



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 03:49 am BST

PDB ID : 4P69  
Title : Acek (D477A) ICDH complex  
Authors : Jimin, Z.; Nan, W.; Shu, W.; Zongchao, J.  
Deposited on : 2014-03-22  
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

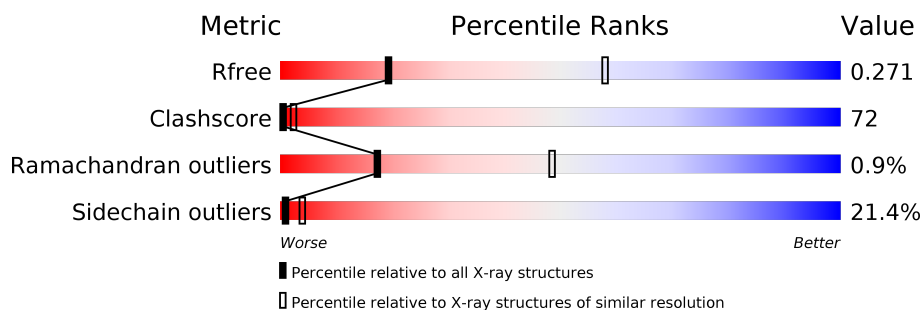
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	568	<div> <div>28%</div> <div>51%</div> <div>18%</div> <div>••</div> </div>
1	B	568	<div> <div>30%</div> <div>53%</div> <div>15%</div> <div>•</div> </div>
2	C	415	<div> <div>37%</div> <div>51%</div> <div>12%</div> </div>
2	D	415	<div> <div>33%</div> <div>53%</div> <div>14%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15755 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 Isocitrate dehydrogenase kinase/phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4575	2946	799	809	21			
1	B	561	Total	C	N	O	S	0	0	0
			4649	2992	815	821	21			

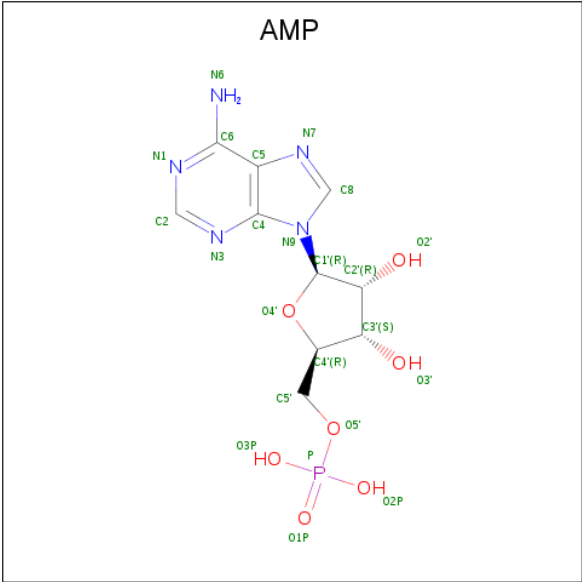
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	477	ALA	ASP	engineered mutation	UNP Q8X607
B	477	ALA	ASP	engineered mutation	UNP Q8X607

- Molecule 2 is a protein called Isocitrate dehydrogenase [NADP].

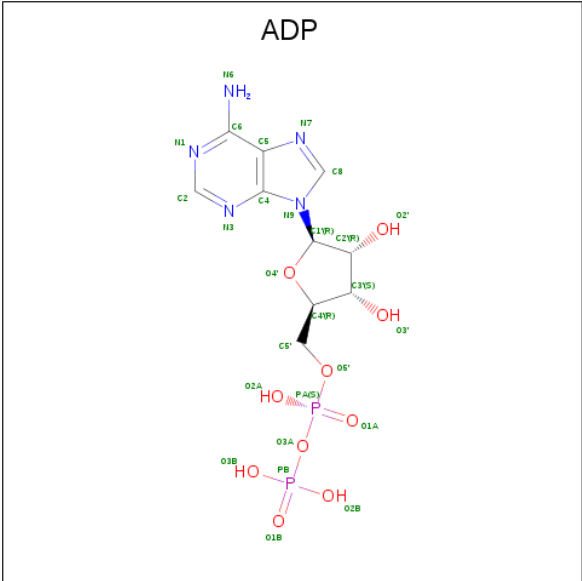
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			
2	D	415	Total	C	N	O	S	0	0	0
			3205	2040	539	608	18			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

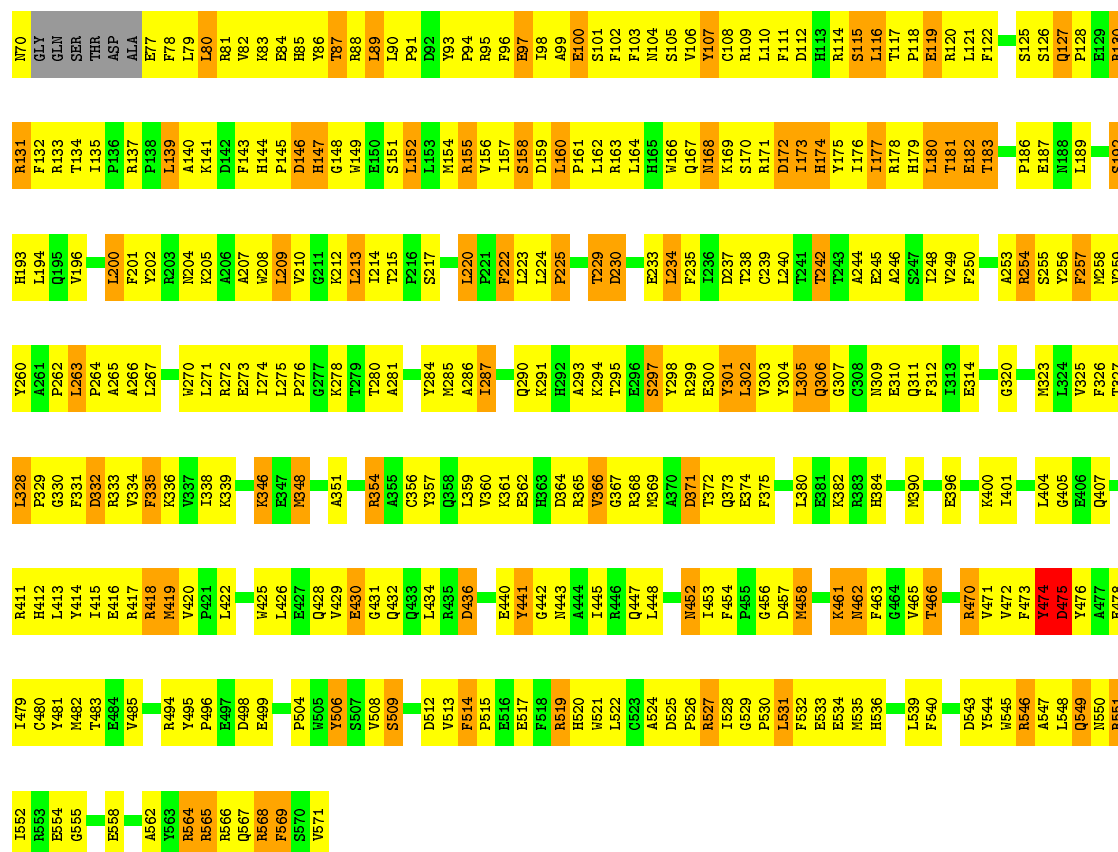
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

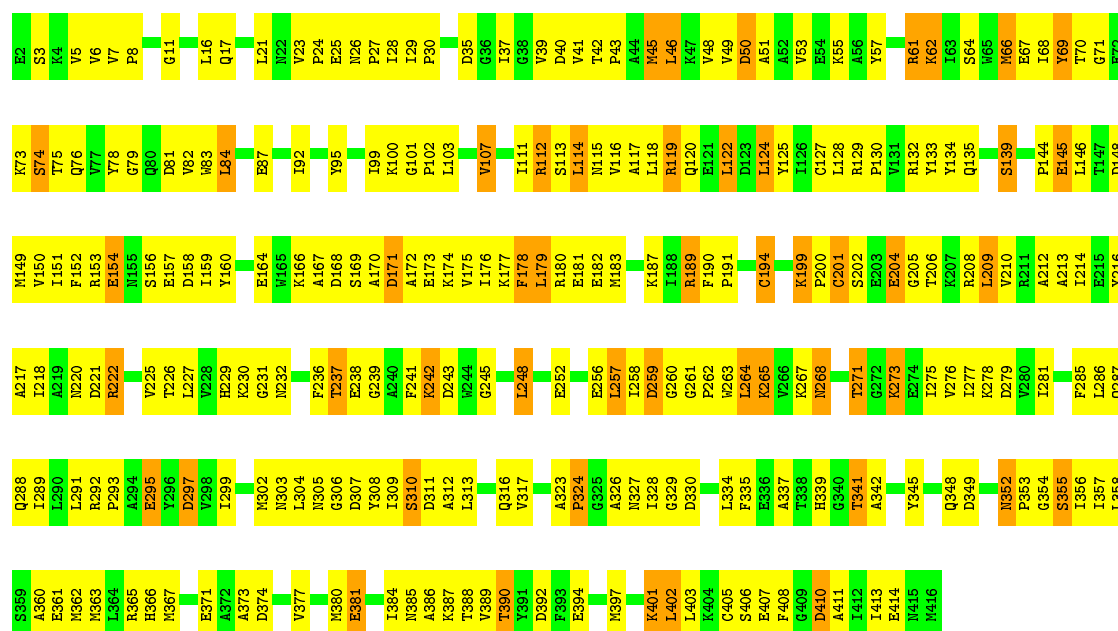
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	4	Total	O	0	0
			4	4		
5	C	7	Total	O	0	0
			7	7		
5	D	7	Total	O	0	0
			7	7		

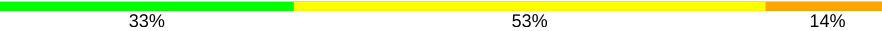


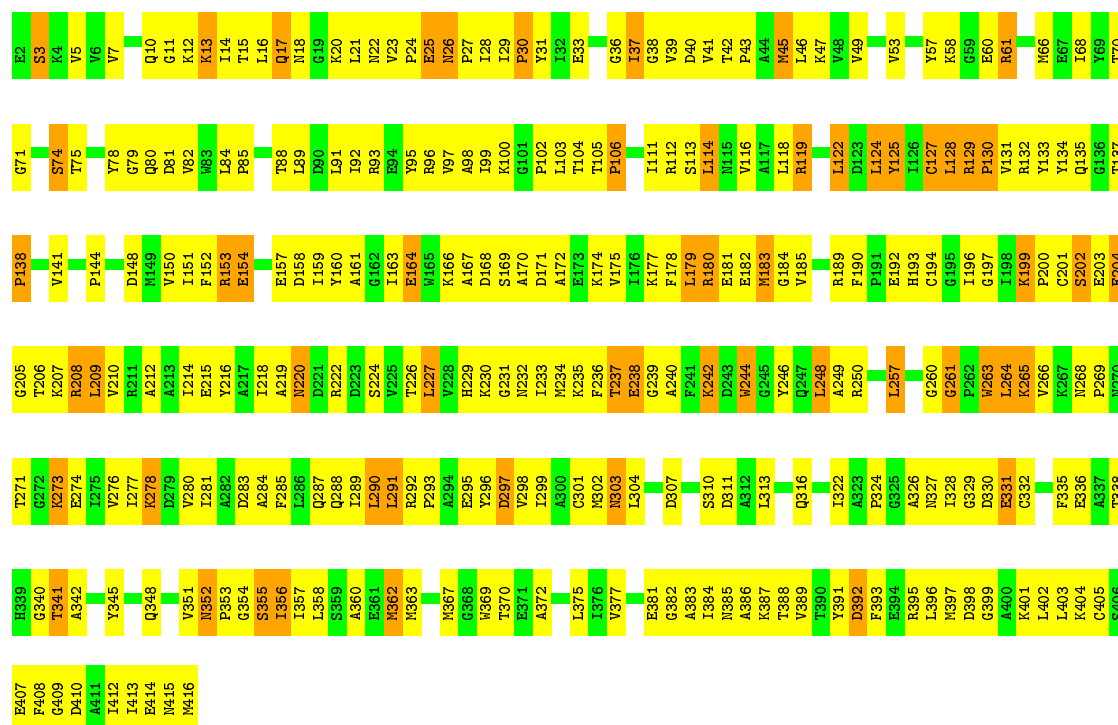


• Molecule 2: Isocitrate dehydrogenase [NADP]



• Molecule 2: Isocitrate dehydrogenase [NADP]

Chain D:  33% 53% 14%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.16Å 198.16Å 156.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 3.30 29.95 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.97-3.30) 99.4 (29.95-3.30)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.177 , 0.247 0.221 , 0.271	Depositor DCC
$R_{free}$ test set	2657 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	99.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 71.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15755	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: AMP, ADP

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	0.91	0/4699	0.74	2/6367 (0.0%)
1	B	0.92	0/4776	0.73	3/6473 (0.0%)
2	C	1.00	0/3266	0.77	2/4417 (0.0%)
2	D	0.93	0/3266	0.79	3/4417 (0.1%)
All	All	0.93	0/16007	0.75	10/21674 (0.0%)

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
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	352	ASN	C-N-CD	-15.54	86.42	120.60
1	B	514	PHE	C-N-CD	-9.84	98.96	120.60
1	A	169	LYS	N-CA-C	-7.42	90.97	111.00
2	C	261	GLY	N-CA-C	-5.92	98.31	113.10
2	D	261	GLY	N-CA-C	-5.88	98.40	113.10
2	C	199	LYS	C-N-CD	-5.84	107.75	120.60
1	B	474	TYR	N-CA-C	5.61	126.14	111.00
1	A	475	ASP	N-CA-C	-5.60	95.87	111.00
1	B	475	ASP	N-CA-C	-5.10	97.23	111.00
2	D	296	TYR	N-CA-C	5.08	124.72	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	GLU	Peptide
2	C	70	THR	Peptide

## 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	4575	0	4464	753	3
1	B	4649	0	4550	688	0
2	C	3205	0	3213	418	2
2	D	3205	0	3211	437	3
3	A	23	0	12	2	0
3	B	23	0	12	6	0
4	A	27	0	12	7	0
4	B	27	0	12	6	0
5	A	3	0	0	0	0
5	B	4	0	0	1	0
5	C	7	0	0	2	0
5	D	7	0	0	2	0
All	All	15755	0	15486	2256	5

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 72.

All (2256) 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)
2:D:261:GLY:HA3	2:D:263:TRP:CZ3	1.26	1.69
1:A:7:LEU:CD1	1:A:85:HIS:CD2	1.76	1.66
1:B:40:TRP:CZ3	1:B:205:LYS:HE2	1.36	1.59
1:A:525:ASP:CB	1:A:528:ILE:HD12	1.31	1.54
2:D:154:GLU:C	2:D:303:ASN:HD21	1.04	1.52
2:D:106:PRO:HB2	2:D:111:ILE:CD1	1.42	1.47
2:D:119:ARG:HA	2:D:124:LEU:CD1	1.44	1.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:240:ALA:O	2:D:244:TRP:CD1	1.69	1.46
1:A:525:ASP:CB	1:A:528:ILE:CD1	1.94	1.44
1:A:525:ASP:CA	1:A:528:ILE:HD11	1.45	1.44
1:A:7:LEU:CD1	1:A:85:HIS:HD2	1.08	1.43
1:A:7:LEU:HD12	1:A:85:HIS:CD2	1.35	1.42
2:C:118:LEU:O	2:C:122:LEU:CD1	1.64	1.41
1:B:365:ARG:NH1	1:B:371:ASP:HB2	1.14	1.40
1:B:169:LYS:O	1:B:173:ILE:CD1	1.67	1.40
1:A:336:LYS:NZ	1:A:416:GLU:CD	1.74	1.39
1:A:444:ALA:O	1:A:448:LEU:CD1	1.73	1.36
2:C:153:ARG:CD	2:C:306:GLY:HA3	1.55	1.36
2:C:100:LYS:NZ	2:C:115:ASN:OD1	1.60	1.35
1:A:23:ARG:NH2	1:B:18:ASP:OD2	1.57	1.34
1:A:254:ARG:NH2	1:A:470:ARG:NH1	1.74	1.34
1:B:176:ILE:O	1:B:180:LEU:HD12	1.16	1.33
2:D:202:SER:OG	2:D:205:GLY:N	1.60	1.33
1:A:219:THR:C	1:A:220:LEU:HD23	1.46	1.33
1:A:509:SER:OG	1:A:512:ASP:CG	1.69	1.31
1:B:237:ASP:OD1	1:B:568:ARG:HD2	1.27	1.30
1:A:7:LEU:O	1:A:11:GLN:HG3	1.33	1.29
2:C:263:TRP:C	2:C:264:LEU:HD23	1.52	1.29
1:A:525:ASP:C	1:A:528:ILE:HD11	1.51	1.29
2:D:106:PRO:CB	2:D:111:ILE:CD1	2.10	1.28
1:B:237:ASP:OD1	1:B:568:ARG:CD	1.81	1.28
1:B:253:ALA:O	1:B:367:GLY:HA2	1.15	1.27
2:C:37:ILE:HG23	2:C:341:THR:O	1.15	1.27
1:A:525:ASP:O	1:A:528:ILE:CD1	1.82	1.27
1:A:422:LEU:O	1:A:426:LEU:HD12	1.34	1.27
2:C:258:ILE:HG22	2:C:259:ASP:OD1	1.29	1.27
2:C:262:PRO:O	2:C:264:LEU:HD21	1.30	1.27
2:C:271:THR:CG2	2:C:273:LYS:HE3	1.64	1.26
2:D:92:ILE:HG22	2:D:332:CYS:SG	1.73	1.26
1:A:163:ARG:O	1:A:164:LEU:HD12	1.10	1.26
1:B:253:ALA:O	1:B:367:GLY:CA	1.82	1.26
1:A:525:ASP:C	1:A:528:ILE:CD1	2.04	1.26
2:C:353:PRO:O	2:C:357:ILE:CD1	1.84	1.26
1:B:229:THR:HG22	1:B:233:GLU:C	1.56	1.26
1:A:294:LYS:C	1:A:297:SER:HG	1.38	1.25
2:C:214:ILE:O	2:C:218:ILE:HD12	1.12	1.25
2:D:261:GLY:CA	2:D:263:TRP:CZ3	2.16	1.25
2:C:353:PRO:O	2:C:357:ILE:HD12	1.15	1.24

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LYS:C	1:A:297:SER:OG	1.76	1.24
2:D:106:PRO:CB	2:D:111:ILE:HD11	1.65	1.24
1:B:192:SER:OG	1:B:215:THR:HA	1.08	1.24
1:B:242:THR:CB	1:B:245:GLU:OE2	1.84	1.24
1:B:229:THR:HG22	1:B:233:GLU:O	1.10	1.24
1:A:525:ASP:HB3	1:A:528:ILE:CD1	1.59	1.23
2:C:124:LEU:HD12	2:C:327:ASN:CB	1.68	1.23
2:C:153:ARG:HD3	2:C:306:GLY:CA	1.68	1.23
2:D:118:LEU:O	2:D:122:LEU:HD12	1.33	1.22
1:A:509:SER:CB	1:A:512:ASP:OD2	1.86	1.22
1:A:7:LEU:HD11	1:A:85:HIS:CD2	1.54	1.22
1:A:368:ARG:NH2	1:A:440:GLU:OE2	1.72	1.22
2:C:262:PRO:O	2:C:264:LEU:CD2	1.86	1.22
1:B:242:THR:OG1	1:B:245:GLU:CD	1.77	1.21
1:B:204:ASN:ND2	1:B:364:ASP:OD2	1.73	1.21
2:C:92:ILE:O	2:C:95:TYR:O	1.56	1.21
2:D:154:GLU:O	2:D:303:ASN:CG	1.77	1.20
1:A:542:ALA:O	1:A:546:ARG:HD2	1.41	1.20
1:A:509:SER:HG	1:A:512:ASP:CG	1.38	1.20
2:C:214:ILE:O	2:C:218:ILE:CD1	1.89	1.20
2:C:124:LEU:CD1	2:C:327:ASN:C	2.11	1.19
2:D:214:ILE:O	2:D:218:ILE:HG13	1.41	1.19
1:B:163:ARG:O	1:B:164:LEU:CD2	1.88	1.19
1:B:551:ARG:NH2	1:B:558:GLU:OE1	1.75	1.19
1:A:294:LYS:CA	1:A:297:SER:OG	1.92	1.18
2:D:203:GLU:HB2	2:D:244:TRP:CZ3	1.77	1.18
2:C:323:ALA:O	2:C:355:SER:OG	1.57	1.18
2:C:222:ARG:NH1	2:C:297:ASP:OD2	1.77	1.18
1:B:192:SER:OG	1:B:215:THR:CA	1.90	1.18
1:B:229:THR:HG21	1:B:233:GLU:CB	1.74	1.17
1:A:551:ARG:O	1:A:554:GLU:N	1.76	1.17
2:D:382:GLY:C	2:D:415:ASN:HD22	1.45	1.17
2:D:119:ARG:CA	2:D:124:LEU:CD1	2.23	1.16
1:B:365:ARG:HH11	1:B:371:ASP:CB	1.57	1.16
1:B:173:ILE:O	1:B:177:ILE:HD11	1.45	1.16
2:C:154:GLU:OE1	2:C:157:GLU:N	1.79	1.16
1:B:176:ILE:O	1:B:180:LEU:CD1	1.92	1.15
1:B:300:GLU:O	1:B:303:VAL:HG22	1.45	1.15
1:B:365:ARG:NH1	1:B:371:ASP:CB	2.10	1.15
1:B:517:GLU:OE2	2:C:107:VAL:HG23	1.42	1.15
1:B:126:SER:OG	1:B:127:GLN:NE2	1.79	1.15

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASP:CA	1:A:528:ILE:CD1	2.16	1.14
1:B:346:LYS:HD3	1:B:348:MET:HE3	1.30	1.14
1:A:439:GLU:O	1:A:443:ASN:ND2	1.79	1.14
2:C:74:SER:OG	2:C:82:VAL:O	1.66	1.14
1:B:40:TRP:CZ3	1:B:205:LYS:CE	2.31	1.13
2:D:382:GLY:C	2:D:415:ASN:ND2	2.01	1.13
2:C:306:GLY:O	2:C:310:SER:OG	1.68	1.12
1:A:163:ARG:O	1:A:164:LEU:CD1	1.97	1.12
1:A:294:LYS:O	1:A:297:SER:OG	1.63	1.12
1:B:89:LEU:O	1:B:93:TYR:CD1	2.03	1.12
2:C:153:ARG:HD3	2:C:306:GLY:HA3	1.13	1.11
2:D:261:GLY:HA3	2:D:263:TRP:CH2	1.85	1.11
2:C:258:ILE:C	2:C:259:ASP:OD1	1.89	1.11
1:B:499:GLU:OE2	2:C:345:TYR:OH	1.67	1.11
1:A:170:SER:H	1:A:173:ILE:CG1	1.62	1.10
1:B:17:PHE:HE1	1:B:98:ILE:HG22	1.13	1.10
1:B:346:LYS:HD3	1:B:348:MET:CE	1.81	1.10
1:A:170:SER:N	1:A:173:ILE:HG12	1.50	1.10
2:D:37:ILE:HG12	2:D:341:THR:O	1.49	1.10
1:A:336:LYS:CE	1:A:416:GLU:OE2	2.00	1.09
1:B:163:ARG:O	1:B:164:LEU:HD23	0.92	1.08
2:D:71:GLY:N	2:D:74:SER:OG	1.67	1.08
1:A:444:ALA:O	1:A:448:LEU:HD12	1.53	1.08
1:B:430:GLU:OE1	1:B:431:GLY:N	1.85	1.08
2:C:78:TYR:OH	2:C:87:GLU:OE2	1.68	1.08
1:A:171:ARG:NH1	1:A:175:TYR:HE2	1.51	1.08
1:B:68:ILE:O	1:B:69:THR:OG1	1.70	1.08
2:C:133:TYR:CE1	2:C:134:TYR:O	2.06	1.08
1:A:100:GLU:OE2	1:A:125:SER:O	1.72	1.08
1:A:444:ALA:O	1:A:448:LEU:HD11	1.34	1.07
1:B:176:ILE:HG22	1:B:180:LEU:HD11	1.09	1.07
1:B:237:ASP:OD1	1:B:568:ARG:NE	1.86	1.07
2:D:157:GLU:OE1	2:D:202:SER:N	1.87	1.07
1:A:140:ALA:HB2	1:A:197:ALA:CA	1.84	1.07
1:B:178:ARG:O	1:B:182:GLU:OE2	1.70	1.07
2:C:271:THR:HG21	2:C:273:LYS:CE	1.85	1.07
1:B:242:THR:HG1	1:B:245:GLU:CD	1.53	1.07
2:D:289:ILE:O	2:D:293:PRO:HG3	1.55	1.07
2:D:80:GLN:O	2:D:81:ASP:OD1	1.71	1.07
1:A:6:GLU:N	1:A:6:GLU:OE1	1.88	1.07
1:B:169:LYS:O	1:B:173:ILE:HD12	1.27	1.06

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:GLU:OE1	2:C:145:GLU:N	1.88	1.06
1:B:167:GLN:HG2	1:B:233:GLU:OE1	1.52	1.06
1:A:542:ALA:C	1:A:546:ARG:HD2	1.74	1.06
1:B:169:LYS:O	1:B:173:ILE:HD13	1.53	1.06
2:C:66:MET:HE1	2:C:95:TYR:CE2	1.91	1.06
1:A:170:SER:H	1:A:173:ILE:HG12	0.93	1.06
2:D:119:ARG:HA	2:D:124:LEU:HD11	1.06	1.06
1:A:422:LEU:O	1:A:426:LEU:CD1	2.04	1.06
1:B:40:TRP:CE3	1:B:205:LYS:HE2	1.89	1.06
1:A:140:ALA:CB	1:A:197:ALA:HA	1.86	1.05
1:A:336:LYS:HZ2	1:A:416:GLU:CD	1.41	1.05
2:C:160:TYR:HB2	2:C:303:ASN:HD22	1.17	1.05
1:A:163:ARG:C	1:A:164:LEU:HD12	1.75	1.05
1:A:177:ILE:O	1:A:181:THR:HG23	1.54	1.05
1:B:80:LEU:HD23	1:B:81:ARG:H	1.20	1.05
2:C:37:ILE:CG2	2:C:341:THR:O	2.05	1.05
1:A:119:GLU:N	1:A:119:GLU:OE2	1.89	1.05
2:D:153:ARG:NH2	2:D:303:ASN:O	1.88	1.05
2:C:258:ILE:CG2	2:C:259:ASP:OD1	2.05	1.05
1:A:166:TRP:HA	1:A:233:GLU:HG3	1.36	1.04
1:A:254:ARG:HH22	1:A:470:ARG:CZ	1.70	1.04
1:A:525:ASP:HB2	1:A:528:ILE:HD12	1.37	1.04
1:B:173:ILE:O	1:B:177:ILE:CD1	2.05	1.04
1:B:179:HIS:HA	1:B:182:GLU:OE2	1.54	1.04
2:C:221:ASP:OD2	2:C:271:THR:HG21	1.53	1.04
1:B:89:LEU:O	1:B:93:TYR:CE1	2.11	1.04
1:A:429:VAL:HG13	1:A:433:GLN:HB2	1.40	1.04
2:C:236:PHE:CD2	2:D:164:GLU:OE1	2.11	1.03
1:B:177:ILE:O	1:B:181:THR:OG1	1.76	1.03
1:B:517:GLU:OE2	2:C:107:VAL:N	1.90	1.03
1:B:253:ALA:C	1:B:367:GLY:HA2	1.77	1.03
2:C:154:GLU:OE2	2:C:156:SER:N	1.89	1.03
1:A:66:ARG:O	1:A:70:ASN:N	1.90	1.03
2:C:124:LEU:HD11	2:C:327:ASN:O	1.59	1.03
1:A:525:ASP:N	1:A:528:ILE:HD11	1.72	1.03
1:B:154:MET:O	1:B:158:SER:OG	1.76	1.03
2:D:106:PRO:HB2	2:D:111:ILE:HD11	1.03	1.03
1:B:229:THR:HG21	1:B:233:GLU:HB2	1.04	1.03
2:D:106:PRO:CB	2:D:111:ILE:HD12	1.88	1.03
2:C:71:GLY:O	2:C:83:TRP:CE3	2.12	1.02
1:A:107:TYR:CE1	1:A:111:PHE:CE2	2.46	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:H	1:B:173:ILE:HD13	1.22	1.02
1:A:525:ASP:O	1:A:528:ILE:HD13	1.55	1.02
1:B:86:TYR:HA	1:B:89:LEU:HD13	1.36	1.02
1:A:176:ILE:HD13	1:A:176:ILE:H	1.24	1.01
1:B:229:THR:CG2	1:B:233:GLU:CA	2.38	1.01
2:C:204:GLU:HB3	2:D:190:PHE:CE2	1.94	1.01
1:B:229:THR:CG2	1:B:233:GLU:O	2.07	1.01
1:A:274:ILE:HG22	1:A:275:LEU:CD2	1.90	1.01
1:A:298:TYR:HE2	1:A:302:LEU:HD11	1.22	1.01
2:D:383:ALA:N	2:D:415:ASN:HD22	1.55	1.01
2:D:154:GLU:C	2:D:303:ASN:ND2	1.79	1.01
2:D:383:ALA:N	2:D:415:ASN:ND2	2.09	1.01
1:A:8:LEU:O	1:A:12:THR:OG1	1.78	1.00
2:C:175:VAL:HG22	2:D:183:MET:HE2	1.39	1.00
2:D:180:ARG:O	2:D:184:GLY:HA2	1.61	1.00
2:C:204:GLU:OE1	2:D:190:PHE:CZ	2.13	1.00
2:C:154:GLU:CD	2:C:157:GLU:H	1.63	1.00
1:B:293:ALA:O	1:B:297:SER:OG	1.78	1.00
1:B:83:LYS:O	1:B:87:THR:N	1.88	1.00
2:C:263:TRP:O	2:C:264:LEU:HD23	1.59	1.00
1:B:176:ILE:CG2	1:B:180:LEU:HD11	1.91	0.99
2:C:118:LEU:O	2:C:122:LEU:HD12	0.83	0.99
2:C:153:ARG:HD3	2:C:306:GLY:C	1.82	0.99
2:C:402:LEU:HD12	2:C:403:LEU:N	1.77	0.99
1:A:525:ASP:O	1:A:528:ILE:HD11	1.49	0.99
1:B:346:LYS:HB3	1:B:348:MET:CE	1.92	0.99
2:D:57:TYR:HE2	2:D:372:ALA:HB2	1.28	0.99
2:C:221:ASP:O	2:C:273:LYS:NZ	1.95	0.99
1:B:229:THR:CG2	1:B:233:GLU:N	2.26	0.98
1:A:294:LYS:HA	1:A:297:SER:OG	1.63	0.98
1:B:375:PHE:CD1	1:B:415:ILE:CD1	2.47	0.98
1:A:219:THR:O	1:A:220:LEU:HD23	1.61	0.98
2:D:353:PRO:HG3	2:D:405:CYS:SG	2.02	0.98
1:A:163:ARG:C	1:A:164:LEU:CD1	2.32	0.98
1:A:7:LEU:HD11	1:A:85:HIS:HD2	0.90	0.98
2:C:124:LEU:CD1	2:C:327:ASN:O	2.10	0.98
1:B:312:PHE:CE1	1:B:328:LEU:CD2	2.47	0.98
2:C:175:VAL:HG22	2:D:183:MET:CE	1.93	0.97
1:A:107:TYR:CE1	1:A:111:PHE:HE2	1.81	0.97
2:D:203:GLU:HB2	2:D:244:TRP:HZ3	1.15	0.97
1:A:452:ASN:O	1:A:452:ASN:ND2	1.95	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ASN:O	1:B:452:ASN:ND2	1.97	0.97
1:B:298:TYR:CE2	3:B:602:AMP:H2	1.82	0.97
1:A:568:ARG:O	1:A:571:VAL:HG23	1.65	0.97
1:B:187:GLU:OE1	1:B:187:GLU:N	1.97	0.96
2:D:230:LYS:H	2:D:238:GLU:HG2	1.25	0.96
1:A:413:LEU:HD12	1:A:414:TYR:N	1.80	0.96
1:A:119:GLU:HG2	1:A:120:ARG:HG2	1.48	0.96
2:C:125:TYR:OH	2:C:330:ASP:OD1	1.82	0.96
1:A:96:PHE:O	1:A:99:ALA:N	1.98	0.96
1:B:229:THR:CG2	1:B:233:GLU:C	2.34	0.96
1:A:254:ARG:HH21	1:A:470:ARG:NH1	1.56	0.96
1:A:298:TYR:CE2	1:A:302:LEU:HD11	1.99	0.96
2:C:171:ASP:O	2:C:175:VAL:HG23	1.66	0.96
2:C:124:LEU:HD12	2:C:327:ASN:C	1.83	0.96
1:B:156:VAL:HG23	1:B:157:ILE:H	1.28	0.95
1:A:166:TRP:CA	1:A:233:GLU:HG3	1.86	0.95
2:C:271:THR:HG21	2:C:273:LYS:HE3	0.99	0.95
2:D:132:ARG:HH11	2:D:132:ARG:HG2	1.31	0.95
2:D:209:LEU:HD23	2:D:210:VAL:N	1.80	0.95
2:D:47:LYS:NZ	2:D:410:ASP:OD1	1.99	0.95
1:B:40:TRP:HZ3	1:B:205:LYS:HE2	1.31	0.95
1:A:149:TRP:CE3	1:A:152:LEU:HD23	2.01	0.95
1:A:303:VAL:O	1:A:306:GLN:HG2	1.66	0.95
2:D:291:LEU:HD12	2:D:291:LEU:H	1.31	0.95
2:D:209:LEU:HD23	2:D:210:VAL:H	1.29	0.95
2:D:129:ARG:NH2	2:D:336:GLU:OE2	2.00	0.95
1:A:140:ALA:HB2	1:A:197:ALA:HA	0.96	0.94
1:B:212:LYS:HG3	1:B:274:ILE:HD11	1.49	0.94
2:C:124:LEU:HD12	2:C:327:ASN:HB3	1.47	0.94
1:A:78:PHE:O	1:A:80:LEU:N	2.00	0.94
2:C:8:PRO:HG3	2:C:28:ILE:HG23	1.47	0.94
1:B:222:PHE:O	1:B:223:LEU:HD12	1.67	0.94
2:D:298:VAL:C	2:D:299:ILE:HD12	1.86	0.94
1:B:17:PHE:HE1	1:B:98:ILE:CG2	1.81	0.94
1:B:169:LYS:C	1:B:173:ILE:HD12	1.80	0.94
2:D:240:ALA:O	2:D:244:TRP:HD1	1.43	0.94
2:D:118:LEU:O	2:D:122:LEU:CD1	2.15	0.94
1:A:149:TRP:HA	1:A:152:LEU:HB3	1.48	0.93
1:B:237:ASP:CG	1:B:568:ARG:HD2	1.88	0.93
1:B:312:PHE:CE1	1:B:328:LEU:HD23	2.02	0.93
1:B:84:GLU:O	1:B:88:ARG:N	2.02	0.93

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLN:O	1:A:436:ASP:OD2	1.86	0.93
1:A:171:ARG:NH1	1:A:175:TYR:CE2	2.37	0.93
1:B:361:LYS:HE2	1:B:372:THR:O	1.69	0.93
1:B:57:HIS:O	1:B:61:VAL:HG23	1.68	0.93
1:B:539:LEU:O	1:B:545:TRP:NE1	2.02	0.93
2:C:236:PHE:HD2	2:D:164:GLU:OE1	1.46	0.93
1:A:448:LEU:H	1:A:448:LEU:HD12	1.33	0.92
1:A:254:ARG:NH2	1:A:470:ARG:HH12	1.60	0.92
1:B:163:ARG:C	1:B:164:LEU:HD23	1.89	0.92
1:B:17:PHE:CE1	1:B:98:ILE:HG22	2.04	0.92
1:A:46:ALA:HA	1:A:49:ASN:OD1	1.70	0.92
1:B:375:PHE:CE1	1:B:415:ILE:HD13	2.04	0.92
1:B:201:PHE:CE1	1:B:210:VAL:HG21	2.05	0.92
2:D:30:PRO:O	2:D:98:ALA:HB1	1.68	0.92
2:C:21:LEU:H	2:C:21:LEU:HD12	1.32	0.92
2:D:199:LYS:HD3	2:D:237:THR:OG1	1.70	0.92
1:A:254:ARG:HH22	1:A:470:ARG:NH1	1.48	0.91
2:C:201:CYS:SG	2:C:237:THR:O	2.28	0.91
1:B:86:TYR:CA	1:B:89:LEU:CD1	2.48	0.91
2:C:66:MET:CE	2:C:95:TYR:CE2	2.53	0.91
2:D:119:ARG:O	2:D:124:LEU:HD12	1.70	0.91
1:A:34:ARG:O	1:A:37:GLN:O	1.88	0.91
1:A:143:PHE:O	1:A:193:HIS:HB2	1.71	0.91
2:C:209:LEU:O	2:C:212:ALA:HB3	1.71	0.91
1:A:91:PRO:HD3	1:A:127:GLN:OE1	1.69	0.91
2:D:240:ALA:O	2:D:244:TRP:NE1	2.04	0.91
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.36	0.91
2:D:240:ALA:C	2:D:244:TRP:NE1	2.24	0.90
1:A:100:GLU:O	1:A:104:ASN:OD1	1.87	0.90
2:D:106:PRO:CA	2:D:111:ILE:HD11	2.01	0.90
1:B:77:GLU:O	1:B:80:LEU:HD22	1.71	0.90
2:C:124:LEU:HD13	2:C:328:ILE:N	1.87	0.90
1:B:253:ALA:O	1:B:367:GLY:N	2.03	0.90
1:B:522:LEU:O	1:B:528:ILE:CD1	2.20	0.90
2:D:57:TYR:CE2	2:D:372:ALA:HB2	2.06	0.90
2:D:106:PRO:HB2	2:D:111:ILE:CG1	2.01	0.90
1:A:192:SER:OG	1:A:215:THR:CA	2.17	0.90
2:D:401:LYS:O	2:D:403:LEU:CD1	2.20	0.90
1:A:322:VAL:HG23	4:A:602:ADP:O1B	1.72	0.89
2:C:361:GLU:OE1	5:C:505:HOH:O	1.90	0.89
1:A:229:THR:OG1	1:A:235:PHE:CE1	2.24	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:ARG:HH11	1:B:546:ARG:HG3	1.38	0.89
2:D:230:LYS:O	2:D:232:ASN:N	2.05	0.89
2:D:384:ILE:O	2:D:387:LYS:N	2.05	0.89
1:A:141:LYS:O	1:A:143:PHE:CE1	2.25	0.89
2:C:71:GLY:O	2:C:83:TRP:CZ3	2.26	0.89
2:D:398:ASP:OD1	2:D:399:GLY:N	2.05	0.89
2:C:160:TYR:HB2	2:C:303:ASN:ND2	1.87	0.89
2:D:45:MET:O	2:D:49:VAL:HG23	1.73	0.89
1:A:149:TRP:O	1:A:152:LEU:N	2.06	0.89
1:A:215:THR:OG1	1:A:216:PRO:HD2	1.71	0.89
1:A:361:LYS:NZ	1:A:371:ASP:OD2	2.06	0.88
1:B:300:GLU:O	1:B:303:VAL:CG2	2.20	0.88
2:C:204:GLU:HB3	2:D:190:PHE:CD2	2.08	0.88
1:A:149:TRP:CE3	1:A:152:LEU:CD2	2.56	0.88
1:A:336:LYS:HZ1	1:A:416:GLU:CD	1.55	0.88
1:A:404:LEU:O	1:A:407:GLN:O	1.92	0.88
1:A:311:GLN:NE2	1:A:383:ARG:O	2.07	0.88
1:A:7:LEU:CD1	1:A:85:HIS:NE2	2.36	0.88
2:D:261:GLY:HA3	2:D:263:TRP:HZ3	1.12	0.88
1:A:223:LEU:O	1:A:224:LEU:HD12	1.72	0.88
1:A:482:MET:HE2	1:A:545:TRP:HE3	1.38	0.88
2:C:268:ASN:OD1	2:C:271:THR:N	1.95	0.88
1:B:346:LYS:HB3	1:B:348:MET:HE2	1.52	0.87
2:D:273:LYS:HG2	2:D:274:GLU:N	1.89	0.87
2:C:124:LEU:HD12	2:C:327:ASN:HB2	1.52	0.87
1:B:145:PRO:HB3	1:B:149:TRP:CE3	2.09	0.87
2:D:132:ARG:NH1	2:D:133:TYR:O	2.08	0.87
2:D:240:ALA:CB	2:D:244:TRP:HE1	1.88	0.87
1:A:170:SER:N	1:A:173:ILE:CG1	2.14	0.87
1:A:543:ASP:HA	1:A:546:ARG:HD3	1.56	0.87
1:A:192:SER:OG	1:A:215:THR:HA	1.75	0.87
1:A:222:PHE:O	1:A:223:LEU:HD12	1.75	0.87
2:D:273:LYS:HG2	2:D:274:GLU:H	1.40	0.87
1:B:86:TYR:HA	1:B:89:LEU:CD1	2.03	0.87
2:D:203:GLU:CB	2:D:244:TRP:CZ3	2.58	0.86
1:B:24:PHE:CZ	1:B:50:ARG:NH2	2.43	0.86
1:B:7:LEU:CB	1:B:85:HIS:CD2	2.59	0.86
1:A:168:ASN:O	1:A:171:ARG:N	2.09	0.86
1:B:229:THR:HG23	1:B:233:GLU:H	1.36	0.86
1:B:167:GLN:CG	1:B:233:GLU:OE1	2.24	0.86
2:C:291:LEU:H	2:C:291:LEU:HD12	1.38	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:ASN:HA	1:B:474:TYR:HE1	1.40	0.86
2:D:240:ALA:C	2:D:244:TRP:CD1	2.49	0.86
2:D:248:LEU:O	2:D:248:LEU:HD12	1.76	0.86
1:A:180:LEU:HD23	1:A:181:THR:HG23	1.56	0.86
1:B:375:PHE:CD1	1:B:415:ILE:HD12	2.11	0.86
1:A:515:PRO:HA	1:A:518:PHE:CE2	2.10	0.85
2:D:158:ASP:OD1	2:D:159:ILE:N	2.07	0.85
1:A:274:ILE:HG22	1:A:275:LEU:HD23	1.57	0.85
1:B:140:ALA:HB1	1:B:196:VAL:O	1.76	0.85
1:A:96:PHE:O	1:A:99:ALA:HB3	1.76	0.85
1:B:192:SER:OG	1:B:214:ILE:O	1.90	0.85
1:B:180:LEU:H	1:B:180:LEU:HD12	1.39	0.85
2:C:133:TYR:HA	2:C:317:VAL:CG1	2.06	0.85
2:D:240:ALA:HB1	2:D:244:TRP:NE1	1.91	0.85
1:A:322:VAL:CG2	4:A:602:ADP:O1B	2.24	0.85
1:A:229:THR:O	1:A:232:GLY:CA	2.25	0.85
1:B:312:PHE:CZ	1:B:328:LEU:HD21	2.12	0.85
2:C:204:GLU:OE1	2:D:190:PHE:CE2	2.29	0.85
2:D:353:PRO:CG	2:D:405:CYS:SG	2.65	0.85
2:C:262:PRO:O	2:C:264:LEU:HD23	1.77	0.85
2:D:71:GLY:O	2:D:74:SER:N	1.98	0.85
1:A:261:ALA:O	1:A:264:PRO:HD3	1.76	0.84
1:B:522:LEU:O	1:B:528:ILE:HD11	1.74	0.84
2:D:119:ARG:HA	2:D:124:LEU:HD13	1.56	0.84
2:D:240:ALA:C	2:D:244:TRP:HE1	1.79	0.84
2:D:127:CYS:SG	2:D:153:ARG:CD	2.64	0.84
1:B:229:THR:HG23	1:B:233:GLU:N	1.90	0.84
1:A:94:PRO:CG	1:B:26:GLU:OE1	2.25	0.84
1:A:287:ILE:HD11	1:A:289:CYS:SG	2.18	0.84
1:B:152:LEU:HD12	1:B:152:LEU:O	1.78	0.84
2:D:235:LYS:O	2:D:239:GLY:CA	2.26	0.84
2:D:409:GLY:O	2:D:413:ILE:HG13	1.78	0.84
1:A:172:ASP:HA	1:A:175:TYR:CD2	2.13	0.83
1:B:169:LYS:C	1:B:173:ILE:CD1	2.27	0.83
1:B:201:PHE:CE1	1:B:210:VAL:CG2	2.61	0.83
1:B:327:THR:HG21	1:B:418:ARG:NH2	1.93	0.83
1:B:80:LEU:HD23	1:B:81:ARG:N	1.92	0.83
1:A:85:HIS:O	1:A:89:LEU:HD11	1.78	0.83
1:B:179:HIS:CA	1:B:182:GLU:OE2	2.26	0.83
1:B:60:LEU:O	1:B:60:LEU:HD12	1.78	0.83
1:B:8:LEU:O	1:B:8:LEU:HD12	1.78	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:413:ILE:O	2:D:416:MET:HB2	1.77	0.83
1:A:525:ASP:HB3	1:A:528:ILE:HD12	0.85	0.83
1:B:166:TRP:CE2	1:B:234:LEU:HD23	2.13	0.83
1:B:189:LEU:HD12	1:B:189:LEU:O	1.79	0.83
1:A:293:ALA:O	1:A:297:SER:OG	1.97	0.83
2:C:213:ALA:O	2:C:216:TYR:N	2.12	0.83
2:C:71:GLY:O	2:C:83:TRP:HE3	1.59	0.83
2:D:235:LYS:O	2:D:239:GLY:HA3	1.77	0.83
1:A:244:ALA:O	1:A:247:SER:OG	1.95	0.83
1:B:312:PHE:CD1	1:B:328:LEU:CD2	2.61	0.83
2:D:240:ALA:HB1	2:D:244:TRP:CE2	2.13	0.83
1:B:127:GLN:HE21	1:B:127:GLN:N	1.77	0.83
1:A:535:MET:HB3	1:A:536:HIS:CD2	2.14	0.83
1:B:149:TRP:O	1:B:152:LEU:HB3	1.78	0.83
1:B:24:PHE:CE1	1:B:50:ARG:NH2	2.47	0.83
2:C:153:ARG:HD2	2:C:306:GLY:HA3	1.61	0.83
2:D:392:ASP:O	2:D:396:LEU:HD12	1.79	0.83
2:D:106:PRO:HB3	2:D:111:ILE:HD12	1.57	0.82
1:A:461:LYS:C	1:A:462:ASN:HD22	1.81	0.82
1:B:89:LEU:O	1:B:93:TYR:HD1	1.59	0.82
1:A:392:LEU:HD12	1:A:392:LEU:O	1.79	0.82
1:A:38:ALA:HA	1:A:40:TRP:CZ3	2.14	0.82
2:C:75:THR:O	2:C:79:GLY:O	1.97	0.82
2:D:322:ILE:O	2:D:358:LEU:HD12	1.78	0.82
2:D:99:ILE:HB	2:D:363:MET:CE	2.09	0.82
1:A:189:LEU:HG	1:A:190:SER:N	1.93	0.82
1:A:257:PHE:HB2	1:A:286:ALA:O	1.80	0.82
2:D:229:HIS:CD2	2:D:242:LYS:HB2	2.14	0.82
2:D:25:GLU:C	2:D:27:PRO:HD3	2.00	0.82
1:B:86:TYR:CA	1:B:89:LEU:HD13	2.08	0.82
1:A:565:ARG:O	1:A:568:ARG:HG2	1.79	0.82
1:A:551:ARG:O	1:A:554:GLU:CA	2.27	0.82
1:B:201:PHE:CD1	1:B:210:VAL:CG2	2.63	0.82
1:B:7:LEU:CA	1:B:85:HIS:HD2	1.92	0.82
2:C:100:LYS:HG2	2:C:101:GLY:O	1.80	0.82
2:D:169:SER:O	2:D:170:ALA:HB3	1.78	0.82
2:D:92:ILE:CG2	2:D:332:CYS:SG	2.64	0.82
1:B:146:ASP:C	1:B:147:HIS:CD2	2.53	0.82
2:C:128:LEU:HD13	2:C:152:PHE:CE1	2.15	0.82
1:A:525:ASP:C	1:A:528:ILE:HD13	1.92	0.81
1:B:212:LYS:CG	1:B:274:ILE:HD11	2.10	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASP:C	1:A:404:LEU:HD13	2.01	0.81
1:A:94:PRO:HG3	1:B:26:GLU:CD	1.99	0.81
1:B:68:ILE:C	1:B:69:THR:HG1	1.81	0.81
1:B:462:ASN:HA	1:B:474:TYR:CE1	2.14	0.81
2:D:268:ASN:OD1	2:D:271:THR:HG22	1.81	0.81
1:A:39:ASP:HB3	1:A:42:ALA:HB3	1.62	0.81
1:A:46:ALA:CA	1:A:49:ASN:OD1	2.28	0.81
1:B:17:PHE:CE1	1:B:98:ILE:CG2	2.61	0.81
1:A:219:THR:C	1:A:220:LEU:CD2	2.41	0.81
1:A:229:THR:OG1	1:A:235:PHE:HE1	1.61	0.81
2:C:166:LYS:O	2:C:169:SER:OG	1.97	0.81
1:B:156:VAL:HG23	1:B:157:ILE:N	1.93	0.81
1:B:222:PHE:C	1:B:223:LEU:HD12	2.01	0.81
2:C:158:ASP:HB3	2:C:303:ASN:HB3	1.62	0.81
2:D:127:CYS:SG	2:D:153:ARG:HD3	2.20	0.81
1:A:429:VAL:HG12	1:A:430:GLU:O	1.81	0.81
1:B:365:ARG:HH12	1:B:371:ASP:HB2	1.41	0.81
2:D:154:GLU:O	2:D:303:ASN:ND2	0.66	0.81
1:A:336:LYS:NZ	1:A:416:GLU:OE2	0.66	0.81
1:B:528:ILE:O	1:B:531:LEU:HD12	1.79	0.81
2:C:160:TYR:OH	2:D:230:LYS:NZ	2.13	0.81
1:A:528:ILE:HD13	1:A:528:ILE:H	1.45	0.80
2:D:356:ILE:HD12	2:D:356:ILE:O	1.81	0.80
1:A:141:LYS:O	1:A:143:PHE:HE1	1.62	0.80
1:A:172:ASP:O	1:A:176:ILE:HD13	1.80	0.80
1:B:141:LYS:NZ	1:B:155:ARG:NH1	2.28	0.80
1:A:26:GLU:O	1:A:29:SER:OG	2.00	0.80
1:A:215:THR:OG1	1:A:216:PRO:CD	2.29	0.80
1:A:107:TYR:CE1	1:A:111:PHE:CD2	2.69	0.80
1:B:23:ARG:NH2	5:B:703:HOH:O	2.14	0.80
1:B:50:ARG:HD2	1:B:258:MET:HE2	1.64	0.80
1:B:173:ILE:CD1	1:B:173:ILE:H	1.95	0.80
2:C:116:VAL:O	2:C:120:GLN:N	2.11	0.80
1:A:322:VAL:HG21	4:A:602:ADP:O2B	1.81	0.80
1:A:482:MET:HE2	1:A:545:TRP:CE3	2.17	0.80
2:C:365:ARG:HG2	2:C:365:ARG:HH11	1.45	0.80
2:D:352:ASN:ND2	2:D:392:ASP:OD2	2.13	0.80
1:B:178:ARG:C	1:B:182:GLU:OE2	2.20	0.79
1:B:192:SER:HG	1:B:215:THR:HA	1.16	0.79
1:B:40:TRP:HA	1:B:43:VAL:HG23	1.63	0.79
2:C:128:LEU:HD13	2:C:152:PHE:CZ	2.17	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ALA:O	1:A:546:ARG:CD	2.28	0.79
1:A:569:PHE:C	1:A:571:VAL:H	1.85	0.79
1:A:104:ASN:ND2	1:A:122:PHE:O	2.15	0.79
1:B:494:ARG:NH1	1:B:498:ASP:OD1	2.15	0.79
2:D:157:GLU:OE2	2:D:205:GLY:HA3	1.82	0.79
2:D:410:ASP:O	2:D:414:GLU:HG3	1.82	0.79
2:C:133:TYR:HA	2:C:317:VAL:HG13	1.64	0.79
1:B:229:THR:HG21	1:B:233:GLU:CA	2.06	0.79
2:C:154:GLU:OE1	2:C:157:GLU:CA	2.29	0.79
2:C:35:ASP:O	2:C:341:THR:HG22	1.83	0.79
2:D:119:ARG:CA	2:D:124:LEU:HD12	2.12	0.79
2:D:179:LEU:HA	2:D:183:MET:HB2	1.65	0.79
1:A:60:LEU:O	1:A:60:LEU:HD12	1.82	0.78
1:A:229:THR:HG1	1:A:235:PHE:HE1	0.80	0.78
1:A:39:ASP:O	1:A:42:ALA:N	2.17	0.78
1:B:5:LEU:O	1:B:8:LEU:HB3	1.83	0.78
2:C:124:LEU:HD13	2:C:327:ASN:C	2.03	0.78
1:A:7:LEU:O	1:A:11:GLN:CG	2.26	0.78
2:C:183:MET:HA	2:C:183:MET:HE3	1.64	0.78
1:A:394:LEU:HD23	1:A:401:ILE:HD11	1.66	0.78
1:B:201:PHE:CD1	1:B:210:VAL:HG23	2.18	0.78
1:B:229:THR:CG2	1:B:233:GLU:H	1.93	0.78
2:D:257:LEU:HD21	2:D:260:GLY:HA2	1.65	0.78
1:B:290:GLN:HG3	1:B:291:LYS:N	1.99	0.78
1:A:189:LEU:HD23	1:A:189:LEU:H	1.49	0.78
1:B:515:PRO:O	1:B:540:PHE:HA	1.83	0.78
1:A:321:MET:HB3	1:A:343:ALA:HB2	1.64	0.77
1:B:253:ALA:CB	1:B:367:GLY:HA2	2.14	0.77
1:B:375:PHE:CE1	1:B:415:ILE:CD1	2.63	0.77
1:A:17:PHE:CE1	1:A:98:ILE:CG2	2.66	0.77
1:A:482:MET:CE	1:A:545:TRP:CE3	2.67	0.77
1:B:149:TRP:O	1:B:152:LEU:N	2.16	0.77
2:C:287:GLN:O	2:C:291:LEU:HD13	1.84	0.77
2:D:307:ASP:OD1	2:D:311:ASP:OD2	2.03	0.77
1:A:119:GLU:CG	1:A:120:ARG:HG2	2.13	0.77
1:B:420:VAL:CG1	1:B:465:VAL:HB	2.13	0.77
2:C:177:LYS:HE2	2:C:181:GLU:OE1	1.82	0.77
2:D:36:GLY:O	2:D:39:VAL:HG12	1.84	0.77
1:A:370:ALA:O	1:A:476:TYR:OH	2.03	0.77
2:C:133:TYR:CD1	2:C:134:TYR:O	2.37	0.77
1:B:525:ASP:OD1	1:B:527:ARG:HG3	1.84	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TYR:OH	1:B:120:ARG:NE	2.18	0.77
2:D:222:ARG:HD2	2:D:297:ASP:OD1	1.83	0.77
1:A:322:VAL:CG2	4:A:602:ADP:O2B	2.32	0.77
1:B:77:GLU:HG3	1:B:78:PHE:H	1.50	0.77
1:A:36:GLU:OE2	1:A:163:ARG:NE	2.18	0.76
1:B:176:ILE:HG22	1:B:180:LEU:CD1	2.04	0.76
2:D:210:VAL:O	2:D:214:ILE:HG13	1.85	0.76
1:A:168:ASN:O	1:A:173:ILE:HD11	1.84	0.76
1:A:525:ASP:HB2	1:A:528:ILE:CD1	2.00	0.76
1:A:94:PRO:HG2	1:B:26:GLU:OE1	1.85	0.76
1:B:32:GLN:O	1:B:36:GLU:HG3	1.83	0.76
2:D:45:MET:CE	2:D:46:LEU:HD23	2.15	0.76
1:B:215:THR:OG1	1:B:217:SER:OG	1.96	0.76
1:B:77:GLU:O	1:B:80:LEU:CD2	2.34	0.76
2:D:240:ALA:HB1	2:D:244:TRP:CZ2	2.20	0.76
2:D:70:THR:C	2:D:74:SER:OG	2.23	0.76
2:D:119:ARG:CA	2:D:124:LEU:HD11	1.99	0.76
1:A:462:ASN:C	1:A:463:PHE:HD1	1.88	0.76
1:B:229:THR:HG22	1:B:233:GLU:CA	2.13	0.76
1:B:474:TYR:HD1	1:B:475:ASP:N	1.82	0.76
1:A:176:ILE:CD1	1:A:176:ILE:H	1.98	0.76
1:A:17:PHE:CE1	1:A:98:ILE:HG22	2.20	0.76
2:D:25:GLU:O	2:D:27:PRO:CD	2.34	0.76
2:D:209:LEU:O	2:D:212:ALA:N	2.19	0.76
1:A:96:PHE:O	1:A:99:ALA:CB	2.33	0.76
2:D:383:ALA:CA	2:D:415:ASN:ND2	2.48	0.76
1:B:176:ILE:C	1:B:180:LEU:CD1	2.54	0.76
1:B:79:LEU:O	1:B:82:VAL:HG22	1.86	0.76
2:C:206:THR:HG23	2:C:241:PHE:CD2	2.20	0.76
1:A:180:LEU:HD22	1:A:180:LEU:H	1.51	0.75
1:A:40:TRP:CD1	1:A:205:LYS:HG2	2.21	0.75
1:B:453:ILE:HG23	1:B:479:ILE:HD11	1.69	0.75
1:B:517:GLU:OE2	2:C:107:VAL:CG2	2.27	0.75
1:B:254:ARG:HG2	1:B:254:ARG:NH1	2.00	0.75
2:C:158:ASP:OD1	2:C:159:ILE:N	2.17	0.75
2:D:249:ALA:HB3	2:D:264:LEU:HD11	1.68	0.75
2:D:383:ALA:HA	2:D:415:ASN:ND2	2.01	0.75
1:A:177:ILE:H	1:A:177:ILE:HD13	1.50	0.75
1:A:20:GLN:NE2	1:A:20:GLN:O	2.19	0.75
2:D:75:THR:O	2:D:79:GLY:O	2.04	0.75
1:A:441:TYR:O	1:A:444:ALA:N	2.18	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:PRO:O	2:C:103:LEU:HD23	1.85	0.75
2:C:124:LEU:HD12	2:C:327:ASN:CA	2.16	0.75
2:C:153:ARG:CG	2:C:306:GLY:HA3	2.16	0.75
2:C:21:LEU:N	2:C:21:LEU:HD12	2.02	0.75
2:C:291:LEU:N	2:C:291:LEU:HD12	2.02	0.75
1:A:119:GLU:CD	1:A:120:ARG:H	1.90	0.74
1:A:419:MET:SD	1:A:472:VAL:CG2	2.74	0.74
1:A:274:ILE:HG22	1:A:275:LEU:HD21	1.66	0.74
2:C:236:PHE:HB2	2:D:164:GLU:OE1	1.86	0.74
1:A:173:ILE:HD12	1:A:173:ILE:H	1.51	0.74
1:A:419:MET:SD	1:A:472:VAL:HG21	2.26	0.74
1:A:66:ARG:O	1:A:69:THR:C	2.09	0.74
1:B:550:ASN:O	1:B:554:GLU:HG3	1.88	0.74
1:A:295:THR:HG23	3:A:601:AMP:O3'	1.86	0.74
1:A:375:PHE:HE2	1:A:415:ILE:HD12	1.52	0.74
1:A:322:VAL:CG2	4:A:602:ADP:PB	2.76	0.74
2:C:135:GLN:OE1	2:C:385:ASN:ND2	2.21	0.74
1:A:375:PHE:CE2	1:A:415:ILE:HD12	2.23	0.74
2:C:124:LEU:HD13	2:C:328:ILE:CA	2.17	0.74
2:D:16:LEU:HD23	2:D:16:LEU:O	1.88	0.74
1:A:171:ARG:HH12	1:A:175:TYR:HE2	1.32	0.74
1:A:473:PHE:HE2	1:A:479:ILE:CD1	2.00	0.74
1:B:13:ILE:HD12	1:B:13:ILE:H	1.51	0.74
2:C:236:PHE:CE1	2:D:166:LYS:HB2	2.23	0.74
1:A:380:LEU:HD12	1:A:380:LEU:N	2.03	0.74
1:A:359:LEU:HD12	1:A:359:LEU:O	1.88	0.74
1:A:365:ARG:C	1:A:366:VAL:CG2	2.57	0.74
2:C:213:ALA:O	2:C:216:TYR:HB3	1.88	0.74
2:D:289:ILE:O	2:D:293:PRO:CG	2.35	0.74
1:A:238:THR:HB	1:A:568:ARG:HA	1.69	0.73
1:A:212:LYS:HD3	1:A:274:ILE:HD13	1.70	0.73
1:A:368:ARG:CZ	1:A:440:GLU:OE2	2.36	0.73
1:A:85:HIS:O	1:A:89:LEU:CD1	2.34	0.73
1:A:94:PRO:HG3	1:B:26:GLU:OE1	1.88	0.73
1:B:361:LYS:CE	1:B:372:THR:O	2.36	0.73
1:B:7:LEU:HA	1:B:85:HIS:HD2	1.52	0.73
2:C:216:TYR:CE1	2:C:220:ASN:ND2	2.56	0.73
1:A:234:LEU:HD12	1:A:234:LEU:N	2.03	0.73
1:B:312:PHE:CE1	1:B:328:LEU:HD21	2.21	0.73
1:B:327:THR:CG2	1:B:418:ARG:NH2	2.50	0.73
2:C:154:GLU:OE1	2:C:157:GLU:CG	2.36	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:O	1:A:220:LEU:CD2	2.35	0.73
1:B:146:ASP:C	1:B:147:HIS:CG	2.62	0.73
2:C:42:THR:HB	2:C:43:PRO:HD3	1.70	0.73
1:A:429:VAL:CG1	1:A:433:GLN:HB2	2.17	0.73
1:B:454:PHE:HB2	1:B:482:MET:HG3	1.68	0.73
1:B:528:ILE:O	1:B:531:LEU:CD1	2.36	0.73
2:D:132:ARG:NH1	2:D:132:ARG:HG2	1.97	0.73
1:B:151:SER:O	1:B:154:MET:HB2	1.87	0.73
1:B:177:ILE:HD13	1:B:177:ILE:N	2.03	0.73
1:B:338:ILE:O	1:B:400:LYS:HE2	1.88	0.73
1:B:546:ARG:NH1	1:B:546:ARG:HG3	1.99	0.73
2:C:264:LEU:HD23	2:C:264:LEU:N	2.03	0.73
2:C:326:ALA:HB2	2:C:335:PHE:HD1	1.53	0.73
2:D:189:ARG:CZ	2:D:190:PHE:HE1	2.01	0.73
1:A:253:ALA:O	1:A:365:ARG:HB2	1.89	0.73
1:A:324:LEU:CD2	1:A:393:LEU:HD23	2.18	0.73
1:A:423:ASN:HD22	1:A:461:LYS:HA	1.52	0.73
1:B:89:LEU:H	1:B:89:LEU:HD12	1.53	0.73
1:B:209:LEU:HD23	1:B:209:LEU:O	1.88	0.73
1:B:254:ARG:NH2	1:B:562:ALA:CB	2.51	0.73
1:A:220:LEU:N	1:A:220:LEU:HD23	2.03	0.73
1:B:527:ARG:O	1:B:531:LEU:HD11	1.88	0.73
2:C:124:LEU:CD1	2:C:328:ILE:N	2.48	0.73
2:D:402:LEU:C	2:D:403:LEU:HD12	2.09	0.73
1:A:21:TYR:OH	1:A:264:PRO:HG3	1.87	0.73
1:A:365:ARG:C	1:A:366:VAL:HG22	2.08	0.73
2:C:37:ILE:HG21	2:C:342:ALA:HB3	1.70	0.73
1:A:83:LYS:O	1:A:87:THR:N	2.19	0.72
1:B:298:TYR:CE2	3:B:602:AMP:C2	2.74	0.72
1:B:17:PHE:CZ	1:B:98:ILE:HB	2.25	0.72
2:D:326:ALA:HB2	2:D:335:PHE:CD2	2.24	0.72
2:D:42:THR:HB	2:D:43:PRO:HD3	1.70	0.72
1:B:179:HIS:O	1:B:183:THR:OG1	2.08	0.72
1:B:254:ARG:NH2	1:B:562:ALA:HA	2.05	0.72
2:D:57:TYR:O	2:D:58:LYS:HB2	1.88	0.72
1:B:290:GLN:HG3	1:B:291:LYS:H	1.54	0.72
2:D:240:ALA:CB	2:D:244:TRP:NE1	2.51	0.72
2:D:404:LYS:HB2	2:D:407:GLU:OE1	1.89	0.72
1:B:117:THR:HG22	1:B:120:ARG:HB2	1.70	0.72
1:B:452:ASN:HD21	1:B:481:TYR:HB3	1.54	0.72
1:B:61:VAL:O	1:B:64:GLN:HB2	1.90	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:LEU:O	2:C:50:ASP:HB2	1.89	0.72
2:D:214:ILE:O	2:D:218:ILE:CG1	2.31	0.72
1:A:173:ILE:N	1:A:173:ILE:HD12	2.05	0.72
1:B:7:LEU:HB2	1:B:85:HIS:CD2	2.23	0.72
2:C:113:SER:HB3	2:C:116:VAL:HG22	1.72	0.72
2:C:365:ARG:HG2	2:C:365:ARG:NH1	2.01	0.72
1:A:551:ARG:O	1:A:554:GLU:HB3	1.89	0.71
2:C:285:PHE:CE2	2:C:289:ILE:CG2	2.73	0.71
1:A:154:MET:O	1:A:158:SER:OG	2.07	0.71
1:A:177:ILE:HG12	1:A:178:ARG:N	2.05	0.71
1:B:119:GLU:OE2	1:B:119:GLU:N	2.23	0.71
1:B:213:LEU:N	1:B:220:LEU:O	2.23	0.71
1:B:311:GLN:HG2	1:B:384:HIS:O	1.90	0.71
1:B:42:ALA:O	1:B:46:ALA:N	2.20	0.71
2:C:271:THR:CG2	2:C:273:LYS:HG2	2.20	0.71
2:C:29:ILE:HG21	2:C:363:MET:CE	2.20	0.71
2:D:353:PRO:O	2:D:357:ILE:HG13	1.89	0.71
1:B:346:LYS:HD3	1:B:348:MET:HE1	1.67	0.71
1:A:117:THR:OG1	1:A:120:ARG:CG	2.38	0.71
2:C:167:ALA:O	2:C:168:ASP:HB2	1.88	0.71
2:D:313:LEU:O	2:D:316:GLN:HB2	1.90	0.71
2:D:392:ASP:O	2:D:396:LEU:CD1	2.39	0.71
2:C:128:LEU:HD11	2:C:150:VAL:CG1	2.19	0.71
2:C:7:VAL:CG1	2:C:8:PRO:HD2	2.20	0.71
2:D:222:ARG:CD	2:D:297:ASP:OD1	2.39	0.71
1:B:133:ARG:HG3	1:B:134:THR:N	2.03	0.71
1:B:50:ARG:HD2	1:B:258:MET:CE	2.20	0.71
2:D:100:LYS:HE3	2:D:336:GLU:HB2	1.71	0.71
1:A:201:PHE:CE1	1:A:210:VAL:HG21	2.26	0.71
1:B:146:ASP:O	1:B:147:HIS:CG	2.43	0.71
1:B:78:PHE:HA	1:B:81:ARG:HG3	1.73	0.71
2:D:79:GLY:HA3	2:D:82:VAL:HG12	1.73	0.71
1:A:168:ASN:HD22	1:A:171:ARG:NH1	1.89	0.71
1:A:380:LEU:HD12	1:A:380:LEU:H	1.56	0.71
1:A:546:ARG:NH1	1:A:546:ARG:HG2	2.06	0.71
1:A:285:MET:O	1:A:288:GLY:N	2.23	0.71
2:C:236:PHE:HD2	2:D:164:GLU:CD	1.93	0.71
1:A:234:LEU:HD12	1:A:234:LEU:H	1.55	0.70
1:B:177:ILE:HD13	1:B:177:ILE:H	1.56	0.70
1:A:177:ILE:N	1:A:177:ILE:HD13	2.06	0.70
1:A:446:ARG:O	1:A:449:ALA:HB3	1.91	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:GLY:HA3	1:A:536:HIS:CE1	2.26	0.70
1:A:546:ARG:O	1:A:550:ASN:CA	2.37	0.70
2:D:133:TYR:HE1	2:D:135:GLN:HA	1.56	0.70
2:D:403:LEU:HD12	2:D:403:LEU:N	2.06	0.70
1:A:546:ARG:HG2	1:A:546:ARG:HH11	1.56	0.70
2:D:157:GLU:OE1	2:D:202:SER:HB3	1.91	0.70
1:B:452:ASN:OD1	1:B:483:THR:HG23	1.91	0.70
2:C:326:ALA:HB2	2:C:362:MET:CE	2.21	0.70
2:D:268:ASN:CG	2:D:271:THR:HG22	2.11	0.70
1:A:149:TRP:CD2	1:A:152:LEU:HD23	2.26	0.70
1:A:441:TYR:O	1:A:444:ALA:HB3	1.91	0.70
1:A:171:ARG:O	1:A:174:HIS:N	2.24	0.70
1:A:462:ASN:O	1:A:463:PHE:CD1	2.45	0.70
1:B:356:CYS:SG	1:B:479:ILE:CG2	2.80	0.70
1:B:522:LEU:O	1:B:528:ILE:HD12	1.90	0.70
1:B:281:ALA:HB2	1:B:300:GLU:OE2	1.91	0.70
1:B:530:PRO:O	1:B:534:GLU:N	2.25	0.70
2:C:352:ASN:CB	2:C:390:THR:HG21	2.21	0.70
2:D:21:LEU:HD12	2:D:21:LEU:O	1.90	0.70
1:A:189:LEU:HD23	1:A:189:LEU:N	2.06	0.69
1:B:212:LYS:HE3	1:B:270:TRP:NE1	2.07	0.69
2:C:133:TYR:CD2	2:C:144:PRO:HB2	2.27	0.69
2:D:102:PRO:O	2:D:103:LEU:HD23	1.92	0.69
1:B:200:LEU:HD12	1:B:202:TYR:OH	1.92	0.69
1:B:254:ARG:CZ	1:B:562:ALA:HB2	2.22	0.69
1:A:163:ARG:C	1:A:164:LEU:HD13	2.13	0.69
1:B:568:ARG:HH21	1:B:568:ARG:HG2	1.57	0.69
1:B:97:GLU:HG2	1:B:98:ILE:H	1.57	0.69
2:C:326:ALA:CB	2:C:362:MET:HE1	2.22	0.69
1:A:422:LEU:CD1	1:A:426:LEU:HD11	2.21	0.69
1:A:528:ILE:H	1:A:528:ILE:CD1	2.05	0.69
1:B:452:ASN:HB2	1:B:552:ILE:HD13	1.73	0.69
1:B:250:PHE:HB3	1:B:278:LYS:NZ	2.07	0.69
2:D:205:GLY:O	2:D:208:ARG:HB2	1.92	0.69
1:B:40:TRP:HA	1:B:43:VAL:CG2	2.23	0.69
2:C:263:TRP:C	2:C:264:LEU:CD2	2.47	0.69
2:C:26:ASN:N	2:C:27:PRO:HD3	2.08	0.69
2:D:326:ALA:CB	2:D:335:PHE:CD2	2.75	0.69
1:A:180:LEU:N	1:A:180:LEU:HD22	2.07	0.69
2:C:139:SER:OG	2:C:316:GLN:O	2.10	0.69
1:A:238:THR:HA	1:A:569:PHE:CZ	2.28	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:HD21	1:A:393:LEU:HD23	1.75	0.69
1:B:114:ARG:O	1:B:115:SER:HB2	1.92	0.69
1:B:201:PHE:CD1	1:B:210:VAL:HG21	2.27	0.69
2:C:210:VAL:O	2:C:214:ILE:HG13	1.91	0.69
2:D:119:ARG:C	2:D:124:LEU:HD12	2.11	0.69
2:C:148:ASP:OD1	2:C:222:ARG:NH2	2.22	0.69
2:C:29:ILE:HG21	2:C:363:MET:HE1	1.74	0.69
2:C:408:PHE:O	2:C:411:ALA:N	2.26	0.69
2:D:326:ALA:HB2	2:D:335:PHE:HD2	1.58	0.69
2:C:99:ILE:HG13	2:C:335:PHE:O	1.93	0.68
1:B:192:SER:HG	1:B:214:ILE:C	1.95	0.68
2:C:5:VAL:HG23	2:C:67:GLU:O	1.93	0.68
2:D:352:ASN:HB2	2:D:392:ASP:OD2	1.93	0.68
2:D:45:MET:HE1	2:D:46:LEU:CD2	2.22	0.68
1:A:58:VAL:HG22	1:A:102:PHE:CE1	2.27	0.68
1:A:303:VAL:O	1:A:306:GLN:CG	2.40	0.68
1:A:561:TYR:HE2	1:A:568:ARG:CZ	2.05	0.68
2:C:21:LEU:H	2:C:21:LEU:CD1	2.06	0.68
1:A:152:LEU:O	1:A:152:LEU:HD12	1.93	0.68
1:B:209:LEU:HD23	1:B:209:LEU:C	2.14	0.68
1:B:166:TRP:CZ2	1:B:234:LEU:HD23	2.29	0.68
1:B:336:LYS:HE2	4:B:601:ADP:C8	2.28	0.68
1:B:442:GLY:HA3	1:B:536:HIS:NE2	2.09	0.68
1:B:7:LEU:CB	1:B:85:HIS:HD2	2.07	0.68
1:A:209:LEU:C	1:A:209:LEU:HD23	2.14	0.68
1:A:482:MET:CE	1:A:545:TRP:CZ3	2.77	0.68
1:B:176:ILE:N	1:B:176:ILE:HD12	2.09	0.68
2:C:133:TYR:HE1	2:C:135:GLN:HA	1.58	0.68
2:C:158:ASP:HB3	2:C:303:ASN:CB	2.24	0.68
2:D:25:GLU:O	2:D:27:PRO:HD2	1.94	0.68
1:A:413:LEU:C	1:A:413:LEU:HD12	2.14	0.68
1:A:473:PHE:CE2	1:A:479:ILE:CD1	2.77	0.68
1:A:528:ILE:HD13	1:A:528:ILE:N	2.08	0.68
1:B:368:ARG:NE	1:B:447:GLN:OE1	2.22	0.68
1:B:504:PRO:HG3	2:C:107:VAL:HG13	1.75	0.68
1:A:435:ARG:NH1	1:A:534:GLU:OE2	2.27	0.68
1:B:351:ALA:O	1:B:354:ARG:HB2	1.94	0.68
2:C:259:ASP:OD1	2:C:259:ASP:N	2.22	0.68
2:C:26:ASN:N	2:C:27:PRO:CD	2.57	0.68
2:D:203:GLU:HA	2:D:244:TRP:CE3	2.29	0.68
1:A:179:HIS:HD2	1:A:239:CYS:HB3	1.58	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLU:O	3:A:601:AMP:N6	2.26	0.68
2:D:49:VAL:O	2:D:53:VAL:HG23	1.93	0.68
2:D:57:TYR:HE2	2:D:372:ALA:CB	2.05	0.68
2:D:10:GLN:O	2:D:26:ASN:ND2	2.26	0.67
2:C:271:THR:HB	2:C:273:LYS:CG	2.24	0.67
1:A:254:ARG:HH11	1:A:254:ARG:HG3	1.59	0.67
1:B:89:LEU:O	1:B:93:TYR:HE1	1.77	0.67
1:A:171:ARG:HH11	1:A:175:TYR:HE2	1.35	0.67
1:A:543:ASP:HA	1:A:546:ARG:CD	2.24	0.67
1:A:85:HIS:O	1:A:88:ARG:HG2	1.94	0.67
1:B:240:LEU:HD22	1:B:245:GLU:HB3	1.76	0.67
2:D:229:HIS:HD2	2:D:242:LYS:HB2	1.58	0.67
1:A:107:TYR:OH	1:A:115:SER:OG	2.10	0.67
1:A:323:MET:HE1	1:A:338:ILE:HG13	1.74	0.67
1:A:365:ARG:O	1:A:366:VAL:HG23	1.93	0.67
1:B:168:ASN:O	1:B:172:ASP:OD1	2.13	0.67
1:A:152:LEU:HD12	1:A:152:LEU:C	2.15	0.67
1:A:229:THR:O	1:A:232:GLY:HA3	1.94	0.67
1:B:141:LYS:HZ2	1:B:155:ARG:HH11	1.42	0.67
1:B:323:MET:HE1	1:B:357:TYR:CE1	2.30	0.67
2:C:179:LEU:HA	2:C:183:MET:HB2	1.77	0.67
2:C:238:GLU:O	2:C:241:PHE:HB3	1.94	0.67
2:C:289:ILE:HD12	2:C:313:LEU:HD23	1.77	0.67
2:D:382:GLY:O	2:D:415:ASN:ND2	2.26	0.67
1:A:17:PHE:HE1	1:A:98:ILE:CG2	2.08	0.67
1:B:141:LYS:HZ2	1:B:155:ARG:NH1	1.91	0.67
2:D:16:LEU:C	2:D:16:LEU:HD23	2.15	0.67
1:A:570:SER:O	1:A:571:VAL:HG13	1.94	0.67
1:A:54:TYR:O	1:A:58:VAL:HG23	1.95	0.67
2:C:172:ALA:O	2:C:176:ILE:HG13	1.95	0.67
2:D:25:GLU:O	2:D:27:PRO:HD3	1.94	0.67
2:D:351:VAL:O	2:D:353:PRO:HD3	1.95	0.67
1:A:111:PHE:O	1:A:114:ARG:HG3	1.95	0.67
1:A:404:LEU:HD22	1:A:409:VAL:HG23	1.76	0.67
1:B:148:GLY:HA3	1:B:151:SER:OG	1.94	0.67
1:B:346:LYS:HB3	1:B:348:MET:HE3	1.77	0.67
1:B:5:LEU:HD23	1:B:5:LEU:C	2.15	0.67
1:A:149:TRP:CE3	1:A:152:LEU:HD21	2.30	0.67
1:A:178:ARG:C	1:A:180:LEU:HD22	2.16	0.67
1:B:133:ARG:HG3	1:B:134:THR:H	1.59	0.67
1:A:326:PHE:CB	1:A:389:LEU:HD21	2.24	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:401:ILE:HD12	1:B:401:ILE:C	2.16	0.66
2:C:42:THR:HB	2:C:43:PRO:CD	2.25	0.66
2:D:388:THR:O	2:D:389:VAL:HG13	1.95	0.66
2:D:84:LEU:HD12	2:D:84:LEU:C	2.15	0.66
1:B:272:ARG:HH22	1:B:280:THR:HG22	1.60	0.66
1:A:35:PHE:HE2	1:A:207:ALA:N	1.93	0.66
1:B:40:TRP:CE3	1:B:205:LYS:CE	2.68	0.66
2:D:230:LYS:C	2:D:232:ASN:H	1.97	0.66
1:A:91:PRO:CD	1:A:127:GLN:OE1	2.43	0.66
2:C:287:GLN:O	2:C:291:LEU:CD1	2.44	0.66
2:D:401:LYS:O	2:D:403:LEU:HD12	1.94	0.66
1:A:212:LYS:HD3	1:A:274:ILE:CD1	2.26	0.66
1:B:351:ALA:O	1:B:354:ARG:N	2.28	0.66
2:C:271:THR:HB	2:C:273:LYS:HG2	1.76	0.66
1:A:272:ARG:HH22	1:A:280:THR:HG22	1.61	0.66
1:A:45:GLN:O	1:A:48:LYS:N	2.29	0.66
1:A:46:ALA:O	1:A:49:ASN:OD1	2.14	0.66
2:D:274:GLU:O	2:D:274:GLU:HG3	1.94	0.66
1:A:322:VAL:HG22	4:A:602:ADP:PB	2.36	0.66
1:B:285:MET:CE	1:B:373:GLN:HE21	2.09	0.66
1:B:365:ARG:HH11	1:B:371:ASP:HB2	0.83	0.66
2:C:206:THR:HG23	2:C:241:PHE:CE2	2.30	0.66
2:C:41:VAL:HB	2:C:353:PRO:HB3	1.78	0.66
2:D:177:LYS:O	2:D:181:GLU:HG2	1.96	0.66
2:D:68:ILE:HD12	2:D:88:THR:HG23	1.77	0.66
1:A:298:TYR:CE2	1:A:302:LEU:CD1	2.78	0.65
1:B:77:GLU:HG3	1:B:78:PHE:N	2.11	0.65
2:C:16:LEU:HD23	2:C:16:LEU:C	2.16	0.65
2:C:221:ASP:OD2	2:C:271:THR:CG2	2.22	0.65
2:D:203:GLU:HA	2:D:244:TRP:CZ3	2.31	0.65
2:D:45:MET:HE2	2:D:46:LEU:N	2.12	0.65
1:A:404:LEU:HD13	1:A:404:LEU:N	2.11	0.65
2:C:236:PHE:CB	2:D:164:GLU:OE1	2.43	0.65
1:B:327:THR:OG1	1:B:418:ARG:NH2	2.29	0.65
2:C:248:LEU:CD1	2:C:252:GLU:HG3	2.26	0.65
2:D:248:LEU:HD12	2:D:248:LEU:C	2.15	0.65
1:A:117:THR:OG1	1:A:120:ARG:HG2	1.96	0.65
1:A:172:ASP:HA	1:A:175:TYR:HD2	1.60	0.65
1:A:452:ASN:HD21	1:A:481:TYR:HB3	1.61	0.65
1:B:54:TYR:O	1:B:58:VAL:HG23	1.97	0.65
2:D:45:MET:HE1	2:D:46:LEU:HD23	1.76	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:HG23	1:A:218:GLY:O	1.95	0.65
1:B:461:LYS:C	1:B:462:ASN:HD22	2.00	0.65
2:C:189:ARG:HH11	2:C:189:ARG:HG3	1.60	0.65
1:A:171:ARG:NH1	1:A:171:ARG:HG2	2.10	0.65
1:A:84:GLU:O	1:A:88:ARG:N	2.27	0.65
1:A:359:LEU:HD21	1:A:481:TYR:CE1	2.31	0.65
1:A:569:PHE:O	1:A:571:VAL:N	2.25	0.65
2:C:158:ASP:CG	2:C:159:ILE:H	1.99	0.65
2:D:171:ASP:O	2:D:174:LYS:HB3	1.95	0.65
1:A:278:LYS:HB3	1:A:282:GLU:HB2	1.78	0.65
1:A:101:SER:OG	1:A:295:THR:OG1	2.13	0.65
1:B:127:GLN:HE21	1:B:127:GLN:CA	2.09	0.65
2:C:171:ASP:O	2:C:175:VAL:N	2.28	0.65
2:D:189:ARG:HH11	2:D:189:ARG:HG3	1.61	0.65
1:A:381:GLU:OE1	1:A:404:LEU:O	2.13	0.65
1:A:570:SER:C	1:A:571:VAL:HG22	2.17	0.65
1:B:420:VAL:HG13	1:B:465:VAL:HB	1.79	0.65
1:A:253:ALA:HB1	1:A:367:GLY:C	2.16	0.65
2:D:99:ILE:HB	2:D:363:MET:HE2	1.78	0.65
1:A:117:THR:OG1	1:A:120:ARG:HG3	1.97	0.64
1:A:179:HIS:CD2	1:A:239:CYS:O	2.50	0.64
2:C:16:LEU:O	2:C:16:LEU:HD23	1.97	0.64
2:D:226:THR:HA	2:D:278:LYS:O	1.96	0.64
1:A:107:TYR:CD1	1:A:111:PHE:CE2	2.85	0.64
1:A:176:ILE:N	1:A:176:ILE:HD13	2.05	0.64
1:B:134:THR:HG22	1:B:135:ILE:N	2.13	0.64
1:A:196:VAL:HG12	1:A:197:ALA:N	2.12	0.64
2:D:25:GLU:C	2:D:27:PRO:CD	2.65	0.64
2:D:265:LYS:HG3	2:D:265:LYS:O	1.96	0.64
1:A:5:LEU:O	1:A:8:LEU:HB3	1.97	0.64
1:B:454:PHE:HB2	1:B:482:MET:CG	2.27	0.64
1:A:515:PRO:HA	1:A:518:PHE:CD2	2.32	0.64
1:B:65:LEU:N	1:B:65:LEU:HD12	2.11	0.64
2:C:238:GLU:O	2:C:241:PHE:CB	2.46	0.64
2:C:133:TYR:CA	2:C:317:VAL:HG13	2.27	0.64
2:D:169:SER:OG	2:D:172:ALA:N	2.29	0.64
1:A:60:LEU:C	1:A:60:LEU:HD12	2.18	0.64
1:B:13:ILE:N	1:B:13:ILE:HD12	2.11	0.64
1:B:222:PHE:C	1:B:223:LEU:CD1	2.65	0.64
2:D:106:PRO:C	2:D:111:ILE:HD11	2.17	0.64
1:A:323:MET:CE	1:A:338:ILE:CG1	2.76	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:LEU:O	2:C:212:ALA:CB	2.46	0.64
1:A:141:LYS:HG3	1:A:143:PHE:CE1	2.32	0.64
1:A:423:ASN:ND2	1:A:461:LYS:HA	2.12	0.64
1:A:462:ASN:C	1:A:463:PHE:CD1	2.70	0.64
1:B:462:ASN:HD22	1:B:462:ASN:N	1.96	0.64
2:C:128:LEU:CD1	2:C:152:PHE:CE1	2.79	0.64
1:A:223:LEU:C	1:A:224:LEU:HD12	2.18	0.64
1:B:173:ILE:HD13	1:B:173:ILE:N	2.06	0.64
2:D:37:ILE:CG1	2:D:341:THR:O	2.38	0.64
1:A:450:ALA:O	1:A:552:ILE:HD11	1.99	0.63
1:B:192:SER:CB	1:B:214:ILE:O	2.45	0.63
2:C:291:LEU:H	2:C:291:LEU:CD1	2.09	0.63
1:A:172:ASP:O	1:A:176:ILE:CD1	2.46	0.63
1:B:346:LYS:CD	1:B:348:MET:HE3	2.19	0.63
1:B:61:VAL:HG12	1:B:65:LEU:HD13	1.79	0.63
2:D:189:ARG:HG3	2:D:189:ARG:NH1	2.13	0.63
2:D:297:ASP:O	2:D:299:ILE:CD1	2.46	0.63
2:D:95:TYR:CZ	5:D:505:HOH:O	2.48	0.63
1:A:107:TYR:CD2	1:A:121:LEU:HD23	2.33	0.63
1:B:568:ARG:NH2	1:B:568:ARG:HG2	2.11	0.63
2:C:402:LEU:HD12	2:C:403:LEU:H	1.61	0.63
1:A:365:ARG:O	1:A:367:GLY:N	2.32	0.63
1:A:551:ARG:C	1:A:554:GLU:H	2.00	0.63
2:C:42:THR:O	2:C:46:LEU:HD12	1.97	0.63
2:D:100:LYS:HE3	2:D:336:GLU:CB	2.28	0.63
2:D:14:ILE:CD1	2:D:23:VAL:HG13	2.29	0.63
1:A:171:ARG:O	1:A:174:HIS:CB	2.46	0.63
1:B:141:LYS:HD2	1:B:143:PHE:CE2	2.34	0.63
2:D:104:THR:HG22	2:D:105:THR:O	1.98	0.63
2:D:175:VAL:O	2:D:179:LEU:HD12	1.98	0.63
1:A:201:PHE:CE1	1:A:210:VAL:CG2	2.81	0.63
1:B:204:ASN:CG	1:B:364:ASP:OD2	2.35	0.63
2:D:89:LEU:O	2:D:93:ARG:HG3	1.99	0.63
1:A:306:GLN:HG3	1:A:307:GLY:N	2.14	0.63
1:A:38:ALA:CB	1:A:40:TRP:HZ3	2.12	0.63
1:A:7:LEU:HD12	1:A:85:HIS:NE2	2.05	0.63
1:B:466:THR:OG1	1:B:470:ARG:O	2.16	0.63
1:B:7:LEU:HA	1:B:85:HIS:CD2	2.33	0.63
1:A:423:ASN:OD1	1:A:424:ILE:N	2.30	0.63
1:B:551:ARG:O	1:B:554:GLU:HB2	1.97	0.63
2:C:116:VAL:HG23	2:C:117:ALA:N	2.14	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASP:N	1:A:142:ASP:OD1	2.29	0.63
1:A:551:ARG:O	1:A:554:GLU:CB	2.46	0.63
1:B:360:VAL:HG21	1:B:476:TYR:CE2	2.34	0.63
2:C:175:VAL:CG2	2:D:183:MET:CE	2.75	0.63
1:A:149:TRP:CA	1:A:152:LEU:HB3	2.28	0.62
1:A:177:ILE:H	1:A:177:ILE:CD1	2.11	0.62
1:A:140:ALA:HA	1:A:198:ASN:OD1	1.98	0.62
2:C:271:THR:HG22	2:C:273:LYS:HE3	1.76	0.62
1:A:46:ALA:C	1:A:49:ASN:OD1	2.37	0.62
1:A:569:PHE:C	1:A:571:VAL:N	2.48	0.62
1:B:306:GLN:HG3	1:B:307:GLY:N	2.14	0.62
1:B:78:PHE:O	1:B:81:ARG:N	2.31	0.62
2:D:169:SER:OG	2:D:172:ALA:CB	2.47	0.62
1:A:456:GLY:HA3	1:A:478:GLU:HB3	1.82	0.62
2:C:358:LEU:O	2:C:361:GLU:HB3	1.99	0.62
2:C:39:VAL:HG13	2:C:40:ASP:N	2.14	0.62
1:A:323:MET:CE	1:A:338:ILE:HG12	2.30	0.62
1:B:310:GLU:HB3	1:B:329:PRO:HG2	1.81	0.62
2:D:95:TYR:O	2:D:96:ARG:HB2	1.98	0.62
1:A:546:ARG:CG	1:A:546:ARG:HH11	2.13	0.62
1:B:141:LYS:HZ3	1:B:155:ARG:NH1	1.96	0.62
1:B:237:ASP:CG	1:B:568:ARG:CD	2.58	0.62
2:C:392:ASP:N	2:C:392:ASP:OD1	2.31	0.62
2:D:119:ARG:CB	2:D:124:LEU:HD13	2.29	0.62
2:D:393:PHE:HA	2:D:396:LEU:HD12	1.82	0.62
1:A:125:SER:O	1:A:126:SER:OG	2.12	0.62
1:B:160:LEU:HD12	1:B:160:LEU:O	1.99	0.62
2:D:203:GLU:CA	2:D:244:TRP:CZ3	2.82	0.62
1:A:274:ILE:C	1:A:275:LEU:HD23	2.19	0.62
1:A:254:ARG:HH21	1:A:470:ARG:HH12	1.30	0.62
2:C:326:ALA:CB	2:C:362:MET:CE	2.77	0.62
2:D:391:TYR:O	2:D:395:ARG:HG3	2.00	0.62
1:B:338:ILE:O	1:B:400:LYS:CE	2.47	0.62
1:B:102:PHE:O	1:B:106:VAL:HG23	1.99	0.62
1:B:462:ASN:OD1	1:B:475:ASP:CB	2.47	0.62
2:C:7:VAL:HG12	2:C:8:PRO:HD2	1.80	0.62
1:A:119:GLU:CD	1:A:120:ARG:HG2	2.20	0.62
2:C:133:TYR:CE1	2:C:134:TYR:C	2.72	0.62
1:A:35:PHE:CD2	1:A:207:ALA:HB2	2.34	0.61
1:B:267:LEU:HD23	1:B:287:ILE:HG21	1.80	0.61
1:B:5:LEU:HD23	1:B:6:GLU:N	2.15	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:209:LEU:CD2	2:D:210:VAL:HG23	2.29	0.61
2:D:389:VAL:N	2:D:403:LEU:HD13	2.14	0.61
1:A:323:MET:HE1	1:A:338:ILE:CG1	2.30	0.61
1:A:481:TYR:HB2	1:A:484:GLU:HG3	1.82	0.61
1:A:89:LEU:HD12	1:A:89:LEU:H	1.64	0.61
1:B:168:ASN:O	1:B:171:ARG:HB3	1.99	0.61
1:B:519:ARG:HH21	1:B:533:GLU:CD	2.03	0.61
2:C:133:TYR:CE1	2:C:135:GLN:HA	2.35	0.61
2:D:39:VAL:O	2:D:43:PRO:HG2	2.00	0.61
1:A:178:ARG:NH2	1:A:182:GLU:OE1	2.34	0.61
2:D:209:LEU:O	2:D:212:ALA:HB3	2.00	0.61
1:A:333:ARG:HH12	1:A:373:GLN:HE22	1.46	0.61
1:B:177:ILE:HA	1:B:180:LEU:HD13	1.81	0.61
1:B:474:TYR:HD1	1:B:475:ASP:H	1.45	0.61
2:C:239:GLY:O	2:C:242:LYS:HG2	2.00	0.61
1:B:564:ARG:CG	1:B:564:ARG:HH11	2.13	0.61
2:C:285:PHE:CE2	2:C:289:ILE:HG21	2.35	0.61
2:C:6:VAL:O	2:C:6:VAL:HG23	2.00	0.61
2:D:169:SER:O	2:D:171:ASP:N	2.29	0.61
2:D:169:SER:HG	2:D:172:ALA:H	1.46	0.61
2:D:351:VAL:O	2:D:353:PRO:CD	2.49	0.61
2:D:352:ASN:CB	2:D:392:ASP:OD2	2.49	0.61
1:A:368:ARG:NE	1:A:447:GLN:OE1	2.31	0.61
1:B:312:PHE:CE2	1:B:328:LEU:HD21	2.34	0.61
2:D:189:ARG:NH1	2:D:190:PHE:CE1	2.68	0.61
2:D:384:ILE:C	2:D:387:LYS:H	2.03	0.61
1:A:364:ASP:OD1	1:A:364:ASP:N	2.30	0.61
1:A:40:TRP:HE1	1:A:205:LYS:HA	1.66	0.61
1:B:244:ALA:O	1:B:248:ILE:HG13	2.01	0.61
1:A:96:PHE:O	1:A:99:ALA:CA	2.48	0.61
1:B:106:VAL:HG12	1:B:110:LEU:HD23	1.83	0.61
1:B:62:VAL:HG23	1:B:63:GLU:N	2.14	0.61
2:D:42:THR:HB	2:D:43:PRO:CD	2.31	0.61
1:A:222:PHE:C	1:A:223:LEU:CD1	2.69	0.61
1:A:482:MET:HE1	1:A:545:TRP:CZ3	2.36	0.61
1:A:509:SER:OG	1:A:512:ASP:OD2	0.62	0.61
1:B:156:VAL:CG2	1:B:157:ILE:H	2.09	0.61
1:B:462:ASN:ND2	4:B:601:ADP:O3B	2.33	0.61
1:B:513:VAL:HG12	1:B:515:PRO:HD3	1.82	0.61
2:D:79:GLY:CA	2:D:82:VAL:HG12	2.30	0.61
1:A:106:VAL:HG12	1:A:110:LEU:HD12	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:O	1:A:183:THR:HG23	2.00	0.61
1:A:35:PHE:CE2	1:A:207:ALA:N	2.69	0.61
1:A:222:PHE:C	1:A:223:LEU:HD12	2.20	0.61
1:A:287:ILE:CD1	1:A:289:CYS:SG	2.89	0.61
1:A:535:MET:CB	1:A:536:HIS:CD2	2.84	0.61
1:B:474:TYR:HA	1:B:476:TYR:HE1	1.64	0.61
1:A:281:ALA:CB	1:A:300:GLU:OE2	2.48	0.60
1:A:365:ARG:O	1:A:366:VAL:CG2	2.48	0.60
1:A:422:LEU:HD12	1:A:426:LEU:HD11	1.82	0.60
1:B:143:PHE:HE1	1:B:155:ARG:HD2	1.66	0.60
1:B:140:ALA:CB	1:B:196:VAL:O	2.48	0.60
1:B:86:TYR:C	1:B:89:LEU:CD1	2.69	0.60
2:C:407:GLU:O	2:C:410:ASP:HB2	2.01	0.60
2:D:242:LYS:HG3	2:D:246:TYR:CE2	2.36	0.60
1:A:114:ARG:O	1:A:115:SER:OG	2.19	0.60
2:C:66:MET:HE1	2:C:95:TYR:HE2	1.58	0.60
2:C:75:THR:HA	2:C:79:GLY:O	2.01	0.60
2:D:157:GLU:O	2:D:157:GLU:HG2	1.99	0.60
2:D:177:LYS:HE2	2:D:181:GLU:OE2	2.01	0.60
1:B:362:GLU:O	1:B:362:GLU:HG3	2.01	0.60
2:C:158:ASP:CB	2:C:303:ASN:HB3	2.32	0.60
2:D:199:LYS:CD	2:D:237:THR:OG1	2.48	0.60
1:A:38:ALA:CB	1:A:40:TRP:CZ3	2.85	0.60
1:B:212:LYS:HE3	1:B:270:TRP:CD1	2.36	0.60
2:C:154:GLU:OE2	2:C:156:SER:OG	2.19	0.60
1:A:189:LEU:H	1:A:189:LEU:CD2	2.14	0.60
1:B:127:GLN:HG3	1:B:128:PRO:HD2	1.83	0.60
1:B:152:LEU:HD12	1:B:152:LEU:C	2.22	0.60
2:D:392:ASP:OD1	2:D:392:ASP:N	2.30	0.60
2:D:45:MET:CE	2:D:46:LEU:CD2	2.79	0.60
1:A:168:ASN:O	1:A:173:ILE:CD1	2.49	0.60
1:A:171:ARG:HH11	1:A:171:ARG:CG	2.15	0.60
1:A:456:GLY:HA3	1:A:478:GLU:CB	2.31	0.60
1:B:272:ARG:HH22	1:B:280:THR:CG2	2.13	0.60
2:C:133:TYR:CE2	2:C:144:PRO:HG2	2.37	0.60
2:C:366:HIS:ND1	2:C:366:HIS:O	2.34	0.60
1:A:326:PHE:HB3	1:A:389:LEU:HD21	1.83	0.60
1:B:143:PHE:CE1	1:B:155:ARG:HB3	2.36	0.60
1:B:263:LEU:HD23	1:B:263:LEU:O	2.00	0.60
1:B:281:ALA:N	1:B:300:GLU:OE2	2.34	0.60
1:B:332:ASP:OD1	1:B:332:ASP:N	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:236:PHE:CG	2:D:164:GLU:OE1	2.55	0.60
1:A:119:GLU:CG	1:A:120:ARG:N	2.64	0.60
1:A:166:TRP:CE2	1:A:234:LEU:HD13	2.36	0.60
1:A:441:TYR:O	1:A:444:ALA:CB	2.50	0.60
2:C:268:ASN:HB2	2:C:275:ILE:CD1	2.32	0.60
2:D:169:SER:O	2:D:170:ALA:CB	2.46	0.60
2:D:299:ILE:N	2:D:299:ILE:HD12	2.16	0.60
1:A:119:GLU:CG	1:A:120:ARG:H	2.15	0.60
1:B:39:ASP:O	1:B:43:VAL:HG23	2.01	0.60
2:C:118:LEU:O	2:C:122:LEU:HD11	1.90	0.60
2:C:82:VAL:O	2:C:82:VAL:HG13	2.02	0.60
2:D:283:ASP:OD1	2:D:284:ALA:N	2.35	0.60
2:D:82:VAL:HG13	2:D:82:VAL:O	2.02	0.60
1:A:66:ARG:O	1:A:69:THR:N	2.18	0.59
1:A:94:PRO:CG	1:B:26:GLU:CD	2.67	0.59
1:B:568:ARG:O	1:B:571:VAL:HG12	2.02	0.59
2:C:263:TRP:O	2:C:264:LEU:CD2	2.42	0.59
2:C:160:TYR:CB	2:C:303:ASN:ND2	2.61	0.59
2:C:352:ASN:HB3	2:C:390:THR:CB	2.32	0.59
2:D:127:CYS:SG	2:D:153:ARG:CG	2.90	0.59
2:D:404:LYS:N	2:D:407:GLU:OE1	2.32	0.59
2:D:382:GLY:CA	2:D:415:ASN:HD22	2.15	0.59
1:B:223:LEU:O	1:B:224:LEU:HD23	2.01	0.59
1:B:531:LEU:H	1:B:531:LEU:HD12	1.65	0.59
2:C:257:LEU:HD23	2:C:260:GLY:HA2	1.83	0.59
2:D:119:ARG:CB	2:D:124:LEU:CD1	2.80	0.59
1:A:176:ILE:HG12	1:A:177:ILE:N	2.17	0.59
1:A:311:GLN:HE21	1:A:384:HIS:HA	1.66	0.59
1:B:28:THR:O	1:B:28:THR:HG22	2.02	0.59
1:A:328:LEU:HB2	1:A:331:PHE:HB2	1.84	0.59
1:B:229:THR:CG2	1:B:233:GLU:CB	2.58	0.59
1:B:254:ARG:NH2	1:B:562:ALA:HB2	2.14	0.59
1:B:86:TYR:C	1:B:89:LEU:HD12	2.22	0.59
2:C:154:GLU:O	2:C:303:ASN:OD1	2.20	0.59
1:A:45:GLN:O	1:A:48:LYS:HB2	2.02	0.59
2:C:35:ASP:HB2	2:C:341:THR:HG21	1.83	0.59
1:A:474:TYR:CD1	1:A:475:ASP:N	2.70	0.59
1:B:200:LEU:HD12	1:B:202:TYR:CZ	2.37	0.59
1:B:21:TYR:HE1	1:B:25:LEU:HD21	1.68	0.59
1:B:90:LEU:N	1:B:91:PRO:HD3	2.18	0.59
2:C:145:GLU:H	2:C:145:GLU:CD	2.00	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:MET:HE1	2:C:299:ILE:HD11	1.84	0.59
2:C:26:ASN:N	2:C:26:ASN:OD1	2.36	0.59
2:D:236:PHE:O	2:D:240:ALA:HB2	2.03	0.59
1:A:560:VAL:HG13	1:A:560:VAL:O	2.03	0.59
1:B:242:THR:OG1	1:B:245:GLU:OE2	0.59	0.59
1:B:54:TYR:CE1	1:B:58:VAL:HG21	2.38	0.59
2:C:149:MET:CE	2:C:299:ILE:HD11	2.33	0.59
2:D:292:ARG:N	2:D:293:PRO:HD3	2.18	0.59
1:A:107:TYR:CD1	1:A:111:PHE:HE2	2.19	0.59
1:A:57:HIS:O	1:A:60:LEU:HB3	2.03	0.59
1:B:143:PHE:CE1	1:B:155:ARG:HD2	2.37	0.59
1:B:272:ARG:O	1:B:276:PRO:HD3	2.03	0.59
1:B:462:ASN:OD1	1:B:475:ASP:HB2	2.03	0.59
2:D:345:TYR:O	2:D:348:GLN:HB2	2.03	0.59
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.66	0.59
1:B:494:ARG:HH11	1:B:498:ASP:CG	2.04	0.59
1:B:508:VAL:HG23	1:B:508:VAL:O	2.02	0.59
1:A:116:LEU:O	1:A:117:THR:HG23	2.03	0.58
1:A:168:ASN:CB	1:A:171:ARG:NE	2.59	0.58
2:C:171:ASP:O	2:C:174:LYS:HB3	2.02	0.58
2:C:158:ASP:CB	2:C:303:ASN:CB	2.81	0.58
2:C:5:VAL:HG21	2:C:68:ILE:HG22	1.85	0.58
1:A:38:ALA:CA	1:A:40:TRP:CZ3	2.85	0.58
1:B:149:TRP:C	1:B:152:LEU:H	2.06	0.58
2:C:154:GLU:OE2	2:C:156:SER:CA	2.51	0.58
2:C:49:VAL:O	2:C:53:VAL:HG23	2.03	0.58
1:A:107:TYR:HE1	1:A:111:PHE:HE2	1.43	0.58
1:A:17:PHE:CE1	1:A:98:ILE:HG21	2.38	0.58
1:A:473:PHE:CE2	1:A:479:ILE:HD12	2.38	0.58
1:B:327:THR:HG1	1:B:418:ARG:NH2	2.01	0.58
1:B:546:ARG:HH11	1:B:546:ARG:CG	2.12	0.58
1:A:551:ARG:HA	1:A:554:GLU:HB3	1.85	0.58
1:A:5:LEU:N	1:A:6:GLU:OE1	2.36	0.58
1:B:246:ALA:HA	1:B:249:VAL:HG12	1.84	0.58
2:C:183:MET:CE	2:C:183:MET:HA	2.34	0.58
2:C:349:ASP:OD1	2:C:405:CYS:HB3	2.02	0.58
2:D:285:PHE:CE1	2:D:289:ILE:CG2	2.86	0.58
1:B:107:TYR:CE1	1:B:111:PHE:CD2	2.92	0.58
1:B:117:THR:OG1	1:B:118:PRO:HD2	2.03	0.58
1:B:275:LEU:N	1:B:276:PRO:HD3	2.19	0.58
1:B:495:TYR:HB3	1:B:496:PRO:HD2	1.84	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:GLU:OE1	2:C:61:ARG:HG2	2.03	0.58
2:C:271:THR:CB	2:C:273:LYS:HG2	2.34	0.58
2:D:189:ARG:HG3	2:D:190:PHE:CD1	2.39	0.58
1:A:296:GLU:O	1:A:300:GLU:HG3	2.03	0.58
1:A:420:VAL:HG13	1:A:420:VAL:O	2.03	0.58
1:A:473:PHE:HE2	1:A:479:ILE:HD12	1.67	0.58
1:B:135:ILE:HD12	1:B:266:ALA:HB2	1.86	0.58
1:B:254:ARG:NH2	1:B:562:ALA:CA	2.67	0.58
2:C:288:GLN:HE22	2:C:292:ARG:HH11	1.51	0.58
2:D:5:VAL:O	2:D:5:VAL:HG23	2.04	0.58
1:A:13:ILE:O	1:A:16:GLY:N	2.35	0.58
1:A:333:ARG:HH22	1:A:373:GLN:HE22	1.50	0.58
1:B:186:PRO:CD	1:B:187:GLU:OE1	2.51	0.58
2:D:57:TYR:OH	2:D:369:TRP:HB3	2.04	0.58
1:B:192:SER:HG	1:B:215:THR:CA	1.91	0.58
2:C:326:ALA:HB2	2:C:335:PHE:CD1	2.38	0.58
2:C:66:MET:O	2:C:66:MET:HG3	2.04	0.58
1:A:106:VAL:HG12	1:A:110:LEU:CD1	2.34	0.57
1:A:426:LEU:H	1:A:426:LEU:HD12	1.68	0.57
1:B:42:ALA:HA	1:B:45:GLN:HB3	1.84	0.57
2:C:24:PRO:O	2:C:27:PRO:HD3	2.04	0.57
1:B:121:LEU:C	1:B:121:LEU:HD12	2.24	0.57
2:D:201:CYS:SG	2:D:206:THR:OG1	2.62	0.57
1:A:375:PHE:CE2	1:A:415:ILE:CD1	2.87	0.57
1:A:462:ASN:N	1:A:462:ASN:HD22	1.99	0.57
1:B:89:LEU:HD12	1:B:89:LEU:N	2.17	0.57
2:C:183:MET:HE3	2:C:183:MET:CA	2.32	0.57
2:C:23:VAL:HG13	2:C:23:VAL:O	2.04	0.57
2:C:124:LEU:CD1	2:C:327:ASN:HB2	2.31	0.57
1:A:368:ARG:NH1	1:A:440:GLU:OE2	2.37	0.57
1:A:404:LEU:O	1:A:407:GLN:N	2.38	0.57
2:C:276:VAL:C	2:C:277:ILE:HD13	2.25	0.57
1:A:554:GLU:HG2	1:A:554:GLU:O	2.05	0.57
1:A:80:LEU:N	1:A:80:LEU:HD12	2.18	0.57
1:A:86:TYR:OH	1:A:99:ALA:O	2.22	0.57
1:B:117:THR:HG23	1:B:120:ARG:H	1.68	0.57
1:B:107:TYR:HH	1:B:120:ARG:HE	1.50	0.57
1:B:366:VAL:HG12	1:B:366:VAL:O	2.04	0.57
1:B:375:PHE:HD1	1:B:415:ILE:HD12	1.64	0.57
2:D:127:CYS:SG	2:D:129:ARG:NH1	2.78	0.57
1:A:167:GLN:HG2	1:A:233:GLU:HB3	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ALA:O	1:A:452:ASN:HB3	2.02	0.57
1:A:506:TYR:N	1:A:506:TYR:CD1	2.73	0.57
1:B:107:TYR:CG	1:B:121:LEU:HD23	2.39	0.57
1:B:147:HIS:CD2	1:B:147:HIS:N	2.72	0.57
1:B:271:LEU:O	1:B:274:ILE:HB	2.05	0.57
2:C:317:VAL:O	2:C:317:VAL:HG12	2.05	0.57
2:C:35:ASP:O	2:C:341:THR:CG2	2.53	0.57
2:D:12:LYS:HG3	2:D:13:LYS:N	2.19	0.57
1:A:168:ASN:HB2	1:A:171:ARG:NE	1.87	0.57
1:A:192:SER:OG	1:A:215:THR:CB	2.52	0.57
1:B:172:ASP:O	1:B:176:ILE:HD13	2.04	0.57
1:A:333:ARG:HH12	1:A:373:GLN:NE2	2.03	0.57
1:A:403:ASP:C	1:A:404:LEU:CD1	2.72	0.57
1:B:271:LEU:O	1:B:274:ILE:N	2.38	0.57
2:C:5:VAL:O	2:C:5:VAL:HG13	2.04	0.57
1:A:189:LEU:CG	1:A:190:SER:N	2.68	0.57
1:A:342:PHE:HD1	1:A:342:PHE:N	2.02	0.57
1:A:561:TYR:HD1	1:A:561:TYR:N	2.02	0.57
1:A:83:LYS:HD3	1:A:87:THR:OG1	2.05	0.57
1:A:88:ARG:CB	1:A:88:ARG:HH11	2.18	0.57
1:A:192:SER:OG	1:A:215:THR:HB	2.03	0.57
1:A:254:ARG:HH11	1:A:254:ARG:CG	2.17	0.57
1:B:275:LEU:N	1:B:276:PRO:CD	2.68	0.57
1:B:332:ASP:O	1:B:417:ARG:HD3	2.05	0.57
2:C:133:TYR:CA	2:C:317:VAL:CG1	2.83	0.57
2:D:125:TYR:N	2:D:125:TYR:CD1	2.73	0.57
1:A:141:LYS:O	1:A:143:PHE:CD1	2.57	0.56
2:D:99:ILE:HB	2:D:363:MET:HE3	1.86	0.56
1:A:335:PHE:N	1:A:335:PHE:CD1	2.73	0.56
1:B:139:LEU:HD12	1:B:139:LEU:H	1.71	0.56
1:B:212:LYS:CE	1:B:270:TRP:NE1	2.68	0.56
1:B:506:TYR:N	1:B:506:TYR:CD1	2.73	0.56
2:C:133:TYR:CD1	2:C:134:TYR:N	2.72	0.56
2:C:248:LEU:HD12	2:C:248:LEU:O	2.04	0.56
1:A:293:ALA:O	1:A:297:SER:N	2.37	0.56
1:A:509:SER:CA	1:A:512:ASP:OD2	2.53	0.56
1:B:157:ILE:O	1:B:160:LEU:CD1	2.54	0.56
1:B:32:GLN:NE2	1:B:162:LEU:HA	2.20	0.56
2:C:157:GLU:OE2	2:C:201:CYS:HA	2.05	0.56
2:D:202:SER:OG	2:D:204:GLU:N	2.38	0.56
2:D:284:ALA:O	2:D:287:GLN:HB2	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:TYR:OH	2:D:369:TRP:CA	2.53	0.56
1:A:499:GLU:HB2	1:A:500:LEU:HD12	1.86	0.56
1:A:536:HIS:CD2	1:A:536:HIS:N	2.73	0.56
1:A:546:ARG:O	1:A:550:ASN:N	2.39	0.56
1:B:335:PHE:CD1	1:B:335:PHE:N	2.72	0.56
2:C:171:ASP:N	2:C:171:ASP:OD1	2.36	0.56
2:D:158:ASP:C	2:D:160:TYR:H	2.07	0.56
2:D:363:MET:O	2:D:367:MET:HG3	2.04	0.56
1:B:301:TYR:CE1	1:B:305:LEU:CD2	2.88	0.56
1:B:82:VAL:HG23	1:B:83:LYS:N	2.20	0.56
2:D:261:GLY:C	2:D:263:TRP:CZ3	2.77	0.56
2:C:213:ALA:O	2:C:216:TYR:CB	2.53	0.56
2:C:29:ILE:CG2	2:C:363:MET:HE3	2.34	0.56
2:D:134:TYR:O	2:D:137:THR:OG1	2.19	0.56
1:A:142:ASP:C	1:A:143:PHE:CD1	2.79	0.56
1:A:168:ASN:ND2	1:A:171:ARG:NH1	2.54	0.56
1:B:256:TYR:OH	1:B:361:LYS:NZ	2.39	0.56
2:C:271:THR:CG2	2:C:273:LYS:CG	2.83	0.56
2:D:148:ASP:OD1	2:D:222:ARG:NH1	2.38	0.56
1:B:13:ILE:CD1	1:B:13:ILE:H	2.19	0.56
1:B:462:ASN:C	1:B:463:PHE:HD1	2.09	0.56
1:B:442:GLY:HA3	1:B:536:HIS:CD2	2.41	0.56
1:B:86:TYR:CD2	1:B:103:PHE:HD2	2.24	0.56
2:C:171:ASP:HA	2:C:174:LYS:HB3	1.87	0.56
2:D:189:ARG:CZ	2:D:190:PHE:CE1	2.87	0.56
2:D:196:ILE:HG22	2:D:197:GLY:N	2.21	0.56
1:A:327:THR:OG1	1:A:328:LEU:N	2.37	0.56
2:C:25:GLU:OE1	2:C:61:ARG:NE	2.36	0.56
2:C:365:ARG:NH2	2:C:374:ASP:OD1	2.35	0.56
2:D:80:GLN:O	2:D:80:GLN:HG3	2.04	0.56
1:A:252:PHE:CD1	1:A:253:ALA:N	2.74	0.56
1:B:253:ALA:HB1	1:B:367:GLY:HA2	1.87	0.56
1:B:61:VAL:HG12	1:B:65:LEU:CD1	2.35	0.56
2:D:289:ILE:HD12	2:D:313:LEU:HD23	1.87	0.56
1:B:172:ASP:O	1:B:176:ILE:CD1	2.53	0.56
1:B:274:ILE:HG22	1:B:275:LEU:HG	1.88	0.56
1:A:143:PHE:N	1:A:143:PHE:CD1	2.73	0.55
1:A:32:GLN:HA	1:A:202:TYR:CZ	2.42	0.55
1:A:88:ARG:HH11	1:A:88:ARG:HB2	1.71	0.55
1:A:97:GLU:HG2	1:A:98:ILE:H	1.70	0.55
1:B:173:ILE:HG12	1:B:174:HIS:N	2.21	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:37:ILE:CG2	2:C:342:ALA:HB3	2.36	0.55
2:D:354:GLY:O	2:D:358:LEU:HG	2.06	0.55
2:D:45:MET:HE3	2:D:46:LEU:HD23	1.86	0.55
1:A:179:HIS:CD2	1:A:239:CYS:HB3	2.39	0.55
1:A:332:ASP:OD1	1:A:332:ASP:N	2.39	0.55
1:B:172:ASP:O	1:B:175:TYR:HB2	2.06	0.55
2:C:78:TYR:HB3	2:C:82:VAL:HG11	1.86	0.55
1:A:459:LEU:HD12	1:A:461:LYS:HE3	1.87	0.55
1:A:78:PHE:CD1	1:A:79:LEU:N	2.70	0.55
1:B:145:PRO:CB	1:B:149:TRP:CE3	2.86	0.55
1:B:176:ILE:HD12	1:B:176:ILE:H	1.69	0.55
1:B:7:LEU:CA	1:B:85:HIS:CD2	2.79	0.55
2:C:258:ILE:HG22	2:C:259:ASP:CG	2.19	0.55
1:A:208:TRP:CE2	1:A:225:PRO:HB3	2.42	0.55
1:A:344:PRO:CD	1:A:345:GLN:H	2.19	0.55
1:B:323:MET:HE1	1:B:357:TYR:CZ	2.41	0.55
1:B:39:ASP:O	1:B:43:VAL:CG2	2.54	0.55
2:D:106:PRO:CA	2:D:111:ILE:CD1	2.74	0.55
2:C:388:THR:C	2:C:389:VAL:HG13	2.26	0.55
1:B:544:TYR:CE1	1:B:548:LEU:HD21	2.42	0.55
2:C:348:GLN:O	2:C:349:ASP:CB	2.55	0.55
2:D:106:PRO:HB2	2:D:111:ILE:HG13	1.84	0.55
2:D:234:MET:HB2	2:D:237:THR:HG23	1.88	0.55
2:D:331:GLU:OE1	2:D:331:GLU:N	2.39	0.55
2:D:351:VAL:C	2:D:353:PRO:HD3	2.27	0.55
1:A:34:ARG:NH2	1:A:258:MET:CE	2.69	0.55
1:B:189:LEU:HD12	1:B:189:LEU:C	2.26	0.55
1:B:201:PHE:O	1:B:208:TRP:HB2	2.07	0.55
1:A:6:GLU:O	1:A:9:ILE:N	2.39	0.55
1:B:90:LEU:N	1:B:91:PRO:CD	2.69	0.55
2:C:116:VAL:O	2:C:120:GLN:HB2	2.07	0.55
2:C:216:TYR:CZ	2:C:220:ASN:ND2	2.75	0.55
2:C:229:HIS:ND1	2:C:229:HIS:O	2.40	0.55
2:C:8:PRO:CG	2:C:28:ILE:HG23	2.31	0.55
2:D:102:PRO:C	2:D:103:LEU:HD23	2.28	0.55
2:D:175:VAL:HG12	2:D:179:LEU:CD1	2.37	0.55
1:A:238:THR:OG1	1:A:239:CYS:N	2.39	0.55
1:A:31:ALA:CB	1:A:202:TYR:CD2	2.90	0.55
1:B:31:ALA:O	1:B:34:ARG:N	2.39	0.55
1:A:104:ASN:OD1	1:A:104:ASN:N	2.37	0.55
1:B:192:SER:OG	1:B:214:ILE:C	2.43	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ARG:HH11	1:B:564:ARG:HG3	1.72	0.55
2:C:258:ILE:O	2:C:259:ASP:OD1	2.22	0.55
1:A:324:LEU:HD23	1:A:393:LEU:HD23	1.89	0.54
2:C:112:ARG:HG2	2:C:113:SER:N	2.20	0.54
2:C:229:HIS:O	2:C:281:ILE:HA	2.07	0.54
2:C:326:ALA:HB3	2:C:362:MET:HE1	1.87	0.54
2:D:209:LEU:HD23	2:D:210:VAL:HG23	1.89	0.54
1:B:7:LEU:HB3	1:B:85:HIS:CD2	2.38	0.54
1:B:97:GLU:HG2	1:B:98:ILE:N	2.23	0.54
2:C:206:THR:O	2:C:210:VAL:HG23	2.06	0.54
2:C:271:THR:HB	2:C:273:LYS:H	1.70	0.54
1:A:561:TYR:CD1	1:A:561:TYR:N	2.73	0.54
1:A:85:HIS:C	1:A:89:LEU:HD11	2.25	0.54
1:B:419:MET:HE1	1:B:472:VAL:HG11	1.89	0.54
2:D:158:ASP:C	2:D:160:TYR:N	2.60	0.54
2:D:235:LYS:O	2:D:239:GLY:N	2.40	0.54
1:A:342:PHE:CD1	1:A:342:PHE:N	2.73	0.54
1:A:38:ALA:HA	1:A:40:TRP:CE3	2.42	0.54
1:B:60:LEU:C	1:B:60:LEU:HD12	2.24	0.54
2:C:8:PRO:HG3	2:C:28:ILE:CG2	2.30	0.54
2:D:356:ILE:HG23	2:D:357:ILE:N	2.22	0.54
1:A:116:LEU:HD12	1:A:116:LEU:N	2.23	0.54
1:B:522:LEU:HD12	1:B:522:LEU:N	2.22	0.54
2:C:183:MET:CE	2:C:183:MET:CA	2.85	0.54
2:D:119:ARG:O	2:D:124:LEU:CD1	2.52	0.54
1:A:17:PHE:HE1	1:A:98:ILE:HG21	1.72	0.54
1:A:189:LEU:HG	1:A:190:SER:H	1.72	0.54
1:A:17:PHE:CZ	1:A:98:ILE:HB	2.43	0.54
1:B:281:ALA:HB2	1:B:300:GLU:CD	2.28	0.54
1:B:323:MET:CE	1:B:357:TYR:OH	2.55	0.54
1:B:254:ARG:CZ	1:B:562:ALA:CB	2.86	0.54
2:D:203:GLU:O	2:D:207:LYS:HG3	2.07	0.54
2:D:261:GLY:C	2:D:263:TRP:CE3	2.81	0.54
2:D:31:TYR:HA	2:D:99:ILE:O	2.07	0.54
2:D:95:TYR:O	2:D:96:ARG:CB	2.56	0.54
1:A:528:ILE:HG12	1:A:529:GLY:N	2.23	0.54
1:B:37:GLN:O	1:B:38:ALA:HB3	2.06	0.54
2:C:151:ILE:HD13	2:C:299:ILE:HG13	1.89	0.54
2:D:45:MET:O	2:D:49:VAL:CG2	2.51	0.54
1:B:531:LEU:O	1:B:534:GLU:N	2.41	0.54
2:C:133:TYR:CZ	2:C:134:TYR:O	2.56	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:GLU:OE1	2:C:157:GLU:HG2	2.08	0.54
2:D:179:LEU:O	2:D:184:GLY:N	2.41	0.54
2:C:133:TYR:HD2	2:C:144:PRO:HB2	1.71	0.53
2:C:135:GLN:HG3	2:C:381:GLU:HG2	1.90	0.53
2:D:415:ASN:C	2:D:416:MET:OXT	2.44	0.53
1:A:305:LEU:HD12	1:A:306:GLN:N	2.22	0.53
1:B:515:PRO:O	1:B:540:PHE:CA	2.56	0.53
2:C:326:ALA:CB	2:C:335:PHE:CD1	2.91	0.53
2:D:132:ARG:HH11	2:D:132:ARG:CG	2.10	0.53
2:C:71:GLY:O	2:C:83:TRP:HZ3	1.87	0.53
2:C:84:LEU:HD12	2:C:84:LEU:C	2.29	0.53
2:D:224:SER:HB2	2:D:276:VAL:O	2.09	0.53
1:A:312:PHE:O	1:A:386:SER:OG	2.27	0.53
2:C:153:ARG:CD	2:C:306:GLY:CA	2.41	0.53
2:D:131:VAL:HG21	2:D:313:LEU:HD13	1.90	0.53
1:A:379:VAL:O	1:A:379:VAL:HG13	2.08	0.53
1:B:312:PHE:CD1	1:B:328:LEU:HD23	2.36	0.53
1:B:325:VAL:HA	1:B:335:PHE:O	2.07	0.53
1:B:440:GLU:HG2	1:B:471:VAL:HG23	1.89	0.53
1:B:485:VAL:HG21	1:B:513:VAL:HG21	1.90	0.53
2:C:160:TYR:CE1	2:C:304:LEU:CD1	2.91	0.53
2:C:7:VAL:HG13	2:C:8:PRO:HD2	1.88	0.53
1:A:229:THR:O	1:A:232:GLY:N	2.41	0.53
1:B:237:ASP:CB	1:B:569:PHE:HE1	1.83	0.53
1:B:59:GLY:O	1:B:62:VAL:HG22	2.09	0.53
2:C:37:ILE:O	2:C:40:ASP:HB2	2.09	0.53
1:A:219:THR:CA	1:A:220:LEU:HD23	2.34	0.53
1:B:13:ILE:O	1:B:16:GLY:N	2.41	0.53
2:C:69:TYR:CD1	2:C:69:TYR:N	2.77	0.53
2:D:130:PRO:HG3	2:D:362:MET:SD	2.49	0.53
2:D:37:ILE:O	2:D:40:ASP:HB2	2.09	0.53
1:B:149:TRP:O	1:B:152:LEU:CB	2.54	0.53
1:B:176:ILE:H	1:B:176:ILE:CD1	2.21	0.53
1:B:257:PHE:HB2	1:B:286:ALA:O	2.08	0.53
1:B:443:ASN:O	1:B:447:GLN:HG3	2.08	0.53
2:C:225:VAL:HB	2:C:277:ILE:HD12	1.91	0.53
2:D:240:ALA:CA	2:D:244:TRP:HE1	2.20	0.53
1:A:14:LEU:HD11	1:A:93:TYR:CE2	2.44	0.53
1:B:21:TYR:CE1	1:B:25:LEU:HD21	2.44	0.53
1:B:281:ALA:CB	1:B:300:GLU:OE2	2.56	0.53
2:C:271:THR:HG21	2:C:273:LYS:CG	2.39	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:VAL:O	2:D:119:ARG:HG3	2.09	0.53
1:A:215:THR:CG2	1:A:218:GLY:O	2.57	0.53
1:B:323:MET:HE3	1:B:357:TYR:OH	2.09	0.53
1:B:253:ALA:CA	1:B:367:GLY:HA2	2.39	0.53
2:C:78:TYR:CB	2:C:82:VAL:HG11	2.39	0.53
2:D:128:LEU:HD13	2:D:152:PHE:CE1	2.44	0.53
2:D:261:GLY:CA	2:D:263:TRP:CH2	2.73	0.53
1:A:31:ALA:CB	1:A:202:TYR:HD2	2.22	0.52
1:A:324:LEU:HB3	1:A:337:VAL:HG13	1.90	0.52
1:A:431:GLY:O	1:A:435:ARG:N	2.39	0.52
2:D:161:ALA:CB	2:D:163:ILE:HG13	2.38	0.52
2:D:189:ARG:NH1	2:D:190:PHE:HE1	2.06	0.52
2:D:196:ILE:CG2	2:D:197:GLY:N	2.72	0.52
1:A:107:TYR:HE1	1:A:111:PHE:CE2	2.17	0.52
1:A:281:ALA:HB3	1:A:300:GLU:OE2	2.09	0.52
1:A:77:GLU:OE2	1:A:78:PHE:HB2	2.09	0.52
1:B:100:GLU:O	1:B:103:PHE:HB3	2.10	0.52
1:B:134:THR:CG2	1:B:135:ILE:N	2.72	0.52
1:A:404:LEU:CD2	1:A:409:VAL:CG2	2.87	0.52
1:A:474:TYR:HD1	1:A:475:ASP:N	2.07	0.52
1:A:561:TYR:CE2	1:A:568:ARG:CZ	2.90	0.52
2:D:307:ASP:OD1	2:D:311:ASP:CG	2.48	0.52
1:A:118:PRO:C	1:A:119:GLU:OE2	2.48	0.52
1:A:254:ARG:CG	1:A:254:ARG:NH1	2.73	0.52
1:B:148:GLY:CA	1:B:151:SER:OG	2.58	0.52
1:B:156:VAL:HG23	1:B:157:ILE:HG13	1.91	0.52
1:B:303:VAL:O	1:B:306:GLN:HG3	2.10	0.52
2:D:227:LEU:N	2:D:227:LEU:CD1	2.73	0.52
1:A:96:PHE:CD1	1:A:96:PHE:N	2.73	0.52
1:B:335:PHE:HA	1:B:414:TYR:O	2.08	0.52
1:B:462:ASN:C	1:B:463:PHE:CD1	2.83	0.52
1:B:494:ARG:C	1:B:495:TYR:CD1	2.83	0.52
2:D:384:ILE:O	2:D:387:LYS:CA	2.56	0.52
1:B:176:ILE:N	1:B:176:ILE:CD1	2.73	0.52
1:B:524:ALA:O	2:C:76:GLN:NE2	2.43	0.52
2:C:352:ASN:CB	2:C:390:THR:OG1	2.58	0.52
2:D:158:ASP:CG	2:D:159:ILE:H	2.08	0.52
1:A:171:ARG:NH1	1:A:171:ARG:CG	2.73	0.52
1:A:551:ARG:HH11	1:A:551:ARG:HB3	1.74	0.52
1:A:87:THR:HG23	1:A:122:PHE:CZ	2.44	0.52
1:B:517:GLU:CD	2:C:107:VAL:HG23	2.24	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:352:ASN:HB2	2:C:390:THR:OG1	2.09	0.52
1:A:149:TRP:C	1:A:152:LEU:H	2.13	0.52
1:A:195:GLN:HG2	1:A:270:TRP:HZ2	1.74	0.52
1:A:509:SER:N	1:A:512:ASP:OD2	2.42	0.52
1:B:117:THR:CG2	1:B:120:ARG:HB2	2.40	0.52
1:B:285:MET:CE	1:B:373:GLN:NE2	2.73	0.52
1:B:41:HIS:O	1:B:45:GLN:HB3	2.09	0.52
2:C:204:GLU:O	2:C:208:ARG:HB2	2.10	0.52
2:C:51:ALA:CB	2:C:413:ILE:CD1	2.88	0.52
2:D:169:SER:C	2:D:171:ASP:N	2.62	0.52
2:D:249:ALA:CB	2:D:264:LEU:HD11	2.37	0.52
2:D:299:ILE:N	2:D:299:ILE:CD1	2.72	0.52
2:D:403:LEU:N	2:D:403:LEU:CD1	2.73	0.52
1:A:223:LEU:N	1:A:223:LEU:CD1	2.73	0.52
1:A:240:LEU:N	1:A:240:LEU:CD1	2.73	0.52
1:B:253:ALA:CB	1:B:367:GLY:CA	2.87	0.52
1:B:528:ILE:C	1:B:531:LEU:HD12	2.29	0.52
2:C:25:GLU:HB3	2:C:61:ARG:HG2	1.90	0.52
2:C:158:ASP:HB2	2:C:303:ASN:HB2	1.92	0.52
2:C:289:ILE:HD12	2:C:313:LEU:CD2	2.40	0.52
2:D:45:MET:HG2	2:D:49:VAL:CG2	2.40	0.52
2:D:75:THR:HG23	2:D:80:GLN:HA	1.90	0.52
1:A:201:PHE:CD2	1:A:259:VAL:HB	2.44	0.52
1:A:88:ARG:CB	1:A:88:ARG:NH1	2.73	0.52
1:B:473:PHE:CZ	1:B:475:ASP:O	2.63	0.52
1:B:88:ARG:HG2	1:B:88:ARG:O	2.10	0.52
2:C:29:ILE:HD12	2:C:363:MET:HE3	1.92	0.52
2:D:261:GLY:CA	2:D:263:TRP:HZ3	1.88	0.52
2:D:45:MET:CE	2:D:46:LEU:N	2.73	0.52
1:A:109:ARG:CG	1:A:109:ARG:HH11	2.22	0.51
1:A:181:THR:O	1:A:184:LEU:O	2.28	0.51
1:B:146:ASP:CB	1:B:147:HIS:CD2	2.91	0.51
1:B:356:CYS:SG	1:B:479:ILE:HG21	2.50	0.51
1:A:21:TYR:O	1:A:24:PHE:HB3	2.09	0.51
1:A:357:TYR:CE1	1:A:476:TYR:HD2	2.27	0.51
1:A:404:LEU:N	1:A:404:LEU:CD1	2.73	0.51
1:A:77:GLU:CG	1:A:78:PHE:N	2.74	0.51
1:B:130:ARG:HD2	1:B:130:ARG:O	2.10	0.51
1:B:68:ILE:O	1:B:69:THR:CB	2.58	0.51
1:A:80:LEU:N	1:A:80:LEU:CD1	2.73	0.51
2:D:166:LYS:O	2:D:169:SER:HB3	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:CD1	1:A:116:LEU:N	2.73	0.51
1:A:213:LEU:N	1:A:220:LEU:O	2.43	0.51
1:A:481:TYR:HB2	1:A:484:GLU:CG	2.41	0.51
1:A:570:SER:O	1:A:571:VAL:HG22	2.10	0.51
1:B:453:ILE:CG2	1:B:479:ILE:HD11	2.40	0.51
1:B:80:LEU:N	1:B:80:LEU:CD2	2.73	0.51
2:C:190:PHE:N	2:C:191:PRO:CD	2.73	0.51
2:C:326:ALA:HB2	2:C:362:MET:HE2	1.90	0.51
2:D:78:TYR:HB3	2:D:82:VAL:HG11	1.91	0.51
1:A:229:THR:O	1:A:232:GLY:HA2	2.09	0.51
1:A:290:GLN:HG3	1:A:291:LYS:N	2.25	0.51
1:B:522:LEU:CD1	1:B:522:LEU:N	2.73	0.51
2:C:160:TYR:CZ	2:C:304:LEU:HD12	2.45	0.51
1:A:97:GLU:HA	1:A:100:GLU:OE1	2.11	0.51
1:A:141:LYS:HG3	1:A:141:LYS:O	2.10	0.51
1:A:201:PHE:CD1	1:A:210:VAL:CG2	2.94	0.51
1:A:422:LEU:HG	1:A:426:LEU:HD11	1.93	0.51
1:B:20:GLN:HG3	1:B:21:TYR:N	2.25	0.51
1:B:304:TYR:OH	1:B:330:GLY:HA3	2.09	0.51
1:B:80:LEU:N	1:B:80:LEU:HD23	2.26	0.51
2:C:146:LEU:O	2:C:293:PRO:HG2	2.10	0.51
2:C:402:LEU:HD12	2:C:402:LEU:C	2.31	0.51
1:B:186:PRO:N	1:B:187:GLU:OE1	2.44	0.51
1:B:401:ILE:HD12	1:B:401:ILE:O	2.09	0.51
1:B:65:LEU:CD1	1:B:65:LEU:N	2.73	0.51
2:D:79:GLY:HA3	2:D:82:VAL:CG1	2.40	0.51
1:B:41:HIS:O	1:B:45:GLN:CB	2.59	0.51
2:C:256:GLU:O	2:C:265:LYS:HG2	2.11	0.51
2:D:26:ASN:N	2:D:27:PRO:CD	2.73	0.51
2:D:238:GLU:OE2	2:D:302:MET:SD	2.69	0.51
1:A:103:PHE:CD2	1:A:122:PHE:HD2	2.29	0.51
1:A:88:ARG:HB3	1:A:88:ARG:NH1	2.25	0.51
2:D:219:ALA:HB3	2:D:220:ASN:ND2	2.25	0.51
1:A:177:ILE:O	1:A:181:THR:N	2.30	0.51
1:A:281:ALA:HB2	1:A:300:GLU:OE2	2.10	0.51
1:A:49:ASN:O	1:A:52:HIS:N	2.40	0.51
1:A:515:PRO:O	1:A:518:PHE:CD2	2.64	0.51
1:B:143:PHE:O	1:B:193:HIS:HB2	2.11	0.51
1:B:144:HIS:HB3	1:B:145:PRO:HD2	1.93	0.51
2:C:214:ILE:HG22	2:C:218:ILE:HD11	1.93	0.51
2:D:153:ARG:HH21	2:D:303:ASN:C	2.01	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:TYR:CG	2:D:61:ARG:HD2	2.46	0.51
1:A:32:GLN:HB2	1:A:202:TYR:OH	2.11	0.50
1:A:482:MET:HE1	1:A:545:TRP:CE3	2.45	0.50
1:B:254:ARG:HH22	1:B:562:ALA:HA	1.76	0.50
2:D:222:ARG:HB3	2:D:297:ASP:OD1	2.11	0.50
2:D:230:LYS:H	2:D:238:GLU:CG	2.10	0.50
2:D:230:LYS:N	2:D:238:GLU:HG2	2.08	0.50
2:D:383:ALA:HA	2:D:415:ASN:HD21	1.75	0.50
2:D:415:ASN:O	2:D:416:MET:OXT	2.30	0.50
1:A:118:PRO:HD2	1:A:119:GLU:H	1.76	0.50
1:A:35:PHE:CE2	1:A:207:ALA:HB2	2.46	0.50
1:A:460:PHE:O	1:A:462:ASN:N	2.44	0.50
1:B:35:PHE:C	1:B:35:PHE:CD1	2.85	0.50
1:B:445:ILE:HG21	1:B:458:MET:HE3	1.93	0.50
1:B:5:LEU:HD23	1:B:6:GLU:CA	2.41	0.50
1:A:100:GLU:O	1:A:103:PHE:HB3	2.11	0.50
1:A:141:LYS:HE2	1:A:143:PHE:CZ	2.46	0.50
1:A:31:ALA:HB3	1:A:202:TYR:CD2	2.46	0.50
1:A:448:LEU:N	1:A:448:LEU:HD12	2.15	0.50
1:B:529:GLY:N	1:B:530:PRO:HD2	2.26	0.50
1:B:8:LEU:C	1:B:8:LEU:HD12	2.25	0.50
2:D:159:ILE:HG12	2:D:199:LYS:HB2	1.93	0.50
2:D:189:ARG:NH1	2:D:190:PHE:CD1	2.80	0.50
2:D:209:LEU:CD2	2:D:210:VAL:N	2.66	0.50
1:A:173:ILE:CD1	1:A:173:ILE:H	2.15	0.50
1:A:180:LEU:CD2	1:A:180:LEU:N	2.73	0.50
1:A:463:PHE:CE1	1:A:473:PHE:CD1	3.00	0.50
1:B:160:LEU:HB2	1:B:161:PRO:HD2	1.93	0.50
1:B:168:ASN:HB2	1:B:171:ARG:HB2	1.93	0.50
1:B:303:VAL:HG23	1:B:304:TYR:N	2.27	0.50
1:B:441:TYR:CD1	1:B:441:TYR:C	2.85	0.50
2:C:175:VAL:HG22	2:D:183:MET:HE3	1.91	0.50
2:D:234:MET:HG3	2:D:238:GLU:CB	2.41	0.50
1:A:35:PHE:CD1	1:A:35:PHE:C	2.85	0.50
1:A:531:LEU:O	1:A:534:GLU:N	2.44	0.50
1:A:56:HIS:CD2	1:A:56:HIS:C	2.85	0.50
1:B:173:ILE:HG12	1:B:174:HIS:H	1.75	0.50
1:B:382:LYS:NZ	1:B:405:GLY:O	2.31	0.50
2:C:48:VAL:HA	2:C:413:ILE:HD11	1.93	0.50
2:D:12:LYS:O	2:D:28:ILE:HG13	2.11	0.50
2:D:7:VAL:HG13	5:D:505:HOH:O	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ALA:O	1:A:552:ILE:CD1	2.59	0.50
1:A:452:ASN:ND2	1:A:482:MET:H	2.10	0.50
1:A:94:PRO:HG3	1:B:26:GLU:OE2	2.12	0.50
1:B:208:TRP:CE3	1:B:225:PRO:HB3	2.47	0.50
1:B:485:VAL:CG2	1:B:513:VAL:HG23	2.42	0.50
2:C:119:ARG:HH11	2:C:119:ARG:CG	2.24	0.50
2:C:158:ASP:CB	2:C:303:ASN:HB2	2.41	0.50
2:C:178:PHE:C	2:C:178:PHE:CD1	2.85	0.50
2:D:150:VAL:HG11	2:D:216:TYR:CE2	2.46	0.50
1:B:97:GLU:O	1:B:100:GLU:HG3	2.12	0.50
1:B:111:PHE:CE2	1:B:120:ARG:NH2	2.79	0.50
1:B:333:ARG:HB3	1:B:416:GLU:O	2.11	0.50
1:B:548:LEU:O	1:B:552:ILE:HG13	2.11	0.50
2:D:141:VAL:HG23	2:D:144:PRO:HB3	1.94	0.50
1:A:177:ILE:CG1	1:A:178:ARG:N	2.75	0.50
1:A:193:HIS:C	1:A:194:LEU:HD12	2.31	0.50
1:A:365:ARG:C	1:A:367:GLY:H	2.14	0.50
1:B:108:CYS:O	1:B:112:ASP:N	2.44	0.50
1:B:357:TYR:CD2	1:B:414:TYR:CE2	3.00	0.50
1:A:312:PHE:CE1	1:A:328:LEU:HG	2.47	0.50
1:A:404:LEU:CD2	1:A:409:VAL:HG23	2.41	0.50
1:B:419:MET:HE3	1:B:472:VAL:HB	1.94	0.50
2:C:357:ILE:O	2:C:360:ALA:HB3	2.11	0.50
2:D:266:VAL:CG2	2:D:277:ILE:CD1	2.90	0.50
1:A:168:ASN:HD22	1:A:171:ARG:CZ	2.25	0.49
1:A:28:THR:HG23	1:A:258:MET:HG3	1.93	0.49
1:A:451:ALA:O	1:A:452:ASN:CB	2.60	0.49
1:B:176:ILE:C	1:B:180:LEU:HD11	2.27	0.49
1:B:235:PHE:CD1	1:B:235:PHE:C	2.85	0.49
1:B:301:TYR:CE2	1:B:302:LEU:HD12	2.47	0.49
1:B:336:LYS:HE2	4:B:601:ADP:H8	1.76	0.49
1:B:525:ASP:HB3	1:B:528:ILE:HG12	1.94	0.49
2:C:133:TYR:C	2:C:133:TYR:CD1	2.85	0.49
2:C:386:ALA:O	2:C:387:LYS:HB2	2.11	0.49
2:D:133:TYR:C	2:D:133:TYR:CD1	2.85	0.49
1:A:220:LEU:HB3	1:A:221:PRO:HD2	1.94	0.49
1:A:77:GLU:HG2	1:A:78:PHE:N	2.27	0.49
2:C:133:TYR:CD1	2:C:134:TYR:C	2.85	0.49
2:C:209:LEU:O	2:C:212:ALA:N	2.45	0.49
2:C:326:ALA:CB	2:C:335:PHE:HD1	2.24	0.49
2:D:401:LYS:O	2:D:403:LEU:HD11	2.08	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:OE2	1:A:163:ARG:HG3	2.12	0.49
1:A:333:ARG:HH22	1:A:373:GLN:NE2	2.10	0.49
1:B:117:THR:HG22	1:B:120:ARG:HD3	1.94	0.49
1:B:132:PHE:CD1	1:B:134:THR:HA	2.48	0.49
1:B:149:TRP:C	1:B:149:TRP:CD1	2.86	0.49
2:D:209:LEU:HD21	2:D:210:VAL:HG23	1.94	0.49
1:A:141:LYS:HE2	1:A:143:PHE:HZ	1.77	0.49
1:A:225:PRO:HG2	1:A:225:PRO:O	2.13	0.49
1:A:31:ALA:HB3	1:A:202:TYR:HD2	1.77	0.49
1:A:321:MET:O	1:A:339:LYS:HE2	2.13	0.49
1:A:323:MET:CE	1:A:338:ILE:HG13	2.37	0.49
1:B:54:TYR:CD1	1:B:54:TYR:C	2.85	0.49
2:C:328:ILE:HG22	2:C:329:GLY:N	2.27	0.49
1:A:107:TYR:CD2	1:A:121:LEU:CD2	2.95	0.49
1:A:565:ARG:O	1:A:568:ARG:CG	2.54	0.49
1:A:56:HIS:O	1:A:60:LEU:N	2.45	0.49
1:B:213:LEU:O	1:B:220:LEU:N	2.28	0.49
1:B:272:ARG:O	1:B:275:LEU:N	2.44	0.49
1:B:323:MET:CE	1:B:357:TYR:CE1	2.96	0.49
1:B:528:ILE:C	1:B:531:LEU:CD1	2.80	0.49
2:C:178:PHE:HD1	2:C:178:PHE:O	1.96	0.49
2:C:271:THR:HB	2:C:273:LYS:HG3	1.93	0.49
1:A:176:ILE:CD1	1:A:176:ILE:N	2.73	0.49
1:A:227:HIS:O	1:A:234:LEU:HA	2.12	0.49
1:A:473:PHE:HE2	1:A:479:ILE:HD13	1.75	0.49
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.93	0.49
1:B:176:ILE:O	1:B:180:LEU:HD11	2.03	0.49
2:C:39:VAL:O	2:C:43:PRO:HG2	2.13	0.49
2:D:189:ARG:O	2:D:189:ARG:NH1	2.44	0.49
1:A:185:GLY:O	1:A:188:ASN:HB2	2.13	0.49
1:A:192:SER:CB	1:A:215:THR:HB	2.43	0.49
1:A:382:LYS:NZ	1:A:405:GLY:O	2.33	0.49
1:A:441:TYR:C	1:A:441:TYR:CD1	2.85	0.49
2:C:28:ILE:HA	2:C:64:SER:O	2.13	0.49
2:C:360:ALA:O	2:C:363:MET:HB3	2.11	0.49
2:D:234:MET:HG3	2:D:238:GLU:HB3	1.95	0.49
2:D:285:PHE:CD1	2:D:285:PHE:C	2.85	0.49
2:D:30:PRO:HD2	2:D:97:VAL:O	2.13	0.49
2:D:407:GLU:HA	2:D:410:ASP:OD2	2.12	0.49
1:A:54:TYR:C	1:A:54:TYR:CD1	2.86	0.49
2:C:189:ARG:NH1	2:C:189:ARG:HG3	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:ASN:N	2:D:220:ASN:ND2	2.60	0.49
1:A:40:TRP:NE1	1:A:205:LYS:HA	2.27	0.49
1:A:274:ILE:CG2	1:A:275:LEU:HD23	2.38	0.49
1:B:525:ASP:HA	2:C:76:GLN:HE22	1.77	0.49
1:B:528:ILE:HA	1:B:531:LEU:CD1	2.42	0.49
2:D:82:VAL:O	2:D:82:VAL:HG22	2.12	0.49
1:A:196:VAL:CG1	1:A:197:ALA:N	2.76	0.49
1:B:17:PHE:CE1	1:B:98:ILE:HB	2.47	0.49
2:C:178:PHE:C	2:C:178:PHE:HD1	2.16	0.49
1:A:298:TYR:O	1:A:301:TYR:HB3	2.13	0.48
1:B:107:TYR:C	1:B:107:TYR:CD1	2.85	0.48
1:B:509:SER:N	1:B:512:ASP:OD2	2.45	0.48
1:B:97:GLU:OE2	1:B:265:ALA:HB2	2.13	0.48
2:C:229:HIS:ND1	2:C:231:GLY:N	2.59	0.48
1:A:153:LEU:O	1:A:157:ILE:HG12	2.13	0.48
1:B:187:GLU:H	1:B:187:GLU:CD	1.94	0.48
2:D:133:TYR:CD2	2:D:144:PRO:HB2	2.48	0.48
2:D:353:PRO:HG2	2:D:405:CYS:SG	2.52	0.48
1:A:359:LEU:HD12	1:A:359:LEU:C	2.32	0.48
1:B:223:LEU:CD1	1:B:223:LEU:N	2.76	0.48
1:B:224:LEU:CD2	1:B:239:CYS:HA	2.44	0.48
1:B:249:VAL:HG22	1:B:249:VAL:O	2.12	0.48
2:C:166:LYS:HG2	2:C:167:ALA:N	2.27	0.48
2:C:357:ILE:O	2:C:360:ALA:N	2.46	0.48
2:D:169:SER:C	2:D:171:ASP:H	2.13	0.48
2:D:14:ILE:HD13	2:D:24:PRO:HD2	1.96	0.48
2:D:266:VAL:HG23	2:D:277:ILE:HD12	1.95	0.48
1:A:271:LEU:O	1:A:274:ILE:N	2.46	0.48
1:B:327:THR:CG2	1:B:418:ARG:HH21	2.26	0.48
1:B:5:LEU:HD23	1:B:6:GLU:HA	1.94	0.48
2:C:271:THR:CB	2:C:273:LYS:CG	2.90	0.48
2:C:352:ASN:HB3	2:C:390:THR:HG21	1.94	0.48
2:D:125:TYR:H	2:D:125:TYR:HD1	1.60	0.48
2:D:45:MET:HG2	2:D:49:VAL:HG23	1.94	0.48
1:A:423:ASN:OD1	1:A:424:ILE:HG13	2.13	0.48
1:B:200:LEU:HB3	1:B:208:TRP:O	2.13	0.48
1:B:208:TRP:HA	1:B:225:PRO:HA	1.95	0.48
1:B:365:ARG:HB3	1:B:369:MET:HB2	1.95	0.48
1:B:485:VAL:HG21	1:B:513:VAL:CG2	2.44	0.48
2:C:307:ASP:O	2:C:311:ASP:HB2	2.13	0.48
1:A:109:ARG:NH1	1:A:109:ARG:CG	2.77	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:HIS:HD2	1:A:239:CYS:CB	2.24	0.48
1:A:230:ASP:OD1	1:A:230:ASP:N	2.46	0.48
1:A:234:LEU:CD1	1:A:234:LEU:H	2.18	0.48
1:A:34:ARG:NH2	1:A:258:MET:HE2	2.28	0.48
1:A:531:LEU:O	1:A:535:MET:N	2.41	0.48
1:B:17:PHE:CE1	1:B:98:ILE:CB	2.97	0.48
1:B:240:LEU:HD22	1:B:245:GLU:CB	2.43	0.48
1:B:552:ILE:O	1:B:555:GLY:N	2.46	0.48
1:A:107:TYR:HB3	1:A:121:LEU:HD23	1.94	0.48
1:A:299:ARG:O	1:A:302:LEU:N	2.46	0.48
1:A:463:PHE:N	1:A:463:PHE:CD1	2.82	0.48
1:B:117:THR:OG1	1:B:118:PRO:CD	2.62	0.48
1:B:422:LEU:N	1:B:463:PHE:O	2.44	0.48
2:D:263:TRP:HB3	2:D:277:ILE:O	2.13	0.48
1:A:107:TYR:CZ	1:A:111:PHE:CD2	3.02	0.48
1:A:334:VAL:HG23	1:A:334:VAL:O	2.13	0.48
1:A:422:LEU:CG	1:A:426:LEU:HD11	2.43	0.48
1:B:127:GLN:CG	1:B:128:PRO:HD2	2.43	0.48
1:B:133:ARG:O	1:B:134:THR:OG1	2.26	0.48
1:B:333:ARG:NH1	1:B:415:ILE:HG21	2.27	0.48
1:B:476:TYR:CD1	1:B:476:TYR:N	2.81	0.48
2:C:133:TYR:CE2	2:C:144:PRO:CG	2.97	0.48
2:C:230:LYS:HE2	2:C:232:ASN:OD1	2.14	0.48
2:D:352:ASN:HA	2:D:353:PRO:HD2	1.37	0.48
1:A:149:TRP:CZ3	1:A:152:LEU:HD21	2.48	0.48
1:A:191:LYS:HA	1:A:191:LYS:HD2	1.60	0.48
1:A:256:TYR:OH	1:A:371:ASP:OD2	2.28	0.48
1:B:145:PRO:CB	1:B:149:TRP:HE3	2.26	0.48
1:B:135:ILE:HD12	1:B:266:ALA:CB	2.43	0.48
1:B:84:GLU:O	1:B:87:THR:CB	2.61	0.48
2:C:257:LEU:CD2	2:C:260:GLY:HA2	2.42	0.48
2:C:39:VAL:CG1	2:C:40:ASP:N	2.77	0.48
2:C:160:TYR:CD1	2:D:233:ILE:HG21	2.48	0.48
2:D:372:ALA:O	2:D:375:LEU:N	2.46	0.48
1:A:293:ALA:O	1:A:297:SER:CB	2.62	0.48
1:A:61:VAL:O	1:A:64:GLN:N	2.47	0.48
1:B:148:GLY:C	1:B:151:SER:OG	2.52	0.48
2:D:328:ILE:HG22	2:D:329:GLY:N	2.28	0.48
1:A:34:ARG:HH21	1:A:258:MET:CE	2.27	0.47
1:A:396:GLU:OE1	1:A:396:GLU:HA	2.13	0.47
2:C:116:VAL:CG2	2:C:117:ALA:N	2.77	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:245:GLY:O	2:C:248:LEU:HB3	2.14	0.47
2:C:365:ARG:HH11	2:C:365:ARG:CG	2.15	0.47
1:B:179:HIS:N	1:B:182:GLU:OE2	2.46	0.47
1:B:192:SER:OG	1:B:215:THR:CB	2.60	0.47
1:B:299:ARG:O	1:B:302:LEU:N	2.47	0.47
1:B:334:VAL:HG13	1:B:418:ARG:HB2	1.96	0.47
2:C:30:PRO:HA	2:C:66:MET:O	2.14	0.47
1:A:344:PRO:HD2	1:A:345:GLN:H	1.79	0.47
1:A:365:ARG:C	1:A:367:GLY:N	2.67	0.47
1:B:434:LEU:C	1:B:436:ASP:N	2.66	0.47
1:B:62:VAL:CG2	1:B:63:GLU:N	2.76	0.47
1:B:80:LEU:CD2	1:B:81:ARG:HG2	2.44	0.47
1:B:97:GLU:CG	1:B:98:ILE:N	2.78	0.47
2:C:133:TYR:CB	2:C:317:VAL:HG13	2.45	0.47
2:D:157:GLU:OE1	2:D:202:SER:CB	2.61	0.47
1:A:31:ALA:HB1	1:A:202:TYR:CD2	2.49	0.47
1:A:229:THR:OG1	1:A:235:PHE:CD1	2.65	0.47
1:B:201:PHE:CE1	1:B:210:VAL:HG23	2.42	0.47
1:B:474:TYR:CD1	1:B:475:ASP:N	2.73	0.47
2:D:167:ALA:O	2:D:168:ASP:HB2	2.14	0.47
1:B:208:TRP:CZ3	1:B:225:PRO:HB3	2.49	0.47
1:A:239:CYS:C	1:A:240:LEU:HD12	2.35	0.47
1:A:321:MET:HB3	1:A:343:ALA:CB	2.39	0.47
1:A:40:TRP:HA	1:A:43:VAL:CG2	2.45	0.47
1:B:329:PRO:O	1:B:418:ARG:NH1	2.48	0.47
1:B:425:TRP:CE2	1:B:429:VAL:HG11	2.50	0.47
1:B:80:LEU:H	1:B:80:LEU:CD2	2.27	0.47
2:C:258:ILE:CA	2:C:259:ASP:OD1	2.60	0.47
1:A:274:ILE:O	1:A:275:LEU:HD23	2.14	0.47
1:A:333:ARG:NH1	1:A:373:GLN:HE22	2.12	0.47
1:A:420:VAL:CG1	1:A:465:VAL:HB	2.44	0.47
1:B:96:PHE:O	1:B:99:ALA:HB3	2.14	0.47
2:D:388:THR:O	2:D:389:VAL:CG1	2.62	0.47
1:A:219:THR:N	1:A:220:LEU:HD23	2.29	0.47
1:B:135:ILE:CD1	1:B:266:ALA:HB2	2.45	0.47
1:B:567:GLN:O	1:B:568:ARG:C	2.50	0.47
1:A:143:PHE:N	1:A:143:PHE:HD1	2.11	0.47
1:A:223:LEU:C	1:A:224:LEU:CD1	2.83	0.47
1:A:460:PHE:C	1:A:462:ASN:N	2.66	0.47
1:A:322:VAL:HG22	4:A:602:ADP:O1B	2.08	0.47
1:B:254:ARG:HG3	1:B:367:GLY:HA3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:HB2	1:B:448:LEU:HD21	1.96	0.47
1:B:550:ASN:O	1:B:554:GLU:CG	2.60	0.47
2:C:285:PHE:HE2	2:C:289:ILE:HG21	1.80	0.47
2:C:352:ASN:CA	2:C:390:THR:HG21	2.45	0.47
2:D:11:GLY:HA3	2:D:28:ILE:HG12	1.97	0.47
1:A:201:PHE:CD1	1:A:210:VAL:HG23	2.50	0.47
1:A:453:ILE:HG23	1:A:479:ILE:CG1	2.44	0.47
1:A:482:MET:CE	1:A:545:TRP:HZ3	2.28	0.47
1:B:178:ARG:O	1:B:182:GLU:HG3	2.15	0.47
1:B:354:ARG:HH21	1:B:412:HIS:CE1	2.33	0.47
2:D:41:VAL:HG23	2:D:42:THR:N	2.29	0.47
1:A:403:ASP:O	1:A:404:LEU:CD1	2.63	0.47
1:A:444:ALA:C	1:A:448:LEU:HD11	2.23	0.47
1:A:238:THR:HA	1:A:569:PHE:CE2	2.50	0.47
1:B:105:SER:OG	3:B:602:AMP:H5'2	2.15	0.47
1:B:360:VAL:HG21	1:B:476:TYR:CD2	2.50	0.47
1:B:223:LEU:C	1:B:224:LEU:HD23	2.35	0.46
2:C:271:THR:HG21	2:C:273:LYS:CD	2.43	0.46
2:C:45:MET:C	2:C:45:MET:SD	2.93	0.46
2:D:161:ALA:HB3	2:D:163:ILE:HG13	1.96	0.46
2:D:185:VAL:HG23	2:D:185:VAL:O	2.14	0.46
1:B:130:ARG:O	1:B:131:ARG:C	2.53	0.46
1:B:346:LYS:CB	1:B:348:MET:CE	2.81	0.46
1:B:61:VAL:O	1:B:65:LEU:HD13	2.16	0.46
2:C:57:TYR:CD1	2:C:61:ARG:CD	2.99	0.46
2:C:75:THR:CA	2:C:79:GLY:O	2.62	0.46
1:A:23:ARG:CG	1:A:23:ARG:HH21	2.27	0.46
1:A:253:ALA:HB1	1:A:367:GLY:O	2.15	0.46
1:B:222:PHE:C	1:B:222:PHE:CD1	2.88	0.46
1:B:208:TRP:CD2	1:B:225:PRO:HB3	2.50	0.46
1:B:327:THR:HG21	1:B:418:ARG:HH21	1.74	0.46
1:B:42:ALA:CA	1:B:45:GLN:HB3	2.45	0.46
1:B:462:ASN:O	1:B:463:PHE:CD1	2.68	0.46
1:B:86:TYR:O	1:B:89:LEU:HD12	2.15	0.46
2:C:133:TYR:HB2	2:C:317:VAL:HG13	1.97	0.46
2:D:229:HIS:NE2	2:D:242:LYS:HD3	2.29	0.46
1:A:313:ILE:O	1:A:327:THR:HG22	2.15	0.46
1:B:254:ARG:HG3	1:B:367:GLY:CA	2.45	0.46
2:D:158:ASP:O	2:D:160:TYR:N	2.48	0.46
2:D:177:LYS:O	2:D:181:GLU:CG	2.63	0.46
2:D:220:ASN:HD22	2:D:220:ASN:N	2.13	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TYR:CE1	1:A:305:LEU:HD23	2.50	0.46
1:A:254:ARG:NH2	1:A:470:ARG:CZ	2.41	0.46
1:A:466:THR:HG22	1:A:470:ARG:O	2.16	0.46
1:A:516:GLU:H	1:A:516:GLU:HG2	1.47	0.46
1:A:238:THR:HA	1:A:569:PHE:CE1	2.49	0.46
1:B:145:PRO:HB3	1:B:149:TRP:CZ3	2.50	0.46
1:B:422:LEU:O	1:B:422:LEU:HD12	2.16	0.46
2:C:204:GLU:OE1	2:D:190:PHE:CE1	2.66	0.46
2:C:292:ARG:HB3	2:C:295:GLU:HG3	1.97	0.46
1:A:173:ILE:HA	1:A:176:ILE:HD12	1.28	0.46
1:A:149:TRP:HZ2	1:A:189:LEU:O	1.98	0.46
1:A:179:HIS:NE2	1:A:239:CYS:O	2.48	0.46
1:A:45:GLN:O	1:A:49:ASN:OD1	2.32	0.46
1:B:132:PHE:CD1	1:B:132:PHE:C	2.88	0.46
1:B:160:LEU:CB	1:B:161:PRO:HD2	2.45	0.46
1:B:259:VAL:HG13	1:B:259:VAL:O	2.14	0.46
1:B:284:TYR:HA	1:B:287:ILE:HD11	1.97	0.46
1:B:332:ASP:C	1:B:333:ARG:HG3	2.35	0.46
2:C:354:GLY:O	2:C:358:LEU:HG	2.16	0.46
1:A:413:LEU:HD12	1:A:414:TYR:CA	2.46	0.46
1:B:107:TYR:CE1	1:B:111:PHE:HD2	2.32	0.46
2:C:112:ARG:CD	5:C:503:HOH:O	2.62	0.46
2:C:154:GLU:CD	2:C:157:GLU:N	2.47	0.46
2:C:166:LYS:CG	2:C:167:ALA:N	2.79	0.46
2:D:257:LEU:CD2	2:D:260:GLY:HA2	2.40	0.46
2:D:266:VAL:HG21	2:D:277:ILE:CD1	2.45	0.46
2:D:99:ILE:CB	2:D:363:MET:CE	2.90	0.46
2:D:37:ILE:O	2:D:40:ASP:N	2.48	0.46
1:A:142:ASP:C	1:A:143:PHE:HD1	2.18	0.46
1:A:166:TRP:HB2	1:A:169:LYS:HG3	1.97	0.46
1:A:304:TYR:OH	1:A:330:GLY:HA3	2.15	0.46
1:A:35:PHE:CE2	1:A:207:ALA:CB	2.98	0.46
1:A:389:LEU:HA	1:A:389:LEU:HD12	1.85	0.46
1:A:118:PRO:CD	1:A:119:GLU:H	2.28	0.46
1:A:303:VAL:HG23	1:A:304:TYR:N	2.31	0.46
1:A:403:ASP:O	1:A:404:LEU:HD12	2.16	0.46
2:C:328:ILE:HG22	2:C:329:GLY:H	1.81	0.46
2:D:351:VAL:O	2:D:405:CYS:HB2	2.16	0.46
1:A:172:ASP:O	1:A:175:TYR:N	2.48	0.46
1:A:239:CYS:C	1:A:240:LEU:CD1	2.84	0.46
1:A:287:ILE:CG1	1:A:289:CYS:SG	3.04	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:O	1:B:177:ILE:CG1	2.63	0.46
2:D:338:THR:HG22	2:D:355:SER:OG	2.16	0.46
1:A:119:GLU:HG2	1:A:120:ARG:N	2.30	0.45
1:A:522:LEU:HD12	1:A:540:PHE:CE1	2.51	0.45
1:B:495:TYR:O	1:B:498:ASP:HB2	2.16	0.45
1:B:54:TYR:HE1	1:B:58:VAL:HG21	1.78	0.45
1:B:78:PHE:H	1:B:78:PHE:HD1	1.64	0.45
2:C:132:ARG:HG2	2:C:133:TYR:O	2.16	0.45
2:C:160:TYR:CE1	2:C:304:LEU:HD12	2.51	0.45
2:D:408:PHE:O	2:D:412:ILE:HG12	2.15	0.45
2:D:82:VAL:HG22	2:D:85:PRO:HD3	1.97	0.45
1:A:229:THR:HG22	1:A:230:ASP:N	2.30	0.45
1:A:378:PHE:O	1:A:409:VAL:HA	2.15	0.45
1:A:453:ILE:HG23	1:A:479:ILE:HG13	1.97	0.45
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.72	0.45
1:A:77:GLU:N	1:A:77:GLU:OE1	2.48	0.45
1:A:94:PRO:CG	1:B:26:GLU:OE2	2.65	0.45
1:B:179:HIS:C	1:B:179:HIS:HD1	2.20	0.45
2:D:31:TYR:CD1	2:D:66:MET:O	2.69	0.45
1:A:123:ILE:HG13	1:A:124:PHE:CD2	2.51	0.45
1:A:222:PHE:C	1:A:223:LEU:HD13	2.37	0.45
1:A:322:VAL:HG21	1:A:477:ALA:HB2	1.98	0.45
1:A:538:ASP:OD1	1:A:538:ASP:N	2.50	0.45
1:B:141:LYS:HD2	1:B:143:PHE:CZ	2.51	0.45
1:B:21:TYR:OH	1:B:264:PRO:CG	2.64	0.45
1:B:312:PHE:CZ	1:B:328:LEU:CD2	2.82	0.45
1:B:61:VAL:O	1:B:64:GLN:N	2.49	0.45
2:C:39:VAL:O	2:C:43:PRO:HD2	2.16	0.45
2:D:297:ASP:O	2:D:299:ILE:HD13	2.13	0.45
2:D:388:THR:C	2:D:389:VAL:HG13	2.37	0.45
2:D:68:ILE:HG22	2:D:91:LEU:HD13	1.97	0.45
1:A:226:ILE:HG22	1:A:227:HIS:N	2.32	0.45
1:B:106:VAL:O	1:B:110:LEU:HD23	2.16	0.45
2:C:217:ALA:O	2:C:221:ASP:N	2.50	0.45
2:D:106:PRO:HG3	2:D:113:SER:CB	2.47	0.45
1:A:101:SER:O	1:A:105:SER:OG	2.31	0.45
1:A:142:ASP:HA	1:A:195:GLN:HA	1.99	0.45
1:A:230:ASP:O	1:A:231:ASP:C	2.54	0.45
1:B:547:ALA:O	1:B:550:ASN:N	2.49	0.45
2:C:326:ALA:HB2	2:C:362:MET:HE1	1.90	0.45
2:C:130:PRO:CD	2:C:362:MET:SD	3.05	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:ARG:N	2:D:293:PRO:CD	2.78	0.45
1:A:213:LEU:HB3	1:A:220:LEU:O	2.17	0.45
1:B:327:THR:CB	1:B:418:ARG:HH21	2.30	0.45
1:B:494:ARG:HB3	1:B:495:TYR:CE1	2.52	0.45
1:B:528:ILE:HG13	1:B:529:GLY:N	2.31	0.45
1:B:78:PHE:CA	1:B:81:ARG:HG3	2.44	0.45
2:C:190:PHE:CD1	2:D:204:GLU:CB	3.00	0.45
2:C:238:GLU:OE1	2:C:302:MET:HG3	2.03	0.45
2:D:29:ILE:HA	2:D:30:PRO:HD3	1.68	0.45
1:A:172:ASP:O	1:A:175:TYR:HB2	2.17	0.45
1:B:118:PRO:HB2	1:B:119:GLU:OE2	2.16	0.45
1:B:253:ALA:HB1	1:B:367:GLY:CA	2.47	0.45
1:B:514:PHE:HA	1:B:515:PRO:HD2	1.67	0.45
2:C:146:LEU:O	2:C:293:PRO:CG	2.65	0.45
2:D:352:ASN:N	2:D:353:PRO:HD3	2.29	0.45
2:D:57:TYR:OH	2:D:369:TRP:CB	2.65	0.45
1:B:132:PHE:CD1	1:B:132:PHE:O	2.70	0.45
1:B:482:MET:O	1:B:549:GLN:NE2	2.49	0.45
2:C:160:TYR:CE1	2:C:304:LEU:HD13	2.50	0.45
2:C:202:SER:OG	2:C:205:GLY:N	2.48	0.45
2:C:373:ALA:O	2:C:377:VAL:HG23	2.16	0.45
2:D:130:PRO:HA	2:D:150:VAL:HA	1.98	0.45
2:D:383:ALA:O	2:D:386:ALA:HB3	2.17	0.45
1:A:526:PRO:O	1:A:530:PRO:HD2	2.16	0.45
1:B:160:LEU:C	1:B:160:LEU:CD1	2.86	0.45
1:B:222:PHE:O	1:B:222:PHE:CD1	2.70	0.45
1:B:254:ARG:CG	1:B:254:ARG:NH1	2.73	0.45
1:B:212:LYS:HG2	1:B:274:ILE:HD11	1.95	0.45
1:B:369:MET:HE1	1:B:453:ILE:HG13	1.99	0.45
1:B:80:LEU:CD2	1:B:81:ARG:N	2.73	0.45
2:C:242:LYS:CG	2:C:243:ASP:N	2.80	0.45
2:D:26:ASN:N	2:D:27:PRO:HD3	2.31	0.45
1:B:246:ALA:HA	1:B:249:VAL:CG1	2.46	0.44
2:C:154:GLU:OE1	2:C:157:GLU:HG3	2.13	0.44
2:D:114:LEU:HD12	2:D:114:LEU:HA	1.78	0.44
2:D:159:ILE:HG22	2:D:159:ILE:O	2.16	0.44
1:A:78:PHE:C	1:A:80:LEU:N	2.67	0.44
1:B:14:LEU:HD12	1:B:14:LEU:O	2.17	0.44
1:B:200:LEU:HG	1:B:200:LEU:H	1.57	0.44
1:B:457:ASP:O	1:B:458:MET:CB	2.65	0.44
1:B:320:GLY:HA3	4:B:601:ADP:O2A	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:286:LEU:O	2:C:289:ILE:HG12	2.17	0.44
2:D:328:ILE:CG2	2:D:329:GLY:N	2.80	0.44
1:A:525:ASP:N	1:A:528:ILE:CD1	2.60	0.44
1:B:230:ASP:N	1:B:230:ASP:OD1	2.50	0.44
1:B:312:PHE:CD1	1:B:328:LEU:HD22	2.50	0.44
1:B:369:MET:CE	1:B:453:ILE:HG13	2.46	0.44
1:B:47:MET:HA	1:B:258:MET:HE1	1.98	0.44
2:C:276:VAL:O	2:C:277:ILE:HD13	2.17	0.44
2:C:352:ASN:CB	2:C:390:THR:CG2	2.94	0.44
1:A:456:GLY:HA3	1:A:478:GLU:HB2	1.99	0.44
1:B:116:LEU:H	1:B:116:LEU:HG	1.57	0.44
1:B:145:PRO:HB3	1:B:149:TRP:HE3	1.73	0.44
1:B:295:THR:OG1	3:B:602:AMP:O3'	1.84	0.44
2:C:113:SER:HB3	2:C:116:VAL:CG2	2.43	0.44
2:C:353:PRO:HG2	2:C:357:ILE:HD11	1.99	0.44
2:D:133:TYR:CE2	2:D:144:PRO:HG2	2.52	0.44
2:D:137:THR:HG22	2:D:138:PRO:N	2.32	0.44
2:D:169:SER:HG	2:D:172:ALA:N	2.12	0.44
1:A:121:LEU:CD1	1:A:121:LEU:C	2.86	0.44
1:A:394:LEU:CD2	1:A:401:ILE:HD11	2.43	0.44
1:A:463:PHE:N	1:A:463:PHE:HD1	2.14	0.44
1:A:78:PHE:CG	1:A:79:LEU:N	2.85	0.44
1:B:143:PHE:HB3	1:B:152:LEU:HD11	1.99	0.44
1:B:35:PHE:CD2	1:B:207:ALA:HB2	2.53	0.44
1:B:274:ILE:CD1	1:B:274:ILE:N	2.81	0.44
1:B:304:TYR:OH	1:B:330:GLY:C	2.56	0.44
1:B:466:THR:OG1	1:B:470:ARG:HB2	2.17	0.44
2:D:307:ASP:O	2:D:311:ASP:HB2	2.18	0.44
1:A:164:LEU:CD1	1:A:164:LEU:N	2.73	0.44
1:A:561:TYR:CE2	1:A:568:ARG:NH1	2.85	0.44
1:A:78:PHE:HA	1:A:81:ARG:HG3	2.00	0.44
1:A:77:GLU:CD	1:A:78:PHE:HB2	2.38	0.44
1:B:103:PHE:CD1	1:B:103:PHE:C	2.91	0.44
1:B:121:LEU:C	1:B:121:LEU:CD1	2.85	0.44
1:B:260:TYR:CD2	1:B:262:PRO:HD3	2.53	0.44
2:C:114:LEU:HD12	2:C:114:LEU:HA	1.84	0.44
1:A:117:THR:HB	1:A:118:PRO:CD	2.48	0.44
1:A:287:ILE:HG13	1:A:289:CYS:SG	2.58	0.44
1:A:365:ARG:CZ	1:A:371:ASP:HB2	2.47	0.44
1:A:452:ASN:HD21	1:A:481:TYR:CB	2.27	0.44
1:A:103:PHE:CD2	1:A:122:PHE:CD2	3.06	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ILE:HG12	1:A:177:ILE:H	1.83	0.44
1:A:209:LEU:C	1:A:209:LEU:CD2	2.85	0.44
1:B:116:LEU:O	1:B:116:LEU:HD12	2.17	0.44
1:B:127:GLN:CB	1:B:128:PRO:HD2	2.47	0.44
1:B:177:ILE:H	1:B:177:ILE:CD1	2.19	0.44
1:B:17:PHE:CD2	1:B:17:PHE:C	2.91	0.44
2:D:357:ILE:O	2:D:360:ALA:HB3	2.18	0.44
1:A:260:TYR:CE2	1:A:262:PRO:HG3	2.52	0.44
1:A:356:CYS:SG	1:A:479:ILE:HG22	2.58	0.44
1:A:551:ARG:O	1:A:554:GLU:C	2.56	0.44
1:B:332:ASP:C	1:B:418:ARG:HB3	2.39	0.44
2:C:308:TYR:O	2:C:312:ALA:HB2	2.18	0.44
2:C:348:GLN:O	2:C:349:ASP:HB2	2.18	0.44
2:C:407:GLU:O	2:C:410:ASP:CB	2.66	0.44
2:D:3:SER:OG	2:D:78:TYR:OH	2.30	0.44
1:A:139:LEU:HG	1:A:139:LEU:H	1.56	0.43
1:A:142:ASP:HA	1:A:194:LEU:O	2.18	0.43
1:A:24:PHE:O	1:A:27:VAL:HG12	2.17	0.43
1:A:280:THR:OG1	1:A:281:ALA:N	2.51	0.43
1:B:23:ARG:HA	1:B:23:ARG:HD2	1.78	0.43
1:B:456:GLY:HA3	1:B:478:GLU:O	2.18	0.43
1:B:543:ASP:O	1:B:546:ARG:HB2	2.18	0.43
2:C:361:GLU:OE2	2:C:365:ARG:HD2	2.18	0.43
2:C:407:GLU:O	2:C:410:ASP:N	2.51	0.43
2:D:127:CYS:SG	2:D:153:ARG:HD2	2.54	0.43
2:D:154:GLU:HG3	2:D:303:ASN:HD22	1.83	0.43
1:A:292:HIS:O	1:A:295:THR:N	2.51	0.43
1:A:359:LEU:HD21	1:A:481:TYR:HE1	1.81	0.43
1:A:422:LEU:CD2	1:A:441:TYR:HD2	2.31	0.43
1:A:238:THR:CA	1:A:569:PHE:CZ	3.00	0.43
2:D:133:TYR:CE1	2:D:135:GLN:HA	2.44	0.43
2:D:31:TYR:HD1	2:D:66:MET:O	2.01	0.43
2:D:45:MET:HE3	2:D:46:LEU:HA	2.00	0.43
1:A:196:VAL:HG12	1:A:197:ALA:H	1.81	0.43
1:A:561:TYR:HD2	1:A:563:TYR:CE1	2.36	0.43
1:A:5:LEU:HD22	1:A:5:LEU:HA	1.86	0.43
1:B:177:ILE:HA	1:B:180:LEU:CD1	2.46	0.43
1:B:425:TRP:NE1	1:B:429:VAL:HG11	2.33	0.43
1:B:420:VAL:HG12	1:B:465:VAL:HB	1.97	0.43
1:B:565:ARG:HD2	1:B:565:ARG:HA	1.81	0.43
2:C:159:ILE:HD12	2:C:199:LYS:HB2	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:GLN:HG2	1:A:233:GLU:CB	2.37	0.43
1:A:39:ASP:O	1:A:41:HIS:N	2.51	0.43
1:A:429:VAL:CG1	1:A:430:GLU:O	2.60	0.43
1:A:446:ARG:HH21	1:A:536:HIS:HB3	1.83	0.43
1:B:100:GLU:HG2	1:B:100:GLU:H	1.58	0.43
1:B:453:ILE:HD13	1:B:453:ILE:HA	1.75	0.43
1:B:517:GLU:O	1:B:521:TRP:CZ3	2.72	0.43
1:B:56:HIS:O	1:B:60:LEU:N	2.40	0.43
2:C:206:THR:CG2	2:C:241:PHE:CD2	2.98	0.43
2:C:241:PHE:CD2	2:C:302:MET:HE3	2.53	0.43
2:C:305:ASN:O	2:C:309:ILE:HG12	2.18	0.43
1:A:174:HIS:HA	1:A:177:ILE:HD12	1.85	0.43
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.83	0.43
1:A:327:THR:OG1	1:A:418:ARG:NH2	2.51	0.43
1:A:460:PHE:C	1:A:462:ASN:H	2.21	0.43
1:B:420:VAL:HG13	1:B:420:VAL:O	2.17	0.43
1:B:461:LYS:NZ	4:B:601:ADP:PB	2.92	0.43
1:B:526:PRO:HD3	2:C:76:GLN:HE22	1.84	0.43
2:C:227:LEU:O	2:C:279:ASP:HA	2.18	0.43
2:C:232:ASN:OD1	2:C:232:ASN:N	2.51	0.43
2:C:241:PHE:CD2	2:C:302:MET:CE	3.01	0.43
2:D:106:PRO:O	2:D:106:PRO:HG2	2.18	0.43
2:D:17:GLN:O	2:D:18:ASN:CB	2.67	0.43
2:D:227:LEU:N	2:D:227:LEU:HD13	2.33	0.43
2:D:151:ILE:HG21	2:D:310:SER:OG	2.18	0.43
1:A:20:GLN:C	1:A:20:GLN:NE2	2.72	0.43
1:A:323:MET:HE3	1:A:338:ILE:HG12	1.99	0.43
1:A:34:ARG:NH2	1:A:258:MET:HE1	2.34	0.43
1:A:352:HIS:C	1:A:352:HIS:HD1	2.21	0.43
1:A:35:PHE:HE2	1:A:207:ALA:H	1.63	0.43
2:C:125:TYR:CE1	2:C:208:ARG:HG2	2.53	0.43
2:D:42:THR:N	2:D:43:PRO:HD2	2.34	0.43
1:A:168:ASN:O	1:A:171:ARG:HB3	2.05	0.43
1:B:284:TYR:O	1:B:287:ILE:HG13	2.19	0.43
2:C:119:ARG:CG	2:C:119:ARG:NH1	2.81	0.43
2:C:149:MET:HA	2:C:297:ASP:O	2.18	0.43
2:C:353:PRO:O	2:C:357:ILE:HD13	2.03	0.43
2:D:229:HIS:ND1	2:D:229:HIS:C	2.72	0.43
2:D:280:VAL:CG2	2:D:285:PHE:HD2	2.32	0.43
2:D:326:ALA:HB1	2:D:335:PHE:CD2	2.54	0.43
2:D:97:VAL:HG13	2:D:97:VAL:O	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TYR:CZ	1:A:111:PHE:HD2	2.36	0.43
1:A:201:PHE:CD1	1:A:210:VAL:HG21	2.53	0.43
1:B:104:ASN:OD1	1:B:122:PHE:HB2	2.18	0.43
1:B:222:PHE:HD1	1:B:222:PHE:O	2.01	0.43
1:B:442:GLY:HA3	1:B:536:HIS:CE1	2.54	0.43
2:C:388:THR:O	2:C:389:VAL:HG13	2.19	0.43
2:D:240:ALA:CA	2:D:244:TRP:NE1	2.79	0.43
2:D:37:ILE:HD11	2:D:340:GLY:O	2.19	0.43
1:A:179:HIS:N	1:A:180:LEU:HD22	2.33	0.43
1:A:294:LYS:O	1:A:297:SER:CB	2.62	0.43
1:A:539:LEU:HD23	1:A:539:LEU:HA	1.80	0.43
1:A:522:LEU:HD12	1:A:540:PHE:HE1	1.82	0.43
1:B:168:ASN:HB2	1:B:171:ARG:CB	2.49	0.43
1:B:413:LEU:HD21	1:B:415:ILE:HG13	2.00	0.43
1:B:462:ASN:OD1	1:B:475:ASP:HB3	2.17	0.43
1:B:320:GLY:CA	4:B:601:ADP:O2A	2.67	0.43
2:C:133:TYR:HA	2:C:317:VAL:HG11	1.98	0.43
2:C:371:GLU:O	2:C:374:ASP:HB2	2.19	0.43
2:C:410:ASP:O	2:C:413:ILE:N	2.52	0.43
2:D:289:ILE:O	2:D:293:PRO:CD	2.66	0.43
1:B:44:GLN:O	1:B:47:MET:HB3	2.18	0.43
2:C:154:GLU:OE1	2:C:157:GLU:CB	2.66	0.43
2:C:191:PRO:O	2:C:194:CYS:HB3	2.19	0.43
2:C:265:LYS:H	2:C:265:LYS:HG2	1.65	0.43
1:A:211:GLY:O	1:A:222:PHE:O	2.37	0.42
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.75	0.42
1:A:551:ARG:CA	1:A:554:GLU:HB3	2.48	0.42
1:B:237:ASP:HB3	1:B:569:PHE:HE1	1.74	0.42
1:A:248:ILE:HG22	1:A:254:ARG:NH1	2.34	0.42
1:A:535:MET:HB3	1:A:536:HIS:NE2	2.34	0.42
1:B:419:MET:CE	1:B:472:VAL:HB	2.49	0.42
2:C:170:ALA:O	2:C:174:LYS:N	2.48	0.42
2:C:248:LEU:HD12	2:C:252:GLU:HG3	1.99	0.42
2:C:388:THR:O	2:C:389:VAL:CG1	2.67	0.42
2:C:26:ASN:HA	2:C:62:LYS:O	2.19	0.42
2:D:169:SER:OG	2:D:172:ALA:HB2	2.18	0.42
2:D:192:GLU:O	2:D:193:HIS:HB2	2.18	0.42
2:D:393:PHE:O	2:D:396:LEU:N	2.52	0.42
1:A:171:ARG:O	1:A:174:HIS:HB2	2.17	0.42
1:A:240:LEU:N	1:A:240:LEU:HD13	2.34	0.42
1:A:543:ASP:CA	1:A:546:ARG:CD	2.96	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:GLN:NE2	1:B:127:GLN:CA	2.80	0.42
1:B:304:TYR:OH	1:B:330:GLY:CA	2.67	0.42
1:B:568:ARG:HH21	1:B:568:ARG:CG	2.23	0.42
2:C:308:TYR:O	2:C:312:ALA:CB	2.67	0.42
2:C:408:PHE:O	2:C:411:ALA:HB3	2.19	0.42
2:C:79:GLY:N	2:C:82:VAL:CG1	2.83	0.42
2:D:384:ILE:O	2:D:387:LYS:HA	2.19	0.42
1:A:293:ALA:C	1:A:297:SER:OG	2.57	0.42
1:A:466:THR:CG2	1:A:470:ARG:HB2	2.48	0.42
2:C:190:PHE:HB3	2:D:202:SER:HB2	2.00	0.42
1:A:215:THR:HG1	1:A:216:PRO:HD2	1.80	0.42
1:A:65:LEU:HB3	1:A:69:THR:HG22	1.99	0.42
1:A:17:PHE:CZ	1:A:98:ILE:CG2	3.02	0.42
1:B:111:PHE:O	1:B:114:ARG:HG2	2.19	0.42
1:B:160:LEU:C	1:B:160:LEU:HD12	2.38	0.42
1:B:166:TRP:CE2	1:B:234:LEU:CD2	2.95	0.42
1:B:82:VAL:CG2	1:B:83:LYS:N	2.83	0.42
2:C:226:THR:HA	2:C:278:LYS:O	2.20	0.42
2:C:366:HIS:ND1	2:C:366:HIS:C	2.73	0.42
2:D:141:VAL:CG2	2:D:144:PRO:HB3	2.49	0.42
2:D:209:LEU:O	2:D:212:ALA:CB	2.65	0.42
1:A:229:THR:HB	1:A:232:GLY:HA2	2.00	0.42
1:A:79:LEU:HA	1:A:79:LEU:HD12	1.88	0.42
1:A:87:THR:HG23	1:A:122:PHE:HZ	1.82	0.42
1:B:238:THR:OG1	1:B:239:CYS:N	2.43	0.42
1:B:380:LEU:O	1:B:407:GLN:HA	2.19	0.42
1:B:9:ILE:O	1:B:13:ILE:HD12	2.20	0.42
2:C:29:ILE:HG23	2:C:363:MET:HE3	2.01	0.42
2:D:30:PRO:O	2:D:98:ALA:CB	2.53	0.42
1:A:34:ARG:HH21	1:A:258:MET:HE2	1.85	0.42
1:A:338:ILE:HG22	1:A:339:LYS:O	2.19	0.42
1:A:54:TYR:CE1	1:A:58:VAL:HG21	2.55	0.42
1:A:91:PRO:O	1:A:92:ASP:CB	2.67	0.42
1:B:301:TYR:CE1	1:B:305:LEU:HD23	2.53	0.42
1:B:204:ASN:OD1	1:B:364:ASP:OD2	2.38	0.42
1:B:520:HIS:C	1:B:520:HIS:ND1	2.72	0.42
2:D:341:THR:O	2:D:342:ALA:C	2.57	0.42
2:D:99:ILE:CB	2:D:363:MET:HE2	2.47	0.42
1:A:104:ASN:ND2	1:A:122:PHE:C	2.73	0.42
1:A:176:ILE:HB	1:A:180:LEU:HD12	1.81	0.42
1:A:213:LEU:HB2	1:A:222:PHE:HB2	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PHE:HD1	1:A:96:PHE:H	1.58	0.42
1:B:356:CYS:SG	1:B:479:ILE:HG22	2.59	0.42
1:B:528:ILE:O	1:B:531:LEU:HD13	2.19	0.42
2:C:229:HIS:ND1	2:C:229:HIS:C	2.73	0.42
2:D:375:LEU:HA	2:D:375:LEU:HD12	1.78	0.42
1:A:143:PHE:CE2	1:A:156:VAL:HG22	2.55	0.42
1:A:179:HIS:C	1:A:179:HIS:ND1	2.73	0.42
1:A:365:ARG:NH1	1:A:371:ASP:HB3	2.35	0.42
1:B:274:ILE:C	1:B:276:PRO:HD3	2.39	0.42
1:B:326:PHE:CD1	1:B:326:PHE:N	2.88	0.42
1:B:425:TRP:O	1:B:429:VAL:HG13	2.19	0.42
1:B:544:TYR:CZ	1:B:548:LEU:HD11	2.55	0.42
2:C:323:ALA:HA	2:C:324:PRO:HD3	1.74	0.42
1:A:344:PRO:CG	1:A:345:GLN:N	2.83	0.42
1:A:514:PHE:O	1:A:517:GLU:HG2	2.19	0.42
1:A:531:LEU:O	1:A:534:GLU:HB3	2.20	0.42
2:C:377:VAL:O	2:C:381:GLU:HB2	2.20	0.42
1:A:414:TYR:N	1:A:414:TYR:CD1	2.88	0.41
1:A:462:ASN:OD1	1:A:475:ASP:CB	2.67	0.41
1:B:295:THR:HG1	3:B:602:AMP:C3'	2.23	0.41
1:B:564:ARG:CG	1:B:564:ARG:NH1	2.73	0.41
2:C:23:VAL:HG21	2:C:367:MET:CE	2.49	0.41
2:C:11:GLY:HA3	2:C:28:ILE:HG12	2.02	0.41
2:D:409:GLY:O	2:D:412:ILE:HB	2.21	0.41
2:D:79:GLY:N	2:D:82:VAL:CG1	2.83	0.41
1:A:237:ASP:OD2	1:A:561:TYR:CE2	2.73	0.41
1:A:490:ILE:O	1:A:490:ILE:HG23	2.20	0.41
1:B:320:GLY:O	1:B:339:LYS:NZ	2.45	0.41
1:B:253:ALA:HB1	1:B:367:GLY:C	2.40	0.41
1:B:298:TYR:CZ	3:B:602:AMP:H2	2.30	0.41
2:C:286:LEU:HD21	2:C:309:ILE:HD13	2.01	0.41
2:C:337:ALA:HB1	2:C:339:HIS:NE2	2.35	0.41
2:D:23:VAL:HG11	2:D:367:MET:CE	2.49	0.41
2:D:38:GLY:HA2	2:D:41:VAL:HG22	2.02	0.41
1:A:119:GLU:OE2	1:A:120:ARG:N	2.51	0.41
1:A:344:PRO:CD	1:A:345:GLN:N	2.83	0.41
1:B:186:PRO:HD2	1:B:187:GLU:OE1	2.18	0.41
1:B:411:ARG:HB2	1:B:411:ARG:HE	1.64	0.41
2:C:149:MET:HE1	2:C:299:ILE:CD1	2.50	0.41
2:D:169:SER:OG	2:D:172:ALA:HB3	2.20	0.41
2:D:291:LEU:CD1	2:D:291:LEU:H	2.09	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:PRO:HA	1:A:189:LEU:HD22	1.13	0.41
1:A:404:LEU:HD21	1:A:409:VAL:HG21	2.02	0.41
1:B:107:TYR:CZ	1:B:111:PHE:CD2	3.08	0.41
1:B:273:GLU:O	1:B:276:PRO:HD3	2.20	0.41
1:B:368:ARG:HA	1:B:368:ARG:HD3	1.91	0.41
1:B:531:LEU:C	1:B:534:GLU:H	2.24	0.41
1:B:53:LEU:HA	1:B:53:LEU:HD12	1.81	0.41
2:C:201:CYS:HB2	2:C:237:THR:HG22	2.02	0.41
2:C:229:HIS:CD2	2:C:242:LYS:HB3	2.56	0.41
2:D:39:VAL:O	2:D:43:PRO:HD2	2.20	0.41
2:D:57:TYR:OH	2:D:369:TRP:HA	2.19	0.41
1:A:561:TYR:HE2	1:A:568:ARG:NE	2.18	0.41
1:B:110:LEU:HA	1:B:110:LEU:HD13	1.85	0.41
1:B:462:ASN:CA	1:B:474:TYR:CE1	2.97	0.41
1:B:24:PHE:HA	1:B:53:LEU:HD23	2.03	0.41
1:B:78:PHE:O	1:B:81:ARG:CB	2.67	0.41
2:C:241:PHE:HD2	2:C:302:MET:HE3	1.85	0.41
2:C:352:ASN:CB	2:C:390:THR:CB	2.98	0.41
2:C:236:PHE:HE1	2:D:166:LYS:HB2	1.79	0.41
2:D:131:VAL:HG21	2:D:313:LEU:CD1	2.49	0.41
2:D:79:GLY:CA	2:D:82:VAL:CG1	2.96	0.41
1:A:281:ALA:HB2	1:A:296:GLU:HB3	2.02	0.41
1:A:404:LEU:HD22	1:A:409:VAL:CG2	2.45	0.41
1:A:463:PHE:CE1	1:A:473:PHE:HD1	2.36	0.41
1:A:47:MET:SD	1:A:47:MET:O	2.79	0.41
1:A:559:ASP:OD1	1:A:559:ASP:N	2.52	0.41
1:A:245:GLU:OE2	1:A:567:GLN:NE2	2.53	0.41
1:A:89:LEU:CD1	1:A:89:LEU:H	2.28	0.41
1:B:172:ASP:OD1	1:B:172:ASP:N	2.44	0.41
1:B:178:ARG:O	1:B:182:GLU:CD	2.51	0.41
2:D:141:VAL:HG22	2:D:316:GLN:O	2.20	0.41
1:A:179:HIS:CD2	1:A:239:CYS:CB	3.01	0.41
1:A:322:VAL:HG11	1:A:477:ALA:HB1	2.03	0.41
1:A:333:ARG:NH2	1:A:373:GLN:HE22	2.15	0.41
1:A:490:ILE:HA	1:A:491:PRO:HD3	1.94	0.41
1:B:166:TRP:NE1	1:B:234:LEU:CD2	2.83	0.41
1:B:359:LEU:HD13	1:B:481:TYR:OH	2.21	0.41
2:C:144:PRO:O	2:C:146:LEU:N	2.54	0.41
2:C:166:LYS:HE3	2:C:166:LYS:HB3	1.76	0.41
2:C:183:MET:HE3	2:C:183:MET:O	2.21	0.41
2:D:161:ALA:HB1	2:D:163:ILE:HG13	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:VAL:HG11	2:D:367:MET:HE2	2.02	0.41
1:B:186:PRO:HA	1:B:189:LEU:HB3	2.02	0.41
1:A:303:VAL:C	1:A:306:GLN:HG2	2.36	0.41
1:A:548:LEU:O	1:A:552:ILE:HG13	2.20	0.41
1:A:97:GLU:HG2	1:A:98:ILE:N	2.34	0.41
1:B:274:ILE:HD12	1:B:274:ILE:N	2.36	0.41
1:B:432:GLN:HG3	1:B:432:GLN:O	2.20	0.41
1:B:356:CYS:HB3	1:B:479:ILE:HG21	2.02	0.41
1:B:452:ASN:ND2	1:B:481:TYR:HD1	2.18	0.41
2:D:266:VAL:HG23	2:D:277:ILE:CD1	2.51	0.41
2:D:391:TYR:O	2:D:395:ARG:CG	2.67	0.41
1:A:121:LEU:HD12	1:A:121:LEU:C	2.42	0.41
1:A:541:ARG:O	1:A:545:TRP:HD1	2.04	0.41
1:B:100:GLU:O	1:B:101:SER:C	2.58	0.41
1:B:485:VAL:CG2	1:B:513:VAL:CG2	2.98	0.41
1:B:84:GLU:O	1:B:87:THR:HB	2.20	0.41
2:C:285:PHE:C	2:C:285:PHE:CD2	2.94	0.41
2:C:337:ALA:HB2	2:C:356:ILE:HD12	2.03	0.41
2:D:119:ARG:HB3	2:D:124:LEU:HD13	2.03	0.41
2:D:127:CYS:O	2:D:127:CYS:SG	2.79	0.41
2:D:281:ILE:O	2:D:285:PHE:HB2	2.21	0.41
2:D:289:ILE:CG1	2:D:290:LEU:N	2.84	0.41
1:A:23:ARG:CG	1:A:23:ARG:NH2	2.81	0.41
1:A:441:TYR:O	1:A:442:GLY:C	2.59	0.41
1:A:570:SER:C	1:A:571:VAL:CG2	2.85	0.41
1:B:94:PRO:HG2	1:B:95:ARG:HG3	2.03	0.41
2:C:361:GLU:HG2	2:C:373:ALA:HB1	2.02	0.41
2:C:388:THR:C	2:C:389:VAL:CG1	2.90	0.41
2:D:377:VAL:O	2:D:381:GLU:HG2	2.21	0.41
1:A:107:TYR:CE1	1:A:111:PHE:HD2	2.29	0.40
1:A:390:MET:O	1:A:390:MET:SD	2.79	0.40
1:A:546:ARG:HA	1:A:549:GLN:HG2	2.02	0.40
1:B:513:VAL:C	1:B:515:PRO:HD3	2.41	0.40
1:B:519:ARG:NE	1:B:533:GLU:OE2	2.51	0.40
1:B:535:MET:H	1:B:535:MET:HG2	1.72	0.40
2:C:286:LEU:CD2	2:C:309:ILE:HD13	2.51	0.40
2:D:298:VAL:O	2:D:299:ILE:HD12	2.19	0.40
1:A:223:LEU:N	1:A:223:LEU:HD13	2.37	0.40
1:A:165:HIS:O	1:A:233:GLU:HA	2.20	0.40
1:A:381:GLU:HG3	1:A:407:GLN:HG3	0.88	0.40
1:A:462:ASN:OD1	1:A:475:ASP:HB2	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:O	1:A:81:ARG:C	2.59	0.40
1:B:127:GLN:HG3	1:B:128:PRO:CD	2.51	0.40
1:B:172:ASP:N	1:B:173:ILE:HD13	2.35	0.40
1:B:472:VAL:HG12	1:B:473:PHE:N	2.36	0.40
1:B:47:MET:SD	1:B:47:MET:O	2.79	0.40
2:C:151:ILE:HD13	2:C:299:ILE:HB	2.02	0.40
2:C:380:MET:O	2:C:384:ILE:HG13	2.21	0.40
2:D:189:ARG:HH11	2:D:189:ARG:CG	2.29	0.40
2:D:14:ILE:HD13	2:D:23:VAL:HG13	2.01	0.40
1:A:179:HIS:O	1:A:179:HIS:ND1	2.54	0.40
1:A:448:LEU:H	1:A:448:LEU:CD1	2.10	0.40
1:B:401:ILE:CD1	1:B:401:ILE:C	2.85	0.40
1:B:372:THR:OG1	1:B:414:TYR:HD2	2.04	0.40
2:D:268:ASN:HA	2:D:269:PRO:HD2	1.84	0.40
1:A:224:LEU:CD1	1:A:224:LEU:N	2.85	0.40
1:A:208:TRP:CD2	1:A:225:PRO:HB3	2.56	0.40
1:A:324:LEU:HD21	1:A:393:LEU:CD2	2.47	0.40
1:A:529:GLY:N	1:A:530:PRO:HD2	2.36	0.40
1:B:170:SER:HA	1:B:173:ILE:HG13	1.80	0.40
1:B:192:SER:HG	1:B:215:THR:N	2.16	0.40
1:B:473:PHE:CE1	1:B:475:ASP:O	2.74	0.40
1:B:69:THR:O	1:B:70:ASN:ND2	2.54	0.40
2:C:154:GLU:OE2	2:C:156:SER:CB	2.70	0.40
2:C:57:TYR:CG	2:C:61:ARG:HD3	2.56	0.40
2:D:288:GLN:HA	2:D:291:LEU:HD13	2.03	0.40
2:D:41:VAL:CG2	2:D:42:THR:N	2.84	0.40
1:A:353:VAL:O	1:A:356:CYS:HB2	2.21	0.40
1:A:514:PHE:N	1:A:514:PHE:CD1	2.89	0.40
1:B:35:PHE:CE2	1:B:207:ALA:HB2	2.56	0.40
2:C:239:GLY:C	2:C:241:PHE:N	2.74	0.40
2:C:326:ALA:HB3	2:C:362:MET:CE	2.50	0.40
2:C:67:GLU:OE2	2:C:73:LYS:NZ	2.54	0.40
2:C:236:PHE:CD1	2:D:166:LYS:HB2	2.56	0.40
2:C:190:PHE:CE1	2:D:204:GLU:HB3	2.56	0.40
2:D:356:ILE:HG23	2:D:357:ILE:H	1.87	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:OE1	2:D:345:TYR:OH[3_555]	1.57	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:SER:OG	2:C:279:ASP:OD1[3_555]	1.61	0.59
2:D:295:GLU:OE2	2:D:398:ASP:OD1[2_455]	1.84	0.36
1:A:520:HIS:NE2	2:D:104:THR:OG1[3_555]	2.09	0.11
2:C:135:GLN:NE2	2:C:401:LYS:N[3_445]	2.18	0.02

## 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	548/568 (96%)	528 (96%)	15 (3%)	5 (1%)	17	48
1	B	557/568 (98%)	548 (98%)	7 (1%)	2 (0%)	34	66
2	C	413/415 (100%)	398 (96%)	13 (3%)	2 (0%)	29	61
2	D	413/415 (100%)	391 (95%)	14 (3%)	8 (2%)	8	34
All	All	1931/1966 (98%)	1865 (97%)	49 (2%)	17 (1%)	17	48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	200	PRO
2	D	200	PRO
1	A	69	THR
1	A	570	SER
2	D	231	GLY
1	B	366	VAL
2	C	324	PRO
2	D	106	PRO
1	A	225	PRO
1	A	366	VAL
1	B	225	PRO
2	D	130	PRO
2	D	324	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	26	ASN
1	A	138	PRO
2	D	138	PRO
2	D	30	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/498 (97%)	370 (76%)	115 (24%)	1	2
1	B	494/498 (99%)	390 (79%)	104 (21%)	1	4
2	C	337/337 (100%)	271 (80%)	66 (20%)	1	5
2	D	337/337 (100%)	269 (80%)	68 (20%)	1	5
All	All	1653/1670 (99%)	1300 (79%)	353 (21%)	1	4

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	LEU
1	A	12	THR
1	A	20	GLN
1	A	23	ARG
1	A	29	SER
1	A	39	ASP
1	A	49	ASN
1	A	53	LEU
1	A	54	TYR
1	A	60	LEU
1	A	66	ARG
1	A	77	GLU
1	A	78	PHE
1	A	79	LEU
1	A	81	ARG
1	A	83	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	84	GLU
1	A	87	THR
1	A	88	ARG
1	A	89	LEU
1	A	96	PHE
1	A	97	GLU
1	A	101	SER
1	A	104	ASN
1	A	109	ARG
1	A	110	LEU
1	A	117	THR
1	A	119	GLU
1	A	121	LEU
1	A	127	GLN
1	A	139	LEU
1	A	142	ASP
1	A	143	PHE
1	A	152	LEU
1	A	158	SER
1	A	167	GLN
1	A	169	LYS
1	A	170	SER
1	A	171	ARG
1	A	172	ASP
1	A	173	ILE
1	A	176	ILE
1	A	177	ILE
1	A	179	HIS
1	A	180	LEU
1	A	181	THR
1	A	191	LYS
1	A	192	SER
1	A	204	ASN
1	A	215	THR
1	A	220	LEU
1	A	223	LEU
1	A	230	ASP
1	A	231	ASP
1	A	234	LEU
1	A	240	LEU
1	A	242	THR
1	A	247	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	254	ARG
1	A	255	SER
1	A	258	MET
1	A	282	GLU
1	A	295	THR
1	A	297	SER
1	A	301	TYR
1	A	323	MET
1	A	331	PHE
1	A	332	ASP
1	A	335	PHE
1	A	345	GLN
1	A	347	GLU
1	A	349	SER
1	A	352	HIS
1	A	356	CYS
1	A	361	LYS
1	A	366	VAL
1	A	371	ASP
1	A	380	LEU
1	A	382	LYS
1	A	386	SER
1	A	390	MET
1	A	392	LEU
1	A	403	ASP
1	A	404	LEU
1	A	406	GLU
1	A	411	ARG
1	A	413	LEU
1	A	435	ARG
1	A	441	TYR
1	A	448	LEU
1	A	452	ASN
1	A	461	LYS
1	A	462	ASN
1	A	470	ARG
1	A	475	ASP
1	A	479	ILE
1	A	480	CYS
1	A	482	MET
1	A	506	TYR
1	A	516	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	525	ASP
1	A	527	ARG
1	A	528	ILE
1	A	532	PHE
1	A	535	MET
1	A	536	HIS
1	A	546	ARG
1	A	549	GLN
1	A	550	ASN
1	A	551	ARG
1	A	553	ARG
1	A	561	TYR
1	A	567	GLN
1	A	571	VAL
1	B	5	LEU
1	B	6	GLU
1	B	7	LEU
1	B	8	LEU
1	B	20	GLN
1	B	54	TYR
1	B	60	LEU
1	B	80	LEU
1	B	87	THR
1	B	89	LEU
1	B	97	GLU
1	B	100	GLU
1	B	107	TYR
1	B	109	ARG
1	B	115	SER
1	B	116	LEU
1	B	119	GLU
1	B	125	SER
1	B	127	GLN
1	B	130	ARG
1	B	131	ARG
1	B	137	ARG
1	B	139	LEU
1	B	146	ASP
1	B	147	HIS
1	B	152	LEU
1	B	155	ARG
1	B	158	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	159	ASP
1	B	160	LEU
1	B	168	ASN
1	B	172	ASP
1	B	173	ILE
1	B	174	HIS
1	B	177	ILE
1	B	180	LEU
1	B	181	THR
1	B	182	GLU
1	B	183	THR
1	B	192	SER
1	B	194	LEU
1	B	200	LEU
1	B	209	LEU
1	B	213	LEU
1	B	220	LEU
1	B	222	PHE
1	B	229	THR
1	B	230	ASP
1	B	234	LEU
1	B	242	THR
1	B	254	ARG
1	B	255	SER
1	B	257	PHE
1	B	263	LEU
1	B	287	ILE
1	B	294	LYS
1	B	297	SER
1	B	301	TYR
1	B	302	LEU
1	B	305	LEU
1	B	306	GLN
1	B	309	ASN
1	B	314	GLU
1	B	328	LEU
1	B	331	PHE
1	B	332	ASP
1	B	335	PHE
1	B	346	LYS
1	B	348	MET
1	B	354	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	371	ASP
1	B	374	GLU
1	B	390	MET
1	B	396	GLU
1	B	404	LEU
1	B	418	ARG
1	B	419	MET
1	B	428	GLN
1	B	430	GLU
1	B	436	ASP
1	B	441	TYR
1	B	452	ASN
1	B	458	MET
1	B	461	LYS
1	B	462	ASN
1	B	466	THR
1	B	470	ARG
1	B	474	TYR
1	B	475	ASP
1	B	480	CYS
1	B	506	TYR
1	B	509	SER
1	B	519	ARG
1	B	527	ARG
1	B	531	LEU
1	B	532	PHE
1	B	546	ARG
1	B	549	GLN
1	B	551	ARG
1	B	564	ARG
1	B	565	ARG
1	B	566	ARG
1	B	568	ARG
1	B	569	PHE
2	C	3	SER
2	C	17	GLN
2	C	45	MET
2	C	46	LEU
2	C	50	ASP
2	C	55	LYS
2	C	61	ARG
2	C	62	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	66	MET
2	C	69	TYR
2	C	74	SER
2	C	81	ASP
2	C	84	LEU
2	C	107	VAL
2	C	111	ILE
2	C	112	ARG
2	C	114	LEU
2	C	119	ARG
2	C	122	LEU
2	C	124	LEU
2	C	127	CYS
2	C	129	ARG
2	C	139	SER
2	C	145	GLU
2	C	154	GLU
2	C	164	GLU
2	C	171	ASP
2	C	173	GLU
2	C	178	PHE
2	C	179	LEU
2	C	180	ARG
2	C	182	GLU
2	C	187	LYS
2	C	189	ARG
2	C	194	CYS
2	C	201	CYS
2	C	204	GLU
2	C	209	LEU
2	C	222	ARG
2	C	237	THR
2	C	242	LYS
2	C	248	LEU
2	C	257	LEU
2	C	259	ASP
2	C	264	LEU
2	C	265	LYS
2	C	267	LYS
2	C	268	ASN
2	C	271	THR
2	C	273	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	295	GLU
2	C	297	ASP
2	C	310	SER
2	C	334	LEU
2	C	341	THR
2	C	352	ASN
2	C	355	SER
2	C	381	GLU
2	C	390	THR
2	C	394	GLU
2	C	397	MET
2	C	401	LYS
2	C	402	LEU
2	C	406	SER
2	C	410	ASP
2	C	414	GLU
2	D	3	SER
2	D	13	LYS
2	D	15	THR
2	D	17	GLN
2	D	20	LYS
2	D	22	ASN
2	D	25	GLU
2	D	33	GLU
2	D	37	ILE
2	D	45	MET
2	D	60	GLU
2	D	61	ARG
2	D	74	SER
2	D	112	ARG
2	D	114	LEU
2	D	119	ARG
2	D	122	LEU
2	D	124	LEU
2	D	125	TYR
2	D	127	CYS
2	D	128	LEU
2	D	129	ARG
2	D	153	ARG
2	D	154	GLU
2	D	164	GLU
2	D	178	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	179	LEU
2	D	180	ARG
2	D	182	GLU
2	D	183	MET
2	D	194	CYS
2	D	199	LYS
2	D	202	SER
2	D	204	GLU
2	D	208	ARG
2	D	209	LEU
2	D	215	GLU
2	D	220	ASN
2	D	227	LEU
2	D	237	THR
2	D	238	GLU
2	D	242	LYS
2	D	244	TRP
2	D	248	LEU
2	D	250	ARG
2	D	257	LEU
2	D	263	TRP
2	D	264	LEU
2	D	265	LYS
2	D	273	LYS
2	D	278	LYS
2	D	290	LEU
2	D	291	LEU
2	D	297	ASP
2	D	301	CYS
2	D	303	ASN
2	D	304	LEU
2	D	327	ASN
2	D	330	ASP
2	D	331	GLU
2	D	341	THR
2	D	355	SER
2	D	356	ILE
2	D	362	MET
2	D	370	THR
2	D	385	ASN
2	D	392	ASP
2	D	397	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	56	HIS
1	A	57	HIS
1	A	64	GLN
1	A	85	HIS
1	A	311	GLN
1	A	373	GLN
1	A	452	ASN
1	A	462	ASN
1	A	536	HIS
1	A	549	GLN
1	A	556	HIS
1	B	64	GLN
1	B	70	ASN
1	B	85	HIS
1	B	127	GLN
1	B	373	GLN
1	B	462	ASN
1	B	549	GLN
2	C	76	GLN
2	C	155	ASN
2	C	287	GLN
2	C	288	GLN
2	C	303	ASN
2	D	18	ASN
2	D	303	ASN
2	D	415	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	AMP	A	601	-	22,25,25	0.92	1 (4%)	25,38,38	1.41	2 (8%)
3	AMP	B	602	-	22,25,25	0.97	2 (9%)	25,38,38	1.38	5 (20%)
4	ADP	A	602	-	24,29,29	1.13	2 (8%)	29,45,45	1.56	6 (20%)
4	ADP	B	601	-	24,29,29	1.34	4 (16%)	29,45,45	2.12	12 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AMP	A	601	-	-	0/6/26/26	0/3/3/3
3	AMP	B	602	-	-	4/6/26/26	0/3/3/3
4	ADP	A	602	-	-	6/12/32/32	0/3/3/3
4	ADP	B	601	-	-	8/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	ADP	C2-N3	2.88	1.36	1.32
4	A	602	ADP	O4'-C1'	2.64	1.44	1.41
4	B	601	ADP	C5-C4	2.61	1.47	1.40
4	B	601	ADP	O4'-C1'	2.47	1.44	1.41
3	A	601	AMP	O4'-C1'	2.24	1.44	1.41
3	B	602	AMP	C5-C4	2.20	1.46	1.40
4	A	602	ADP	C5-C4	2.16	1.46	1.40
4	B	601	ADP	C5-N7	-2.07	1.32	1.39
3	B	602	AMP	O4'-C1'	2.04	1.43	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	ADP	O3B-PB-O3A	-5.50	86.18	104.64
3	A	601	AMP	N3-C2-N1	-3.91	122.57	128.68
4	B	601	ADP	O3B-PB-O1B	3.51	124.42	110.68
4	A	602	ADP	O3B-PB-O1B	3.40	124.00	110.68
4	B	601	ADP	C4-C5-N7	-3.11	106.15	109.40
4	B	601	ADP	N3-C2-N1	-3.11	123.81	128.68
4	A	602	ADP	PA-O3A-PB	-3.06	122.34	132.83
4	B	601	ADP	C2'-C3'-C4'	2.98	108.44	102.64
4	A	602	ADP	N3-C2-N1	-2.97	124.04	128.68
4	B	601	ADP	C3'-C2'-C1'	2.88	105.31	100.98
4	B	601	ADP	C1'-N9-C4	2.86	131.66	126.64
4	B	601	ADP	O5'-C5'-C4'	2.83	118.73	108.99
3	B	602	AMP	N3-C2-N1	-2.81	124.28	128.68
4	A	602	ADP	N6-C6-N1	2.68	124.13	118.57
3	A	601	AMP	C3'-C2'-C1'	2.61	104.90	100.98
3	B	602	AMP	O3P-P-O2P	2.54	117.34	107.64
4	B	601	ADP	O2B-PB-O3A	2.42	112.74	104.64
4	B	601	ADP	N6-C6-N1	2.31	123.36	118.57
3	B	602	AMP	C1'-N9-C4	-2.28	122.64	126.64
4	A	602	ADP	O5'-PA-O1A	-2.27	100.20	109.07
4	B	601	ADP	O2B-PB-O1B	-2.23	101.96	110.68
4	A	602	ADP	C2-N1-C6	2.18	122.48	118.75
3	B	602	AMP	O3P-P-O5'	-2.17	100.96	106.73
3	B	602	AMP	C3'-C2'-C1'	-2.12	97.79	100.98
4	B	601	ADP	O4'-C4'-C5'	2.09	116.26	109.37

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	AMP	C5'-O5'-P-O2P
3	B	602	AMP	C5'-O5'-P-O3P
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	O4'-C4'-C5'-O5'
4	A	602	ADP	C3'-C4'-C5'-O5'
4	B	601	ADP	PA-O3A-PB-O2B
4	B	601	ADP	C4'-C5'-O5'-PA
4	B	601	ADP	C3'-C4'-C5'-O5'
4	B	601	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	C5'-O5'-PA-O2A
4	B	601	ADP	PB-O3A-PA-O1A
3	B	602	AMP	O4'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	601	ADP	PA-O3A-PB-O1B
3	B	602	AMP	C5'-O5'-P-O1P
4	A	602	ADP	PB-O3A-PA-O2A
4	B	601	ADP	PB-O3A-PA-O2A
4	B	601	ADP	C5'-O5'-PA-O2A

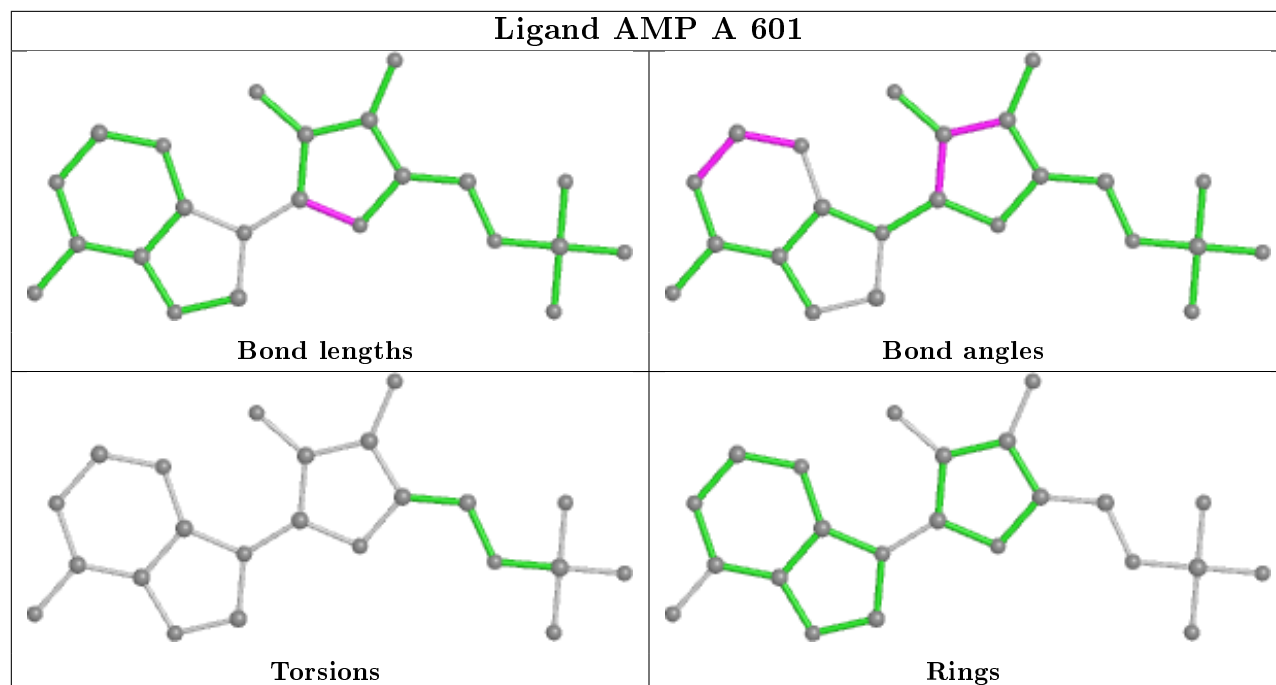
There are no ring outliers.

4 monomers are involved in 21 short contacts:

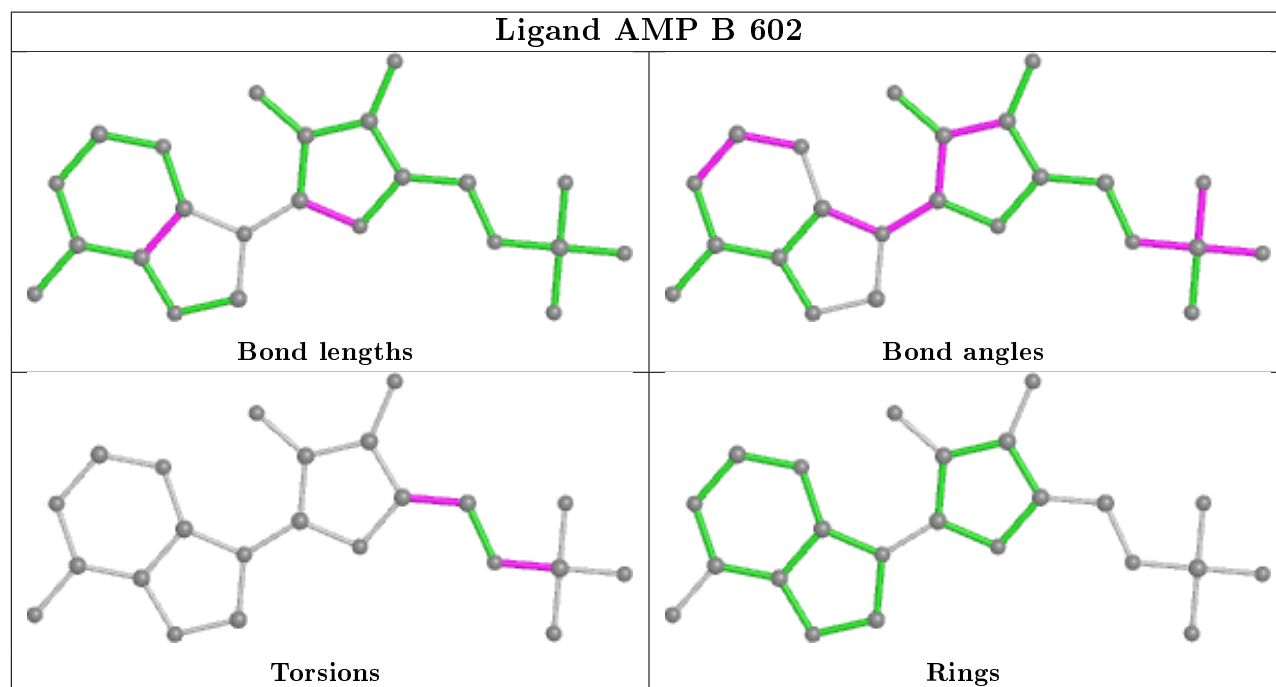
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	AMP	2	0
3	B	602	AMP	6	0
4	A	602	ADP	7	0
4	B	601	ADP	6	0

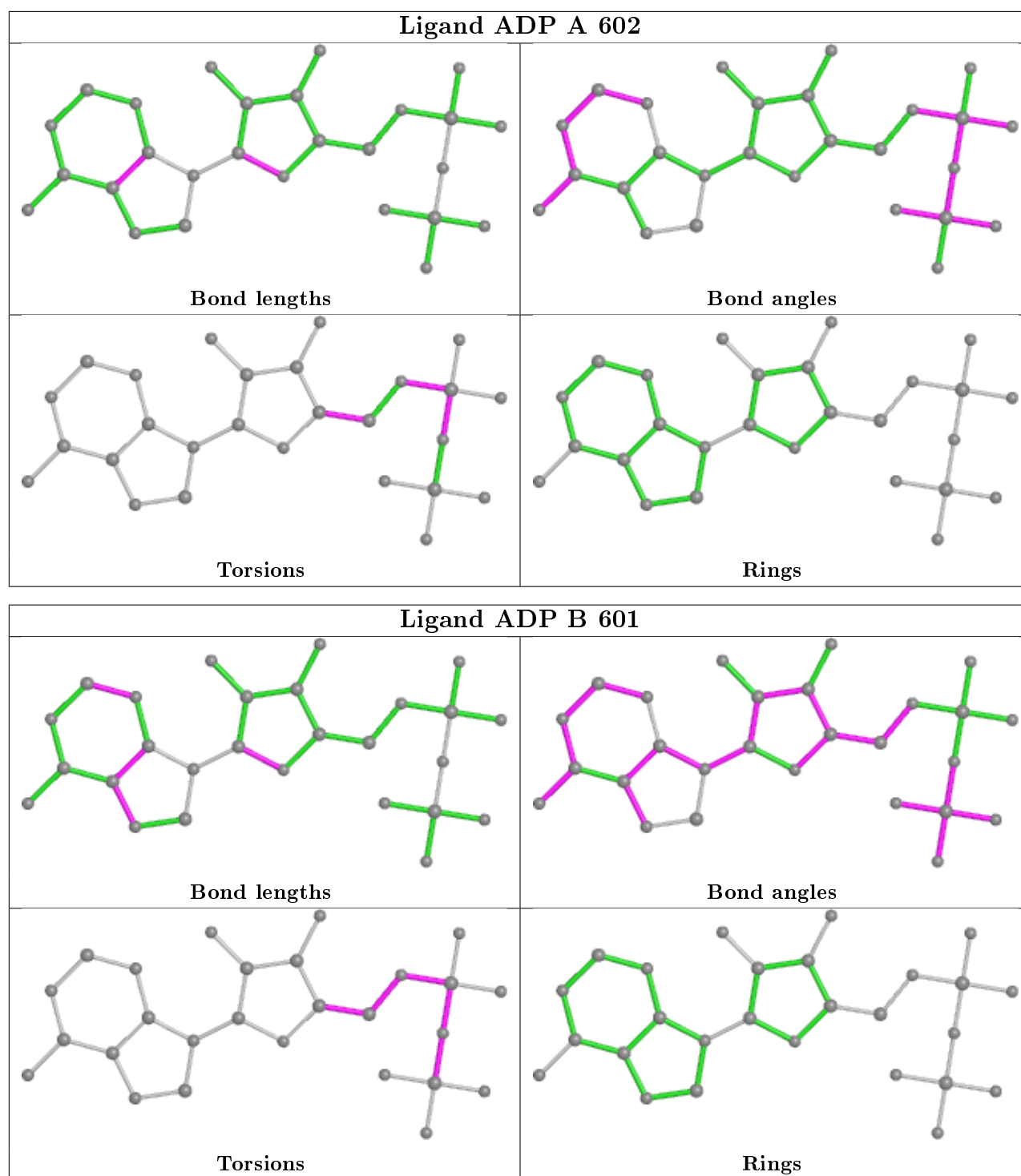
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand AMP A 601



## Ligand AMP B 602





## 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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

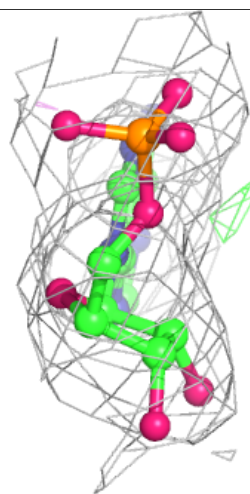
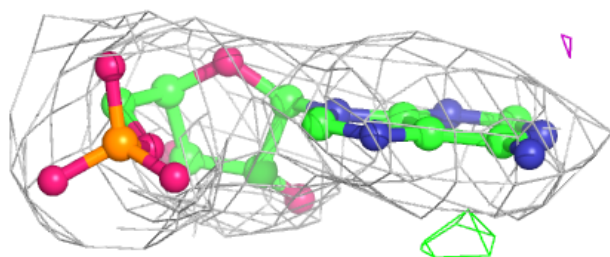
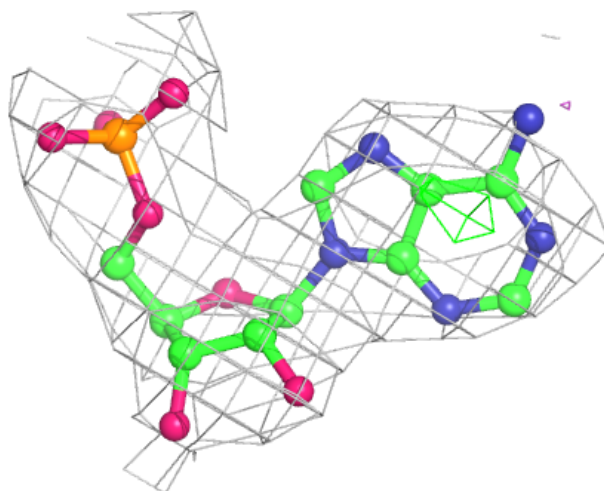
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

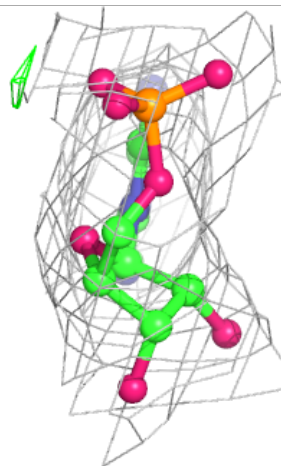
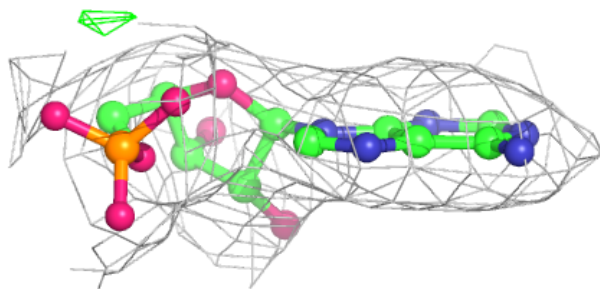
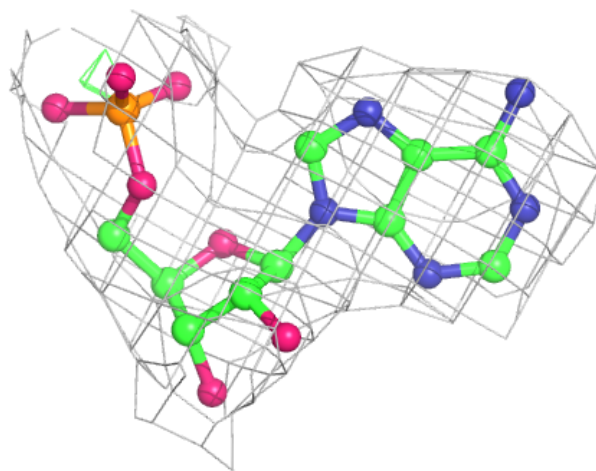
**Electron density around AMP A 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



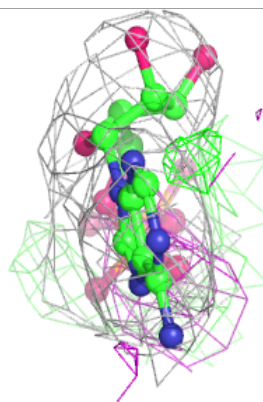
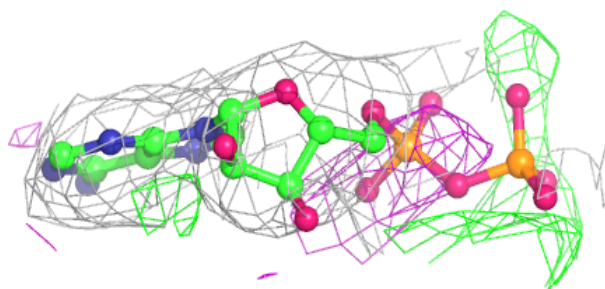
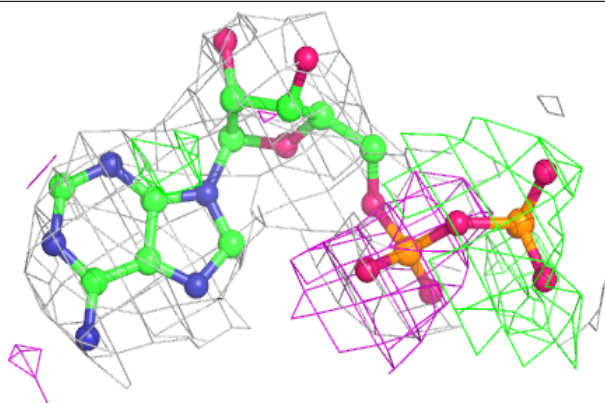
**Electron density around AMP B 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

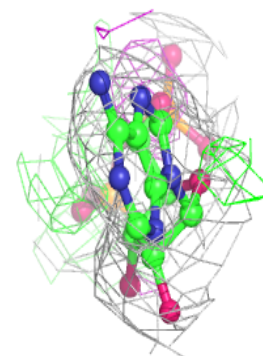
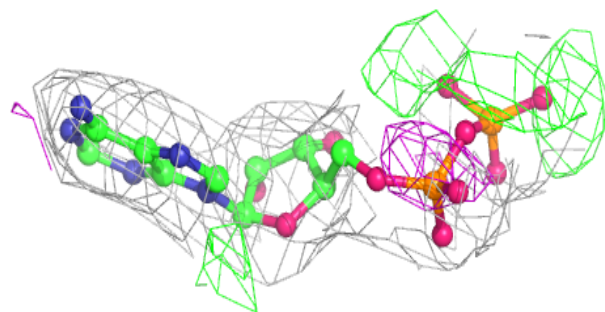
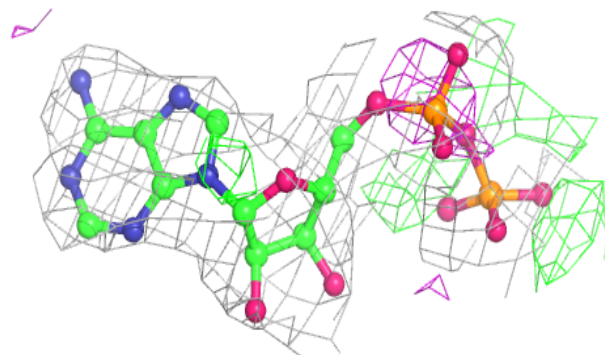


**Electron density around ADP A 602:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP B 601:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.