:166:GLU:H	2.21	0.44
1:G:280:ASN:HB3	1:G:286:SER:HA	1.99	0.44
1:G:248:TRP:HD1	1:G:431:LEU:CD2	2.25	0.44
1:G:547:LEU:N	1:G:547:LEU:CD2	2.81	0.44
1:G:299:LEU:HD12	1:G:300:PRO:CD	2.48	0.44
1:G:276:VAL:H	1:G:391:VAL:HG12	1.81	0.44
1:E:126:ILE:N	1:E:126:ILE:CD1	2.80	0.44
1:C:354:THR:N	1:C:374:SER:CB	2.80	0.44
1:G:236:PHE:HB3	1:G:504:ILE:HG21	2.00	0.44
2:F:613:ARG:NH1	3:R:4:U:C6	2.85	0.44
1:A:156:ASN:N	1:A:206:TYR:O	2.50	0.44
1:A:120:GLN:CD	1:A:208:LEU:HB3	2.38	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:HA3	1:A:532:GLU:N	2.33	0.44
2:D:565:ALA:O	2:D:568:GLY:N	2.51	0.44
1:G:143:TRP:NE1	1:G:498:ILE:HG22	2.32	0.44
1:G:197:PHE:CZ	1:G:201:TRP:HB3	2.53	0.44
1:G:408:LEU:HD21	1:G:458:PHE:O	2.17	0.44
1:G:407:ARG:CZ	1:G:478:ARG:O	2.66	0.44
1:G:440:ILE:HA	1:G:549:GLY:O	2.18	0.44
1:G:341:ILE:HG23	1:G:396:VAL:CG1	2.48	0.44
1:A:419:GLU:O	1:A:423:ASN:N	2.51	0.44
1:C:359:MET:CE	1:C:367:VAL:HG11	2.48	0.44
1:A:534:ASP:O	1:A:537:VAL:HG22	2.18	0.44
1:E:407:ARG:NE	1:E:478:ARG:O	2.51	0.44
1:E:275:THR:HG22	1:E:478:ARG:HH12	1.82	0.44
1:G:178:GLN:CD	1:G:182:ASN:ND2	2.71	0.44
1:G:160:LEU:HA	1:G:203:TYR:HA	2.00	0.44
1:G:407:ARG:HG3	1:G:460:GLY:C	2.38	0.44
1:A:297:THR:HG23	1:A:478:ARG:CZ	2.47	0.44
1:E:416:THR:C	1:E:418:GLU:N	2.71	0.44
1:G:543:LEU:O	1:G:544:GLN:C	2.56	0.44
1:E:121:ARG:HA	1:E:508:THR:O	2.17	0.44
2:H:561:VAL:C	2:H:563:ALA:N	2.70	0.44
1:G:435:SER:C	1:G:437:GLY:N	2.69	0.44
1:A:343:ALA:C	1:A:344:GLU:HG2	2.38	0.44
1:A:225:THR:HB	1:E:255:PRO:O	2.18	0.43
2:B:577:ALA:O	2:B:578:THR:C	2.54	0.43
2:B:579:PRO:HA	2:B:582:ILE:HD12	2.00	0.43
1:C:162:ASN:ND2	1:C:164:ASN:O	2.51	0.43
1:C:242:THR:HA	1:C:245:ASP:OD2	2.18	0.43
1:C:245:ASP:O	1:C:246:GLN:C	2.56	0.43
1:C:84:TRP:O	1:C:85:PHE:C	2.57	0.43
2:D:567:ILE:CG2	2:D:568:GLY:H	2.31	0.43
1:E:173:ARG:HG2	1:E:177:ILE:HD11	2.00	0.43
1:C:257:LYS:CB	1:E:456:GLU:OE2	2.66	0.43
1:G:537:VAL:HG12	1:G:541:ASN:HD21	1.83	0.43
1:E:250:VAL:HG13	1:E:429:GLN:HB2	1.99	0.43
1:C:90:ASP:C	1:C:92:ALA:H	2.21	0.43
1:G:146:SER:OG	1:G:494:HIS:ND1	2.50	0.43
1:C:337:ALA:O	1:C:351:GLU:O	2.35	0.43
1:G:139:ASP:O	1:G:139:ASP:OD1	2.35	0.43
1:A:443:TYR:HH	1:C:112:LEU:HA	1.82	0.43
1:C:111:LEU:O	1:C:111:LEU:HG	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLN:CB	1:C:455:GLU:HG3	2.43	0.43
1:E:184:THR:HG21	1:E:295:SER:OG	2.17	0.43
1:G:240:ALA:HB1	1:G:241:PRO:HD2	2.00	0.43
1:A:470:PRO:HB2	1:C:403:GLU:HB3	2.00	0.43
1:G:307:THR:OG1	1:G:334:THR:HG22	2.19	0.43
1:E:300:PRO:O	1:E:338:PRO:HG2	2.18	0.43
1:A:128:CYS:HA	1:A:143:TRP:CH2	2.53	0.43
2:F:588:GLN:O	2:F:591:GLY:N	2.51	0.43
1:E:77:PRO:HB2	1:E:82:VAL:CG2	2.47	0.43
1:A:440:ILE:O	1:A:440:ILE:HG13	2.18	0.43
1:A:208:LEU:O	1:A:209:PRO:C	2.56	0.43
2:B:564:LEU:CD1	2:B:589:ALA:O	2.66	0.43
1:C:140:GLY:HA3	1:G:138:LEU:CD2	2.47	0.43
1:C:167:ALA:O	1:C:201:TRP:HZ2	2.01	0.43
1:E:364:ALA:O	1:E:387:LYS:HE3	2.18	0.43
1:E:520:SER:C	1:E:522:VAL:H	2.20	0.43
2:F:574:LYS:HG2	2:F:575:SER:N	2.33	0.43
1:A:276:VAL:HG22	1:A:294:TRP:CB	2.46	0.43
2:F:563:ALA:O	2:F:566:SER:HB3	2.18	0.43
1:G:248:TRP:CH2	1:G:250:VAL:HB	2.54	0.43
1:E:248:TRP:CB	1:E:431:LEU:HA	2.48	0.43
1:E:120:GLN:NE2	1:E:211:THR:HG23	2.34	0.43
1:G:373:SER:C	1:G:375:LEU:N	2.71	0.43
1:C:126:ILE:N	1:C:126:ILE:CD1	2.81	0.43
1:G:146:SER:CB	1:G:494:HIS:ND1	2.82	0.43
1:C:178:GLN:HB3	1:C:472:ASN:ND2	2.33	0.43
1:E:253:HIS:HA	1:E:491:ALA:HB2	1.99	0.43
1:E:253:HIS:HB3	1:E:489:SER:OG	2.18	0.43
1:A:178:GLN:NE2	1:A:391:VAL:N	2.67	0.43
1:C:295:SER:HA	1:C:322:SER:HA	2.01	0.43
1:C:398:VAL:CB	1:C:400:ILE:HD13	2.43	0.43
1:G:185:ASN:O	1:G:187:ARG:N	2.51	0.43
1:A:169:THR:HG23	1:A:172:THR:H	1.82	0.43
1:A:495:PHE:CG	1:A:498:ILE:HD11	2.54	0.43
1:E:371:VAL:HB	1:E:381:ILE:HB	2.00	0.43
1:A:227:PHE:CD1	1:A:228:ARG:N	2.86	0.43
2:B:578:THR:HG22	2:B:580:SER:H	1.83	0.43
2:B:582:ILE:O	2:B:583:LYS:C	2.56	0.43
1:C:136:LEU:C	1:C:136:LEU:HD12	2.39	0.43
1:C:153:PHE:CE2	1:C:211:THR:HG23	2.54	0.43
1:C:544:GLN:O	1:C:545:MET:C	2.57	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ALA:O	1:C:82:VAL:C	2.57	0.43
1:G:224:VAL:CG1	1:G:225:THR:N	2.81	0.43
2:F:567:ILE:HG13	2:F:568:GLY:N	2.34	0.43
1:G:554:ASP:O	1:G:555:ASP:OD2	2.37	0.43
1:G:274:MET:O	1:G:274:MET:HG3	2.17	0.43
1:A:183:ILE:HG22	1:A:186:TRP:HA	2.00	0.43
1:A:137:PRO:O	1:A:137:PRO:CG	2.65	0.43
1:G:375:LEU:HD23	1:G:376:THR:O	2.19	0.43
1:A:97:SER:O	1:A:99:LYS:N	2.51	0.43
1:C:170:LEU:O	1:C:171:GLU:C	2.57	0.43
1:A:224:VAL:HG13	1:A:515:THR:O	2.18	0.43
1:E:408:LEU:HD12	1:E:461:PHE:CE2	2.53	0.43
1:A:122:PRO:HB3	1:A:209:PRO:CG	2.49	0.43
1:A:253:HIS:CE1	1:A:491:ALA:HB2	2.54	0.43
1:A:538:GLN:OE1	1:A:542:ARG:NH1	2.47	0.43
1:C:442:HIS:O	1:C:443:TYR:HB3	2.17	0.43
1:C:75:ILE:HD12	1:C:535:GLU:HG3	2.00	0.43
2:D:578:THR:HB	2:D:581:VAL:CG2	2.47	0.43
1:C:254:ILE:CG2	1:E:225:THR:HG21	2.48	0.43
1:A:111:LEU:HD13	1:E:448:PRO:HA	2.01	0.43
1:E:537:VAL:HG12	1:E:541:ASN:HD21	1.83	0.43
1:A:532:GLU:HG2	1:E:542:ARG:NH2	2.34	0.43
1:G:122:PRO:HB3	1:G:209:PRO:CG	2.48	0.43
1:G:178:GLN:HA	1:G:468:TYR:OH	2.17	0.43
1:C:299:LEU:HA	1:C:300:PRO:HD3	1.92	0.43
1:A:407:ARG:O	1:A:408:LEU:HD23	2.19	0.43
1:E:130:THR:OG1	1:E:163:ILE:HG12	2.18	0.43
1:A:240:ALA:O	1:A:241:PRO:C	2.57	0.43
1:E:470:PRO:C	1:E:472:ASN:N	2.70	0.43
1:G:74:SER:O	1:G:75:ILE:HG23	2.19	0.43
1:C:431:LEU:HD23	1:C:431:LEU:HA	1.90	0.43
1:E:396:VAL:HG12	1:E:397:THR:N	2.32	0.43
1:E:555:ASP:O	1:E:556:ASN:O	2.37	0.43
1:G:142:LEU:HB3	1:G:499:SER:HA	2.01	0.43
1:G:217:ILE:HG23	1:G:319:LYS:HZ2	1.84	0.43
1:E:249:TRP:HB3	1:E:495:PHE:CD2	2.54	0.43
1:E:291:ARG:HG2	1:E:291:ARG:O	2.18	0.43
1:A:108:PRO:HG2	1:A:537:VAL:HG12	2.01	0.43
1:C:144:ARG:O	1:C:161:ALA:HA	2.19	0.43
1:C:234:ILE:HG22	1:C:508:THR:HB	2.00	0.43
1:C:246:GLN:HE22	1:C:499:SER:CB	2.31	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:SER:O	1:C:371:VAL:HA	2.19	0.43
1:C:229:LYS:CB	1:C:485:GLU:HG3	2.49	0.43
1:C:74:SER:C	1:C:75:ILE:HG23	2.39	0.43
1:E:174:ASN:OD1	1:E:468:TYR:HA	2.19	0.43
1:A:475:LEU:HA	1:A:475:LEU:HD12	1.76	0.43
1:A:269:PHE:CE1	1:A:399:GLY:HA2	2.54	0.43
1:A:171:GLU:O	1:A:172:THR:C	2.55	0.43
1:G:304:VAL:CG1	1:G:323:VAL:HG21	2.46	0.43
1:E:245:ASP:N	1:E:245:ASP:OD1	2.52	0.43
1:C:187:ARG:C	1:C:189:LEU:N	2.71	0.43
1:C:230:VAL:O	1:C:231:TYR:HB3	2.19	0.43
2:D:579:PRO:HG2	1:E:535:GLU:CD	2.38	0.43
1:E:109:ASP:O	1:E:110:GLY:C	2.56	0.43
1:E:117:ASP:O	1:E:118:ALA:HB2	2.19	0.43
1:E:304:VAL:HA	1:E:334:THR:O	2.19	0.43
1:G:130:THR:HG22	1:G:282:ILE:HG21	2.01	0.43
1:G:256:VAL:HG12	1:G:410:ILE:HG23	2.01	0.43
1:E:87:LYS:NZ	1:E:95:VAL:CG2	2.81	0.43
1:G:339:ALA:O	1:G:341:ILE:HG13	2.18	0.43
1:E:248:TRP:CZ3	1:E:250:VAL:HG23	2.53	0.43
1:C:360:THR:HB	1:C:368:VAL:HG11	1.99	0.43
1:G:48:LEU:HD22	1:G:54:VAL:HG21	2.01	0.43
1:A:116:VAL:HG22	1:A:526:ALA:HB2	2.01	0.43
1:A:537:VAL:O	1:A:538:GLN:C	2.57	0.43
1:A:85:PHE:CE2	2:B:565:ALA:HB1	2.54	0.43
1:A:256:VAL:HG22	1:C:225:THR:CG2	2.49	0.43
1:C:291:ARG:NE	1:C:324:GLU:OE1	2.45	0.43
1:C:370:SER:HB2	1:C:381:ILE:O	2.19	0.43
1:E:228:ARG:CB	1:E:452:MET:CE	2.92	0.43
1:G:522:VAL:O	1:G:525:PHE:N	2.48	0.43
1:A:198:ALA:HB3	1:A:201:TRP:CB	2.35	0.43
1:A:279:SER:OG	1:A:291:ARG:NH2	2.52	0.43
1:A:282:ILE:O	1:A:283:PHE:CB	2.66	0.43
1:A:290:ALA:HB2	1:A:387:LYS:HZ1	1.84	0.43
1:E:79:GLU:HB3	1:E:101:LEU:CD1	2.45	0.43
1:A:435:SER:OG	1:A:552:GLN:HG2	2.19	0.43
1:C:148:ILE:N	1:C:148:ILE:CD1	2.79	0.43
1:E:146:SER:O	1:E:160:LEU:HD23	2.19	0.43
1:A:97:SER:C	1:A:99:LYS:N	2.73	0.43
1:A:152:ALA:HA	1:A:483:THR:O	2.19	0.42
1:C:82:VAL:HB	1:C:101:LEU:HD11	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:MET:HE1	1:C:113:ARG:HB2	2.00	0.42
1:C:142:LEU:O	1:C:143:TRP:CB	2.67	0.42
1:C:451:GLU:HG2	1:C:452:MET:H	1.83	0.42
1:C:88:TYR:OH	1:C:443:TYR:HB2	2.19	0.42
2:D:580:SER:O	2:D:583:LYS:HB3	2.18	0.42
1:G:460:GLY:O	1:G:461:PHE:C	2.57	0.42
1:A:398:VAL:HG12	1:A:399:GLY:N	2.34	0.42
1:E:144:ARG:NH1	1:E:201:TRP:HH2	2.17	0.42
1:C:87:LYS:HE3	1:C:94:ALA:HB3	2.02	0.42
1:G:539:LEU:O	1:G:543:LEU:N	2.52	0.42
2:H:582:ILE:O	2:H:585:ILE:HB	2.19	0.42
1:G:292:ILE:HD13	1:G:325:ILE:O	2.19	0.42
1:G:292:ILE:HG12	1:G:325:ILE:CG1	2.49	0.42
1:A:456:GLU:HG2	1:A:457:ASN:H	1.83	0.42
2:F:593:VAL:CG1	2:F:594:GLN:N	2.81	0.42
1:A:485:GLU:HG3	1:A:487:ASN:H	1.83	0.42
1:A:256:VAL:HG22	1:C:225:THR:HG21	2.00	0.42
1:C:447:ASN:C	1:C:449:VAL:N	2.73	0.42
1:C:503:THR:C	1:C:504:ILE:HD12	2.40	0.42
1:C:82:VAL:O	1:C:83:GLY:C	2.56	0.42
1:E:178:GLN:C	1:E:178:GLN:OE1	2.58	0.42
1:A:359:MET:HA	1:A:369:TYR:HA	2.02	0.42
1:G:87:LYS:HG3	1:G:104:PHE:CD1	2.53	0.42
1:A:375:LEU:CG	1:A:378:SER:HB3	2.49	0.42
1:A:240:ALA:HB2	1:A:502:ALA:HB1	2.00	0.42
1:C:492:VAL:CG1	1:C:494:HIS:NE2	2.81	0.42
1:E:343:ALA:O	1:E:344:GLU:C	2.58	0.42
1:E:267:GLU:O	1:E:401:ASP:OD2	2.37	0.42
1:A:121:ARG:HG2	1:A:509:TYR:CE2	2.54	0.42
1:C:176:PHE:HB2	1:C:197:PHE:CE1	2.53	0.42
1:C:535:GLU:CD	1:C:535:GLU:N	2.71	0.42
1:E:480:ILE:HG22	1:E:481:VAL:N	2.34	0.42
1:G:155:LEU:HD12	1:G:156:ASN:H	1.85	0.42
1:E:116:VAL:HG22	1:G:525:PHE:HE2	1.85	0.42
1:A:405:VAL:HG12	1:A:477:LEU:HD13	2.01	0.42
1:G:442:HIS:H	1:G:442:HIS:CD2	2.37	0.42
2:H:588:GLN:C	2:H:590:VAL:N	2.73	0.42
1:G:274:MET:HA	1:G:296:ILE:HA	2.01	0.42
1:G:276:VAL:HG22	1:G:294:TRP:CD1	2.54	0.42
1:G:299:LEU:HA	1:G:300:PRO:HD3	1.83	0.42
1:E:207:VAL:HB	1:E:212:TYR:CB	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:GLU:HG3	1:E:472:ASN:N	2.34	0.42
1:A:143:TRP:HB2	1:A:162:ASN:O	2.19	0.42
1:C:107:VAL:HG23	1:C:230:VAL:HG22	1.99	0.42
1:E:178:GLN:HE22	1:E:391:VAL:HG23	1.84	0.42
1:E:284:GLN:OE1	1:E:284:GLN:N	2.41	0.42
1:G:154:ARG:O	1:G:208:LEU:HG	2.19	0.42
2:F:567:ILE:HD12	2:F:567:ILE:O	2.20	0.42
1:E:60:ARG:NH2	1:E:64:ASP:OD1	2.52	0.42
1:A:482:ASP:CG	1:A:483:THR:H	2.22	0.42
1:E:178:GLN:CA	1:E:181:ASN:HD22	2.33	0.42
1:G:178:GLN:NE2	1:G:182:ASN:ND2	2.67	0.42
1:G:176:PHE:HB2	1:G:197:PHE:HE1	1.83	0.42
1:G:196:GLN:HG2	1:G:197:PHE:N	2.34	0.42
1:A:370:SER:CB	1:A:381:ILE:O	2.61	0.42
1:G:299:LEU:HD13	1:G:341:ILE:HD11	2.00	0.42
1:E:270:SER:CB	1:E:402:THR:OG1	2.68	0.42
1:C:375:LEU:CB	1:C:378:SER:HB3	2.42	0.42
1:C:248:TRP:CE2	1:G:505:VAL:HG11	2.54	0.42
1:E:160:LEU:N	1:E:160:LEU:CD2	2.82	0.42
1:A:114:TYR:HA	1:A:528:THR:HA	2.00	0.42
1:E:400:ILE:HG23	1:E:400:ILE:O	2.19	0.42
1:C:272:GLY:HA3	1:C:298:PRO:CG	2.49	0.42
1:A:485:GLU:HG2	1:A:488:PHE:HB2	2.00	0.42
1:C:198:ALA:O	1:C:199:PRO:C	2.58	0.42
1:C:211:THR:HA	1:C:214:MET:SD	2.59	0.42
1:C:241:PRO:HG2	1:C:244:ILE:CG1	2.50	0.42
1:C:140:GLY:HA3	1:G:138:LEU:HD21	2.01	0.42
1:G:177:ILE:CD1	1:G:465:TYR:HB2	2.49	0.42
1:G:194:TRP:HE3	1:G:204:SER:HB2	1.80	0.42
1:G:224:VAL:CG1	1:G:225:THR:H	2.32	0.42
1:E:95:VAL:HG13	1:G:63:MET:CB	2.50	0.42
1:C:287:ASN:HA	1:C:363:THR:C	2.39	0.42
1:G:89:MET:HE2	1:G:543:LEU:HD23	2.02	0.42
1:G:79:GLU:C	1:G:81:ALA:N	2.73	0.42
1:G:263:ILE:O	1:G:404:ALA:HA	2.19	0.42
1:A:349:ALA:HA	1:A:353:ASP:OD2	2.19	0.42
1:C:326:ASP:O	1:C:333:TRP:HZ2	2.02	0.42
1:G:453:THR:HG23	1:G:487:ASN:ND2	2.35	0.42
1:A:83:GLY:HA3	1:A:104:PHE:HB3	2.00	0.42
1:C:187:ARG:C	1:C:189:LEU:H	2.22	0.42
1:C:548:THR:HB	1:C:550:VAL:CG2	2.50	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:LYS:HE3	1:E:115:SER:OG	2.20	0.42
1:E:542:ARG:O	1:E:543:LEU:C	2.57	0.42
1:G:238:PHE:CE2	1:G:240:ALA:HB3	2.55	0.42
1:C:259:GLN:HG2	1:E:406:ASN:HD21	1.84	0.42
1:G:544:GLN:O	1:G:545:MET:C	2.57	0.42
2:D:594:GLN:CD	1:E:41:ALA:CB	2.87	0.42
1:C:306:LEU:HD11	1:C:310:THR:O	2.20	0.42
1:C:238:PHE:CD1	1:C:432:CYS:HB3	2.55	0.42
1:A:329:VAL:HG13	1:A:330:ASN:N	2.31	0.42
1:A:334:THR:CG2	1:A:354:THR:HG22	2.49	0.42
1:A:150:PHE:C	1:A:152:ALA:H	2.22	0.42
1:C:132:SER:C	1:C:134:SER:N	2.73	0.42
1:C:334:THR:HG22	1:C:356:SER:CA	2.49	0.42
1:C:254:ILE:O	1:C:490:SER:O	2.37	0.42
1:C:556:ASN:C	1:C:556:ASN:ND2	2.72	0.42
2:D:565:ALA:C	2:D:567:ILE:N	2.71	0.42
1:E:180:LEU:HD12	1:E:180:LEU:N	2.35	0.42
1:E:524:GLN:HG3	1:E:525:PHE:CD1	2.54	0.42
2:F:583:LYS:O	2:F:587:GLN:HG3	2.19	0.42
1:C:141:LYS:NZ	1:G:133:GLU:O	2.53	0.42
1:G:208:LEU:HA	1:G:209:PRO:HD2	1.68	0.42
1:A:395:PRO:CB	1:C:268:ARG:HB2	2.50	0.42
1:E:424:VAL:HG12	1:E:427:TYR:HB3	2.01	0.42
2:H:562:SER:HA	2:H:565:ALA:CB	2.49	0.42
1:A:164:ASN:C	1:A:166:GLU:N	2.73	0.42
1:A:85:PHE:O	1:A:89:MET:HG2	2.19	0.42
1:C:194:TRP:CZ3	1:C:204:SER:OG	2.72	0.42
1:E:111:LEU:HD23	1:E:228:ARG:NH2	2.35	0.42
1:E:272:GLY:CA	1:E:298:PRO:HD3	2.50	0.42
1:G:196:GLN:HB2	1:G:202:TYR:CD2	2.54	0.42
1:E:43:ILE:HG22	1:E:44:LEU:N	2.34	0.42
2:H:580:SER:O	2:H:581:VAL:C	2.58	0.42
1:E:134:SER:HB3	1:E:139:ASP:HB2	2.02	0.42
1:G:313:THR:HA	1:G:325:ILE:HG22	2.02	0.42
1:G:307:THR:N	1:G:332:VAL:O	2.53	0.42
1:E:548:THR:C	1:E:550:VAL:H	2.21	0.42
2:F:584:GLY:O	2:F:588:GLN:HB2	2.20	0.42
1:C:553:ALA:C	1:C:555:ASP:N	2.73	0.42
1:E:82:VAL:O	1:E:83:GLY:C	2.57	0.42
1:E:65:PRO:HA	1:E:66:PRO:HD2	1.74	0.42
2:F:570:GLY:O	2:F:573:GLY:N	2.53	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:GLY:C	1:E:475:LEU:HD12	2.41	0.42
1:G:138:LEU:HD22	1:G:244:ILE:HD11	2.02	0.42
1:G:282:ILE:O	1:G:283:PHE:HB2	2.19	0.42
1:A:357:PHE:CE1	1:A:369:TYR:HB2	2.55	0.42
1:E:197:PHE:HD2	1:E:203:TYR:CD2	2.38	0.42
1:E:93:GLY:C	1:E:97:SER:HB2	2.39	0.42
1:C:87:LYS:O	1:C:91:PRO:CD	2.63	0.42
1:G:280:ASN:HD22	1:G:280:ASN:H	1.62	0.42
1:A:239:ASN:OD1	1:A:503:THR:OG1	2.38	0.42
1:A:180:LEU:HA	1:A:183:ILE:HG13	2.01	0.42
1:C:313:THR:CG2	1:C:314:ASN:N	2.82	0.42
1:A:185:ASN:O	1:A:187:ARG:N	2.53	0.42
1:G:350:GLU:HG3	1:G:375:LEU:HD12	2.01	0.42
2:H:572:LEU:O	2:H:574:LYS:N	2.52	0.42
1:E:149:SER:OG	1:E:442:HIS:CE1	2.73	0.42
2:F:569:LEU:HD13	2:F:569:LEU:C	2.40	0.42
1:C:297:THR:CB	1:C:298:PRO:CD	2.98	0.41
1:A:74:SER:O	1:A:75:ILE:CB	2.65	0.41
1:C:499:SER:O	1:C:502:ALA:N	2.47	0.41
2:D:562:SER:O	2:D:565:ALA:HB3	2.20	0.41
1:E:304:VAL:HG22	1:E:321:PHE:HE1	1.85	0.41
1:G:143:TRP:CD1	1:G:498:ILE:HG22	2.54	0.41
1:G:162:ASN:HB2	1:G:201:TRP:CD2	2.55	0.41
1:G:444:LYS:O	1:G:444:LYS:CD	2.68	0.41
1:G:464:HIS:ND1	1:G:464:HIS:C	2.73	0.41
1:C:313:THR:OG1	1:C:333:TRP:CD1	2.73	0.41
1:A:249:TRP:HB3	1:A:495:PHE:CD2	2.55	0.41
1:C:148:ILE:HG12	1:C:412:MET:CE	2.50	0.41
1:E:232:LYS:HG2	1:E:442:HIS:HD2	1.85	0.41
1:C:174:ASN:OD1	1:C:468:TYR:HA	2.19	0.41
1:E:114:TYR:CD1	1:E:114:TYR:C	2.93	0.41
1:A:542:ARG:NE	2:B:583:LYS:HA	2.32	0.41
1:C:450:PHE:C	1:C:451:GLU:O	2.57	0.41
1:E:393:ILE:HG22	1:E:395:PRO:HD3	2.01	0.41
1:E:539:LEU:O	1:E:540:ALA:C	2.58	0.41
1:G:208:LEU:O	1:G:210:ASN:N	2.52	0.41
1:G:444:LYS:O	1:G:444:LYS:HD3	2.20	0.41
1:C:306:LEU:HA	1:C:333:TRP:HA	2.03	0.41
1:G:292:ILE:CG1	1:G:325:ILE:HG13	2.50	0.41
1:A:235:THR:HG23	1:A:507:LYS:CB	2.50	0.41
1:A:118:ALA:HB3	1:A:512:TRP:CE2	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:LEU:O	1:G:245:ASP:OD1	2.38	0.41
1:C:394:THR:O	1:C:395:PRO:C	2.57	0.41
1:A:230:VAL:O	1:A:231:TYR:CB	2.68	0.41
1:A:543:LEU:O	1:A:547:LEU:HB2	2.21	0.41
1:C:176:PHE:O	1:C:177:ILE:C	2.59	0.41
1:C:232:LYS:O	1:C:233:GLY:O	2.37	0.41
1:C:235:THR:HG22	1:C:439:TYR:CG	2.54	0.41
1:C:245:ASP:O	1:C:247:GLY:N	2.54	0.41
1:C:421:THR:HG21	1:G:123:ILE:CG1	2.49	0.41
1:E:276:VAL:HG11	1:E:369:TYR:CE2	2.55	0.41
1:C:448:PRO:CG	1:E:449:VAL:CG1	2.98	0.41
1:E:522:VAL:O	1:E:525:PHE:N	2.50	0.41
1:G:163:ILE:C	1:G:165:ASN:N	2.74	0.41
1:E:90:ASP:HB2	2:F:561:VAL:CG1	2.51	0.41
1:G:281:ALA:HB3	1:G:284:GLN:CG	2.29	0.41
1:G:110:GLY:H	1:G:531:GLU:C	2.24	0.41
1:A:193:GLN:HG2	1:A:194:TRP:O	2.20	0.41
1:E:217:ILE:HD13	1:E:217:ILE:H	1.85	0.41
1:A:539:LEU:O	1:A:540:ALA:C	2.59	0.41
2:B:583:LYS:HE2	2:B:583:LYS:HB3	1.89	0.41
1:C:106:LYS:HE3	1:C:115:SER:HG	1.83	0.41
1:C:107:VAL:O	1:C:530:ALA:HB3	2.21	0.41
1:C:450:PHE:O	1:C:451:GLU:O	2.39	0.41
1:A:532:GLU:HB3	1:E:542:ARG:NH1	2.36	0.41
1:C:405:VAL:HG13	1:C:406:ASN:N	2.35	0.41
1:E:63:MET:CE	1:G:101:LEU:HD23	2.50	0.41
1:A:248:TRP:CZ3	1:A:250:VAL:CG2	3.04	0.41
1:A:131:VAL:CG2	1:A:500:GLN:HB3	2.49	0.41
1:A:293:VAL:HG22	1:A:324:GLU:CG	2.51	0.41
1:C:539:LEU:O	1:C:540:ALA:C	2.59	0.41
1:C:106:LYS:HG3	1:C:117:ASP:CB	2.49	0.41
1:A:113:ARG:NH2	1:E:443:TYR:HD2	2.17	0.41
1:E:474:ALA:HB1	1:E:478:ARG:HH11	1.86	0.41
1:G:133:GLU:N	1:G:283:PHE:CE2	2.66	0.41
1:A:178:GLN:O	1:A:182:ASN:ND2	2.54	0.41
1:A:289:VAL:HG13	1:A:327:GLY:CA	2.50	0.41
1:G:84:TRP:NE1	1:G:230:VAL:HG12	2.35	0.41
2:H:582:ILE:O	2:H:583:LYS:C	2.59	0.41
1:A:460:GLY:CA	1:A:481:VAL:HG22	2.50	0.41
2:F:607:ILE:CA	2:F:610:VAL:HG23	2.49	0.41
1:G:469:ASP:C	1:G:471:GLU:N	2.72	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:614:LEU:HD23	2:F:617:SER:OG	2.21	0.41
1:G:150:PHE:O	1:G:152:ALA:N	2.48	0.41
1:A:158:ILE:HG22	1:A:159:ALA:N	2.35	0.41
1:A:156:ASN:ND2	1:A:508:THR:HG21	2.36	0.41
2:D:565:ALA:O	2:D:567:ILE:N	2.54	0.41
1:E:274:MET:HE2	1:E:294:TRP:NE1	2.32	0.41
1:E:534:ASP:HA	1:E:537:VAL:HB	2.02	0.41
1:G:237:GLU:HB2	1:G:507:LYS:HE3	2.01	0.41
1:A:299:LEU:HD11	1:A:338:PRO:HD2	2.02	0.41
1:A:369:TYR:OH	1:A:392:SER:HB3	2.20	0.41
1:E:195:ALA:O	1:E:203:TYR:CD2	2.73	0.41
1:C:286:SER:O	1:C:364:ALA:HA	2.21	0.41
1:E:554:ASP:O	2:F:557:PHE:N	2.54	0.41
1:G:332:VAL:CG2	1:G:358:SER:HB2	2.49	0.41
1:G:412:MET:SD	1:G:413:PRO:CD	3.04	0.41
1:C:250:VAL:CG2	1:C:429:GLN:HB3	2.50	0.41
1:E:149:SER:OG	1:E:442:HIS:NE2	2.43	0.41
2:B:563:ALA:C	2:B:565:ALA:N	2.73	0.41
1:C:181:ASN:OD1	1:C:463:PHE:N	2.53	0.41
1:E:253:HIS:HD2	1:E:549:GLY:CA	2.27	0.41
1:E:304:VAL:CG2	1:E:321:PHE:HE1	2.33	0.41
1:E:306:LEU:HD21	1:E:309:GLY:O	2.20	0.41
1:A:217:ILE:HD11	1:E:465:TYR:O	2.21	0.41
1:G:137:PRO:HG2	1:G:140:GLY:HA3	2.03	0.41
1:G:174:ASN:O	1:G:175:THR:C	2.59	0.41
1:A:182:ASN:OD1	1:A:474:ALA:N	2.53	0.41
1:A:410:ILE:O	1:A:463:PHE:HA	2.20	0.41
2:F:562:SER:O	2:F:566:SER:HB2	2.19	0.41
1:C:363:THR:CG2	1:C:365:ASP:H	2.12	0.41
1:C:363:THR:HG21	1:C:365:ASP:OD2	2.20	0.41
1:C:366:THR:HA	1:C:386:THR:HA	2.01	0.41
1:G:429:GLN:C	1:G:430:PHE:CD1	2.94	0.41
1:G:449:VAL:HG22	1:G:450:PHE:H	1.86	0.41
1:G:537:VAL:O	1:G:538:GLN:C	2.59	0.41
1:G:263:ILE:O	1:G:263:ILE:HG22	2.20	0.41
1:E:250:VAL:CG1	1:E:427:TYR:CD2	3.03	0.41
1:A:420:VAL:HG21	1:A:494:HIS:CD2	2.56	0.41
1:C:90:ASP:O	1:C:92:ALA:N	2.54	0.41
1:A:334:THR:HG23	1:A:355:THR:O	2.21	0.41
1:A:348:PHE:CZ	1:A:372:SER:HA	2.55	0.41
1:C:297:THR:CG2	1:C:298:PRO:HD3	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LYS:CG	1:A:117:ASP:HB3	2.50	0.41
1:A:267:GLU:HG2	1:E:475:LEU:HD11	2.03	0.41
1:A:447:ASN:OD1	1:A:447:ASN:C	2.59	0.41
1:C:177:ILE:O	1:C:181:ASN:ND2	2.48	0.41
1:C:453:THR:HG22	1:C:485:GLU:OE1	2.20	0.41
1:C:446:ASN:ND2	1:E:226:GLN:OE1	2.54	0.41
1:E:296:ILE:HB	1:E:321:PHE:HD2	1.86	0.41
1:G:197:PHE:CG	1:G:198:ALA:N	2.89	0.41
1:A:262:THR:HG22	1:A:263:ILE:N	2.36	0.41
1:E:79:GLU:CB	1:E:101:LEU:HD12	2.44	0.41
2:F:564:LEU:C	2:F:564:LEU:HD23	2.41	0.41
1:C:362:ILE:O	1:C:362:ILE:CG2	2.69	0.41
1:G:248:TRP:CD1	1:G:431:LEU:CD2	2.97	0.41
1:G:249:TRP:NE1	1:G:430:PHE:HB2	2.35	0.41
1:G:537:VAL:HG12	1:G:541:ASN:ND2	2.36	0.41
1:G:552:GLN:O	1:G:554:ASP:N	2.49	0.41
1:A:422:THR:O	1:A:422:THR:CG2	2.67	0.41
1:C:413:PRO:HB2	1:C:492:VAL:CG2	2.50	0.41
1:A:162:ASN:HA	1:A:200:GLY:O	2.19	0.41
2:F:569:LEU:O	2:F:569:LEU:HD13	2.20	0.41
1:G:150:PHE:HB3	1:G:484:PHE:CE1	2.56	0.41
1:G:400:ILE:HG12	1:G:401:ASP:N	2.35	0.41
1:C:297:THR:CG2	1:C:298:PRO:CD	2.97	0.41
1:A:485:GLU:C	1:A:487:ASN:N	2.74	0.41
2:B:582:ILE:O	2:B:585:ILE:HB	2.21	0.41
1:C:453:THR:CG2	1:C:485:GLU:OE1	2.68	0.41
1:E:460:GLY:HA2	1:E:480:ILE:O	2.20	0.41
1:E:535:GLU:OE2	2:F:577:ALA:HB3	2.21	0.41
1:A:151:PRO:HB2	1:A:485:GLU:CB	2.44	0.41
1:C:117:ASP:N	1:C:117:ASP:OD2	2.53	0.41
1:C:210:ASN:O	1:C:214:MET:HG3	2.20	0.41
1:C:535:GLU:O	1:C:538:GLN:HB3	2.19	0.41
1:E:116:VAL:HG22	1:E:117:ASP:N	2.36	0.41
1:E:182:ASN:O	1:E:478:ARG:HD3	2.21	0.41
1:G:160:LEU:HD11	1:G:201:TRP:CZ3	2.56	0.41
1:A:325:ILE:HB	1:A:333:TRP:CE2	2.56	0.41
1:A:359:MET:CE	1:A:367:VAL:HG11	2.51	0.41
1:C:89:MET:HB2	1:C:89:MET:HE2	1.83	0.41
1:C:266:ALA:HB3	1:C:270:SER:CB	2.47	0.41
1:C:429:GLN:HE22	1:E:58:GLY:C	2.24	0.41
1:E:235:THR:O	1:E:506:CYS:HA	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:ASP:OD2	1:C:471:GLU:CB	2.69	0.41
1:C:342:LEU:HD23	1:C:347:PRO:HA	2.02	0.41
1:E:354:THR:H	1:E:374:SER:HG	1.59	0.41
1:E:528:THR:HG22	1:E:529:GLY:N	2.35	0.41
1:A:436:GLY:N	1:A:554:ASP:OD1	2.54	0.41
1:C:481:VAL:O	1:C:481:VAL:HG12	2.19	0.41
1:A:425:PRO:HG3	1:C:526:ALA:O	2.21	0.41
1:A:267:GLU:HG2	1:E:475:LEU:HG	2.03	0.41
1:A:545:MET:C	1:A:547:LEU:N	2.75	0.41
1:A:542:ARG:HD2	2:B:582:ILE:HG22	2.02	0.41
1:C:213:ALA:O	1:C:215:ALA:N	2.54	0.41
1:C:241:PRO:O	1:C:242:THR:C	2.60	0.41
1:C:253:HIS:CE1	1:C:442:HIS:HA	2.56	0.41
1:C:445:MET:O	1:C:445:MET:CG	2.67	0.41
1:C:178:GLN:HB3	1:C:472:ASN:HD21	1.85	0.41
1:C:145:VAL:CG1	1:C:495:PHE:HB2	2.50	0.41
1:E:177:ILE:O	1:E:179:THR:N	2.54	0.41
1:G:182:ASN:OD1	1:G:474:ALA:N	2.54	0.41
1:A:178:GLN:HE22	1:A:390:GLY:HA2	1.84	0.41
1:C:87:LYS:HZ1	1:C:95:VAL:HG23	1.85	0.41
2:F:557:PHE:O	2:F:558:ALA:C	2.57	0.41
1:G:362:ILE:HG22	1:G:367:VAL:CG1	2.41	0.41
1:G:541:ASN:C	1:G:543:LEU:N	2.75	0.41
1:C:296:ILE:HD12	1:C:299:LEU:HD22	2.03	0.41
1:G:269:PHE:CB	1:G:397:THR:HG23	2.51	0.41
1:G:265:ALA:HB2	1:G:404:ALA:HB2	2.01	0.41
1:E:120:GLN:C	1:E:122:PRO:HD2	2.40	0.41
1:A:248:TRP:NE1	1:A:496:TRP:CE3	2.85	0.41
1:A:455:GLU:C	1:E:259:GLN:HG2	2.42	0.41
2:B:581:VAL:CG1	2:B:585:ILE:HD11	2.50	0.40
1:C:251:GLY:O	1:C:252:ALA:HB2	2.21	0.40
1:C:439:TYR:CD2	1:C:556:ASN:HA	2.55	0.40
1:G:121:ARG:HH11	1:G:121:ARG:CG	2.28	0.40
1:G:142:LEU:C	1:G:165:ASN:ND2	2.75	0.40
1:G:183:ILE:HG21	1:G:186:TRP:HA	2.03	0.40
1:G:172:THR:HG21	1:G:201:TRP:CE2	2.57	0.40
1:G:174:ASN:ND2	1:G:468:TYR:HD1	2.12	0.40
1:G:275:THR:HG23	1:G:478:ARG:NH1	2.36	0.40
1:A:198:ALA:CB	1:A:199:PRO:HD2	2.33	0.40
1:A:201:TRP:C	1:A:202:TYR:CD1	2.94	0.40
1:A:181:ASN:O	1:A:478:ARG:HB2	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:GLN:C	1:E:554:ASP:N	2.74	0.40
1:G:386:THR:O	1:G:387:LYS:C	2.59	0.40
1:C:435:SER:C	1:C:437:GLY:N	2.74	0.40
1:G:453:THR:HG21	1:G:486:ASN:N	2.36	0.40
2:H:564:LEU:C	2:H:566:SER:N	2.73	0.40
2:H:568:GLY:O	2:H:569:LEU:C	2.58	0.40
1:A:255:PRO:HB3	1:A:445:MET:SD	2.61	0.40
1:A:82:VAL:O	1:A:85:PHE:HB3	2.21	0.40
1:C:101:LEU:HD12	1:C:101:LEU:O	2.22	0.40
1:E:278:ALA:HB2	1:E:385:VAL:CG2	2.45	0.40
1:E:275:THR:HG22	1:E:478:ARG:HH22	1.86	0.40
1:G:164:ASN:HD21	1:G:166:GLU:CD	2.25	0.40
1:A:412:MET:HG2	1:A:463:PHE:CB	2.50	0.40
1:A:412:MET:HA	1:A:413:PRO:HD2	1.81	0.40
1:E:40:GLN:N	1:E:71:CYS:HB2	2.36	0.40
1:A:148:ILE:HG23	1:A:492:VAL:HG12	2.02	0.40
2:F:605:LYS:HG2	2:F:610:VAL:HG21	2.03	0.40
1:G:380:VAL:HG12	1:G:381:ILE:N	2.36	0.40
1:E:342:LEU:O	1:E:343:ALA:CB	2.68	0.40
1:G:420:VAL:O	1:G:422:THR:N	2.55	0.40
2:B:565:ALA:O	2:B:566:SER:C	2.59	0.40
2:B:580:SER:HB2	1:C:75:ILE:HG22	2.03	0.40
1:C:164:ASN:HD21	1:C:200:GLY:HA3	1.81	0.40
1:C:209:PRO:HG2	1:C:210:ASN:OD1	2.21	0.40
1:C:277:SER:OG	1:C:293:VAL:HB	2.22	0.40
1:E:272:GLY:HA2	1:E:297:THR:CG2	2.51	0.40
1:E:228:ARG:CG	1:E:452:MET:HE1	2.50	0.40
1:G:156:ASN:HB2	1:G:208:LEU:CD2	2.49	0.40
1:G:158:ILE:HG22	1:G:159:ALA:O	2.22	0.40
1:G:282:ILE:HG22	1:G:283:PHE:CD1	2.57	0.40
1:G:522:VAL:O	1:G:523:GLY:C	2.58	0.40
1:G:526:ALA:O	1:G:527:HIS:HB3	2.21	0.40
1:A:198:ALA:HB3	1:A:201:TRP:CD1	2.56	0.40
1:C:87:LYS:HZ1	1:C:95:VAL:CG2	2.34	0.40
1:G:542:ARG:HD3	2:H:583:LYS:HA	2.02	0.40
1:G:185:ASN:HD21	1:G:320:PHE:H	1.70	0.40
1:G:299:LEU:HD23	1:G:321:PHE:CB	2.51	0.40
1:G:185:ASN:HD21	1:G:320:PHE:HB2	1.86	0.40
1:G:397:THR:O	1:G:397:THR:HG22	2.21	0.40
1:G:49:LEU:HB2	1:G:52:GLU:CG	2.45	0.40
1:E:191:THR:OG1	1:E:193:GLN:HG2	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:SER:CB	1:C:381:ILE:O	2.70	0.40
1:C:85:PHE:HE2	2:D:565:ALA:HB1	1.86	0.40
1:E:412:MET:O	1:E:465:TYR:CE1	2.74	0.40
1:E:484:PHE:O	1:E:486:ASN:N	2.55	0.40
2:F:578:THR:O	2:F:580:SER:N	2.55	0.40
1:G:133:GLU:O	1:G:135:ASP:N	2.55	0.40
1:G:183:ILE:CG2	1:G:186:TRP:HA	2.50	0.40
1:E:169:THR:HB	1:E:172:THR:CB	2.49	0.40
2:F:588:GLN:HG3	2:F:594:GLN:HB3	2.03	0.40
1:A:451:GLU:HG3	1:E:447:ASN:OD1	2.21	0.40
1:A:445:MET:O	1:C:111:LEU:HD11	2.21	0.40
1:C:421:THR:HB	1:G:121:ARG:O	2.21	0.40
1:A:262:THR:HG23	1:A:406:ASN:HB3	2.03	0.40
1:G:70:ILE:HD12	1:G:82:VAL:HG21	2.03	0.40
2:H:582:ILE:O	2:H:585:ILE:N	2.53	0.40
2:D:594:GLN:CG	1:E:41:ALA:HB1	2.52	0.40
1:E:250:VAL:HG13	1:E:427:TYR:CD2	2.56	0.40
1:E:429:GLN:C	1:E:429:GLN:CD	2.79	0.40
1:A:528:THR:OG1	1:E:426:LYS:NZ	2.54	0.40
1:E:528:THR:CG2	1:E:529:GLY:N	2.84	0.40
1:C:510:ASP:OD1	1:C:511:GLY:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	A	482/556 (87%)	357 (74%)	80 (17%)	45 (9%)	1	15
1	C	482/556 (87%)	358 (74%)	74 (15%)	50 (10%)	1	12
1	E	515/556 (93%)	379 (74%)	95 (18%)	41 (8%)	1	19
1	G	516/556 (93%)	373 (72%)	87 (17%)	56 (11%)	0	11

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	37/75 (49%)	21 (57%)	12 (32%)	4 (11%)	0	11
2	D	38/75 (51%)	30 (79%)	6 (16%)	2 (5%)	2	30
2	F	65/75 (87%)	47 (72%)	12 (18%)	6 (9%)	1	16
2	H	36/75 (48%)	16 (44%)	16 (44%)	4 (11%)	0	10
All	All	2171/2524 (86%)	1581 (73%)	382 (18%)	208 (10%)	1	14

All (208) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	PRO
1	A	297	THR
1	A	318	GLY
1	A	405	VAL
1	A	455	GLU
1	A	474	ALA
1	C	209	PRO
1	C	260	SER
1	C	286	SER
1	C	351	GLU
1	C	486	ASN
1	C	536	VAL
1	E	223	SER
1	E	395	PRO
1	E	475	LEU
1	E	476	GLY
1	E	537	VAL
2	F	577	ALA
2	F	618	ILE
1	G	133	GLU
1	G	135	ASP
1	G	387	LYS
1	G	475	LEU
1	G	476	GLY
1	G	528	THR
1	A	129	PRO
1	A	214	MET
1	A	231	TYR
1	A	282	ILE
1	A	311	GLY
1	A	414	ALA
1	A	418	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	436	GLY
1	A	534	ASP
1	A	538	GLN
1	A	540	ALA
1	A	554	ASP
2	B	576	SER
2	B	582	ILE
1	C	143	TRP
1	C	176	PHE
1	C	177	ILE
1	C	210	ASN
1	C	218	GLY
1	C	225	THR
1	C	233	GLY
1	C	353	ASP
1	C	436	GLY
1	C	444	LYS
1	C	451	GLU
1	C	485	GLU
1	C	523	GLY
1	E	66	PRO
1	E	110	GLY
1	E	132	SER
1	E	140	GLY
1	E	209	PRO
1	E	434	GLU
1	E	436	GLY
1	E	444	LYS
1	E	485	GLU
2	F	602	GLY
1	G	56	PRO
1	G	57	SER
1	G	110	GLY
1	G	126	ILE
1	G	289	VAL
1	G	329	VAL
1	G	420	VAL
1	G	421	THR
1	G	436	GLY
1	G	454	GLY
1	G	456	GLU
1	G	482	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	590	VAL
1	A	186	TRP
1	A	351	GLU
1	A	422	THR
1	A	446	ASN
1	A	456	GLU
1	A	545	MET
1	A	546	GLU
2	B	572	LEU
2	B	589	ALA
1	C	126	ILE
1	C	184	THR
1	C	214	MET
1	C	242	THR
1	C	250	VAL
1	C	285	PRO
1	C	287	ASN
1	C	414	ALA
1	C	450	PHE
1	C	488	PHE
1	C	532	GLU
1	C	554	ASP
2	D	572	LEU
1	E	50	PRO
1	E	91	PRO
1	E	177	ILE
1	E	199	PRO
1	E	231	TYR
1	E	242	THR
1	E	316	THR
1	E	329	VAL
1	E	343	ALA
1	E	375	LEU
1	E	417	THR
1	E	455	GLU
1	E	519	GLY
1	E	523	GLY
1	E	534	ASP
2	F	620	ALA
1	G	85	PHE
1	G	160	LEU
1	G	182	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	186	TRP
1	G	197	PHE
1	G	209	PRO
1	G	231	TYR
1	G	244	ILE
1	G	285	PRO
1	G	286	SER
1	G	486	ASN
1	G	527	HIS
2	H	573	GLY
1	A	85	PHE
1	A	115	SER
1	A	170	LEU
1	A	177	ILE
1	A	178	GLN
1	A	184	THR
1	A	210	ASN
1	A	264	PRO
1	A	486	ASN
1	C	88	TYR
1	C	91	PRO
1	C	231	TYR
1	C	252	ALA
1	C	305	ALA
1	C	425	PRO
1	C	501	SER
2	D	564	LEU
1	E	64	ASP
1	E	94	ALA
1	E	226	GLN
2	F	596	ASN
1	G	91	PRO
1	G	141	LYS
1	G	219	ASP
1	G	245	ASP
1	G	303	THR
1	G	443	TYR
1	G	544	GLN
2	H	577	ALA
1	A	75	ILE
1	A	134	SER
1	A	173	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	285	PRO
1	A	387	LYS
1	C	82	VAL
1	C	139	ASP
1	C	162	ASN
1	C	199	PRO
1	C	318	GLY
1	C	534	ASP
1	E	103	GLU
1	E	118	ALA
1	E	297	THR
1	E	451	GLU
1	E	536	VAL
1	E	553	ALA
1	G	73	GLN
1	G	82	VAL
1	G	84	TRP
1	G	118	ALA
1	G	134	SER
1	G	164	ASN
1	G	165	ASN
1	G	217	ILE
1	G	297	THR
1	G	318	GLY
1	G	388	GLY
1	G	523	GLY
1	G	553	ALA
1	A	77	PRO
1	A	280	ASN
1	A	524	GLN
1	C	297	THR
2	F	558	ALA
1	G	334	THR
1	G	537	VAL
1	A	217	ILE
1	A	345	GLY
1	E	467	GLY
1	G	163	ILE
1	G	208	LEU
1	E	298	PRO
1	G	466	PRO
1	A	98	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	311	GLY
1	C	312	GLY
1	C	347	PRO
1	E	121	ARG
1	C	98	GLY
1	C	129	PRO
1	G	276	VAL
2	H	581	VAL

### 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	A	403/466 (86%)	339 (84%)	64 (16%)	3	23
1	C	403/466 (86%)	348 (86%)	55 (14%)	5	30
1	E	429/466 (92%)	385 (90%)	44 (10%)	9	42
1	G	430/466 (92%)	376 (87%)	54 (13%)	5	32
2	B	25/49 (51%)	22 (88%)	3 (12%)	6	34
2	D	26/49 (53%)	21 (81%)	5 (19%)	2	13
2	F	43/49 (88%)	36 (84%)	7 (16%)	3	21
2	H	25/49 (51%)	21 (84%)	4 (16%)	3	22
All	All	1784/2060 (87%)	1548 (87%)	236 (13%)	5	31

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	79	GLU
1	A	113	ARG
1	A	121	ARG
1	A	124	VAL
1	A	127	GLU
1	A	136	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	142	LEU
1	A	160	LEU
1	A	163	ILE
1	A	165	ASN
1	A	171	GLU
1	A	178	GLN
1	A	181	ASN
1	A	184	THR
1	A	191	THR
1	A	193	GLN
1	A	204	SER
1	A	207	VAL
1	A	210	ASN
1	A	221	THR
1	A	225	THR
1	A	228	ARG
1	A	231	TYR
1	A	235	THR
1	A	243	LEU
1	A	246	GLN
1	A	258	PRO
1	A	261	GLU
1	A	264	PRO
1	A	282	ILE
1	A	284	GLN
1	A	294	TRP
1	A	295	SER
1	A	307	THR
1	A	310	THR
1	A	315	ASN
1	A	329	VAL
1	A	356	SER
1	A	366	THR
1	A	369	TYR
1	A	371	VAL
1	A	382	VAL
1	A	383	ARG
1	A	386	THR
1	A	401	ASP
1	A	402	THR
1	A	403	GLU
1	A	406	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	412	MET
1	A	417	THR
1	A	433	LYS
1	A	443	TYR
1	A	447	ASN
1	A	461	PHE
1	A	486	ASN
1	A	508	THR
1	A	510	ASP
1	A	532	GLU
1	A	534	ASP
1	A	539	LEU
1	A	545	MET
1	A	554	ASP
1	A	556	ASN
2	B	567	ILE
2	B	580	SER
2	B	590	VAL
1	C	75	ILE
1	C	76	ASP
1	C	79	GLU
1	C	96	GLU
1	C	101	LEU
1	C	104	PHE
1	C	113	ARG
1	C	121	ARG
1	C	124	VAL
1	C	127	GLU
1	C	136	LEU
1	C	139	ASP
1	C	154	ARG
1	C	155	LEU
1	C	156	ASN
1	C	160	LEU
1	C	165	ASN
1	C	178	GLN
1	C	204	SER
1	C	234	ILE
1	C	244	ILE
1	C	245	ASP
1	C	246	GLN
1	C	262	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	263	ILE
1	C	267	GLU
1	C	288	THR
1	C	291	ARG
1	C	292	ILE
1	C	315	ASN
1	C	316	THR
1	C	328	ASN
1	C	336	THR
1	C	359	MET
1	C	361	THR
1	C	369	TYR
1	C	371	VAL
1	C	401	ASP
1	C	403	GLU
1	C	405	VAL
1	C	407	ARG
1	C	416	THR
1	C	453	THR
1	C	455	GLU
1	C	457	ASN
1	C	483	THR
1	C	485	GLU
1	C	488	PHE
1	C	501	SER
1	C	525	PHE
1	C	542	ARG
1	C	545	MET
1	C	548	THR
1	C	551	TYR
1	C	556	ASN
2	D	557	PHE
2	D	564	LEU
2	D	574	LYS
2	D	593	VAL
2	D	594	GLN
1	E	48	LEU
1	E	76	ASP
1	E	104	PHE
1	E	114	TYR
1	E	121	ARG
1	E	124	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	157	PHE
1	E	178	GLN
1	E	189	LEU
1	E	194	TRP
1	E	209	PRO
1	E	217	ILE
1	E	223	SER
1	E	243	LEU
1	E	245	ASP
1	E	246	GLN
1	E	255	PRO
1	E	259	GLN
1	E	275	THR
1	E	283	PHE
1	E	292	ILE
1	E	297	THR
1	E	313	THR
1	E	323	VAL
1	E	360	THR
1	E	361	THR
1	E	366	THR
1	E	374	SER
1	E	386	THR
1	E	394	THR
1	E	412	MET
1	E	429	GLN
1	E	430	PHE
1	E	440	ILE
1	E	444	LYS
1	E	452	MET
1	E	462	GLN
1	E	494	HIS
1	E	508	THR
1	E	515	THR
1	E	533	GLU
1	E	548	THR
1	E	551	TYR
1	E	556	ASN
2	F	564	LEU
2	F	567	ILE
2	F	574	LYS
2	F	594	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	F	601	GLU
2	F	605	LYS
2	F	622	ARG
1	G	39	GLU
1	G	57	SER
1	G	63	MET
1	G	79	GLU
1	G	95	VAL
1	G	99	LYS
1	G	121	ARG
1	G	143	TRP
1	G	144	ARG
1	G	168	LEU
1	G	169	THR
1	G	178	GLN
1	G	188	ASP
1	G	189	LEU
1	G	191	THR
1	G	194	TRP
1	G	210	ASN
1	G	217	ILE
1	G	220	ARG
1	G	229	LYS
1	G	269	PHE
1	G	274	MET
1	G	280	ASN
1	G	291	ARG
1	G	292	ILE
1	G	301	VAL
1	G	308	THR
1	G	313	THR
1	G	315	ASN
1	G	355	THR
1	G	356	SER
1	G	371	VAL
1	G	376	THR
1	G	383	ARG
1	G	386	THR
1	G	405	VAL
1	G	417	THR
1	G	429	GLN
1	G	444	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	446	ASN
1	G	456	GLU
1	G	458	PHE
1	G	461	PHE
1	G	464	HIS
1	G	486	ASN
1	G	500	GLN
1	G	508	THR
1	G	524	GLN
1	G	527	HIS
1	G	528	THR
1	G	544	GLN
1	G	545	MET
1	G	546	GLU
1	G	547	LEU
2	H	564	LEU
2	H	571	LEU
2	H	578	THR
2	H	590	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	259	GLN
1	C	120	GLN
1	C	181	ASN
1	C	462	GLN
1	C	464	HIS
1	G	47	GLN
1	G	120	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	3/4 (75%)	3 (100%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	2	U
3	R	3	U
3	R	4	U

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	A	484/556 (87%)	-0.27	1 (0%) 95 91	7, 20, 30, 48	0
1	C	484/556 (87%)	-0.27	0 100 100	8, 19, 30, 43	0
1	E	517/556 (92%)	-0.28	0 100 100	7, 21, 33, 52	0
1	G	518/556 (93%)	-0.28	0 100 100	7, 20, 31, 53	0
2	B	39/75 (52%)	-0.21	0 100 100	10, 20, 36, 40	0
2	D	40/75 (53%)	-0.26	0 100 100	10, 21, 35, 40	0
2	F	67/75 (89%)	-0.16	0 100 100	13, 20, 35, 39	0
2	H	38/75 (50%)	-0.35	0 100 100	11, 18, 29, 38	0
3	R	4/4 (100%)	0.56	0 100 100	54, 56, 57, 61	0
All	All	2191/2528 (86%)	-0.27	1 (0%) 100 100	7, 20, 32, 61	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	SER	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	557	1/1	0.95	0.09	-4.91	44,44,44,44	0
4	CA	G	557	1/1	0.99	0.08	-	73,73,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.