



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2017 – 09:28 PM EST

PDB ID : 1NR1  
Title : Crystal structure of the R463A mutant of human Glutamate dehydrogenase  
Authors : Banerjee, S.; Schmidt, T.; Fang, J.; Stanley, C.A.; Smith, T.J.  
Deposited on : 2003-01-23  
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

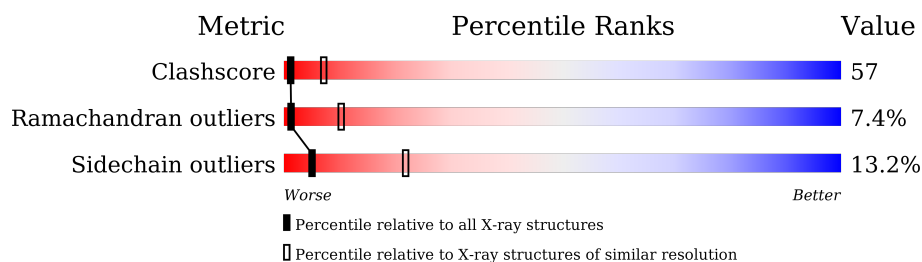
# 1 Overall quality at a glance

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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	496	
1	B	496	
1	C	496	
1	D	496	
1	E	496	
1	F	496	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23208 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 Glutamate dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	B	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	C	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	D	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	E	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			
1	F	496	Total	C	N	O	S	0	0	0
			3868	2447	676	726	19			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	GLN	HIS	CONFLICT	UNP P00367
A	89	HIS	GLN	CONFLICT	UNP P00367
A	463	ALA	ARG	ENGINEERED	UNP P00367
B	88	GLN	HIS	CONFLICT	UNP P00367
B	89	HIS	GLN	CONFLICT	UNP P00367
B	463	ALA	ARG	ENGINEERED	UNP P00367
C	88	GLN	HIS	CONFLICT	UNP P00367
C	89	HIS	GLN	CONFLICT	UNP P00367
C	463	ALA	ARG	ENGINEERED	UNP P00367
D	88	GLN	HIS	CONFLICT	UNP P00367
D	89	HIS	GLN	CONFLICT	UNP P00367
D	463	ALA	ARG	ENGINEERED	UNP P00367
E	88	GLN	HIS	CONFLICT	UNP P00367
E	89	HIS	GLN	CONFLICT	UNP P00367
E	463	ALA	ARG	ENGINEERED	UNP P00367
F	88	GLN	HIS	CONFLICT	UNP P00367
F	89	HIS	GLN	CONFLICT	UNP P00367

*Continued on next page...*

*Continued from previous page...*

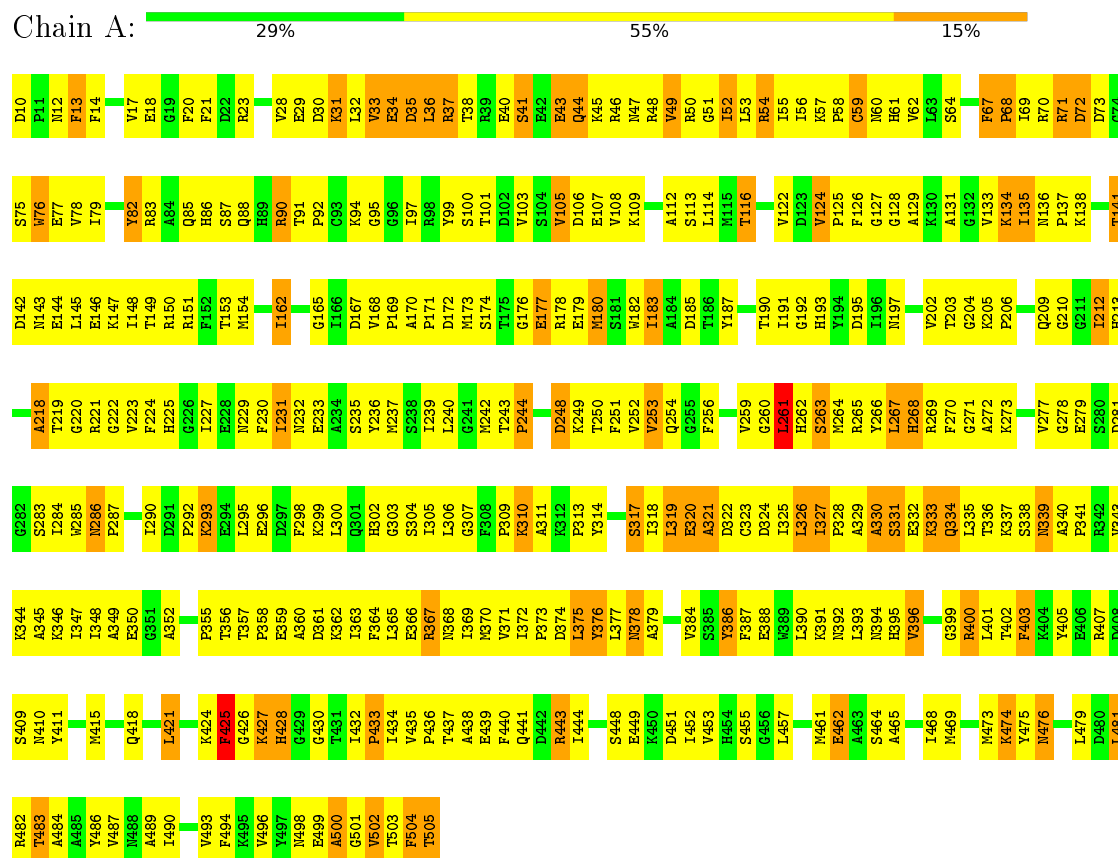
Chain	Residue	Modelled	Actual	Comment	Reference
F	463	ALA	ARG	ENGINEERED	UNP P00367

### 3 Residue-property plots

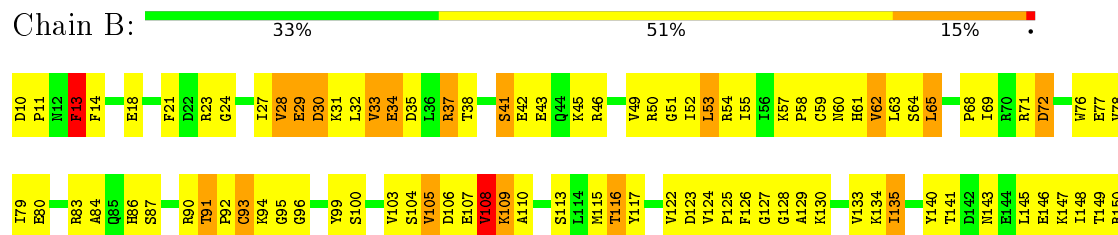
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

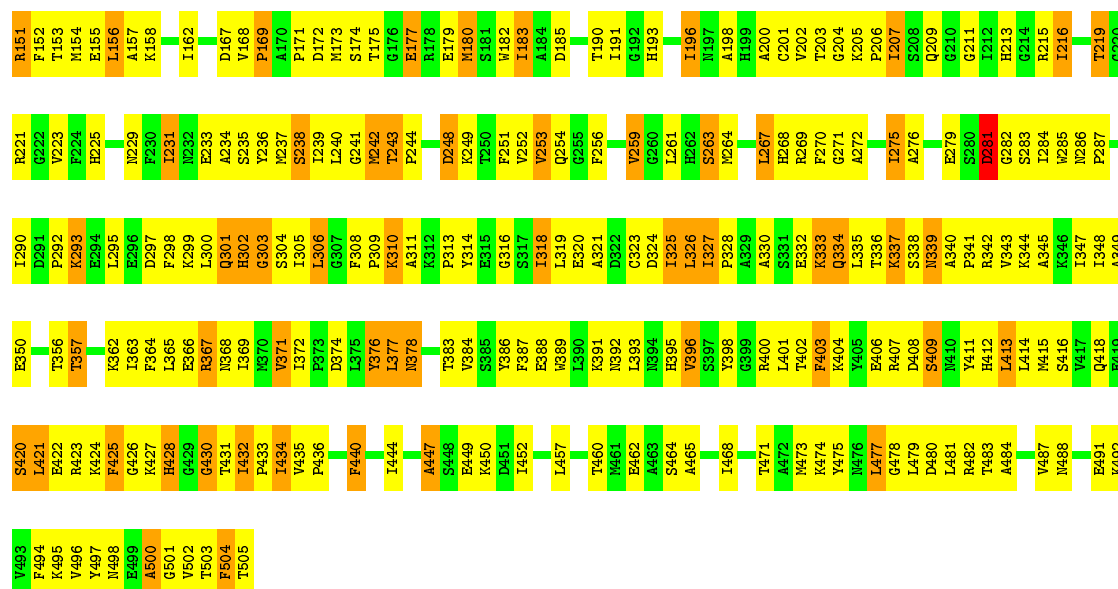
Note EDS was not executed.

#### • Molecule 1: Glutamate dehydrogenase 1



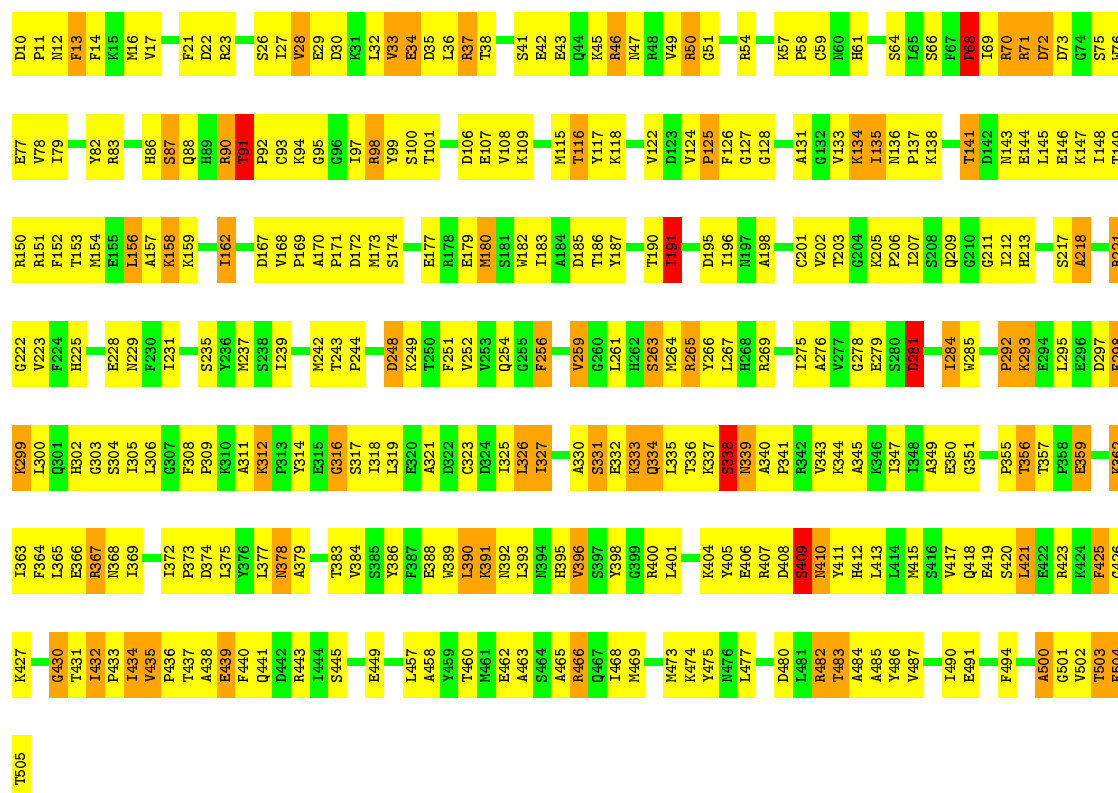
#### • Molecule 1: Glutamate dehydrogenase 1





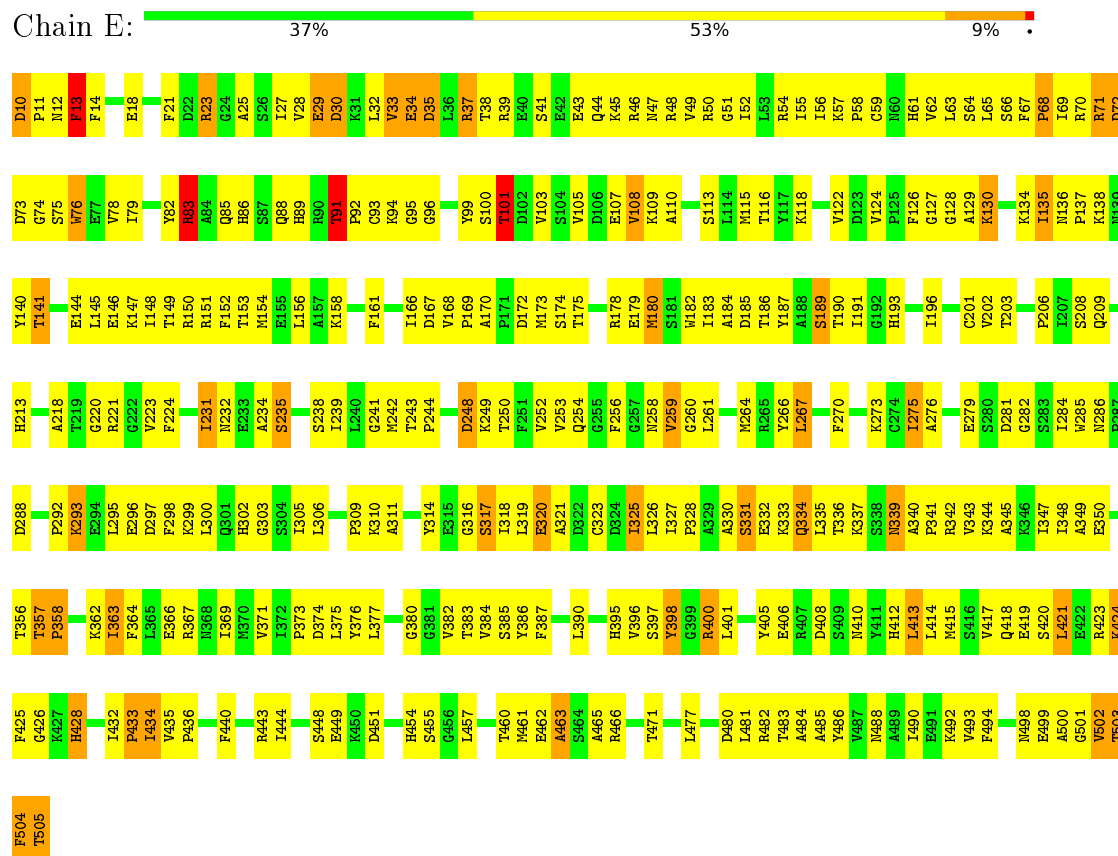
### • Molecule 1: Glutamate dehydrogenase 1

Chain C: 37% 49% 13%



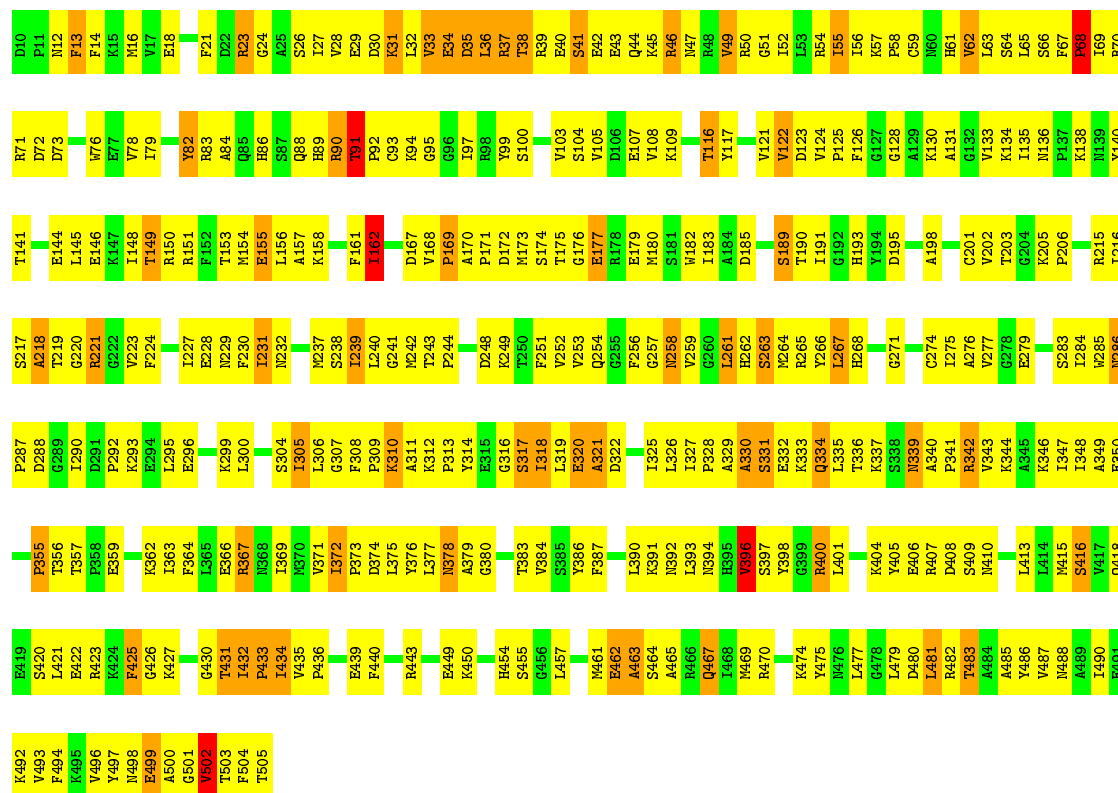
### • Molecule 1: Glutamate dehydrogenase 1

Chain D: 28% 57% 13%



• Molecule 1: Glutamate dehydrogenase 1

Chain F:  31% 55% 12%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.92Å 98.64Å 124.26Å 86.48° 69.69° 60.87°	Depositor
Resolution (Å)	19.99 – 3.30	Depositor
% Data completeness (in resolution range)	90.9 (19.99-3.30)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23208	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.68	1/3952 (0.0%)	0.85	1/5333 (0.0%)
1	B	0.65	1/3952 (0.0%)	0.86	5/5333 (0.1%)
1	C	0.66	2/3952 (0.1%)	0.86	6/5333 (0.1%)
1	D	0.66	1/3952 (0.0%)	0.87	5/5333 (0.1%)
1	E	0.63	0/3952	0.85	4/5333 (0.1%)
1	F	0.64	0/3952	0.85	3/5333 (0.1%)
All	All	0.65	5/23712 (0.0%)	0.86	24/31998 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	E	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	CYS	CB-SG	9.46	1.98	1.82
1	C	59	CYS	CB-SG	8.70	1.97	1.82
1	D	59	CYS	CB-SG	7.67	1.95	1.82
1	C	93	CYS	CB-SG	-6.07	1.72	1.82
1	B	93	CYS	CB-SG	-5.53	1.72	1.81

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	240	LEU	CA-CB-CG	6.75	130.84	115.30
1	D	326	LEU	CA-CB-CG	6.73	130.78	115.30
1	C	316	GLY	N-CA-C	-6.33	97.27	113.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	PHE	N-CA-C	-6.12	94.47	111.00
1	C	503	THR	N-CA-C	-6.04	94.68	111.00
1	C	66	SER	N-CA-C	-6.03	94.71	111.00
1	D	504	PHE	N-CA-C	-6.00	94.79	111.00
1	B	504	PHE	N-CA-C	-5.92	95.02	111.00
1	C	504	PHE	N-CA-C	-5.88	95.13	111.00
1	B	316	GLY	N-CA-C	-5.81	98.58	113.10
1	F	393	LEU	CA-CB-CG	5.74	128.49	115.30
1	E	504	PHE	N-CA-C	-5.62	95.83	111.00
1	B	243	THR	N-CA-C	-5.58	95.93	111.00
1	B	326	LEU	CA-CB-CG	5.57	128.12	115.30
1	E	83	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	300	LEU	CA-CB-CG	5.44	127.82	115.30
1	F	66	SER	N-CA-C	-5.44	96.31	111.00
1	F	396	VAL	CB-CA-C	-5.20	101.53	111.40
1	B	127	GLY	N-CA-C	-5.13	100.28	113.10
1	E	503	THR	N-CA-C	-5.12	97.19	111.00
1	C	91	THR	C-N-CD	5.07	139.04	128.40
1	E	39	ARG	N-CA-C	-5.03	97.43	111.00
1	C	191	ILE	CG1-CB-CG2	-5.02	100.36	111.40
1	D	243	THR	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	266	TYR	Sidechain
1	D	459	TYR	Sidechain
1	E	187	TYR	Sidechain
1	E	398	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3868	0	3833	532	0
1	B	3868	0	3833	437	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3868	0	3833	430	0
1	D	3868	0	3833	506	0
1	E	3868	0	3833	415	0
1	F	3868	0	3833	487	0
All	All	23208	0	22998	2635	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 57.

All (2635) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LYS:HE3	1:C:359:GLU:HG3	1.26	1.16
1:E:190:THR:HG22	1:E:191:ILE:H	1.09	1.15
1:A:251:PHE:HB3	1:A:325:ILE:HG13	1.29	1.14
1:A:71:ARG:HH11	1:A:71:ARG:HB3	1.07	1.13
1:D:86:HIS:CD2	1:D:116:THR:HG21	1.83	1.11
1:E:116:THR:HG22	1:E:128:GLY:N	1.66	1.10
1:D:99:TYR:OH	1:D:149:THR:HG22	1.49	1.10
1:C:327:ILE:HG22	1:C:349:ALA:HB3	1.33	1.09
1:F:277:VAL:HB	1:F:284:ILE:HD12	1.27	1.09
1:A:37:ARG:HB2	1:A:37:ARG:HH11	0.99	1.08
1:E:116:THR:HG22	1:E:128:GLY:H	0.95	1.08
1:C:37:ARG:HH21	1:C:49:VAL:HG11	1.14	1.07
1:A:10:ASP:HB2	1:A:333:LYS:HE2	1.31	1.07
1:E:38:THR:HG23	1:E:41:SER:HB3	1.38	1.06
1:B:190:THR:HG22	1:B:191:ILE:H	1.17	1.05
1:F:251:PHE:HB3	1:F:325:ILE:HG13	1.37	1.05
1:A:71:ARG:HB3	1:A:71:ARG:NH1	1.72	1.05
1:C:99:TYR:OH	1:C:149:THR:HG22	1.56	1.04
1:E:284:ILE:HG23	1:E:311:ALA:HB1	1.38	1.03
1:D:325:ILE:HG22	1:D:347:ILE:HB	1.40	1.03
1:F:86:HIS:CD2	1:F:116:THR:HG21	1.93	1.02
1:F:333:LYS:HE3	1:F:357:THR:HG22	1.40	1.02
1:C:325:ILE:HG22	1:C:347:ILE:HB	1.42	1.02
1:D:348:ILE:HB	1:D:371:VAL:HG22	1.36	1.02
1:E:190:THR:HG22	1:E:191:ILE:N	1.74	1.02
1:E:34:GLU:HA	1:E:38:THR:HB	1.39	1.01
1:D:284:ILE:HG23	1:D:311:ALA:HB1	1.41	1.01
1:A:185:ASP:OD1	1:F:505:THR:HG23	1.61	1.01
1:A:37:ARG:HB2	1:A:37:ARG:NH1	1.75	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:THR:HG23	1:F:41:SER:HB3	1.37	1.01
1:E:320:GLU:HG2	1:E:342:ARG:HG2	1.43	1.01
1:F:327:ILE:HG22	1:F:349:ALA:HB3	1.40	1.01
1:F:486:TYR:O	1:F:490:ILE:HG12	1.62	1.00
1:B:116:THR:HG22	1:B:128:GLY:H	1.25	1.00
1:B:37:ARG:HB2	1:B:37:ARG:HH11	1.22	1.00
1:F:334:GLN:HE21	1:F:334:GLN:HA	1.23	0.99
1:A:99:TYR:OH	1:A:149:THR:HG22	1.62	0.99
1:D:37:ARG:HH11	1:D:37:ARG:HB2	1.24	0.99
1:C:141:THR:HG23	1:C:144:GLU:HG3	1.45	0.99
1:F:43:GLU:HB3	1:F:45:LYS:HG3	1.44	0.99
1:A:237:MET:HE2	1:A:240:LEU:HD12	1.45	0.99
1:B:505:THR:HG23	1:F:185:ASP:OD1	1.62	0.98
1:B:37:ARG:NH1	1:B:37:ARG:HB2	1.79	0.98
1:A:116:THR:HG22	1:A:128:GLY:HA3	1.45	0.98
1:C:71:ARG:HB3	1:C:71:ARG:HH11	1.23	0.97
1:E:37:ARG:HB2	1:E:37:ARG:NH1	1.79	0.97
1:B:116:THR:HG22	1:B:128:GLY:N	1.80	0.97
1:C:83:ARG:HD3	1:C:131:ALA:HB2	1.46	0.97
1:E:418:GLN:HB2	1:E:433:PRO:HD2	1.47	0.97
1:C:185:ASP:OD1	1:E:505:THR:HG23	1.65	0.96
1:B:418:GLN:HB2	1:B:433:PRO:HD2	1.46	0.95
1:D:86:HIS:HD2	1:D:116:THR:HG21	1.22	0.95
1:D:372:ILE:HG21	1:D:377:LEU:HD13	1.47	0.95
1:A:91:THR:HB	1:A:92:PRO:HD3	1.49	0.95
1:F:243:THR:N	1:F:244:PRO:HD3	1.80	0.94
1:C:284:ILE:HG13	1:C:311:ALA:HB1	1.47	0.94
1:B:327:ILE:HG22	1:B:349:ALA:HB3	1.50	0.94
1:F:86:HIS:HD2	1:F:116:THR:HG21	1.23	0.94
1:A:86:HIS:CD2	1:A:116:THR:HG21	2.02	0.94
1:B:190:THR:HG22	1:B:191:ILE:N	1.81	0.94
1:A:13:PHE:HD1	1:A:14:PHE:H	1.13	0.93
1:E:327:ILE:HG22	1:E:349:ALA:HB3	1.47	0.93
1:D:41:SER:HA	1:D:46:ARG:HE	1.31	0.93
1:B:343:VAL:HG21	1:B:364:PHE:HE1	1.34	0.93
1:A:61:HIS:HD2	1:A:88:GLN:HE22	1.17	0.93
1:A:23:ARG:HE	1:A:483:THR:HG21	1.32	0.92
1:C:243:THR:N	1:C:244:PRO:HD3	1.84	0.92
1:A:284:ILE:HG23	1:A:311:ALA:HB1	1.48	0.92
1:B:100:SER:O	1:B:103:VAL:HG13	1.69	0.92
1:C:396:VAL:HG13	1:E:386:TYR:OH	1.70	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ARG:HG2	1:C:221:ARG:HH11	1.34	0.92
1:E:86:HIS:CD2	1:E:116:THR:HG21	2.05	0.92
1:F:61:HIS:HD2	1:F:88:GLN:HE22	1.12	0.92
1:C:252:VAL:HG13	1:C:276:ALA:HB3	1.50	0.92
1:A:319:LEU:H	1:A:319:LEU:HD12	1.35	0.92
1:F:24:GLY:O	1:F:28:VAL:HG23	1.70	0.91
1:E:99:TYR:OH	1:E:149:THR:HG22	1.69	0.91
1:A:243:THR:N	1:A:244:PRO:HD3	1.85	0.91
1:C:145:LEU:O	1:C:149:THR:HG23	1.71	0.91
1:C:86:HIS:CD2	1:C:116:THR:HG21	2.05	0.90
1:C:144:GLU:O	1:C:148:ILE:HG13	1.72	0.90
1:B:76:TRP:HE1	1:D:502:VAL:HG11	1.37	0.90
1:D:427:LYS:HD3	1:D:430:GLY:HA3	1.52	0.90
1:D:83:ARG:HD2	1:D:131:ALA:HB2	1.52	0.90
1:E:336:THR:H	1:E:339:ASN:HD21	1.15	0.90
1:D:154:MET:SD	1:D:190:THR:HG21	2.11	0.90
1:B:281:ASP:HB2	1:B:306:LEU:HD11	1.54	0.89
1:F:325:ILE:HG22	1:F:347:ILE:HB	1.55	0.89
1:B:116:THR:HG22	1:B:128:GLY:CA	2.03	0.89
1:B:251:PHE:HB3	1:B:325:ILE:HG13	1.55	0.89
1:D:505:THR:HG23	1:E:185:ASP:OD1	1.73	0.89
1:F:251:PHE:CB	1:F:325:ILE:HG13	2.03	0.89
1:F:343:VAL:HG21	1:F:364:PHE:HE1	1.37	0.88
1:A:83:ARG:HD3	1:A:131:ALA:HB2	1.53	0.88
1:A:37:ARG:HH11	1:A:37:ARG:CB	1.84	0.88
1:D:251:PHE:HB3	1:D:325:ILE:HG12	1.54	0.88
1:E:71:ARG:HB3	1:E:71:ARG:HH11	1.37	0.88
1:B:86:HIS:CD2	1:B:116:THR:HG21	2.08	0.88
1:C:333:LYS:HD3	1:C:357:THR:HG22	1.54	0.87
1:E:41:SER:HA	1:E:46:ARG:HD2	1.56	0.87
1:B:43:GLU:HB3	1:B:45:LYS:HG3	1.55	0.87
1:C:169:PRO:O	1:C:202:VAL:HG23	1.74	0.87
1:A:116:THR:HG22	1:A:128:GLY:CA	2.03	0.87
1:D:91:THR:HB	1:D:92:PRO:HD3	1.53	0.87
1:A:54:ARG:O	1:A:58:PRO:HD2	1.75	0.87
1:D:227:ILE:HD11	1:D:349:ALA:HB2	1.55	0.87
1:C:116:THR:HG22	1:C:128:GLY:HA3	1.56	0.87
1:A:502:VAL:HG11	1:E:76:TRP:NE1	1.90	0.87
1:C:13:PHE:CZ	1:C:107:GLU:HG3	2.10	0.87
1:F:146:GLU:O	1:F:150:ARG:HG3	1.73	0.86
1:E:100:SER:O	1:E:103:VAL:HG13	1.75	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:THR:N	1:D:244:PRO:HD3	1.89	0.86
1:D:34:GLU:HA	1:D:38:THR:HB	1.56	0.86
1:D:425:PHE:CE1	1:D:427:LYS:HE2	2.10	0.86
1:D:97:ILE:HD13	1:D:131:ALA:HB3	1.56	0.86
1:E:135:ILE:HD11	1:E:140:TYR:OH	1.75	0.86
1:F:332:GLU:HG2	1:F:333:LYS:HG3	1.57	0.86
1:C:229:ASN:ND2	1:C:462:GLU:HA	1.90	0.85
1:F:91:THR:HB	1:F:92:PRO:HD3	1.59	0.85
1:A:103:VAL:HA	1:A:107:GLU:OE2	1.77	0.85
1:C:433:PRO:O	1:C:435:VAL:N	2.09	0.85
1:D:63:LEU:HD21	1:D:65:LEU:HD21	1.56	0.85
1:F:83:ARG:HD2	1:F:131:ALA:HB2	1.58	0.85
1:F:61:HIS:CD2	1:F:88:GLN:HE22	1.94	0.85
1:A:285:TRP:HB2	1:A:314:TYR:HB2	1.57	0.85
1:E:206:PRO:HD2	1:E:209:GLN:HB2	1.59	0.85
1:F:135:ILE:HD11	1:F:140:TYR:OH	1.76	0.85
1:E:433:PRO:O	1:E:435:VAL:N	2.09	0.84
1:B:362:LYS:O	1:B:366:GLU:HG3	1.77	0.84
1:C:505:THR:HG23	1:D:185:ASP:OD1	1.77	0.84
1:E:72:ASP:OD1	1:E:144:GLU:HG3	1.77	0.84
1:C:254:GLN:HE22	1:C:334:GLN:HG2	1.40	0.84
1:D:285:TRP:HB2	1:D:314:TYR:HB2	1.57	0.84
1:B:146:GLU:O	1:B:150:ARG:HG3	1.78	0.84
1:B:205:LYS:NZ	1:B:392:ASN:HD21	1.75	0.83
1:D:105:VAL:O	1:D:109:LYS:HG3	1.79	0.83
1:D:502:VAL:HG23	1:D:503:THR:H	1.44	0.83
1:A:410:ASN:ND2	1:B:413:LEU:HD21	1.93	0.83
1:C:76:TRP:HE1	1:F:502:VAL:HG11	1.43	0.83
1:A:171:PRO:HG3	1:A:180:MET:SD	2.20	0.82
1:A:504:PHE:HE1	1:E:151:ARG:NH2	1.76	0.82
1:A:71:ARG:CB	1:A:71:ARG:HH11	1.91	0.82
1:D:327:ILE:N	1:D:327:ILE:HD13	1.94	0.82
1:A:146:GLU:O	1:A:150:ARG:HG3	1.78	0.82
1:E:466:ARG:HG3	1:E:466:ARG:HH11	1.44	0.82
1:F:319:LEU:HD12	1:F:319:LEU:H	1.43	0.82
1:C:97:ILE:CD1	1:C:131:ALA:HB3	2.09	0.82
1:F:13:PHE:HD1	1:F:14:PHE:N	1.77	0.82
1:F:433:PRO:O	1:F:435:VAL:N	2.12	0.82
1:D:483:THR:O	1:D:487:VAL:HG23	1.79	0.82
1:A:122:VAL:HG11	1:A:379:ALA:HB1	1.60	0.82
1:B:244:PRO:HG2	1:B:248:ASP:N	1.94	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLU:HB3	1:D:45:LYS:HG3	1.62	0.81
1:E:147:LYS:O	1:E:151:ARG:HG3	1.80	0.81
1:E:146:GLU:O	1:E:150:ARG:HG3	1.80	0.81
1:A:319:LEU:CD1	1:A:319:LEU:H	1.93	0.81
1:A:502:VAL:HG23	1:A:503:THR:H	1.44	0.81
1:C:325:ILE:HG22	1:C:347:ILE:CB	2.10	0.81
1:A:23:ARG:NE	1:A:483:THR:HG21	1.95	0.81
1:B:502:VAL:HG23	1:B:503:THR:H	1.43	0.81
1:F:350:GLU:HG2	1:F:355:PRO:HG3	1.62	0.81
1:A:318:ILE:HD12	1:A:319:LEU:N	1.96	0.81
1:C:86:HIS:HD2	1:C:116:THR:HG21	1.45	0.81
1:C:337:LYS:CE	1:C:359:GLU:HG3	2.09	0.81
1:F:94:LYS:HD3	1:F:126:PHE:CE1	2.15	0.81
1:A:505:THR:HG23	1:B:185:ASP:OD1	1.81	0.81
1:D:227:ILE:HD11	1:D:349:ALA:CB	2.10	0.81
1:F:398:TYR:HB2	1:F:449:GLU:HG3	1.63	0.81
1:F:50:ARG:O	1:F:50:ARG:HG3	1.79	0.81
1:C:339:ASN:HD22	1:C:340:ALA:N	1.80	0.80
1:B:172:ASP:O	1:B:174:SER:N	2.14	0.80
1:E:343:VAL:HG21	1:E:364:PHE:HE1	1.47	0.80
1:F:350:GLU:OE1	1:F:373:PRO:HA	1.80	0.80
1:F:57:LYS:N	1:F:58:PRO:HD2	1.97	0.80
1:A:503:THR:HG21	1:E:151:ARG:HD3	1.63	0.80
1:B:339:ASN:HD22	1:B:339:ASN:H	1.28	0.80
1:D:172:ASP:O	1:D:174:SER:N	2.15	0.80
1:C:77:GLU:HA	1:F:54:ARG:NH2	1.96	0.80
1:B:76:TRP:NE1	1:D:502:VAL:HG11	1.97	0.80
1:B:11:PRO:O	1:B:333:LYS:HE2	1.80	0.79
1:E:418:GLN:OE1	1:E:432:ILE:HA	1.82	0.79
1:E:61:HIS:HD2	1:E:88:GLN:HE22	1.29	0.79
1:F:340:ALA:HB3	1:F:341:PRO:HD3	1.64	0.79
1:A:34:GLU:HA	1:A:38:THR:HB	1.63	0.79
1:C:34:GLU:HA	1:C:38:THR:HB	1.63	0.79
1:D:324:ASP:HB2	1:D:325:ILE:HD13	1.64	0.79
1:C:486:TYR:O	1:C:490:ILE:HG12	1.81	0.79
1:D:326:LEU:HD12	1:D:348:ILE:CD1	2.13	0.79
1:D:38:THR:HG23	1:D:41:SER:HB3	1.64	0.79
1:E:243:THR:N	1:E:244:PRO:HD3	1.95	0.79
1:D:326:LEU:HD12	1:D:348:ILE:HD12	1.63	0.79
1:A:143:ASN:HD21	1:C:70:ARG:HH22	1.29	0.79
1:E:400:ARG:HH11	1:E:400:ARG:HG3	1.48	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:GLU:OE2	1:F:355:PRO:HD2	1.83	0.79
1:A:86:HIS:HD2	1:A:116:THR:HG21	1.47	0.79
1:C:190:THR:HG22	1:C:191:ILE:N	1.97	0.79
1:A:281:ASP:HB2	1:A:306:LEU:HD11	1.62	0.78
1:B:243:THR:N	1:B:244:PRO:HD3	1.97	0.78
1:F:29:GLU:O	1:F:33:VAL:HG23	1.82	0.78
1:B:34:GLU:HA	1:B:38:THR:HB	1.64	0.78
1:D:37:ARG:HB2	1:D:37:ARG:NH1	1.97	0.78
1:A:38:THR:HG23	1:A:41:SER:HB3	1.66	0.78
1:E:400:ARG:HH11	1:E:400:ARG:CG	1.96	0.78
1:D:252:VAL:HG22	1:D:275:ILE:CG2	2.14	0.78
1:F:240:LEU:HB3	1:F:346:LYS:HD2	1.66	0.78
1:F:418:GLN:HB2	1:F:433:PRO:HD2	1.66	0.78
1:A:168:VAL:HG13	1:A:202:VAL:HA	1.64	0.78
1:C:141:THR:HG23	1:C:144:GLU:CG	2.13	0.78
1:D:348:ILE:CB	1:D:371:VAL:HG22	2.14	0.78
1:B:502:VAL:HG11	1:D:76:TRP:HE1	1.49	0.78
1:F:179:GLU:O	1:F:183:ILE:HG13	1.84	0.78
1:A:76:TRP:NE1	1:E:502:VAL:HG11	1.98	0.77
1:B:69:ILE:HA	1:B:151:ARG:NH1	1.98	0.77
1:D:145:LEU:O	1:D:149:THR:HG23	1.85	0.77
1:A:61:HIS:CD2	1:A:88:GLN:HE22	2.03	0.77
1:F:253:VAL:HG13	1:F:277:VAL:HG13	1.66	0.77
1:F:355:PRO:HG2	1:F:356:THR:HG23	1.66	0.77
1:D:394:ASN:O	1:D:396:VAL:HG23	1.84	0.77
1:F:37:ARG:HH11	1:F:37:ARG:HB2	1.47	0.77
1:F:409:SER:O	1:F:413:LEU:HD23	1.84	0.77
1:A:284:ILE:HD12	1:A:305:ILE:HD12	1.67	0.77
1:A:427:LYS:HA	1:A:427:LYS:HE2	1.65	0.77
1:B:116:THR:HG22	1:B:128:GLY:HA3	1.67	0.77
1:F:285:TRP:CD1	1:F:287:PRO:HD3	2.20	0.77
1:F:61:HIS:HD2	1:F:88:GLN:NE2	1.82	0.77
1:A:352:ALA:O	1:A:355:PRO:HD3	1.85	0.77
1:D:327:ILE:H	1:D:327:ILE:HD13	1.50	0.77
1:E:502:VAL:HG23	1:E:503:THR:H	1.48	0.77
1:A:370:MET:HB2	1:A:479:LEU:HD23	1.67	0.77
1:A:440:PHE:CD2	1:B:412:HIS:HB3	2.20	0.77
1:D:116:THR:HG22	1:D:128:GLY:HA3	1.66	0.77
1:F:334:GLN:HE21	1:F:334:GLN:CA	1.95	0.77
1:D:337:LYS:NZ	1:D:337:LYS:HB3	1.98	0.77
1:F:23:ARG:HE	1:F:27:ILE:HD11	1.48	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:GLU:HG3	1:A:46:ARG:HH12	1.49	0.76
1:A:190:THR:HG22	1:A:191:ILE:N	2.00	0.76
1:E:340:ALA:HB3	1:E:341:PRO:HD3	1.66	0.76
1:E:47:ASN:O	1:E:50:ARG:HG2	1.86	0.76
1:C:254:GLN:OE1	1:C:319:LEU:HD11	1.85	0.76
1:C:502:VAL:HG11	1:F:76:TRP:NE1	1.99	0.76
1:A:281:ASP:HB3	1:A:306:LEU:HD21	1.65	0.76
1:B:99:TYR:OH	1:B:149:THR:HG22	1.86	0.76
1:F:69:ILE:HA	1:F:151:ARG:CZ	2.15	0.76
1:A:360:ALA:HB1	1:A:364:PHE:HE2	1.47	0.76
1:C:222:GLY:HA2	1:C:457:LEU:HD21	1.68	0.76
1:C:502:VAL:HG23	1:C:503:THR:H	1.50	0.76
1:D:323:CYS:O	1:D:345:ALA:HA	1.85	0.76
1:D:223:VAL:HG13	1:D:377:LEU:HD21	1.68	0.76
1:A:372:ILE:HG22	1:A:377:LEU:HB2	1.67	0.76
1:A:145:LEU:O	1:A:149:THR:HG23	1.85	0.76
1:E:71:ARG:HB3	1:E:71:ARG:NH1	2.01	0.76
1:B:293:LYS:HA	1:B:293:LYS:HE2	1.66	0.76
1:D:432:ILE:HG13	1:D:432:ILE:O	1.85	0.76
1:E:434:ILE:O	1:E:436:PRO:HD3	1.86	0.76
1:E:172:ASP:O	1:E:174:SER:N	2.19	0.75
1:F:343:VAL:HG21	1:F:364:PHE:CE1	2.21	0.75
1:B:104:SER:O	1:B:107:GLU:N	2.19	0.75
1:D:331:SER:HB2	1:D:334:GLN:OE1	1.86	0.75
1:F:93:CYS:HB2	1:F:167:ASP:OD1	1.86	0.75
1:F:28:VAL:HG22	1:F:487:VAL:HG13	1.68	0.75
1:A:340:ALA:HB3	1:A:341:PRO:HD3	1.69	0.75
1:B:154:MET:SD	1:B:190:THR:HG21	2.26	0.75
1:B:34:GLU:HG3	1:B:35:ASP:OD2	1.86	0.75
1:E:486:TYR:O	1:E:490:ILE:HG12	1.84	0.75
1:B:365:LEU:HD23	1:B:366:GLU:N	2.00	0.75
1:C:157:ALA:HB1	1:C:191:ILE:HG21	1.68	0.75
1:C:61:HIS:CD2	1:C:88:GLN:HE22	2.05	0.75
1:A:348:ILE:HD11	1:A:364:PHE:CE1	2.22	0.75
1:E:83:ARG:HG2	1:E:161:PHE:HD1	1.52	0.75
1:A:325:ILE:HG22	1:A:347:ILE:CG2	2.17	0.75
1:C:190:THR:HG22	1:C:191:ILE:H	1.52	0.75
1:D:320:GLU:HG3	1:D:342:ARG:HG2	1.69	0.75
1:C:78:VAL:H	1:F:54:ARG:HH22	1.33	0.75
1:D:23:ARG:HG3	1:D:23:ARG:HH11	1.49	0.75
1:A:122:VAL:HG11	1:A:379:ALA:CB	2.16	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:THR:CB	1:F:92:PRO:HD3	2.17	0.75
1:D:252:VAL:HG23	1:D:323:CYS:SG	2.26	0.74
1:F:363:ILE:O	1:F:367:ARG:HG2	1.86	0.74
1:B:325:ILE:HG22	1:B:347:ILE:CG2	2.17	0.74
1:D:29:GLU:O	1:D:33:VAL:HG23	1.86	0.74
1:D:501:GLY:N	1:D:505:THR:HA	2.02	0.74
1:E:501:GLY:N	1:E:505:THR:HA	2.02	0.74
1:B:505:THR:OXT	1:F:150:ARG:NH2	2.18	0.74
1:C:264:MET:HE1	1:C:292:PRO:HA	1.69	0.74
1:D:251:PHE:CB	1:D:325:ILE:HG12	2.18	0.74
1:A:363:ILE:HG23	1:A:367:ARG:HD3	1.69	0.74
1:D:252:VAL:HG22	1:D:275:ILE:HG23	1.70	0.74
1:D:350:GLU:CD	1:D:482:ARG:HH22	1.90	0.74
1:B:502:VAL:N	1:B:505:THR:HB	2.02	0.74
1:C:69:ILE:HA	1:C:151:ARG:NH1	2.03	0.74
1:E:86:HIS:HD2	1:E:116:THR:HG21	1.53	0.74
1:A:57:LYS:HB3	1:A:58:PRO:CD	2.18	0.73
1:B:52:ILE:HD12	1:B:497:TYR:HB3	1.70	0.73
1:E:96:GLY:O	1:E:130:LYS:HD2	1.89	0.73
1:F:13:PHE:CZ	1:F:107:GLU:HA	2.22	0.73
1:F:284:ILE:HG23	1:F:311:ALA:HB1	1.70	0.73
1:F:34:GLU:HA	1:F:38:THR:HB	1.69	0.73
1:A:336:THR:HG22	1:A:357:THR:HG21	1.70	0.73
1:F:501:GLY:N	1:F:505:THR:HA	2.03	0.73
1:E:190:THR:CG2	1:E:191:ILE:N	2.48	0.73
1:D:275:ILE:HG23	1:D:276:ALA:H	1.53	0.73
1:E:418:GLN:CB	1:E:433:PRO:HD2	2.18	0.73
1:B:483:THR:O	1:B:487:VAL:HG23	1.88	0.73
1:F:154:MET:SD	1:F:190:THR:HG21	2.28	0.73
1:A:13:PHE:HD1	1:A:14:PHE:N	1.86	0.73
1:C:38:THR:HG23	1:C:41:SER:HB3	1.69	0.73
1:C:436:PRO:HB3	1:C:440:PHE:HD1	1.53	0.73
1:E:37:ARG:HB2	1:E:37:ARG:HH11	1.53	0.73
1:E:480:ASP:OD1	1:E:483:THR:HG22	1.89	0.73
1:B:259:VAL:O	1:B:263:SER:HB2	1.88	0.73
1:C:79:ILE:HD12	1:C:135:ILE:HD11	1.70	0.73
1:D:264:MET:CE	1:D:292:PRO:HA	2.19	0.73
1:E:116:THR:CG2	1:E:128:GLY:H	1.89	0.73
1:F:135:ILE:HD11	1:F:140:TYR:CZ	2.24	0.73
1:F:223:VAL:HG11	1:F:263:SER:OG	1.88	0.73
1:C:378:ASN:HD22	1:C:378:ASN:C	1.93	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:ALA:O	1:D:364:PHE:CD2	2.42	0.72
1:E:335:LEU:HB2	1:E:356:THR:HG22	1.71	0.72
1:F:243:THR:N	1:F:244:PRO:CD	2.50	0.72
1:C:502:VAL:HG11	1:F:76:TRP:HE1	1.53	0.72
1:A:10:ASP:HB2	1:A:333:LYS:CE	2.15	0.72
1:A:348:ILE:HB	1:A:371:VAL:HG22	1.71	0.72
1:A:386:TYR:OH	1:B:396:VAL:HG13	1.89	0.72
1:E:23:ARG:HG3	1:E:23:ARG:HH11	1.52	0.72
1:F:251:PHE:HB3	1:F:325:ILE:CG1	2.16	0.72
1:B:86:HIS:HD2	1:B:116:THR:HG21	1.53	0.72
1:C:71:ARG:CB	1:C:71:ARG:HH11	1.99	0.72
1:F:307:GLY:O	1:F:309:PRO:HD3	1.90	0.72
1:D:94:LYS:HB2	1:D:126:PHE:CD1	2.25	0.72
1:E:154:MET:SD	1:E:190:THR:HG21	2.28	0.72
1:E:339:ASN:H	1:E:339:ASN:HD22	1.35	0.72
1:F:432:ILE:HD13	1:F:432:ILE:N	2.05	0.72
1:A:150:ARG:NH1	1:F:505:THR:OXT	2.23	0.72
1:B:319:LEU:HD12	1:B:319:LEU:N	2.03	0.72
1:F:334:GLN:NE2	1:F:334:GLN:HA	1.99	0.72
1:A:333:LYS:HA	1:A:355:PRO:O	1.89	0.72
1:F:501:GLY:CA	1:F:505:THR:HA	2.20	0.72
1:F:57:LYS:O	1:F:86:HIS:HE1	1.72	0.72
1:A:254:GLN:HB2	1:A:318:ILE:HD11	1.72	0.72
1:C:501:GLY:CA	1:C:505:THR:HA	2.20	0.72
1:D:99:TYR:HH	1:D:149:THR:HG22	1.55	0.72
1:B:309:PRO:O	1:B:310:LYS:HB2	1.90	0.72
1:D:304:SER:HB3	1:D:306:LEU:HD13	1.72	0.72
1:A:69:ILE:HG12	1:A:79:ILE:HD11	1.72	0.71
1:A:427:LYS:HG3	1:A:428:HIS:H	1.54	0.71
1:B:339:ASN:H	1:B:339:ASN:ND2	1.88	0.71
1:B:416:SER:O	1:B:420:SER:HB2	1.90	0.71
1:B:480:ASP:OD1	1:B:483:THR:HG23	1.91	0.71
1:F:243:THR:H	1:F:244:PRO:HD3	1.54	0.71
1:A:319:LEU:N	1:A:319:LEU:HD12	2.06	0.71
1:A:359:GLU:HA	1:A:362:LYS:HD3	1.72	0.71
1:B:151:ARG:HD3	1:D:503:THR:HG21	1.70	0.71
1:E:339:ASN:ND2	1:E:339:ASN:H	1.89	0.71
1:E:13:PHE:HD1	1:E:14:PHE:N	1.88	0.71
1:C:76:TRP:NE1	1:F:502:VAL:HG11	2.06	0.71
1:B:221:ARG:HG2	1:B:225:HIS:HE1	1.56	0.71
1:B:319:LEU:CD1	1:B:319:LEU:H	2.04	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ASP:O	1:C:174:SER:N	2.23	0.71
1:A:378:ASN:HD22	1:A:378:ASN:H	1.38	0.71
1:A:501:GLY:N	1:A:505:THR:HA	2.06	0.70
1:C:168:VAL:HG13	1:C:202:VAL:HA	1.72	0.70
1:C:436:PRO:HA	1:D:416:SER:HB3	1.73	0.70
1:C:501:GLY:N	1:C:505:THR:HA	2.06	0.70
1:C:404:LYS:NZ	1:C:407:ARG:HH21	1.90	0.70
1:D:158:LYS:HD3	1:F:193:HIS:CE1	2.26	0.70
1:A:150:ARG:NH2	1:F:505:THR:OXT	2.23	0.70
1:A:72:ASP:OD1	1:A:144:GLU:HG3	1.91	0.70
1:B:143:ASN:HD21	1:E:70:ARG:HH12	1.37	0.70
1:A:154:MET:SD	1:A:190:THR:HG21	2.32	0.70
1:D:275:ILE:HG23	1:D:276:ALA:N	2.06	0.70
1:D:372:ILE:HG22	1:D:377:LEU:HB2	1.73	0.70
1:D:205:LYS:HZ1	1:D:392:ASN:HD21	1.38	0.70
1:E:398:TYR:HB2	1:E:449:GLU:HG3	1.73	0.70
1:C:77:GLU:HA	1:F:54:ARG:HH22	1.55	0.70
1:A:279:GLU:HG3	1:A:305:ILE:HG12	1.73	0.70
1:B:248:ASP:OD2	1:B:249:LYS:HG3	1.90	0.70
1:B:378:ASN:H	1:B:378:ASN:HD22	1.38	0.70
1:C:393:LEU:O	1:C:395:HIS:HD2	1.74	0.70
1:F:144:GLU:O	1:F:148:ILE:HG13	1.91	0.70
1:B:104:SER:O	1:B:106:ASP:N	2.24	0.70
1:C:502:VAL:N	1:C:505:THR:HB	2.06	0.70
1:F:176:GLY:O	1:F:180:MET:HG2	1.90	0.70
1:C:243:THR:N	1:C:244:PRO:CD	2.54	0.70
1:E:13:PHE:HD1	1:E:14:PHE:H	1.38	0.70
1:C:205:LYS:HD2	1:C:209:GLN:O	1.91	0.70
1:D:325:ILE:N	1:D:325:ILE:HD13	2.05	0.70
1:D:94:LYS:HD3	1:D:126:PHE:CE1	2.27	0.70
1:E:59:CYS:SG	1:E:109:LYS:O	2.50	0.70
1:E:428:HIS:CD2	1:E:428:HIS:N	2.60	0.70
1:A:374:ASP:O	1:A:378:ASN:ND2	2.25	0.69
1:B:93:CYS:HB2	1:B:167:ASP:OD1	1.91	0.69
1:D:325:ILE:CG2	1:D:347:ILE:HB	2.20	0.69
1:F:256:PHE:CE2	1:F:295:LEU:HG	2.26	0.69
1:B:51:GLY:HA2	1:B:54:ARG:HG3	1.72	0.69
1:E:61:HIS:CD2	1:E:88:GLN:HE22	2.10	0.69
1:A:427:LYS:HG3	1:A:428:HIS:N	2.06	0.69
1:D:243:THR:H	1:D:244:PRO:HD3	1.55	0.69
1:F:13:PHE:CD1	1:F:14:PHE:N	2.58	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:ILE:HG22	1:F:285:TRP:N	2.08	0.69
1:A:343:VAL:HG21	1:A:364:PHE:HE1	1.58	0.69
1:B:116:THR:CG2	1:B:128:GLY:H	2.04	0.69
1:B:440:PHE:HE2	1:B:444:ILE:HD11	1.57	0.69
1:D:34:GLU:HA	1:D:38:THR:CB	2.23	0.69
1:D:190:THR:HG22	1:D:191:ILE:N	2.08	0.69
1:E:221:ARG:HE	1:E:454:HIS:CE1	2.10	0.69
1:F:68:PRO:O	1:F:151:ARG:NH1	2.25	0.69
1:B:335:LEU:CD1	1:B:348:ILE:HD13	2.23	0.69
1:F:242:MET:HE2	1:F:242:MET:HA	1.73	0.69
1:C:12:ASN:ND2	1:C:14:PHE:HB3	2.08	0.69
1:C:136:ASN:OD1	1:C:138:LYS:HB2	1.92	0.69
1:E:122:VAL:HG23	1:E:124:VAL:HG23	1.73	0.69
1:F:38:THR:O	1:F:38:THR:HG22	1.93	0.69
1:A:240:LEU:HA	1:A:346:LYS:NZ	2.08	0.69
1:A:304:SER:OG	1:A:305:ILE:N	2.25	0.69
1:A:251:PHE:CB	1:A:325:ILE:HG13	2.17	0.69
1:C:28:VAL:HG13	1:C:32:LEU:HD22	1.75	0.69
1:D:418:GLN:HB2	1:D:433:PRO:HD2	1.73	0.69
1:F:400:ARG:O	1:F:400:ARG:HD2	1.92	0.69
1:A:57:LYS:HB3	1:A:58:PRO:HD3	1.74	0.69
1:A:64:SER:HB2	1:E:62:VAL:CG1	2.23	0.69
1:D:61:HIS:HD2	1:D:88:GLN:HE22	1.37	0.69
1:E:252:VAL:HG22	1:E:275:ILE:HG22	1.73	0.69
1:A:418:GLN:HB2	1:A:433:PRO:HD2	1.74	0.68
1:B:264:MET:HG2	1:B:292:PRO:HG3	1.75	0.68
1:D:281:ASP:HB2	1:D:306:LEU:HD11	1.75	0.68
1:A:76:TRP:HZ3	1:E:49:VAL:HG23	1.58	0.68
1:A:281:ASP:CB	1:A:306:LEU:HD21	2.23	0.68
1:B:62:VAL:HG11	1:B:109:LYS:NZ	2.07	0.68
1:C:243:THR:HG23	1:C:243:THR:O	1.93	0.68
1:C:501:GLY:HA3	1:C:504:PHE:O	1.92	0.68
1:E:367:ARG:HH11	1:E:367:ARG:HB3	1.56	0.68
1:A:243:THR:N	1:A:244:PRO:CD	2.56	0.68
1:D:325:ILE:HD13	1:D:325:ILE:H	1.59	0.68
1:E:362:LYS:O	1:E:366:GLU:HG3	1.93	0.68
1:C:460:THR:HG23	1:D:400:ARG:HH21	1.58	0.68
1:D:264:MET:HE3	1:D:292:PRO:HA	1.75	0.68
1:E:336:THR:N	1:E:339:ASN:HD21	1.89	0.68
1:F:335:LEU:HB2	1:F:356:THR:HG22	1.76	0.68
1:C:116:THR:HG22	1:C:128:GLY:CA	2.22	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:SER:O	1:D:267:LEU:HD23	1.94	0.68
1:F:348:ILE:HB	1:F:371:VAL:HG22	1.75	0.68
1:A:133:VAL:O	1:A:135:ILE:N	2.26	0.68
1:D:242:MET:HA	1:D:244:PRO:HG3	1.76	0.68
1:E:34:GLU:HA	1:E:38:THR:CB	2.22	0.68
1:A:337:LYS:HE3	1:A:359:GLU:HG3	1.75	0.68
1:C:436:PRO:HB3	1:C:440:PHE:CD1	2.28	0.68
1:E:153:THR:OG1	1:E:183:ILE:HG23	1.93	0.68
1:E:281:ASP:HB2	1:E:306:LEU:HD11	1.75	0.68
1:A:427:LYS:HG2	1:A:430:GLY:HA3	1.76	0.68
1:B:10:ASP:OD2	1:B:10:ASP:O	2.12	0.68
1:D:350:GLU:CD	1:D:482:ARG:NH2	2.48	0.68
1:F:317:SER:HB2	1:F:319:LEU:HD13	1.75	0.68
1:B:23:ARG:HE	1:B:483:THR:HG21	1.59	0.67
1:C:29:GLU:O	1:C:33:VAL:HG23	1.94	0.67
1:D:37:ARG:C	1:D:37:ARG:HD3	2.13	0.67
1:B:500:ALA:C	1:B:505:THR:HA	2.14	0.67
1:D:332:GLU:HG2	1:D:333:LYS:HG2	1.74	0.67
1:A:221:ARG:O	1:A:224:PHE:HB3	1.95	0.67
1:B:205:LYS:HZ2	1:B:392:ASN:ND2	1.93	0.67
1:C:319:LEU:HD23	1:C:335:LEU:HD23	1.76	0.67
1:D:28:VAL:HG22	1:D:487:VAL:HG13	1.75	0.67
1:F:314:TYR:HE2	1:F:318:ILE:HA	1.59	0.67
1:F:427:LYS:HG2	1:F:430:GLY:HA3	1.77	0.67
1:A:237:MET:HE2	1:A:240:LEU:CD1	2.24	0.67
1:B:427:LYS:HG3	1:B:428:HIS:H	1.58	0.67
1:D:91:THR:HB	1:D:92:PRO:CD	2.24	0.67
1:F:285:TRP:HB2	1:F:314:TYR:HB2	1.76	0.67
1:A:14:PHE:O	1:A:18:GLU:HB2	1.94	0.67
1:A:332:GLU:HG2	1:A:333:LYS:HG2	1.74	0.67
1:A:240:LEU:HA	1:A:346:LYS:HZ2	1.59	0.67
1:B:122:VAL:HB	1:B:460:THR:HG21	1.75	0.67
1:B:319:LEU:HD12	1:B:319:LEU:H	1.59	0.67
1:B:103:VAL:HA	1:B:107:GLU:OE2	1.94	0.67
1:B:190:THR:CG2	1:B:191:ILE:N	2.54	0.67
1:B:501:GLY:N	1:B:505:THR:HA	2.09	0.67
1:E:37:ARG:HB2	1:E:37:ARG:CZ	2.24	0.67
1:B:332:GLU:HG2	1:B:333:LYS:HG2	1.77	0.67
1:E:34:GLU:CA	1:E:38:THR:HB	2.22	0.67
1:F:427:LYS:NZ	1:F:430:GLY:HA2	2.10	0.67
1:F:436:PRO:HB3	1:F:440:PHE:CD1	2.29	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:HIS:CD2	1:F:116:THR:CG2	2.76	0.67
1:E:243:THR:HG23	1:E:243:THR:O	1.95	0.67
1:F:180:MET:HE3	1:F:202:VAL:CG2	2.25	0.67
1:F:436:PRO:HB3	1:F:440:PHE:HD1	1.60	0.67
1:F:91:THR:HB	1:F:92:PRO:CD	2.24	0.67
1:B:146:GLU:HA	1:B:182:TRP:CE3	2.30	0.67
1:C:34:GLU:HA	1:C:38:THR:CB	2.24	0.67
1:D:252:VAL:HG13	1:D:276:ALA:HB3	1.76	0.67
1:D:501:GLY:CA	1:D:505:THR:HA	2.25	0.67
1:A:436:PRO:HB3	1:A:440:PHE:HD1	1.60	0.66
1:A:464:SER:O	1:A:468:ILE:HG12	1.95	0.66
1:B:13:PHE:HD1	1:B:14:PHE:N	1.92	0.66
1:B:251:PHE:CB	1:B:325:ILE:HG13	2.25	0.66
1:B:372:ILE:HG21	1:B:377:LEU:HD13	1.77	0.66
1:D:433:PRO:O	1:D:435:VAL:N	2.28	0.66
1:F:319:LEU:HD23	1:F:335:LEU:HD23	1.77	0.66
1:F:500:ALA:C	1:F:505:THR:HA	2.15	0.66
1:D:59:CYS:SG	1:D:109:LYS:O	2.45	0.66
1:D:327:ILE:CG2	1:D:349:ALA:HB3	2.26	0.66
1:E:33:VAL:O	1:E:34:GLU:O	2.14	0.66
1:F:172:ASP:O	1:F:174:SER:N	2.28	0.66
1:A:76:TRP:HE1	1:E:502:VAL:HG11	1.60	0.66
1:B:243:THR:O	1:B:243:THR:HG23	1.94	0.66
1:D:190:THR:HG23	1:F:190:THR:HG23	1.76	0.66
1:B:221:ARG:HG2	1:B:225:HIS:CE1	2.29	0.66
1:B:95:GLY:O	1:B:169:PRO:HA	1.95	0.66
1:B:169:PRO:HB2	1:B:202:VAL:HG23	1.75	0.66
1:C:374:ASP:OD2	1:C:375:LEU:N	2.28	0.66
1:B:38:THR:HG23	1:B:41:SER:HB3	1.76	0.66
1:A:243:THR:HG23	1:A:243:THR:O	1.95	0.66
1:A:69:ILE:HG12	1:A:79:ILE:CD1	2.26	0.66
1:C:279:GLU:HG3	1:C:305:ILE:HG12	1.77	0.66
1:E:501:GLY:CA	1:E:505:THR:HA	2.25	0.66
1:F:223:VAL:HG22	1:F:377:LEU:HG	1.77	0.66
1:F:326:LEU:HD12	1:F:348:ILE:HD12	1.76	0.66
1:B:374:ASP:O	1:B:378:ASN:ND2	2.29	0.66
1:D:360:ALA:O	1:D:364:PHE:HD2	1.78	0.66
1:D:502:VAL:N	1:D:505:THR:HB	2.11	0.66
1:A:367:ARG:O	1:A:369:ILE:HG12	1.95	0.66
1:A:78:VAL:HG23	1:A:78:VAL:O	1.95	0.66
1:D:100:SER:O	1:D:103:VAL:HG13	1.95	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG23	1:D:134:LYS:HE2	1.76	0.66
1:E:462:GLU:O	1:E:463:ALA:C	2.31	0.66
1:A:97:ILE:HD13	1:A:131:ALA:HB3	1.78	0.65
1:C:221:ARG:HH11	1:C:221:ARG:CG	2.08	0.65
1:C:50:ARG:HD2	1:C:50:ARG:O	1.96	0.65
1:D:345:ALA:O	1:D:369:ILE:HD12	1.96	0.65
1:D:418:GLN:OE1	1:D:434:ILE:HG12	1.97	0.65
1:E:206:PRO:HD2	1:E:209:GLN:CB	2.25	0.65
1:C:154:MET:SD	1:C:190:THR:HG21	2.36	0.65
1:A:125:PRO:O	1:A:126:PHE:CD2	2.49	0.65
1:C:327:ILE:HD13	1:C:327:ILE:H	1.61	0.65
1:E:264:MET:HE3	1:E:292:PRO:HA	1.77	0.65
1:E:33:VAL:O	1:E:37:ARG:HG3	1.97	0.65
1:F:259:VAL:O	1:F:263:SER:HB2	1.97	0.65
1:F:475:TYR:O	1:F:477:LEU:HD23	1.96	0.65
1:A:146:GLU:HG2	1:A:150:ARG:HD2	1.76	0.65
1:B:59:CYS:SG	1:B:109:LYS:O	2.45	0.65
1:B:145:LEU:O	1:B:149:THR:HG23	1.97	0.65
1:E:116:THR:HG22	1:E:128:GLY:CA	2.26	0.65
1:A:64:SER:HB2	1:E:62:VAL:HG12	1.77	0.65
1:A:47:ASN:HD21	1:A:50:ARG:CZ	2.09	0.65
1:F:239:ILE:HG22	1:F:239:ILE:O	1.97	0.65
1:F:285:TRP:HB2	1:F:314:TYR:CB	2.27	0.65
1:C:202:VAL:O	1:C:205:LYS:NZ	2.29	0.65
1:D:390:LEU:HD13	1:E:396:VAL:HG21	1.78	0.65
1:F:327:ILE:CG2	1:F:349:ALA:HB3	2.21	0.65
1:F:376:TYR:OH	1:F:465:ALA:HB2	1.96	0.65
1:A:17:VAL:CG2	1:A:114:LEU:HD13	2.27	0.65
1:C:350:GLU:CD	1:C:482:ARG:HH22	1.99	0.65
1:F:63:LEU:HD22	1:F:161:PHE:CE2	2.32	0.65
1:D:362:LYS:O	1:D:366:GLU:HG3	1.97	0.65
1:F:261:LEU:O	1:F:261:LEU:HD12	1.97	0.65
1:F:217:SER:HA	1:F:262:HIS:CD2	2.31	0.65
1:B:231:ILE:HD13	1:B:237:MET:SD	2.36	0.65
1:E:67:PHE:CE1	1:E:79:ILE:HB	2.32	0.65
1:F:177:GLU:HB2	1:F:206:PRO:HG3	1.77	0.65
1:A:179:GLU:HA	1:A:182:TRP:CE3	2.31	0.65
1:A:79:ILE:HD12	1:A:79:ILE:N	2.11	0.65
1:B:332:GLU:O	1:B:334:GLN:NE2	2.30	0.65
1:C:404:LYS:HZ3	1:C:407:ARG:HH21	1.45	0.65
1:E:55:ILE:O	1:E:58:PRO:HD2	1.98	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:GLY:CA	1:B:505:THR:HA	2.27	0.64
1:C:390:LEU:O	1:C:393:LEU:N	2.29	0.64
1:C:43:GLU:HB3	1:C:45:LYS:HG3	1.78	0.64
1:F:362:LYS:O	1:F:366:GLU:HG3	1.97	0.64
1:F:49:VAL:O	1:F:52:ILE:HG12	1.96	0.64
1:A:317:SER:HB2	1:A:319:LEU:HD13	1.79	0.64
1:A:500:ALA:CA	1:A:505:THR:O	2.45	0.64
1:C:251:PHE:HB3	1:C:325:ILE:HG13	1.79	0.64
1:E:325:ILE:HG23	1:E:347:ILE:CG2	2.27	0.64
1:E:502:VAL:N	1:E:505:THR:HB	2.13	0.64
1:A:146:GLU:HG2	1:A:150:ARG:HH11	1.60	0.64
1:B:418:GLN:CB	1:B:433:PRO:HD2	2.23	0.64
1:B:93:CYS:CB	1:B:167:ASP:OD1	2.45	0.64
1:D:404:LYS:CE	1:D:407:ARG:HH21	2.10	0.64
1:A:502:VAL:HG23	1:A:503:THR:N	2.13	0.64
1:C:92:PRO:HG2	1:C:389:TRP:CZ2	2.32	0.64
1:D:256:PHE:HE2	1:D:264:MET:HE2	1.62	0.64
1:D:320:GLU:O	1:D:321:ALA:O	2.14	0.64
1:E:435:VAL:O	1:E:435:VAL:HG13	1.98	0.64
1:A:292:PRO:O	1:A:296:GLU:HB2	1.98	0.64
1:B:256:PHE:HE2	1:B:264:MET:HE2	1.61	0.64
1:F:418:GLN:CB	1:F:433:PRO:HD2	2.28	0.64
1:A:343:VAL:HG21	1:A:364:PHE:CE1	2.32	0.64
1:B:28:VAL:HG23	1:B:487:VAL:HG13	1.80	0.64
1:B:264:MET:CE	1:B:292:PRO:HA	2.28	0.64
1:B:205:LYS:HZ1	1:B:392:ASN:HD21	1.44	0.64
1:C:97:ILE:HD12	1:C:131:ALA:HB3	1.78	0.64
1:D:227:ILE:HD13	1:D:372:ILE:HD12	1.80	0.64
1:D:350:GLU:OE1	1:D:482:ARG:NH2	2.31	0.64
1:E:349:ALA:HB1	1:E:377:LEU:HD21	1.79	0.64
1:F:170:ALA:HA	1:F:180:MET:HE2	1.78	0.64
1:A:249:LYS:HD2	1:A:271:GLY:O	1.98	0.64
1:A:327:ILE:HG23	1:A:349:ALA:HB3	1.77	0.64
1:C:285:TRP:CB	1:C:314:TYR:HB2	2.27	0.64
1:C:76:TRP:HE1	1:F:502:VAL:CG1	2.09	0.64
1:F:205:LYS:NZ	1:F:392:ASN:HD21	1.95	0.64
1:A:133:VAL:O	1:A:135:ILE:HB	1.97	0.64
1:A:259:VAL:HG13	1:A:260:GLY:N	2.13	0.64
1:B:150:ARG:O	1:B:153:THR:N	2.30	0.64
1:D:243:THR:N	1:D:244:PRO:CD	2.54	0.64
1:F:205:LYS:HZ1	1:F:392:ASN:ND2	1.96	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ARG:CD	1:F:503:THR:HG21	2.27	0.64
1:A:205:LYS:NZ	1:A:392:ASN:HD21	1.96	0.64
1:B:77:GLU:HA	1:D:54:ARG:NH1	2.12	0.64
1:C:79:ILE:HD12	1:C:135:ILE:CD1	2.28	0.64
1:C:330:ALA:O	1:C:331:SER:O	2.15	0.64
1:C:474:LYS:HD3	1:C:475:TYR:CE2	2.33	0.64
1:E:343:VAL:HG21	1:E:364:PHE:CE1	2.32	0.64
1:F:253:VAL:HA	1:F:327:ILE:HG13	1.80	0.64
1:A:240:LEU:HB3	1:A:346:LYS:HD2	1.79	0.64
1:A:427:LYS:NZ	1:A:428:HIS:H	1.96	0.64
1:B:61:HIS:ND1	1:D:159:LYS:HE3	2.13	0.64
1:F:108:VAL:HG23	1:F:109:LYS:N	2.13	0.64
1:C:229:ASN:HD21	1:C:462:GLU:HA	1.59	0.63
1:C:362:LYS:O	1:C:366:GLU:HG3	1.98	0.63
1:D:343:VAL:HG21	1:D:364:PHE:HE1	1.62	0.63
1:D:502:VAL:HG23	1:D:503:THR:N	2.11	0.63
1:C:427:LYS:HG2	1:C:430:GLY:HA3	1.80	0.63
1:C:95:GLY:O	1:C:169:PRO:HA	1.97	0.63
1:F:501:GLY:HA3	1:F:505:THR:HA	1.80	0.63
1:D:242:MET:O	1:D:243:THR:HG22	1.98	0.63
1:F:243:THR:O	1:F:243:THR:HG23	1.97	0.63
1:D:411:TYR:O	1:D:415:MET:HB2	1.98	0.63
1:E:376:TYR:OH	1:E:465:ALA:HB2	1.98	0.63
1:A:205:LYS:NZ	1:A:392:ASN:ND2	2.46	0.63
1:A:295:LEU:HD11	1:A:305:ILE:HB	1.81	0.63
1:B:145:LEU:HA	1:B:148:ILE:HD12	1.80	0.63
1:B:204:GLY:HA2	1:B:215:ARG:HD2	1.79	0.63
1:B:295:LEU:HD11	1:B:305:ILE:HG22	1.79	0.63
1:B:393:LEU:O	1:B:395:HIS:CD2	2.51	0.63
1:D:500:ALA:C	1:D:505:THR:HA	2.19	0.63
1:A:205:LYS:HZ1	1:A:392:ASN:ND2	1.97	0.63
1:C:61:HIS:CD2	1:C:88:GLN:NE2	2.66	0.63
1:D:224:PHE:CD2	1:D:266:TYR:HB3	2.33	0.63
1:D:337:LYS:HG2	1:D:337:LYS:O	1.97	0.63
1:E:221:ARG:NE	1:E:454:HIS:CE1	2.67	0.63
1:A:285:TRP:O	1:A:286:ASN:HB2	1.98	0.63
1:A:394:ASN:O	1:A:396:VAL:HG23	1.98	0.63
1:B:427:LYS:HG2	1:B:430:GLY:HA3	1.79	0.63
1:C:284:ILE:HG13	1:C:311:ALA:CB	2.24	0.63
1:C:340:ALA:HB3	1:C:341:PRO:HD3	1.79	0.63
1:E:440:PHE:O	1:E:444:ILE:HG13	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:LYS:HD2	1:F:271:GLY:O	1.98	0.63
1:A:461:MET:HA	1:A:461:MET:HE3	1.81	0.63
1:A:47:ASN:ND2	1:A:50:ARG:CZ	2.61	0.63
1:C:393:LEU:O	1:C:395:HIS:CD2	2.52	0.63
1:F:483:THR:O	1:F:487:VAL:HG23	1.99	0.63
1:A:172:ASP:O	1:A:174:SER:N	2.32	0.63
1:D:284:ILE:HG23	1:D:311:ALA:CB	2.25	0.63
1:E:73:ASP:OD1	1:E:73:ASP:O	2.17	0.63
1:F:285:TRP:NE1	1:F:287:PRO:HD3	2.13	0.63
1:B:391:LYS:HD2	1:B:449:GLU:OE2	1.98	0.62
1:B:477:LEU:HD12	1:B:484:ALA:HB2	1.81	0.62
1:C:223:VAL:HA	1:C:377:LEU:CD1	2.29	0.62
1:D:133:VAL:HG12	1:D:133:VAL:O	1.99	0.62
1:F:90:ARG:HG3	1:F:125:PRO:C	2.20	0.62
1:A:259:VAL:HG13	1:A:260:GLY:H	1.65	0.62
1:F:51:GLY:HA2	1:F:54:ARG:HG2	1.81	0.62
1:B:146:GLU:HA	1:B:182:TRP:CZ3	2.33	0.62
1:C:223:VAL:HA	1:C:377:LEU:HD11	1.82	0.62
1:C:418:GLN:OE1	1:C:433:PRO:HD2	1.99	0.62
1:D:95:GLY:O	1:D:169:PRO:HA	2.00	0.62
1:E:336:THR:HA	1:E:357:THR:HG23	1.81	0.62
1:F:168:VAL:HG13	1:F:201:CYS:O	1.99	0.62
1:F:242:MET:O	1:F:243:THR:HG22	2.00	0.62
1:F:274:CYS:O	1:F:290:ILE:HD12	2.00	0.62
1:A:314:TYR:HE2	1:A:318:ILE:HA	1.65	0.62
1:B:243:THR:N	1:B:244:PRO:CD	2.63	0.62
1:B:284:ILE:HG23	1:B:311:ALA:HB1	1.81	0.62
1:C:221:ARG:HD2	1:C:225:HIS:CE1	2.35	0.62
1:C:264:MET:HE3	1:C:292:PRO:HG3	1.82	0.62
1:D:370:MET:HG3	1:D:479:LEU:HB3	1.81	0.62
1:D:480:ASP:OD2	1:D:483:THR:HG23	2.00	0.62
1:B:90:ARG:HB3	1:B:125:PRO:O	1.99	0.62
1:D:281:ASP:HB3	1:D:306:LEU:HD21	1.80	0.62
1:E:73:ASP:O	1:E:75:SER:N	2.33	0.62
1:F:242:MET:HA	1:F:244:PRO:HG3	1.82	0.62
1:A:224:PHE:CD1	1:A:225:HIS:N	2.68	0.62
1:A:325:ILE:HG22	1:A:347:ILE:HB	1.81	0.62
1:B:69:ILE:HG12	1:B:79:ILE:HD11	1.82	0.62
1:C:390:LEU:O	1:C:392:ASN:N	2.32	0.62
1:F:23:ARG:NE	1:F:27:ILE:HD11	2.12	0.62
1:F:350:GLU:HG2	1:F:355:PRO:CG	2.28	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:HD3	1:A:126:PHE:CE1	2.35	0.62
1:C:502:VAL:HG23	1:C:503:THR:N	2.14	0.62
1:D:63:LEU:HD22	1:D:161:PHE:CD2	2.35	0.62
1:D:21:PHE:CE2	1:D:57:LYS:HB2	2.34	0.62
1:E:256:PHE:HE2	1:E:264:MET:HE2	1.64	0.62
1:A:268:HIS:CD2	1:A:292:PRO:HD3	2.35	0.62
1:B:238:SER:O	1:B:241:GLY:N	2.31	0.62
1:C:57:LYS:HB3	1:C:58:PRO:HD3	1.80	0.62
1:D:86:HIS:CG	1:D:116:THR:HG21	2.35	0.62
1:D:116:THR:HG22	1:D:128:GLY:CA	2.29	0.62
1:F:431:THR:C	1:F:432:ILE:HD13	2.20	0.62
1:B:54:ARG:HB3	1:B:54:ARG:NH1	2.15	0.62
1:D:443:ARG:HG3	1:D:443:ARG:HH11	1.63	0.62
1:E:248:ASP:OD2	1:E:249:LYS:HG3	1.99	0.62
1:F:202:VAL:HG22	1:F:203:THR:N	2.15	0.62
1:A:443:ARG:HH21	1:B:409:SER:CB	2.12	0.62
1:F:435:VAL:O	1:F:435:VAL:HG13	2.00	0.62
1:D:34:GLU:CA	1:D:38:THR:HB	2.29	0.61
1:E:264:MET:CE	1:E:292:PRO:HA	2.29	0.61
1:E:400:ARG:HG3	1:E:400:ARG:NH1	2.14	0.61
1:C:421:LEU:HD11	1:E:421:LEU:CD2	2.28	0.61
1:B:34:GLU:CA	1:B:38:THR:HB	2.31	0.61
1:C:439:GLU:CD	1:C:439:GLU:H	2.03	0.61
1:D:239:ILE:O	1:D:239:ILE:HG22	1.99	0.61
1:D:34:GLU:O	1:D:38:THR:HB	2.00	0.61
1:D:205:LYS:NZ	1:D:392:ASN:HD21	1.98	0.61
1:D:52:ILE:O	1:D:56:ILE:HG13	1.99	0.61
1:F:23:ARG:O	1:F:27:ILE:HG13	2.00	0.61
1:A:501:GLY:CA	1:A:505:THR:HA	2.30	0.61
1:A:57:LYS:O	1:A:86:HIS:HE1	1.83	0.61
1:D:243:THR:O	1:D:243:THR:HG23	2.00	0.61
1:F:350:GLU:C	1:F:377:LEU:HD23	2.21	0.61
1:C:343:VAL:HG21	1:C:364:PHE:CE1	2.36	0.61
1:C:78:VAL:N	1:F:54:ARG:HH22	1.97	0.61
1:D:224:PHE:CD1	1:D:225:HIS:N	2.68	0.61
1:D:224:PHE:HD1	1:D:225:HIS:N	1.98	0.61
1:B:122:VAL:HB	1:B:460:THR:CG2	2.31	0.61
1:B:376:TYR:OH	1:B:465:ALA:HB2	2.00	0.61
1:F:330:ALA:O	1:F:331:SER:O	2.19	0.61
1:A:262:HIS:HA	1:A:265:ARG:HG3	1.83	0.61
1:A:284:ILE:CD1	1:A:305:ILE:HD12	2.29	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:MET:HA	1:C:244:PRO:HG3	1.81	0.61
1:C:37:ARG:NH2	1:C:49:VAL:HG11	2.00	0.61
1:E:21:PHE:CE2	1:E:57:LYS:HB2	2.36	0.61
1:F:180:MET:HE3	1:F:202:VAL:HG21	1.81	0.61
1:A:259:VAL:O	1:A:263:SER:HB2	2.00	0.61
1:A:91:THR:HB	1:A:92:PRO:CD	2.26	0.61
1:B:318:ILE:HD13	1:B:318:ILE:H	1.64	0.61
1:C:334:GLN:HE21	1:C:334:GLN:CA	2.12	0.61
1:D:336:THR:C	1:D:338:SER:H	2.03	0.61
1:E:65:LEU:HD12	1:E:152:PHE:CE1	2.36	0.61
1:F:71:ARG:HB3	1:F:71:ARG:NH1	2.16	0.61
1:A:372:ILE:CG2	1:A:377:LEU:HB2	2.31	0.61
1:B:285:TRP:HB2	1:B:314:TYR:HB2	1.83	0.61
1:B:31:LYS:HG3	1:B:475:TYR:HE1	1.66	0.61
1:C:337:LYS:HE3	1:C:359:GLU:CG	2.18	0.61
1:A:30:ASP:O	1:A:34:GLU:HG2	2.00	0.61
1:A:427:LYS:CG	1:A:430:GLY:H	2.14	0.61
1:B:179:GLU:O	1:B:183:ILE:HD13	2.00	0.61
1:A:70:ARG:HH12	1:C:143:ASN:ND2	1.99	0.61
1:C:505:THR:O	1:D:185:ASP:OD1	2.19	0.61
1:D:240:LEU:HD23	1:D:479:LEU:HD21	1.81	0.61
1:E:367:ARG:NH1	1:E:367:ARG:HB3	2.15	0.61
1:F:21:PHE:CE1	1:F:490:ILE:HD12	2.36	0.61
1:F:374:ASP:O	1:F:378:ASN:ND2	2.34	0.61
1:C:503:THR:HG21	1:F:151:ARG:CD	2.31	0.61
1:D:319:LEU:H	1:D:319:LEU:HD12	1.66	0.61
1:D:371:VAL:HG11	1:D:482:ARG:HH21	1.65	0.61
1:E:336:THR:H	1:E:339:ASN:ND2	1.95	0.61
1:A:323:CYS:O	1:A:345:ALA:HA	2.01	0.60
1:B:180:MET:HG2	1:B:203:THR:O	2.01	0.60
1:B:425:PHE:CD1	1:B:427:LYS:HB2	2.36	0.60
1:C:72:ASP:OD1	1:C:144:GLU:CG	2.49	0.60
1:C:325:ILE:HG22	1:C:347:ILE:CG2	2.31	0.60
1:D:54:ARG:O	1:D:58:PRO:HD2	2.01	0.60
1:F:268:HIS:CD2	1:F:292:PRO:HD3	2.36	0.60
1:A:248:ASP:OD2	1:A:249:LYS:HG3	2.02	0.60
1:C:505:THR:O	1:D:185:ASP:CG	2.40	0.60
1:C:50:ARG:C	1:C:50:ARG:HD2	2.22	0.60
1:D:421:LEU:CD2	1:E:421:LEU:HD11	2.31	0.60
1:E:168:VAL:HG13	1:E:201:CYS:O	2.02	0.60
1:D:12:ASN:HD21	1:D:14:PHE:HB3	1.66	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:ARG:NH1	1:D:443:ARG:HG3	2.17	0.60
1:E:243:THR:N	1:E:244:PRO:CD	2.64	0.60
1:E:375:LEU:HD23	1:E:485:ALA:HB1	1.83	0.60
1:F:285:TRP:CB	1:F:314:TYR:HB2	2.30	0.60
1:A:51:GLY:O	1:A:54:ARG:N	2.35	0.60
1:B:42:GLU:HB2	1:B:46:ARG:HH22	1.65	0.60
1:E:319:LEU:HD23	1:E:335:LEU:HD23	1.83	0.60
1:E:480:ASP:CG	1:E:483:THR:HG22	2.21	0.60
1:F:237:MET:HE1	1:F:240:LEU:HD12	1.83	0.60
1:F:502:VAL:HG23	1:F:503:THR:H	1.65	0.60
1:A:346:LYS:O	1:A:347:ILE:HG13	2.00	0.60
1:C:261:LEU:O	1:C:261:LEU:HD12	2.01	0.60
1:A:143:ASN:ND2	1:C:70:ARG:HH22	1.99	0.60
1:D:343:VAL:HG21	1:D:364:PHE:CE1	2.36	0.60
1:D:348:ILE:HB	1:D:371:VAL:CG2	2.22	0.60
1:D:193:HIS:CE1	1:F:158:LYS:HD3	2.36	0.60
1:A:384:VAL:O	1:A:387:PHE:HB2	2.02	0.60
1:B:343:VAL:HG21	1:B:364:PHE:CE1	2.25	0.60
1:C:151:ARG:HD3	1:F:503:THR:HG21	1.84	0.60
1:C:263:SER:O	1:C:267:LEU:HD23	2.01	0.60
1:C:72:ASP:OD1	1:C:144:GLU:HG3	2.02	0.60
1:D:327:ILE:HG22	1:D:349:ALA:HB3	1.83	0.60
1:B:147:LYS:HE3	1:D:504:PHE:CZ	2.37	0.60
1:F:279:GLU:HG3	1:F:305:ILE:HG12	1.83	0.60
1:A:375:LEU:HD22	1:A:486:TYR:CE2	2.36	0.60
1:E:348:ILE:HB	1:E:371:VAL:HG22	1.84	0.60
1:E:466:ARG:HG3	1:E:466:ARG:NH1	2.15	0.60
1:B:242:MET:O	1:B:243:THR:HG22	2.00	0.60
1:B:256:PHE:HE2	1:B:264:MET:CE	2.14	0.60
1:B:264:MET:HE3	1:B:292:PRO:HA	1.82	0.60
1:C:83:ARG:CD	1:C:131:ALA:HB2	2.28	0.60
1:C:362:LYS:HA	1:C:362:LYS:HE3	1.84	0.60
1:D:32:LEU:HD11	1:D:494:PHE:CE2	2.37	0.60
1:D:342:ARG:HH11	1:D:342:ARG:HB2	1.67	0.60
1:B:404:LYS:HZ3	1:B:407:ARG:HH21	1.50	0.60
1:D:133:VAL:O	1:D:135:ILE:N	2.34	0.60
1:F:56:ILE:HD13	1:F:493:VAL:CG1	2.32	0.60
1:A:473:MET:O	1:A:476:ASN:N	2.29	0.60
1:D:410:ASN:ND2	1:E:413:LEU:HD21	2.17	0.60
1:A:168:VAL:HG13	1:A:202:VAL:CA	2.31	0.59
1:A:411:TYR:O	1:A:415:MET:HB2	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:HB3	1:B:71:ARG:NH1	2.17	0.59
1:D:370:MET:HB2	1:D:479:LEU:HD23	1.84	0.59
1:A:337:LYS:HE3	1:A:359:GLU:CG	2.31	0.59
1:C:13:PHE:O	1:C:17:VAL:HG23	2.01	0.59
1:C:312:LYS:HG3	1:C:312:LYS:O	2.01	0.59
1:C:437:THR:HG23	1:D:416:SER:HA	1.83	0.59
1:C:465:ALA:O	1:C:469:MET:HG3	2.02	0.59
1:C:501:GLY:HA3	1:C:505:THR:HA	1.84	0.59
1:D:500:ALA:HB1	1:D:505:THR:OG1	2.03	0.59
1:A:72:ASP:CG	1:A:141:THR:HG21	2.23	0.59
1:A:285:TRP:CB	1:A:314:TYR:HB2	2.32	0.59
1:C:264:MET:CE	1:C:292:PRO:HA	2.32	0.59
1:C:350:GLU:OE2	1:C:356:THR:HG23	2.01	0.59
1:D:382:VAL:HG12	1:D:382:VAL:O	2.02	0.59
1:E:500:ALA:HB1	1:E:505:THR:C	2.23	0.59
1:A:483:THR:O	1:A:487:VAL:HG23	2.02	0.59
1:B:168:VAL:HG13	1:B:201:CYS:O	2.02	0.59
1:B:60:ASN:HB3	1:B:61:HIS:HD2	1.65	0.59
1:E:285:TRP:HB2	1:E:314:TYR:HB2	1.85	0.59
1:B:319:LEU:CD1	1:B:319:LEU:N	2.64	0.59
1:B:372:ILE:CG2	1:B:377:LEU:HD13	2.32	0.59
1:D:240:LEU:HD12	1:D:242:MET:HG3	1.84	0.59
1:D:312:LYS:HD2	1:D:313:PRO:HD2	1.84	0.59
1:E:339:ASN:N	1:E:339:ASN:HD22	1.94	0.59
1:A:343:VAL:HG22	1:A:367:ARG:NH2	2.17	0.59
1:A:378:ASN:N	1:A:378:ASN:HD22	1.95	0.59
1:B:249:LYS:HD2	1:B:271:GLY:O	2.02	0.59
1:B:252:VAL:HG23	1:B:323:CYS:SG	2.42	0.59
1:B:367:ARG:O	1:B:369:ILE:HG12	2.03	0.59
1:B:502:VAL:HG23	1:B:503:THR:N	2.17	0.59
1:C:278:GLY:HA3	1:C:318:ILE:HD13	1.85	0.59
1:C:421:LEU:HD11	1:E:421:LEU:HD21	1.83	0.59
1:C:61:HIS:HE1	1:F:155:GLU:HG3	1.68	0.59
1:D:136:ASN:O	1:D:138:LYS:N	2.36	0.59
1:D:238:SER:O	1:D:241:GLY:N	2.29	0.59
1:D:251:PHE:HB3	1:D:325:ILE:CG1	2.31	0.59
1:E:110:ALA:O	1:E:113:SER:HB3	2.03	0.59
1:F:238:SER:O	1:F:241:GLY:N	2.25	0.59
1:A:190:THR:HG22	1:A:191:ILE:H	1.65	0.59
1:B:14:PHE:O	1:B:18:GLU:HB2	2.02	0.59
1:C:98:ARG:NH2	1:C:107:GLU:OE1	2.36	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ASP:OD2	1:C:249:LYS:HG3	2.03	0.59
1:F:261:LEU:C	1:F:261:LEU:HD12	2.22	0.59
1:B:30:ASP:O	1:B:34:GLU:HG2	2.03	0.59
1:B:94:LYS:HB2	1:B:126:PHE:CD1	2.37	0.59
1:B:151:ARG:CD	1:D:503:THR:HG21	2.33	0.59
1:E:424:LYS:HB3	1:E:424:LYS:NZ	2.16	0.59
1:E:91:THR:CB	1:E:92:PRO:HD3	2.33	0.59
1:F:57:LYS:N	1:F:58:PRO:CD	2.66	0.59
1:D:169:PRO:HB2	1:D:202:VAL:HG23	1.85	0.59
1:E:129:ALA:O	1:E:130:LYS:HB2	2.03	0.59
1:F:14:PHE:O	1:F:18:GLU:HB2	2.03	0.59
1:F:205:LYS:NZ	1:F:392:ASN:ND2	2.50	0.59
1:B:94:LYS:NZ	1:B:203:THR:OG1	2.29	0.58
1:E:339:ASN:HD22	1:E:340:ALA:N	2.01	0.58
1:B:63:LEU:HG	1:B:65:LEU:HD23	1.85	0.58
1:D:337:LYS:HB3	1:D:337:LYS:HZ3	1.68	0.58
1:D:505:THR:O	1:E:185:ASP:OD1	2.21	0.58
1:D:339:ASN:H	1:D:339:ASN:HD22	1.50	0.58
1:E:103:VAL:HG23	1:E:103:VAL:O	2.03	0.58
1:E:151:ARG:O	1:E:154:MET:HB2	2.03	0.58
1:F:205:LYS:HZ3	1:F:392:ASN:HD21	1.52	0.58
1:A:378:ASN:ND2	1:A:378:ASN:H	1.99	0.58
1:A:40:GLU:HG3	1:A:46:ARG:NH1	2.18	0.58
1:A:32:LEU:HD21	1:A:494:PHE:CD1	2.37	0.58
1:A:500:ALA:HA	1:A:505:THR:O	2.03	0.58
1:E:336:THR:HG22	1:E:357:THR:HG21	1.84	0.58
1:F:217:SER:OG	1:F:454:HIS:NE2	2.25	0.58
1:F:23:ARG:HH11	1:F:23:ARG:HG3	1.67	0.58
1:D:16:MET:HE1	1:D:333:LYS:HE3	1.85	0.58
1:D:433:PRO:O	1:D:434:ILE:C	2.41	0.58
1:B:77:GLU:HA	1:D:54:ARG:HH12	1.68	0.58
1:E:72:ASP:CG	1:E:141:THR:HG21	2.23	0.58
1:F:384:VAL:O	1:F:387:PHE:N	2.37	0.58
1:B:430:GLY:O	1:B:432:ILE:HG13	2.03	0.58
1:E:284:ILE:CG2	1:E:311:ALA:HB1	2.25	0.58
1:B:505:THR:OXT	1:F:185:ASP:OD1	2.22	0.58
1:F:264:MET:CE	1:F:292:PRO:HA	2.34	0.58
1:F:72:ASP:OD1	1:F:144:GLU:HG2	2.03	0.58
1:A:418:GLN:HB2	1:A:433:PRO:CD	2.34	0.58
1:D:293:LYS:HA	1:D:293:LYS:HE2	1.84	0.58
1:D:284:ILE:HG13	1:D:305:ILE:HD12	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:SER:HA	1:D:46:ARG:NE	2.12	0.58
1:D:78:VAL:O	1:D:78:VAL:HG23	2.03	0.58
1:B:243:THR:H	1:B:244:PRO:HD3	1.69	0.58
1:B:261:LEU:HD12	1:B:261:LEU:C	2.24	0.58
1:B:414:LEU:HB3	1:B:434:ILE:HA	1.86	0.58
1:D:253:VAL:HA	1:D:327:ILE:HG12	1.84	0.58
1:E:23:ARG:HG3	1:E:23:ARG:NH1	2.19	0.58
1:E:349:ALA:HB1	1:E:377:LEU:CD2	2.34	0.58
1:A:293:LYS:HA	1:A:293:LYS:HE2	1.85	0.58
1:B:168:VAL:HG13	1:B:201:CYS:C	2.25	0.58
1:D:206:PRO:HD2	1:D:209:GLN:HB2	1.86	0.58
1:D:86:HIS:CD2	1:D:116:THR:CG2	2.74	0.58
1:E:168:VAL:HG13	1:E:201:CYS:C	2.24	0.58
1:E:213:HIS:HB2	1:E:449:GLU:HB3	1.86	0.58
1:F:99:TYR:OH	1:F:149:THR:HB	2.04	0.58
1:B:233:GLU:HG2	1:B:236:TYR:HD1	1.69	0.58
1:C:185:ASP:OD1	1:E:505:THR:CG2	2.47	0.58
1:C:438:ALA:O	1:C:439:GLU:C	2.43	0.58
1:C:179:GLU:OE2	1:C:179:GLU:N	2.33	0.57
1:C:477:LEU:HD12	1:C:484:ALA:HB2	1.85	0.57
1:E:384:VAL:O	1:E:387:PHE:HB2	2.03	0.57
1:F:238:SER:O	1:F:240:LEU:N	2.36	0.57
1:F:56:ILE:HD13	1:F:493:VAL:HG12	1.86	0.57
1:A:336:THR:HG22	1:A:357:THR:CG2	2.34	0.57
1:B:252:VAL:HG13	1:B:276:ALA:O	2.04	0.57
1:D:346:LYS:HA	1:D:369:ILE:HD13	1.86	0.57
1:D:375:LEU:HD23	1:D:485:ALA:HB1	1.84	0.57
1:E:86:HIS:ND1	1:E:113:SER:HA	2.19	0.57
1:A:90:ARG:NH1	1:A:496:VAL:HG21	2.19	0.57
1:A:70:ARG:HH12	1:C:143:ASN:HD21	1.52	0.57
1:C:367:ARG:O	1:C:369:ILE:HG12	2.04	0.57
1:D:319:LEU:HD12	1:D:319:LEU:N	2.19	0.57
1:E:500:ALA:C	1:E:505:THR:HA	2.25	0.57
1:F:238:SER:C	1:F:240:LEU:H	2.07	0.57
1:C:90:ARG:HG2	1:C:125:PRO:HA	1.86	0.57
1:D:227:ILE:HD13	1:D:372:ILE:CD1	2.34	0.57
1:E:339:ASN:HD22	1:E:340:ALA:H	1.53	0.57
1:A:13:PHE:CD1	1:A:14:PHE:N	2.67	0.57
1:A:376:TYR:C	1:A:376:TYR:CD1	2.78	0.57
1:A:449:GLU:O	1:A:453:VAL:HG23	2.04	0.57
1:B:23:ARG:HH11	1:B:23:ARG:HG3	1.70	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:LYS:O	1:B:337:LYS:HG2	2.04	0.57
1:B:336:THR:HG22	1:B:357:THR:CG2	2.35	0.57
1:C:212:ILE:HB	1:C:388:GLU:HG3	1.86	0.57
1:C:327:ILE:N	1:C:327:ILE:HD13	2.19	0.57
1:D:146:GLU:O	1:D:150:ARG:HG3	2.04	0.57
1:D:427:LYS:CD	1:D:430:GLY:HA3	2.28	0.57
1:D:77:GLU:HG2	1:D:79:ILE:HD13	1.86	0.57
1:F:156:LEU:HB3	1:F:162:ILE:HB	1.87	0.57
1:F:190:THR:HG22	1:F:191:ILE:N	2.19	0.57
1:F:336:THR:HG22	1:F:357:THR:CG2	2.34	0.57
1:B:321:ALA:O	1:B:344:LYS:HB2	2.04	0.57
1:E:108:VAL:HG23	1:E:109:LYS:H	1.69	0.57
1:F:462:GLU:O	1:F:464:SER:N	2.37	0.57
1:A:205:LYS:HZ3	1:A:392:ASN:HD21	1.50	0.57
1:B:350:GLU:OE2	1:B:356:THR:HG23	2.05	0.57
1:C:30:ASP:O	1:C:34:GLU:HG2	2.04	0.57
1:F:170:ALA:HA	1:F:180:MET:CE	2.34	0.57
1:A:359:GLU:O	1:A:362:LYS:HB2	2.04	0.57
1:B:339:ASN:N	1:B:339:ASN:HD22	1.92	0.57
1:B:348:ILE:HB	1:B:371:VAL:HG13	1.85	0.57
1:D:318:ILE:HD12	1:D:318:ILE:C	2.25	0.57
1:D:333:LYS:HA	1:D:355:PRO:O	2.05	0.57
1:D:200:ALA:HA	1:D:392:ASN:HD22	1.70	0.57
1:E:482:ARG:HH11	1:E:482:ARG:HG3	1.69	0.57
1:A:116:THR:HG22	1:A:128:GLY:N	2.20	0.57
1:A:337:LYS:HE3	1:A:359:GLU:CD	2.25	0.57
1:A:223:VAL:O	1:A:377:LEU:HD11	2.04	0.57
1:A:432:ILE:HG13	1:A:432:ILE:O	2.05	0.57
1:A:47:ASN:HD21	1:A:50:ARG:NH2	2.03	0.57
1:D:14:PHE:O	1:D:18:GLU:HB2	2.05	0.57
1:E:21:PHE:CE1	1:E:490:ILE:HD12	2.39	0.57
1:A:76:TRP:CZ3	1:E:49:VAL:HG23	2.38	0.57
1:A:136:ASN:OD1	1:A:138:LYS:HB2	2.03	0.57
1:A:67:PHE:N	1:A:67:PHE:CD2	2.73	0.57
1:B:150:ARG:O	1:B:152:PHE:N	2.38	0.57
1:B:275:ILE:HD12	1:B:287:PRO:HA	1.86	0.57
1:C:383:THR:O	1:C:386:TYR:HB3	2.05	0.57
1:E:284:ILE:HG22	1:E:285:TRP:N	2.19	0.57
1:F:427:LYS:NZ	1:F:430:GLY:CA	2.68	0.57
1:F:230:PHE:CE2	1:F:481:LEU:HD21	2.40	0.57
1:A:400:ARG:O	1:A:400:ARG:HD2	2.04	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:VAL:HG11	1:B:109:LYS:HZ3	1.68	0.56
1:E:32:LEU:HD11	1:E:494:PHE:CE2	2.39	0.56
1:F:326:LEU:HB3	1:F:348:ILE:HD13	1.87	0.56
1:A:99:TYR:CZ	1:A:149:THR:HG22	2.41	0.56
1:B:180:MET:HE2	1:B:180:MET:HA	1.87	0.56
1:B:309:PRO:O	1:B:310:LYS:CB	2.53	0.56
1:D:376:TYR:CD1	1:D:376:TYR:C	2.78	0.56
1:D:54:ARG:O	1:D:58:PRO:CD	2.53	0.56
1:F:13:PHE:CE1	1:F:107:GLU:HA	2.40	0.56
1:A:304:SER:OG	1:A:306:LEU:HD13	2.05	0.56
1:A:336:THR:O	1:A:340:ALA:HB2	2.05	0.56
1:D:161:PHE:O	1:D:167:ASP:HB3	2.03	0.56
1:D:350:GLU:OE1	1:D:373:PRO:HA	2.04	0.56
1:D:223:VAL:HA	1:D:377:LEU:HG	1.86	0.56
1:E:410:ASN:N	1:E:410:ASN:ND2	2.53	0.56
1:A:149:THR:HB	1:A:183:ILE:HD11	1.87	0.56
1:A:504:PHE:CE1	1:E:151:ARG:NH2	2.66	0.56
1:C:28:VAL:HG12	1:C:29:GLU:N	2.20	0.56
1:C:441:GLN:O	1:C:441:GLN:HG3	2.05	0.56
1:D:336:THR:HG22	1:D:357:THR:HG21	1.87	0.56
1:F:103:VAL:HA	1:F:107:GLU:OE1	2.06	0.56
1:A:146:GLU:HG3	1:A:182:TRP:CE2	2.40	0.56
1:A:393:LEU:O	1:A:395:HIS:HD2	1.88	0.56
1:A:418:GLN:HA	1:A:433:PRO:HG2	1.88	0.56
1:B:256:PHE:CZ	1:B:261:LEU:HD13	2.41	0.56
1:B:79:ILE:N	1:B:79:ILE:HD12	2.20	0.56
1:C:180:MET:HG3	1:C:202:VAL:HG21	1.87	0.56
1:C:400:ARG:O	1:C:400:ARG:HD2	2.05	0.56
1:C:73:ASP:OD1	1:C:75:SER:N	2.36	0.56
1:D:238:SER:C	1:D:240:LEU:H	2.09	0.56
1:D:24:GLY:O	1:D:28:VAL:HG23	2.05	0.56
1:E:43:GLU:HB3	1:E:45:LYS:HG3	1.87	0.56
1:B:275:ILE:HG22	1:B:276:ALA:N	2.20	0.56
1:B:295:LEU:HD11	1:B:305:ILE:CG2	2.36	0.56
1:C:281:ASP:HB2	1:C:306:LEU:HD11	1.87	0.56
1:D:106:ASP:HA	1:D:109:LYS:HD3	1.87	0.56
1:D:440:PHE:CE2	1:D:444:ILE:HD11	2.40	0.56
1:A:337:LYS:CE	1:A:359:GLU:HG3	2.35	0.56
1:A:433:PRO:HD2	1:A:434:ILE:H	1.70	0.56
1:B:436:PRO:HA	1:F:416:SER:OG	2.04	0.56
1:C:77:GLU:HA	1:F:54:ARG:CZ	2.35	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ILE:CD1	1:A:364:PHE:CE1	2.88	0.56
1:A:60:ASN:HA	1:E:66:SER:OG	2.05	0.56
1:A:69:ILE:HA	1:A:151:ARG:NH1	2.21	0.56
1:C:437:THR:CG2	1:D:416:SER:HA	2.35	0.56
1:D:416:SER:O	1:D:420:SER:HB2	2.06	0.56
1:A:231:ILE:HG22	1:A:232:ASN:N	2.20	0.56
1:C:254:GLN:NE2	1:C:334:GLN:HG2	2.14	0.56
1:C:285:TRP:HB2	1:C:314:TYR:HB2	1.86	0.56
1:D:92:PRO:HG2	1:D:389:TRP:CZ2	2.40	0.56
1:F:367:ARG:HH11	1:F:367:ARG:CB	2.19	0.56
1:A:265:ARG:HH11	1:A:265:ARG:HG3	1.70	0.56
1:A:327:ILE:CG2	1:A:349:ALA:HB3	2.36	0.56
1:B:205:LYS:NZ	1:B:392:ASN:ND2	2.49	0.56
1:C:333:LYS:HZ2	1:C:357:THR:HA	1.71	0.56
1:C:41:SER:HA	1:C:46:ARG:HD2	1.88	0.56
1:D:339:ASN:HD22	1:D:339:ASN:N	2.01	0.56
1:D:350:GLU:HG2	1:D:355:PRO:CG	2.35	0.56
1:D:355:PRO:HG2	1:D:356:THR:HG23	1.88	0.56
1:D:384:VAL:HG22	1:D:453:VAL:HG12	1.88	0.56
1:E:410:ASN:HD22	1:E:410:ASN:N	2.02	0.56
1:C:146:GLU:OE1	1:E:504:PHE:HB3	2.05	0.56
1:A:17:VAL:HG22	1:A:114:LEU:HD13	1.88	0.56
1:A:237:MET:CE	1:A:347:ILE:HD11	2.36	0.56
1:D:32:LEU:HD12	1:D:32:LEU:O	2.06	0.56
1:E:135:ILE:HD11	1:E:140:TYR:CZ	2.40	0.56
1:E:136:ASN:OD1	1:E:138:LYS:HG2	2.06	0.56
1:E:46:ARG:O	1:E:49:VAL:HG12	2.05	0.56
1:A:205:LYS:HE2	1:A:210:GLY:O	2.06	0.55
1:A:278:GLY:O	1:A:279:GLU:HG2	2.07	0.55
1:A:325:ILE:HG22	1:A:347:ILE:HG21	1.87	0.55
1:A:425:PHE:C	1:A:425:PHE:CD1	2.80	0.55
1:C:179:GLU:O	1:C:183:ILE:HG13	2.06	0.55
1:C:304:SER:HB3	1:C:306:LEU:HD13	1.88	0.55
1:D:314:TYR:HE2	1:D:318:ILE:HA	1.71	0.55
1:E:185:ASP:O	1:E:189:SER:OG	2.23	0.55
1:A:325:ILE:HG22	1:A:347:ILE:CB	2.37	0.55
1:B:162:ILE:O	1:B:162:ILE:HG23	2.04	0.55
1:C:339:ASN:HD22	1:C:340:ALA:H	1.54	0.55
1:B:502:VAL:CG1	1:D:76:TRP:HE1	2.19	0.55
1:F:295:LEU:HD11	1:F:305:ILE:CG2	2.36	0.55
1:F:339:ASN:C	1:F:339:ASN:HD22	2.09	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:O	1:A:183:ILE:HD13	2.06	0.55
1:A:318:ILE:C	1:A:318:ILE:HD12	2.26	0.55
1:A:443:ARG:HH21	1:B:409:SER:HB2	1.71	0.55
1:C:180:MET:HE2	1:C:183:ILE:HD12	1.87	0.55
1:E:175:THR:HG22	1:E:179:GLU:HG2	1.87	0.55
1:E:259:VAL:HG22	1:E:260:GLY:N	2.21	0.55
1:E:309:PRO:O	1:E:310:LYS:HB2	2.06	0.55
1:A:363:ILE:O	1:A:367:ARG:HG2	2.06	0.55
1:A:386:TYR:HE2	1:A:390:LEU:HD21	1.71	0.55
1:A:418:GLN:CA	1:A:433:PRO:HG2	2.37	0.55
1:B:190:THR:CG2	1:B:191:ILE:H	1.94	0.55
1:B:268:HIS:ND1	1:B:292:PRO:HD2	2.21	0.55
1:B:92:PRO:HG2	1:B:389:TRP:CZ2	2.41	0.55
1:C:409:SER:O	1:C:410:ASN:C	2.44	0.55
1:A:125:PRO:O	1:A:126:PHE:HD2	1.88	0.55
1:A:264:MET:CE	1:A:292:PRO:HA	2.36	0.55
1:A:213:HIS:O	1:A:453:VAL:HG21	2.06	0.55
1:D:264:MET:HE3	1:D:292:PRO:CA	2.37	0.55
1:A:256:PHE:CZ	1:A:261:LEU:HD13	2.42	0.55
1:A:320:GLU:O	1:A:344:LYS:HG2	2.07	0.55
1:E:72:ASP:OD2	1:E:141:THR:HG21	2.07	0.55
1:E:14:PHE:O	1:E:18:GLU:HB2	2.07	0.55
1:E:284:ILE:HG12	1:E:305:ILE:HD12	1.89	0.55
1:D:390:LEU:CD2	1:E:396:VAL:HG23	2.37	0.55
1:F:319:LEU:HD23	1:F:335:LEU:CD2	2.36	0.55
1:B:31:LYS:HG3	1:B:475:TYR:CE1	2.41	0.55
1:D:240:LEU:CD2	1:D:479:LEU:HD21	2.36	0.55
1:D:264:MET:HE3	1:D:292:PRO:HB3	1.89	0.55
1:D:325:ILE:HG22	1:D:347:ILE:CB	2.26	0.55
1:E:316:GLY:O	1:E:317:SER:C	2.45	0.55
1:E:501:GLY:HA3	1:E:504:PHE:O	2.05	0.55
1:A:224:PHE:CD2	1:A:266:TYR:HB3	2.42	0.55
1:D:238:SER:O	1:D:240:LEU:N	2.40	0.55
1:D:251:PHE:CE1	1:D:267:LEU:HB3	2.42	0.55
1:E:256:PHE:CE2	1:E:264:MET:HE2	2.41	0.55
1:E:350:GLU:OE1	1:E:373:PRO:HA	2.06	0.55
1:F:180:MET:CE	1:F:202:VAL:HG21	2.36	0.55
1:F:285:TRP:O	1:F:286:ASN:HB2	2.07	0.55
1:A:251:PHE:CZ	1:A:267:LEU:HB3	2.42	0.55
1:A:253:VAL:HG13	1:A:277:VAL:HG22	1.89	0.55
1:A:440:PHE:CD2	1:B:412:HIS:CB	2.89	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:503:THR:HG21	1:F:151:ARG:HD3	1.88	0.55
1:D:157:ALA:HA	1:D:162:ILE:HG22	1.89	0.55
1:E:122:VAL:HG23	1:E:122:VAL:O	2.06	0.55
1:E:29:GLU:O	1:E:33:VAL:HG23	2.06	0.55
1:F:162:ILE:O	1:F:162:ILE:HD13	2.06	0.55
1:A:94:LYS:HD3	1:A:126:PHE:CD1	2.42	0.55
1:C:251:PHE:HB3	1:C:325:ILE:CG1	2.37	0.55
1:D:17:VAL:HA	1:D:20:PHE:CD1	2.42	0.55
1:F:295:LEU:HD11	1:F:305:ILE:HG22	1.89	0.55
1:B:501:GLY:HA3	1:B:504:PHE:O	2.07	0.54
1:C:278:GLY:HA3	1:C:318:ILE:CD1	2.37	0.54
1:C:396:VAL:HG13	1:E:386:TYR:HH	1.71	0.54
1:E:94:LYS:HG2	1:E:126:PHE:CD1	2.42	0.54
1:E:141:THR:HG23	1:E:144:GLU:H	1.72	0.54
1:F:38:THR:HG23	1:F:41:SER:CB	2.25	0.54
1:A:252:VAL:HG23	1:A:323:CYS:SG	2.47	0.54
1:A:87:SER:O	1:A:127:GLY:HA3	2.07	0.54
1:C:298:PHE:O	1:C:300:LEU:N	2.40	0.54
1:D:404:LYS:HE3	1:D:407:ARG:HH21	1.71	0.54
1:D:435:VAL:HG13	1:E:420:SER:OG	2.07	0.54
1:F:502:VAL:N	1:F:505:THR:HB	2.21	0.54
1:A:355:PRO:HG2	1:A:356:THR:HG23	1.90	0.54
1:A:34:GLU:CA	1:A:38:THR:HB	2.36	0.54
1:A:386:TYR:CE2	1:A:390:LEU:HD21	2.42	0.54
1:A:49:VAL:O	1:A:52:ILE:HG12	2.06	0.54
1:B:110:ALA:O	1:B:113:SER:HB3	2.07	0.54
1:B:254:GLN:HE22	1:B:334:GLN:HG2	1.72	0.54
1:C:153:THR:HG22	1:C:154:MET:N	2.22	0.54
1:C:430:GLY:O	1:C:432:ILE:HG12	2.07	0.54
1:E:363:ILE:HG22	1:E:364:PHE:N	2.22	0.54
1:E:45:LYS:HE2	1:E:48:ARG:HH11	1.72	0.54
1:A:251:PHE:HB3	1:A:325:ILE:CG1	2.21	0.54
1:A:331:SER:HB2	1:A:334:GLN:NE2	2.22	0.54
1:A:360:ALA:HB1	1:A:364:PHE:CE2	2.36	0.54
1:A:418:GLN:OE1	1:A:433:PRO:HD2	2.07	0.54
1:A:502:VAL:CG2	1:A:503:THR:H	2.19	0.54
1:D:226:GLY:HA3	1:D:377:LEU:HD12	1.89	0.54
1:D:240:LEU:CD2	1:D:479:LEU:CD2	2.86	0.54
1:F:253:VAL:CG1	1:F:277:VAL:HG13	2.37	0.54
1:F:431:THR:O	1:F:433:PRO:HD3	2.08	0.54
1:B:323:CYS:O	1:B:345:ALA:HA	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:CD2	1:B:387:PHE:N	2.75	0.54
1:B:400:ARG:HH11	1:B:400:ARG:HG2	1.73	0.54
1:B:58:PRO:O	1:B:59:CYS:C	2.46	0.54
1:F:217:SER:OG	1:F:218:ALA:N	2.40	0.54
1:F:373:PRO:CD	1:F:481:LEU:HB3	2.36	0.54
1:E:13:PHE:CD1	1:E:14:PHE:N	2.72	0.54
1:F:257:GLY:O	1:F:258:ASN:C	2.46	0.54
1:F:433:PRO:O	1:F:434:ILE:C	2.45	0.54
1:A:146:GLU:CG	1:A:150:ARG:HH11	2.20	0.54
1:A:395:HIS:O	1:A:396:VAL:HG22	2.08	0.54
1:C:133:VAL:O	1:C:135:ILE:N	2.41	0.54
1:D:363:ILE:HD13	1:D:363:ILE:N	2.23	0.54
1:D:79:ILE:HD13	1:D:79:ILE:N	2.23	0.54
1:F:33:VAL:O	1:F:34:GLU:O	2.25	0.54
1:A:113:SER:O	1:A:116:THR:HG23	2.08	0.54
1:B:404:LYS:NZ	1:B:407:ARG:HH21	2.06	0.54
1:B:57:LYS:N	1:B:58:PRO:HD2	2.23	0.54
1:D:17:VAL:HA	1:D:20:PHE:HD1	1.72	0.54
1:D:501:GLY:HA3	1:D:505:THR:HA	1.89	0.54
1:E:69:ILE:HA	1:E:151:ARG:CZ	2.38	0.54
1:E:396:VAL:HG12	1:E:397:SER:N	2.22	0.54
1:F:108:VAL:HG23	1:F:109:LYS:H	1.71	0.54
1:D:158:LYS:HD3	1:F:193:HIS:ND1	2.23	0.54
1:F:256:PHE:HZ	1:F:296:GLU:HA	1.72	0.54
1:A:23:ARG:HE	1:A:483:THR:CG2	2.15	0.54
1:A:264:MET:HE3	1:A:292:PRO:HA	1.90	0.54
1:A:372:ILE:N	1:A:372:ILE:HD12	2.23	0.54
1:B:256:PHE:CE2	1:B:264:MET:HE2	2.41	0.54
1:B:501:GLY:HA3	1:B:505:THR:HA	1.89	0.54
1:C:285:TRP:HB3	1:C:314:TYR:HB2	1.89	0.54
1:D:180:MET:HE3	1:D:183:ILE:HD12	1.89	0.54
1:D:424:LYS:O	1:D:425:PHE:HB2	2.08	0.54
1:E:145:LEU:O	1:E:149:THR:HG23	2.08	0.54
1:A:62:VAL:HG13	1:E:64:SER:HB2	1.90	0.54
1:E:79:ILE:N	1:E:79:ILE:HD12	2.22	0.54
1:E:91:THR:OG1	1:E:92:PRO:HD3	2.07	0.54
1:F:145:LEU:O	1:F:149:THR:CG2	2.55	0.54
1:A:17:VAL:HA	1:A:20:PHE:CD1	2.43	0.54
1:C:162:ILE:HG23	1:C:162:ILE:O	2.07	0.54
1:C:252:VAL:O	1:C:327:ILE:HD13	2.07	0.54
1:C:57:LYS:HB3	1:C:58:PRO:CD	2.37	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LYS:N	1:C:58:PRO:HD2	2.23	0.54
1:D:418:GLN:CB	1:D:433:PRO:HD2	2.38	0.54
1:F:261:LEU:HD11	1:F:296:GLU:OE1	2.08	0.54
1:F:16:MET:SD	1:F:333:LYS:NZ	2.80	0.54
1:F:439:GLU:H	1:F:439:GLU:CD	2.12	0.54
1:F:457:LEU:HD23	1:F:461:MET:HG2	1.90	0.54
1:B:434:ILE:O	1:B:436:PRO:HD3	2.08	0.53
1:C:221:ARG:CD	1:C:225:HIS:CE1	2.92	0.53
1:D:254:GLN:OE1	1:D:334:GLN:HG2	2.09	0.53
1:E:21:PHE:O	1:E:25:ALA:HB2	2.08	0.53
1:F:336:THR:HG22	1:F:357:THR:HG21	1.90	0.53
1:F:500:ALA:CA	1:F:505:THR:O	2.56	0.53
1:D:502:VAL:CG2	1:D:503:THR:H	2.20	0.53
1:E:45:LYS:HE2	1:E:48:ARG:NH1	2.23	0.53
1:E:65:LEU:HD12	1:E:152:PHE:HE1	1.73	0.53
1:F:155:GLU:HA	1:F:155:GLU:OE1	2.08	0.53
1:F:261:LEU:O	1:F:265:ARG:HG2	2.07	0.53
1:F:350:GLU:O	1:F:377:LEU:HD23	2.08	0.53
1:F:410:ASN:O	1:F:413:LEU:HB2	2.08	0.53
1:A:285:TRP:NE1	1:A:287:PRO:HD3	2.23	0.53
1:A:437:THR:HG23	1:B:416:SER:HA	1.90	0.53
1:A:95:GLY:O	1:A:169:PRO:HA	2.07	0.53
1:B:14:PHE:HD1	1:B:110:ALA:HB2	1.73	0.53
1:C:143:ASN:O	1:C:147:LYS:HG3	2.09	0.53
1:C:71:ARG:HB3	1:C:71:ARG:NH1	2.08	0.53
1:D:480:ASP:CG	1:D:483:THR:HG23	2.29	0.53
1:E:221:ARG:HG2	1:E:221:ARG:HH11	1.72	0.53
1:A:105:VAL:O	1:A:109:LYS:HG3	2.08	0.53
1:A:150:ARG:CZ	1:F:505:THR:OXT	2.56	0.53
1:A:183:ILE:N	1:A:183:ILE:HD13	2.23	0.53
1:B:383:THR:O	1:B:386:TYR:HB3	2.08	0.53
1:B:42:GLU:HB2	1:B:46:ARG:NH2	2.22	0.53
1:D:336:THR:H	1:D:339:ASN:HD21	1.54	0.53
1:D:485:ALA:O	1:D:488:ASN:N	2.41	0.53
1:F:251:PHE:CE1	1:F:267:LEU:HB3	2.43	0.53
1:B:13:PHE:HD1	1:B:14:PHE:H	1.57	0.53
1:B:341:PRO:HG3	1:B:363:ILE:HG21	1.91	0.53
1:C:384:VAL:HG23	1:C:457:LEU:HD12	1.90	0.53
1:D:135:ILE:CD1	1:D:148:ILE:HD13	2.38	0.53
1:E:423:ARG:HH11	1:E:423:ARG:HG3	1.74	0.53
1:F:231:ILE:HG23	1:F:232:ASN:ND2	2.24	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:PHE:CE1	1:F:299:LYS:HG2	2.43	0.53
1:A:32:LEU:HD21	1:A:494:PHE:CE1	2.44	0.53
1:A:363:ILE:HG22	1:A:364:PHE:N	2.23	0.53
1:B:335:LEU:HD11	1:B:348:ILE:HD13	1.89	0.53
1:C:293:LYS:HE2	1:C:297:ASP:OD2	2.09	0.53
1:C:350:GLU:HG2	1:C:355:PRO:HG2	1.89	0.53
1:C:423:ARG:HH21	1:E:435:VAL:HG11	1.74	0.53
1:F:122:VAL:O	1:F:124:VAL:HG23	2.08	0.53
1:F:418:GLN:CG	1:F:433:PRO:HD2	2.39	0.53
1:A:433:PRO:HA	1:B:420:SER:OG	2.08	0.53
1:B:105:VAL:O	1:B:109:LYS:HG3	2.08	0.53
1:B:285:TRP:CB	1:B:314:TYR:HB2	2.38	0.53
1:C:180:MET:HG3	1:C:202:VAL:CG2	2.39	0.53
1:C:203:THR:HA	1:C:388:GLU:OE1	2.09	0.53
1:D:300:LEU:HD13	1:D:301:GLN:N	2.23	0.53
1:D:410:ASN:O	1:D:414:LEU:HG	2.08	0.53
1:E:224:PHE:HD2	1:E:267:LEU:HD22	1.73	0.53
1:F:502:VAL:HG23	1:F:504:PHE:H	1.74	0.53
1:A:239:ILE:HG22	1:A:239:ILE:O	2.07	0.53
1:A:339:ASN:H	1:A:339:ASN:ND2	2.07	0.53
1:A:212:ILE:HD11	1:A:453:VAL:HG22	1.91	0.53
1:A:500:ALA:HB1	1:A:505:THR:O	2.08	0.53
1:A:47:ASN:O	1:A:50:ARG:CG	2.57	0.53
1:C:78:VAL:O	1:C:78:VAL:HG23	2.08	0.53
1:D:23:ARG:HG3	1:D:23:ARG:NH1	2.22	0.53
1:F:180:MET:CE	1:F:202:VAL:CG2	2.87	0.53
1:A:133:VAL:HG12	1:A:133:VAL:O	2.07	0.53
1:A:251:PHE:CE1	1:A:267:LEU:HB3	2.44	0.53
1:D:251:PHE:HD2	1:D:327:ILE:HD11	1.74	0.53
1:D:275:ILE:CG2	1:D:276:ALA:H	2.21	0.53
1:D:400:ARG:HG3	1:D:400:ARG:HH11	1.74	0.53
1:D:68:PRO:O	1:D:151:ARG:HD2	2.07	0.53
1:E:296:GLU:O	1:E:296:GLU:HG2	2.09	0.53
1:E:295:LEU:HD11	1:E:305:ILE:HB	1.90	0.53
1:F:329:ALA:O	1:F:330:ALA:HB2	2.08	0.53
1:F:122:VAL:HG11	1:F:379:ALA:HB3	1.91	0.53
1:F:427:LYS:HE2	1:F:430:GLY:N	2.24	0.53
1:B:13:PHE:CZ	1:B:107:GLU:HG3	2.43	0.53
1:B:50:ARG:HG3	1:B:50:ARG:O	2.09	0.53
1:C:34:GLU:O	1:C:36:LEU:N	2.41	0.53
1:D:281:ASP:CB	1:D:306:LEU:HD21	2.38	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ASP:OD1	1:E:141:THR:HG21	2.08	0.53
1:E:72:ASP:OD1	1:E:144:GLU:CG	2.54	0.53
1:A:218:ALA:O	1:A:219:THR:C	2.48	0.52
1:A:373:PRO:HG3	1:A:482:ARG:N	2.24	0.52
1:A:73:ASP:OD1	1:A:75:SER:OG	2.25	0.52
1:B:243:THR:CG2	1:B:243:THR:O	2.55	0.52
1:C:293:LYS:O	1:C:293:LYS:HG3	2.09	0.52
1:D:190:THR:CG2	1:D:191:ILE:N	2.71	0.52
1:D:23:ARG:O	1:D:27:ILE:HG12	2.08	0.52
1:D:314:TYR:HD2	1:D:318:ILE:HG22	1.74	0.52
1:D:317:SER:HB2	1:D:319:LEU:HD13	1.91	0.52
1:E:23:ARG:O	1:E:27:ILE:HG13	2.10	0.52
1:F:32:LEU:HD21	1:F:494:PHE:CG	2.44	0.52
1:A:501:GLY:O	1:A:502:VAL:HG13	2.09	0.52
1:A:85:GLN:NE2	1:A:167:ASP:HB2	2.24	0.52
1:B:500:ALA:CA	1:B:505:THR:O	2.58	0.52
1:D:424:LYS:O	1:D:425:PHE:CB	2.57	0.52
1:F:117:TYR:O	1:F:121:VAL:HG23	2.08	0.52
1:F:309:PRO:O	1:F:310:LYS:HB2	2.09	0.52
1:A:17:VAL:HG21	1:A:114:LEU:HD13	1.91	0.52
1:A:240:LEU:HD21	1:A:479:LEU:HD21	1.91	0.52
1:A:501:GLY:HA3	1:A:504:PHE:O	2.10	0.52
1:B:435:VAL:O	1:B:435:VAL:HG13	2.09	0.52
1:C:195:ASP:HB3	1:C:198:ALA:HB2	1.91	0.52
1:E:285:TRP:CB	1:E:314:TYR:HB2	2.38	0.52
1:F:363:ILE:CG2	1:F:367:ARG:HD3	2.39	0.52
1:F:367:ARG:HB2	1:F:367:ARG:HH11	1.73	0.52
1:B:335:LEU:HD13	1:B:348:ILE:HD13	1.91	0.52
1:C:71:ARG:NH1	1:C:144:GLU:OE2	2.42	0.52
1:C:500:ALA:C	1:C:505:THR:HA	2.29	0.52
1:F:195:ASP:HB3	1:F:198:ALA:HB2	1.90	0.52
1:A:350:GLU:OE2	1:A:356:THR:HG23	2.09	0.52
1:A:362:LYS:O	1:A:365:LEU:HB3	2.10	0.52
1:A:69:ILE:HD13	1:A:148:ILE:HG12	1.92	0.52
1:A:99:TYR:OH	1:A:149:THR:CG2	2.46	0.52
1:B:283:SER:O	1:B:284:ILE:HD12	2.10	0.52
1:C:231:ILE:HD12	1:C:237:MET:SD	2.49	0.52
1:C:334:GLN:NE2	1:C:334:GLN:CA	2.71	0.52
1:E:180:MET:HG2	1:E:203:THR:O	2.09	0.52
1:F:105:VAL:O	1:F:108:VAL:HG22	2.10	0.52
1:F:146:GLU:HG2	1:F:150:ARG:HD2	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:ALA:HA	1:F:372:ILE:HG13	1.90	0.52
1:A:427:LYS:C	1:A:428:HIS:HD1	2.13	0.52
1:B:28:VAL:CG1	1:B:32:LEU:HD22	2.39	0.52
1:B:400:ARG:NH1	1:B:400:ARG:HG2	2.24	0.52
1:B:425:PHE:HD1	1:B:427:LYS:HB2	1.74	0.52
1:B:427:LYS:HG3	1:B:428:HIS:N	2.24	0.52
1:D:12:ASN:OD1	1:D:15:LYS:HG2	2.10	0.52
1:D:83:ARG:HG2	1:D:161:PHE:HB3	1.91	0.52
1:D:234:ALA:O	1:D:235:SER:C	2.48	0.52
1:D:372:ILE:CG2	1:D:377:LEU:HD13	2.30	0.52
1:B:299:LYS:HD2	1:B:304:SER:HA	1.92	0.52
1:B:440:PHE:CE2	1:B:444:ILE:HD11	2.42	0.52
1:C:180:MET:HE2	1:C:180:MET:HA	1.92	0.52
1:C:336:THR:OG1	1:C:338:SER:HB3	2.10	0.52
1:C:61:HIS:CE1	1:F:155:GLU:HG3	2.45	0.52
1:A:183:ILE:HD13	1:A:183:ILE:H	1.75	0.52
1:A:285:TRP:CD1	1:A:286:ASN:N	2.78	0.52
1:C:221:ARG:NH1	1:C:221:ARG:CG	2.70	0.52
1:C:86:HIS:CD2	1:C:116:THR:CG2	2.88	0.52
1:D:350:GLU:HG2	1:D:355:PRO:HG2	1.92	0.52
1:E:284:ILE:HG23	1:E:311:ALA:CB	2.26	0.52
1:A:122:VAL:O	1:A:122:VAL:HG23	2.10	0.52
1:A:248:ASP:CG	1:A:249:LYS:HG3	2.29	0.52
1:B:95:GLY:HA3	1:B:129:ALA:O	2.09	0.52
1:C:187:TYR:CE1	1:C:191:ILE:HG22	2.45	0.52
1:C:231:ILE:O	1:C:237:MET:HG3	2.09	0.52
1:C:409:SER:O	1:C:411:TYR:N	2.43	0.52
1:D:399:GLY:HA3	1:D:403:PHE:CE1	2.44	0.52
1:F:427:LYS:HZ3	1:F:430:GLY:CA	2.23	0.52
1:A:481:LEU:H	1:A:481:LEU:CD1	2.23	0.52
1:B:363:ILE:O	1:B:367:ARG:HG2	2.10	0.52
1:B:65:LEU:O	1:B:80:GLU:HA	2.10	0.52
1:C:475:TYR:OH	1:C:491:GLU:OE2	2.26	0.52
1:D:105:VAL:O	1:D:108:VAL:HG22	2.09	0.52
1:E:141:THR:HG22	1:E:144:GLU:CD	2.30	0.52
1:E:332:GLU:HG2	1:E:333:LYS:HG2	1.92	0.52
1:F:145:LEU:O	1:F:149:THR:HG22	2.10	0.52
1:F:349:ALA:HB1	1:F:377:LEU:HD21	1.91	0.52
1:A:108:VAL:O	1:A:109:LYS:C	2.47	0.51
1:A:265:ARG:HG3	1:A:265:ARG:NH1	2.25	0.51
1:A:34:GLU:O	1:A:36:LEU:N	2.39	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:PRO:HA	1:A:367:ARG:HE	1.74	0.51
1:A:427:LYS:C	1:A:428:HIS:ND1	2.63	0.51
1:B:488:ASN:O	1:B:492:LYS:HG3	2.10	0.51
1:D:197:ASN:O	1:D:200:ALA:HB3	2.10	0.51
1:D:501:GLY:HA3	1:D:504:PHE:O	2.10	0.51
1:D:96:GLY:HA2	1:D:170:ALA:O	2.10	0.51
1:C:401:LEU:HD13	1:E:398:TYR:CE2	2.44	0.51
1:E:428:HIS:HD2	1:E:428:HIS:N	2.07	0.51
1:E:51:GLY:O	1:E:54:ARG:HG2	2.09	0.51
1:F:265:ARG:HG3	1:F:265:ARG:HH11	1.75	0.51
1:F:319:LEU:CD1	1:F:319:LEU:H	2.19	0.51
1:A:326:LEU:O	1:A:328:PRO:HD3	2.10	0.51
1:A:53:LEU:CD1	1:A:494:PHE:HD1	2.23	0.51
1:C:101:THR:HG22	1:C:101:THR:O	2.09	0.51
1:C:38:THR:HG22	1:C:38:THR:O	2.10	0.51
1:C:418:GLN:OE1	1:C:432:ILE:HA	2.09	0.51
1:D:268:HIS:O	1:D:270:PHE:N	2.43	0.51
1:E:224:PHE:CZ	1:E:270:PHE:CD2	2.99	0.51
1:F:94:LYS:HD3	1:F:126:PHE:CD1	2.44	0.51
1:F:284:ILE:HG13	1:F:305:ILE:HD12	1.91	0.51
1:F:326:LEU:HB3	1:F:348:ILE:CD1	2.39	0.51
1:A:284:ILE:HG23	1:A:311:ALA:CB	2.31	0.51
1:A:47:ASN:O	1:A:50:ARG:HG2	2.11	0.51
1:B:398:TYR:HB2	1:B:449:GLU:HG3	1.93	0.51
1:B:63:LEU:HG	1:B:65:LEU:CD2	2.40	0.51
1:D:256:PHE:CE2	1:D:264:MET:HE2	2.44	0.51
1:D:440:PHE:CZ	1:D:444:ILE:HD11	2.45	0.51
1:F:359:GLU:O	1:F:362:LYS:HB2	2.09	0.51
1:F:425:PHE:CE1	1:F:427:LYS:HB2	2.46	0.51
1:A:223:VAL:HG11	1:A:263:SER:OG	2.11	0.51
1:C:170:ALA:HB1	1:C:171:PRO:CD	2.40	0.51
1:D:365:LEU:C	1:D:365:LEU:HD23	2.31	0.51
1:E:32:LEU:HD21	1:E:494:PHE:CD1	2.45	0.51
1:E:501:GLY:HA3	1:E:505:THR:HA	1.92	0.51
1:A:178:ARG:HB3	1:A:179:GLU:OE2	2.10	0.51
1:A:285:TRP:HB2	1:A:314:TYR:CB	2.35	0.51
1:A:424:LYS:NZ	1:A:424:LYS:O	2.35	0.51
1:B:38:THR:HG22	1:B:38:THR:O	2.10	0.51
1:C:13:PHE:HD1	1:C:14:PHE:N	2.08	0.51
1:D:171:PRO:HG3	1:D:180:MET:SD	2.51	0.51
1:E:293:LYS:NZ	1:E:297:ASP:OD1	2.44	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:PHE:CD2	1:F:266:TYR:HB3	2.45	0.51
1:A:285:TRP:CD1	1:A:287:PRO:HD3	2.46	0.51
1:A:396:VAL:CG2	1:F:390:LEU:CD2	2.88	0.51
1:B:404:LYS:NZ	1:B:408:ASP:OD2	2.33	0.51
1:D:309:PRO:O	1:D:310:LYS:CB	2.58	0.51
1:D:34:GLU:C	1:D:38:THR:HB	2.31	0.51
1:D:404:LYS:HE3	1:D:407:ARG:NH2	2.25	0.51
1:D:77:GLU:HG2	1:D:79:ILE:CD1	2.41	0.51
1:F:252:VAL:HG22	1:F:276:ALA:HB3	1.91	0.51
1:F:37:ARG:NE	1:F:46:ARG:HD3	2.25	0.51
1:F:46:ARG:NE	1:F:46:ARG:HA	2.26	0.51
1:F:55:ILE:O	1:F:58:PRO:HD2	2.10	0.51
1:A:440:PHE:CE1	1:A:444:ILE:HD11	2.45	0.51
1:B:400:ARG:HG3	1:B:401:LEU:HD12	1.92	0.51
1:B:46:ARG:O	1:B:49:VAL:HG12	2.10	0.51
1:B:69:ILE:HG12	1:B:79:ILE:CD1	2.40	0.51
1:C:42:GLU:O	1:C:43:GLU:HB2	2.10	0.51
1:E:316:GLY:O	1:E:317:SER:O	2.29	0.51
1:E:433:PRO:O	1:E:434:ILE:C	2.49	0.51
1:E:466:ARG:NH1	1:E:466:ARG:CG	2.74	0.51
1:F:427:LYS:HZ3	1:F:430:GLY:HA3	1.76	0.51
1:A:21:PHE:CE2	1:A:57:LYS:HB2	2.46	0.51
1:A:227:ILE:HD11	1:A:349:ALA:CB	2.41	0.51
1:B:21:PHE:C	1:B:21:PHE:CD2	2.85	0.51
1:B:502:VAL:HG11	1:D:76:TRP:NE1	2.20	0.51
1:E:400:ARG:CG	1:E:400:ARG:NH1	2.65	0.51
1:A:29:GLU:O	1:A:33:VAL:HG23	2.10	0.51
1:B:378:ASN:HD22	1:B:378:ASN:N	2.04	0.51
1:D:336:THR:HG22	1:D:357:THR:CG2	2.41	0.51
1:D:363:ILE:O	1:D:367:ARG:HG2	2.10	0.51
1:F:350:GLU:OE2	1:F:482:ARG:NH2	2.44	0.51
1:F:21:PHE:CE2	1:F:57:LYS:HB2	2.46	0.51
1:A:149:THR:HG21	1:A:179:GLU:HG3	1.91	0.51
1:B:57:LYS:HB3	1:B:58:PRO:HD3	1.93	0.51
1:D:309:PRO:O	1:D:310:LYS:HB2	2.11	0.51
1:D:321:ALA:O	1:D:344:LYS:HB2	2.11	0.51
1:D:324:ASP:HB2	1:D:325:ILE:CD1	2.39	0.51
1:D:374:ASP:OD2	1:D:375:LEU:N	2.44	0.51
1:F:157:ALA:HB2	1:F:162:ILE:HG21	1.93	0.51
1:A:86:HIS:CG	1:A:116:THR:HG21	2.44	0.50
1:A:190:THR:CG2	1:A:191:ILE:N	2.67	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:CD2	1:A:292:PRO:CD	2.94	0.50
1:A:309:PRO:O	1:A:310:LYS:HB2	2.12	0.50
1:A:349:ALA:HA	1:A:372:ILE:HB	1.93	0.50
1:A:38:THR:O	1:A:38:THR:CG2	2.59	0.50
1:C:153:THR:HG21	1:C:186:THR:HB	1.93	0.50
1:C:298:PHE:CZ	1:C:302:HIS:HE1	2.29	0.50
1:C:502:VAL:CG2	1:C:503:THR:H	2.23	0.50
1:C:86:HIS:HB3	1:C:116:THR:HG21	1.94	0.50
1:E:108:VAL:HG23	1:E:109:LYS:N	2.26	0.50
1:F:37:ARG:C	1:F:39:ARG:H	2.15	0.50
1:A:407:ARG:NH1	1:A:411:TYR:CD2	2.79	0.50
1:A:500:ALA:C	1:A:505:THR:HA	2.31	0.50
1:C:237:MET:O	1:C:242:MET:N	2.36	0.50
1:D:327:ILE:HG23	1:D:349:ALA:HB3	1.92	0.50
1:C:417:VAL:HG21	1:E:417:VAL:HG21	1.93	0.50
1:F:318:ILE:HD12	1:F:319:LEU:HD12	1.92	0.50
1:F:500:ALA:HB1	1:F:505:THR:OG1	2.11	0.50
1:B:318:ILE:N	1:B:318:ILE:HD13	2.26	0.50
1:B:84:ALA:O	1:B:129:ALA:HB1	2.10	0.50
1:B:86:HIS:CD2	1:B:116:THR:CG2	2.88	0.50
1:C:168:VAL:CG1	1:C:202:VAL:HA	2.40	0.50
1:C:433:PRO:O	1:C:434:ILE:C	2.49	0.50
1:D:83:ARG:NH2	1:D:167:ASP:OD1	2.44	0.50
1:E:254:GLN:OE1	1:E:319:LEU:HD11	2.11	0.50
1:A:327:ILE:N	1:A:327:ILE:HD13	2.27	0.50
1:A:343:VAL:HG22	1:A:367:ARG:HH21	1.77	0.50
1:C:206:PRO:HD2	1:C:209:GLN:HB2	1.93	0.50
1:D:47:ASN:O	1:D:50:ARG:HG2	2.11	0.50
1:E:146:GLU:CG	1:E:150:ARG:HH11	2.23	0.50
1:E:96:GLY:HA2	1:E:170:ALA:O	2.12	0.50
1:E:462:GLU:O	1:E:463:ALA:O	2.29	0.50
1:F:32:LEU:HD21	1:F:494:PHE:CD2	2.47	0.50
1:B:376:TYR:CD2	1:B:376:TYR:C	2.84	0.50
1:C:86:HIS:CG	1:C:116:THR:HG21	2.45	0.50
1:C:146:GLU:HG2	1:C:150:ARG:HD2	1.93	0.50
1:C:251:PHE:CB	1:C:325:ILE:HG13	2.41	0.50
1:D:144:GLU:O	1:D:148:ILE:HG13	2.11	0.50
1:D:224:PHE:CD1	1:D:224:PHE:C	2.84	0.50
1:E:141:THR:HG22	1:E:144:GLU:OE1	2.11	0.50
1:F:242:MET:HE1	1:F:244:PRO:HG2	1.93	0.50
1:F:83:ARG:HH21	1:F:167:ASP:CG	2.14	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:HIS:O	1:A:302:HIS:ND1	2.45	0.50
1:A:331:SER:HB2	1:A:334:GLN:HE22	1.76	0.50
1:B:23:ARG:HE	1:B:483:THR:CG2	2.25	0.50
1:C:100:SER:O	1:C:134:LYS:HA	2.11	0.50
1:E:118:LYS:HD3	1:E:382:VAL:HG21	1.94	0.50
1:E:116:THR:CG2	1:E:128:GLY:HA3	2.42	0.50
1:E:175:THR:CG2	1:E:179:GLU:HG2	2.42	0.50
1:F:47:ASN:O	1:F:50:ARG:HG2	2.11	0.50
1:A:503:THR:CA	1:A:505:THR:HG22	2.42	0.50
1:B:325:ILE:HG22	1:B:347:ILE:HG22	1.94	0.50
1:C:409:SER:O	1:C:412:HIS:N	2.43	0.50
1:D:176:GLY:N	1:D:179:GLU:OE1	2.30	0.50
1:D:318:ILE:HD12	1:D:319:LEU:N	2.27	0.50
1:D:485:ALA:O	1:D:487:VAL:N	2.44	0.50
1:F:157:ALA:HA	1:F:162:ILE:HG22	1.93	0.50
1:A:46:ARG:O	1:A:49:VAL:HG12	2.11	0.50
1:A:505:THR:OXT	1:B:150:ARG:NH2	2.44	0.50
1:A:47:ASN:O	1:A:50:ARG:CD	2.59	0.50
1:B:29:GLU:HG2	1:B:30:ASP:N	2.26	0.50
1:B:474:LYS:NZ	1:B:491:GLU:OE2	2.43	0.50
1:C:141:THR:HG23	1:C:144:GLU:CD	2.32	0.50
1:C:418:GLN:OE1	1:C:433:PRO:CD	2.60	0.50
1:D:390:LEU:HD22	1:E:396:VAL:HG23	1.93	0.50
1:D:413:LEU:O	1:D:417:VAL:HG23	2.11	0.50
1:E:256:PHE:CZ	1:E:261:LEU:HD13	2.46	0.50
1:F:349:ALA:HB1	1:F:377:LEU:CD2	2.42	0.50
1:F:364:PHE:HB3	1:F:369:ILE:HB	1.92	0.50
1:A:425:PHE:C	1:A:425:PHE:HD1	2.15	0.50
1:A:433:PRO:CD	1:A:434:ILE:H	2.22	0.50
1:B:146:GLU:HG3	1:B:182:TRP:CE2	2.46	0.50
1:B:335:LEU:HD13	1:B:364:PHE:CZ	2.47	0.50
1:D:153:THR:HG23	1:D:162:ILE:HD13	1.94	0.50
1:E:190:THR:CG2	1:E:191:ILE:H	1.91	0.50
1:E:396:VAL:CG1	1:E:397:SER:N	2.75	0.50
1:F:170:ALA:CA	1:F:180:MET:HE2	2.42	0.50
1:C:77:GLU:CA	1:F:54:ARG:HH22	2.25	0.50
1:A:240:LEU:HD21	1:A:479:LEU:CD2	2.42	0.49
1:A:502:VAL:HG11	1:E:76:TRP:HE1	1.71	0.49
1:A:502:VAL:N	1:A:505:THR:HB	2.27	0.49
1:A:79:ILE:CD1	1:A:79:ILE:N	2.74	0.49
1:B:179:GLU:H	1:B:179:GLU:CD	2.15	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:LEU:CD1	1:B:306:LEU:H	2.25	0.49
1:B:427:LYS:HG3	1:B:430:GLY:H	1.77	0.49
1:C:97:ILE:HD13	1:C:131:ALA:HB3	1.92	0.49
1:C:252:VAL:HB	1:C:326:LEU:HD23	1.93	0.49
1:E:336:THR:HG22	1:E:357:THR:CG2	2.41	0.49
1:E:502:VAL:O	1:E:505:THR:CG2	2.60	0.49
1:F:284:ILE:HG22	1:F:285:TRP:H	1.76	0.49
1:F:56:ILE:CD1	1:F:493:VAL:HG12	2.42	0.49
1:A:237:MET:HE1	1:A:347:ILE:HD11	1.94	0.49
1:B:340:ALA:O	1:B:343:VAL:HG22	2.12	0.49
1:B:350:GLU:CD	1:B:482:ARG:HH22	2.14	0.49
1:F:171:PRO:HG3	1:F:180:MET:HG3	1.94	0.49
1:F:309:PRO:O	1:F:310:LYS:CB	2.60	0.49
1:F:67:PHE:CE1	1:F:79:ILE:HB	2.47	0.49
1:A:190:THR:CG2	1:A:191:ILE:H	2.24	0.49
1:A:360:ALA:O	1:A:361:ASP:C	2.51	0.49
1:A:386:TYR:CE2	1:A:390:LEU:HD11	2.47	0.49
1:C:28:VAL:HG13	1:C:32:LEU:CD2	2.40	0.49
1:C:390:LEU:O	1:C:391:LYS:C	2.48	0.49
1:D:337:LYS:NZ	1:D:337:LYS:CB	2.72	0.49
1:E:418:GLN:O	1:E:419:GLU:C	2.47	0.49
1:F:51:GLY:O	1:F:54:ARG:HG2	2.12	0.49
1:A:307:GLY:O	1:A:309:PRO:HD3	2.13	0.49
1:A:331:SER:CB	1:A:334:GLN:HE22	2.25	0.49
1:A:337:LYS:NZ	1:A:359:GLU:HG3	2.27	0.49
1:B:339:ASN:N	1:B:339:ASN:ND2	2.52	0.49
1:B:34:GLU:O	1:B:38:THR:HB	2.11	0.49
1:C:108:VAL:O	1:C:109:LYS:C	2.48	0.49
1:D:12:ASN:ND2	1:D:14:PHE:HB3	2.27	0.49
1:A:54:ARG:NH1	1:E:78:VAL:HG13	2.27	0.49
1:F:239:ILE:O	1:F:239:ILE:CG2	2.60	0.49
1:F:343:VAL:CG2	1:F:364:PHE:HE1	2.19	0.49
1:A:427:LYS:CG	1:A:428:HIS:H	2.25	0.49
1:B:28:VAL:O	1:B:29:GLU:C	2.50	0.49
1:C:316:GLY:O	1:C:317:SER:C	2.50	0.49
1:C:37:ARG:HH21	1:C:49:VAL:CG1	2.04	0.49
1:C:480:ASP:CG	1:C:483:THR:HG23	2.32	0.49
1:C:21:PHE:CE1	1:C:490:ILE:HD12	2.47	0.49
1:F:149:THR:O	1:F:153:THR:OG1	2.27	0.49
1:A:203:THR:HB	1:A:388:GLU:OE2	2.13	0.49
1:A:233:GLU:HG2	1:A:236:TYR:CD1	2.47	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LYS:HD3	1:A:35:ASP:OD2	2.13	0.49
1:A:387:PHE:N	1:A:387:PHE:CD2	2.80	0.49
1:C:23:ARG:HH11	1:C:23:ARG:HG3	1.76	0.49
1:D:115:MET:O	1:D:116:THR:C	2.49	0.49
1:F:220:GLY:O	1:F:223:VAL:N	2.45	0.49
1:F:418:GLN:HG3	1:F:431:THR:O	2.13	0.49
1:A:349:ALA:HB1	1:A:377:LEU:CD2	2.42	0.49
1:A:418:GLN:OE1	1:A:433:PRO:CD	2.60	0.49
1:B:108:VAL:O	1:B:110:ALA:N	2.45	0.49
1:B:425:PHE:O	1:B:427:LYS:N	2.46	0.49
1:C:94:LYS:HD3	1:C:126:PHE:CE1	2.47	0.49
1:C:482:ARG:O	1:C:485:ALA:N	2.44	0.49
1:D:136:ASN:C	1:D:138:LYS:H	2.16	0.49
1:D:44:GLN:C	1:D:46:ARG:H	2.16	0.49
1:D:73:ASP:OD2	1:D:75:SER:N	2.33	0.49
1:F:171:PRO:HB3	1:F:175:THR:O	2.12	0.49
1:F:227:ILE:O	1:F:231:ILE:HB	2.13	0.49
1:B:487:VAL:O	1:B:491:GLU:HG3	2.13	0.49
1:B:52:ILE:HG21	1:B:494:PHE:CD1	2.48	0.49
1:D:314:TYR:CD2	1:D:318:ILE:HG22	2.48	0.49
1:E:115:MET:HB3	1:E:128:GLY:HA2	1.94	0.49
1:E:408:ASP:O	1:E:412:HIS:HD2	1.96	0.49
1:E:92:PRO:HA	1:E:166:ILE:O	2.12	0.49
1:F:116:THR:HG22	1:F:128:GLY:HA3	1.94	0.49
1:A:72:ASP:OD1	1:A:144:GLU:OE2	2.30	0.49
1:A:396:VAL:HG22	1:F:390:LEU:HD11	1.95	0.49
1:B:433:PRO:HA	1:F:420:SER:HB3	1.93	0.49
1:B:64:SER:HB2	1:D:62:VAL:HG13	1.94	0.49
1:C:68:PRO:O	1:C:151:ARG:NH1	2.40	0.49
1:D:251:PHE:O	1:D:275:ILE:HG22	2.13	0.49
1:F:215:ARG:O	1:F:218:ALA:HB3	2.13	0.49
1:F:284:ILE:CG2	1:F:285:TRP:N	2.75	0.49
1:F:322:ASP:OD1	1:F:344:LYS:HB3	2.13	0.49
1:F:477:LEU:HD13	1:F:480:ASP:OD2	2.12	0.49
1:C:151:ARG:CZ	1:F:503:THR:OG1	2.60	0.49
1:B:28:VAL:O	1:B:29:GLU:O	2.31	0.49
1:C:284:ILE:HG23	1:C:285:TRP:N	2.28	0.49
1:C:432:ILE:HG22	1:C:434:ILE:CG1	2.43	0.49
1:D:386:TYR:CE2	1:D:390:LEU:HD11	2.48	0.49
1:F:319:LEU:HD21	1:F:334:GLN:HG3	1.95	0.49
1:F:427:LYS:HZ1	1:F:430:GLY:HA2	1.77	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HB2	1:A:206:PRO:HG3	1.94	0.48
1:A:273:LYS:HD3	1:A:287:PRO:O	2.12	0.48
1:B:320:GLU:HG2	1:B:342:ARG:O	2.13	0.48
1:B:407:ARG:NH1	1:B:411:TYR:CE2	2.81	0.48
1:C:168:VAL:HG13	1:C:202:VAL:CA	2.40	0.48
1:D:331:SER:HB2	1:D:334:GLN:NE2	2.28	0.48
1:D:390:LEU:CD2	1:E:396:VAL:CG2	2.91	0.48
1:D:480:ASP:OD1	1:D:483:THR:HG23	2.13	0.48
1:D:51:GLY:O	1:D:54:ARG:HG2	2.13	0.48
1:F:30:ASP:O	1:F:34:GLU:HG2	2.13	0.48
1:F:378:ASN:C	1:F:378:ASN:HD22	2.15	0.48
1:B:398:TYR:CE2	1:F:401:LEU:HD13	2.47	0.48
1:B:298:PHE:CZ	1:B:302:HIS:HE1	2.30	0.48
1:C:33:VAL:O	1:C:34:GLU:O	2.31	0.48
1:C:222:GLY:CA	1:C:457:LEU:HD21	2.40	0.48
1:C:91:THR:CB	1:C:92:PRO:HD3	2.43	0.48
1:D:298:PHE:CE1	1:D:309:PRO:HD3	2.48	0.48
1:D:28:VAL:O	1:D:32:LEU:HB3	2.13	0.48
1:D:331:SER:HB2	1:D:334:GLN:HE22	1.78	0.48
1:E:146:GLU:HG2	1:E:150:ARG:HD2	1.93	0.48
1:E:95:GLY:O	1:E:169:PRO:HA	2.13	0.48
1:F:116:THR:HB	1:F:128:GLY:H	1.78	0.48
1:A:427:LYS:HG3	1:A:430:GLY:H	1.78	0.48
1:B:219:THR:O	1:B:223:VAL:HG23	2.13	0.48
1:B:440:PHE:CE1	1:F:413:LEU:HD22	2.49	0.48
1:D:85:GLN:OE1	1:D:88:GLN:NE2	2.46	0.48
1:F:202:VAL:CG2	1:F:203:THR:N	2.76	0.48
1:A:339:ASN:H	1:A:339:ASN:HD22	1.61	0.48
1:A:34:GLU:HA	1:A:38:THR:CB	2.39	0.48
1:A:399:GLY:HA3	1:A:403:PHE:CE1	2.49	0.48
1:A:501:GLY:HA3	1:A:505:THR:HA	1.96	0.48
1:B:237:MET:CE	1:B:237:MET:HA	2.43	0.48
1:E:244:PRO:HB2	1:E:248:ASP:H	1.77	0.48
1:E:254:GLN:OE1	1:E:334:GLN:HG2	2.13	0.48
1:F:153:THR:CG2	1:F:183:ILE:HG23	2.43	0.48
1:A:443:ARG:NH2	1:B:409:SER:HB2	2.28	0.48
1:B:21:PHE:HD1	1:B:117:TYR:CZ	2.32	0.48
1:D:254:GLN:HE22	1:D:334:GLN:CD	2.17	0.48
1:D:91:THR:HG22	1:D:165:GLY:O	2.13	0.48
1:E:317:SER:OG	1:E:320:GLU:OE1	2.30	0.48
1:F:326:LEU:HD13	1:F:328:PRO:HD3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:68:PRO:O	1:F:151:ARG:HD2	2.14	0.48
1:B:146:GLU:CA	1:B:182:TRP:CZ3	2.97	0.48
1:B:150:ARG:O	1:B:151:ARG:C	2.52	0.48
1:D:16:MET:CE	1:D:333:LYS:HE3	2.43	0.48
1:E:323:CYS:O	1:E:345:ALA:HA	2.13	0.48
1:E:383:THR:O	1:E:386:TYR:HB3	2.13	0.48
1:D:390:LEU:CD1	1:E:396:VAL:HG21	2.42	0.48
1:E:428:HIS:HD2	1:E:428:HIS:H	1.61	0.48
1:F:105:VAL:O	1:F:108:VAL:CG2	2.62	0.48
1:F:421:LEU:C	1:F:423:ARG:H	2.17	0.48
1:F:469:MET:O	1:F:470:ARG:C	2.51	0.48
1:F:78:VAL:C	1:F:79:ILE:HD12	2.33	0.48
1:B:135:ILE:HG12	1:B:140:TYR:CE2	2.49	0.48
1:B:175:THR:HG22	1:B:179:GLU:HG2	1.96	0.48
1:B:29:GLU:O	1:B:30:ASP:C	2.52	0.48
1:A:435:VAL:HG12	1:B:420:SER:OG	2.13	0.48
1:C:122:VAL:HG11	1:C:379:ALA:HB3	1.96	0.48
1:C:99:TYR:HB2	1:C:174:SER:HB2	1.96	0.48
1:D:331:SER:HB2	1:D:334:GLN:CD	2.34	0.48
1:F:21:PHE:HE1	1:F:490:ILE:HD12	1.78	0.48
1:F:380:GLY:O	1:F:383:THR:HB	2.13	0.48
1:F:46:ARG:HE	1:F:46:ARG:N	2.12	0.48
1:F:21:PHE:CD1	1:F:490:ILE:HD12	2.49	0.48
1:A:185:ASP:OD1	1:F:505:THR:CG2	2.46	0.48
1:A:231:ILE:O	1:A:237:MET:HG3	2.13	0.48
1:B:267:LEU:O	1:B:272:ALA:HB3	2.14	0.48
1:C:86:HIS:HB3	1:C:116:THR:CG2	2.44	0.48
1:F:231:ILE:CG2	1:F:232:ASN:ND2	2.77	0.48
1:F:35:ASP:CG	1:F:36:LEU:H	2.16	0.48
1:F:404:LYS:O	1:F:405:TYR:C	2.50	0.48
1:A:12:ASN:ND2	1:A:14:PHE:HB3	2.29	0.48
1:B:223:VAL:HG13	1:B:377:LEU:HD21	1.96	0.48
1:B:238:SER:O	1:B:240:LEU:N	2.46	0.48
1:B:253:VAL:O	1:B:253:VAL:HG22	2.13	0.48
1:C:152:PHE:CE2	1:C:156:LEU:HD21	2.48	0.48
1:C:223:VAL:HG11	1:C:263:SER:OG	2.13	0.48
1:C:349:ALA:HB1	1:C:377:LEU:CD2	2.43	0.48
1:D:166:ILE:HG22	1:D:167:ASP:N	2.28	0.48
1:F:122:VAL:HG23	1:F:124:VAL:HG23	1.95	0.48
1:A:146:GLU:O	1:A:147:LYS:C	2.52	0.48
1:A:179:GLU:O	1:A:182:TRP:HB2	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ILE:H	1:A:55:ILE:CD1	2.27	0.48
1:C:264:MET:HG2	1:C:292:PRO:HG3	1.95	0.48
1:D:275:ILE:CG2	1:D:276:ALA:N	2.74	0.48
1:D:33:VAL:HG12	1:D:38:THR:OG1	2.13	0.48
1:D:421:LEU:HD21	1:E:421:LEU:HD11	1.96	0.48
1:F:215:ARG:O	1:F:218:ALA:CB	2.61	0.48
1:A:204:GLY:N	1:A:388:GLU:OE2	2.40	0.47
1:B:108:VAL:O	1:B:109:LYS:C	2.51	0.47
1:B:147:LYS:HE3	1:D:504:PHE:HZ	1.77	0.47
1:B:264:MET:HE3	1:B:292:PRO:CA	2.44	0.47
1:A:433:PRO:HA	1:B:420:SER:CB	2.44	0.47
1:C:378:ASN:C	1:C:378:ASN:ND2	2.64	0.47
1:F:502:VAL:O	1:F:505:THR:CG2	2.62	0.47
1:F:94:LYS:HB2	1:F:126:PHE:CD1	2.48	0.47
1:A:82:TYR:O	1:A:131:ALA:HA	2.14	0.47
1:A:309:PRO:O	1:A:310:LYS:CB	2.62	0.47
1:A:387:PHE:HD2	1:A:387:PHE:N	2.11	0.47
1:A:57:LYS:CB	1:A:58:PRO:CD	2.88	0.47
1:C:281:ASP:CB	1:C:306:LEU:HD21	2.44	0.47
1:C:500:ALA:CA	1:C:505:THR:OXT	2.62	0.47
1:D:150:ARG:O	1:D:153:THR:N	2.47	0.47
1:D:278:GLY:O	1:D:279:GLU:HG2	2.13	0.47
1:D:481:LEU:O	1:D:482:ARG:C	2.53	0.47
1:F:467:GLN:HG3	1:F:470:ARG:HH12	1.79	0.47
1:F:97:ILE:CD1	1:F:131:ALA:HB3	2.45	0.47
1:A:108:VAL:HG23	1:A:109:LYS:N	2.28	0.47
1:A:94:LYS:HB2	1:A:126:PHE:CD1	2.50	0.47
1:A:149:THR:HG1	1:A:182:TRP:HE3	1.59	0.47
1:B:179:GLU:C	1:B:183:ILE:HD13	2.33	0.47
1:B:325:ILE:HG22	1:B:347:ILE:HB	1.96	0.47
1:A:193:HIS:CE1	1:C:158:LYS:HG2	2.50	0.47
1:C:281:ASP:HB3	1:C:306:LEU:HD21	1.96	0.47
1:C:433:PRO:C	1:C:435:VAL:N	2.68	0.47
1:C:51:GLY:HA2	1:C:54:ARG:HG2	1.95	0.47
1:D:409:SER:O	1:D:413:LEU:HD23	2.15	0.47
1:D:481:LEU:O	1:D:484:ALA:N	2.47	0.47
1:E:122:VAL:HB	1:E:460:THR:CG2	2.43	0.47
1:A:69:ILE:HD13	1:A:148:ILE:CG1	2.43	0.47
1:A:153:THR:HG23	1:A:162:ILE:HD13	1.96	0.47
1:A:378:ASN:N	1:A:378:ASN:ND2	2.60	0.47
1:A:28:VAL:HG23	1:A:487:VAL:HG13	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:PHE:O	1:B:365:LEU:C	2.52	0.47
1:B:501:GLY:C	1:B:505:THR:HB	2.34	0.47
1:C:243:THR:H	1:C:244:PRO:HD3	1.73	0.47
1:D:112:ALA:O	1:D:115:MET:HB2	2.14	0.47
1:D:428:HIS:N	1:D:428:HIS:ND1	2.62	0.47
1:E:238:SER:O	1:E:241:GLY:N	2.47	0.47
1:E:284:ILE:CG2	1:E:285:TRP:N	2.77	0.47
1:E:330:ALA:O	1:E:331:SER:O	2.32	0.47
1:F:256:PHE:O	1:F:256:PHE:HD1	1.95	0.47
1:F:415:MET:SD	1:F:434:ILE:CG2	3.02	0.47
1:A:242:MET:O	1:A:243:THR:HG22	2.14	0.47
1:B:168:VAL:HG13	1:B:202:VAL:HA	1.96	0.47
1:C:252:VAL:HG23	1:C:323:CYS:SG	2.54	0.47
1:C:350:GLU:HG2	1:C:355:PRO:CG	2.43	0.47
1:D:320:GLU:O	1:D:344:LYS:HB2	2.15	0.47
1:D:350:GLU:OE2	1:D:355:PRO:HD2	2.13	0.47
1:D:505:THR:C	1:E:150:ARG:HH22	2.17	0.47
1:E:410:ASN:H	1:E:410:ASN:ND2	2.12	0.47
1:E:91:THR:HB	1:E:92:PRO:HD3	1.95	0.47
1:F:334:GLN:NE2	1:F:334:GLN:CA	2.69	0.47
1:A:277:VAL:HG23	1:A:290:ILE:HD12	1.96	0.47
1:B:13:PHE:CD1	1:B:14:PHE:N	2.79	0.47
1:B:275:ILE:CD1	1:B:287:PRO:HA	2.44	0.47
1:C:500:ALA:C	1:C:505:THR:OXT	2.52	0.47
1:D:70:ARG:O	1:D:147:LYS:NZ	2.38	0.47
1:E:180:MET:HG3	1:E:202:VAL:CG2	2.45	0.47
1:E:321:ALA:O	1:E:344:LYS:HB2	2.13	0.47
1:F:464:SER:O	1:F:465:ALA:C	2.52	0.47
1:C:243:THR:CG2	1:C:243:THR:O	2.62	0.47
1:C:425:PHE:HD1	1:C:427:LYS:HB2	1.80	0.47
1:D:327:ILE:CD1	1:D:327:ILE:N	2.66	0.47
1:D:346:LYS:HA	1:D:369:ILE:CD1	2.45	0.47
1:D:94:LYS:CB	1:D:126:PHE:CD1	2.95	0.47
1:E:135:ILE:HD12	1:E:135:ILE:HA	1.62	0.47
1:E:136:ASN:O	1:E:140:TYR:HD2	1.98	0.47
1:A:28:VAL:O	1:A:32:LEU:CB	2.62	0.47
1:A:37:ARG:C	1:A:37:ARG:HD3	2.35	0.47
1:B:393:LEU:O	1:B:395:HIS:HD2	1.95	0.47
1:B:433:PRO:O	1:B:435:VAL:N	2.47	0.47
1:D:254:GLN:HE22	1:D:334:GLN:HG2	1.78	0.47
1:D:43:GLU:C	1:D:45:LYS:N	2.68	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:VAL:HG12	1:E:38:THR:OG1	2.14	0.47
1:E:69:ILE:HA	1:E:151:ARG:NH1	2.30	0.47
1:B:223:VAL:HG13	1:B:377:LEU:CD2	2.45	0.47
1:C:365:LEU:O	1:C:365:LEU:HD23	2.14	0.47
1:C:460:THR:CG2	1:D:400:ARG:HH21	2.26	0.47
1:F:350:GLU:O	1:F:377:LEU:HB3	2.14	0.47
1:A:396:VAL:CG2	1:F:390:LEU:HD21	2.45	0.47
1:A:237:MET:O	1:A:242:MET:N	2.43	0.47
1:B:116:THR:CG2	1:B:128:GLY:HA3	2.39	0.47
1:B:349:ALA:HB1	1:B:377:LEU:CD2	2.45	0.47
1:F:256:PHE:O	1:F:256:PHE:CD1	2.68	0.47
1:A:407:ARG:NH1	1:A:411:TYR:CE2	2.83	0.47
1:B:133:VAL:HG12	1:B:135:ILE:HB	1.97	0.47
1:B:145:LEU:HD23	1:B:148:ILE:HD12	1.97	0.47
1:B:54:ARG:HB3	1:B:54:ARG:CZ	2.45	0.47
1:C:135:ILE:HD13	1:C:148:ILE:HD13	1.96	0.47
1:C:221:ARG:NH1	1:C:221:ARG:HG2	2.13	0.47
1:C:221:ARG:HE	1:C:225:HIS:CE1	2.33	0.47
1:C:22:ASP:O	1:C:23:ARG:C	2.53	0.47
1:C:212:ILE:HD12	1:C:388:GLU:HA	1.96	0.47
1:C:46:ARG:O	1:C:49:VAL:HG12	2.14	0.47
1:D:38:THR:O	1:D:38:THR:CG2	2.62	0.47
1:D:42:GLU:O	1:D:43:GLU:HB2	2.15	0.47
1:C:420:SER:HB3	1:E:433:PRO:HA	1.97	0.47
1:E:56:ILE:CD1	1:E:493:VAL:HG12	2.45	0.47
1:A:136:ASN:O	1:A:137:PRO:C	2.52	0.46
1:A:77:GLU:HA	1:E:54:ARG:NH1	2.30	0.46
1:C:223:VAL:HG22	1:C:377:LEU:HG	1.97	0.46
1:C:405:TYR:CE1	1:E:443:ARG:NH2	2.83	0.46
1:D:259:VAL:O	1:D:263:SER:HB2	2.15	0.46
1:D:339:ASN:N	1:D:339:ASN:ND2	2.63	0.46
1:D:342:ARG:NH1	1:D:342:ARG:HB2	2.29	0.46
1:D:415:MET:CE	1:D:419:GLU:HG3	2.45	0.46
1:E:141:THR:HG23	1:E:144:GLU:HB2	1.96	0.46
1:E:243:THR:O	1:E:243:THR:CG2	2.63	0.46
1:E:503:THR:CA	1:E:505:THR:HG22	2.45	0.46
1:F:367:ARG:HB2	1:F:367:ARG:NH1	2.29	0.46
1:A:262:HIS:CD2	1:A:265:ARG:HH12	2.33	0.46
1:A:358:PRO:O	1:A:361:ASP:HB2	2.15	0.46
1:A:43:GLU:C	1:A:45:LYS:H	2.18	0.46
1:B:104:SER:O	1:B:105:VAL:C	2.52	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:LEU:O	1:B:328:PRO:HD3	2.16	0.46
1:B:407:ARG:HH11	1:B:407:ARG:HG2	1.80	0.46
1:D:264:MET:HE3	1:D:292:PRO:CB	2.45	0.46
1:E:250:THR:O	1:E:323:CYS:HB2	2.15	0.46
1:A:401:LEU:HD21	1:F:387:PHE:CE2	2.50	0.46
1:A:401:LEU:HD13	1:F:398:TYR:CE2	2.50	0.46
1:A:220:GLY:O	1:A:221:ARG:C	2.53	0.46
1:A:254:GLN:HB2	1:A:318:ILE:CD1	2.43	0.46
1:A:322:ASP:HA	1:A:344:LYS:HB2	1.96	0.46
1:A:486:TYR:O	1:A:490:ILE:HG13	2.15	0.46
1:B:54:ARG:O	1:B:58:PRO:CD	2.63	0.46
1:C:150:ARG:O	1:C:153:THR:HB	2.15	0.46
1:D:125:PRO:O	1:D:126:PHE:CD2	2.67	0.46
1:D:86:HIS:HD2	1:D:116:THR:CG2	2.10	0.46
1:F:391:LYS:HE3	1:F:397:SER:HA	1.97	0.46
1:C:151:ARG:HD3	1:F:503:THR:CG2	2.45	0.46
1:A:103:VAL:HG21	1:A:134:LYS:N	2.30	0.46
1:A:233:GLU:HG2	1:A:236:TYR:HD1	1.79	0.46
1:A:283:SER:HB2	1:A:314:TYR:O	2.16	0.46
1:A:124:VAL:HG22	1:A:386:TYR:CD1	2.51	0.46
1:A:372:ILE:HA	1:A:481:LEU:HD23	1.98	0.46
1:A:48:ARG:C	1:A:50:ARG:H	2.17	0.46
1:B:407:ARG:HG2	1:B:407:ARG:NH1	2.30	0.46
1:B:478:GLY:C	1:B:480:ASP:H	2.17	0.46
1:C:306:LEU:N	1:C:306:LEU:HD12	2.31	0.46
1:C:69:ILE:HD13	1:C:148:ILE:HG12	1.96	0.46
1:D:146:GLU:CD	1:D:150:ARG:HH11	2.19	0.46
1:D:146:GLU:HG3	1:D:182:TRP:CE2	2.50	0.46
1:E:152:PHE:CE2	1:E:156:LEU:HD21	2.50	0.46
1:E:242:MET:O	1:E:243:THR:C	2.54	0.46
1:E:252:VAL:HG13	1:E:276:ALA:HB3	1.97	0.46
1:E:336:THR:HA	1:E:357:THR:CG2	2.43	0.46
1:F:394:ASN:O	1:F:396:VAL:HG22	2.15	0.46
1:F:42:GLU:O	1:F:43:GLU:HB2	2.14	0.46
1:F:457:LEU:CD2	1:F:461:MET:HG2	2.45	0.46
1:F:51:GLY:CA	1:F:54:ARG:HG2	2.45	0.46
1:A:401:LEU:HD21	1:F:387:PHE:CD2	2.51	0.46
1:A:451:ASP:O	1:A:455:SER:OG	2.32	0.46
1:A:47:ASN:ND2	1:A:50:ARG:NH2	2.64	0.46
1:B:384:VAL:O	1:B:387:PHE:HB2	2.16	0.46
1:B:96:GLY:O	1:B:130:LYS:HD2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:VAL:O	1:C:435:VAL:HG12	2.15	0.46
1:D:133:VAL:HG12	1:D:135:ILE:HB	1.97	0.46
1:D:25:ALA:HB1	1:D:53:LEU:HD23	1.98	0.46
1:E:94:LYS:HA	1:E:94:LYS:HD2	1.76	0.46
1:F:69:ILE:HG23	1:F:79:ILE:HD13	1.96	0.46
1:A:54:ARG:CZ	1:A:54:ARG:HB2	2.45	0.46
1:C:78:VAL:H	1:F:54:ARG:NH2	2.07	0.46
1:D:179:GLU:HA	1:D:182:TRP:CE3	2.51	0.46
1:E:94:LYS:HB2	1:E:126:PHE:HB3	1.97	0.46
1:F:95:GLY:O	1:F:169:PRO:HA	2.16	0.46
1:F:51:GLY:O	1:F:54:ARG:CG	2.64	0.46
1:F:71:ARG:HB3	1:F:71:ARG:HH11	1.79	0.46
1:A:224:PHE:CD1	1:A:224:PHE:C	2.88	0.46
1:A:267:LEU:HD13	1:A:267:LEU:HA	1.68	0.46
1:B:94:LYS:HD2	1:B:168:VAL:O	2.14	0.46
1:B:196:ILE:O	1:B:395:HIS:CE1	2.68	0.46
1:B:424:LYS:O	1:B:425:PHE:CB	2.63	0.46
1:B:502:VAL:O	1:B:505:THR:CG2	2.63	0.46
1:E:325:ILE:HG23	1:E:347:ILE:HG21	1.96	0.46
1:F:231:ILE:O	1:F:237:MET:HG3	2.16	0.46
1:F:46:ARG:NE	1:F:46:ARG:CA	2.79	0.46
1:A:106:ASP:O	1:A:107:GLU:C	2.54	0.46
1:B:193:HIS:O	1:B:193:HIS:CG	2.69	0.46
1:B:425:PHE:O	1:B:425:PHE:CD1	2.69	0.46
1:C:349:ALA:HB1	1:C:377:LEU:HD21	1.98	0.46
1:D:306:LEU:HD12	1:D:306:LEU:N	2.31	0.46
1:D:28:VAL:CG2	1:D:487:VAL:HG13	2.44	0.46
1:E:218:ALA:CB	1:E:384:VAL:HG21	2.46	0.46
1:F:171:PRO:HG3	1:F:180:MET:CG	2.46	0.46
1:F:339:ASN:ND2	1:F:339:ASN:C	2.69	0.46
1:F:38:THR:O	1:F:38:THR:CG2	2.62	0.46
1:A:249:LYS:HB2	1:A:272:ALA:HA	1.97	0.46
1:A:427:LYS:HG2	1:A:430:GLY:CA	2.43	0.46
1:C:408:ASP:O	1:C:409:SER:O	2.34	0.46
1:D:238:SER:C	1:D:240:LEU:N	2.70	0.46
1:E:428:HIS:H	1:E:428:HIS:CD2	2.33	0.46
1:E:56:ILE:C	1:E:58:PRO:HD2	2.36	0.46
1:F:91:THR:CB	1:F:92:PRO:CD	2.84	0.46
1:A:72:ASP:OD2	1:A:141:THR:HG21	2.16	0.46
1:A:339:ASN:HD22	1:A:339:ASN:N	2.14	0.46
1:B:304:SER:OG	1:B:305:ILE:N	2.47	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLU:C	1:D:45:LYS:H	2.18	0.46
1:E:85:GLN:NE2	1:E:167:ASP:OD2	2.49	0.46
1:F:304:SER:OG	1:F:305:ILE:N	2.49	0.46
1:A:265:ARG:O	1:A:268:HIS:HB3	2.16	0.45
1:A:500:ALA:CB	1:A:505:THR:O	2.64	0.45
1:A:52:ILE:O	1:A:56:ILE:HG13	2.16	0.45
1:B:349:ALA:HB1	1:B:377:LEU:HD21	1.97	0.45
1:C:146:GLU:O	1:C:150:ARG:HG3	2.17	0.45
1:D:172:ASP:C	1:D:172:ASP:OD1	2.53	0.45
1:D:319:LEU:H	1:D:319:LEU:CD1	2.28	0.45
1:E:108:VAL:O	1:E:109:LYS:C	2.55	0.45
1:E:178:ARG:O	1:E:179:GLU:C	2.53	0.45
1:E:382:VAL:O	1:E:385:SER:OG	2.31	0.45
1:F:418:GLN:HA	1:F:433:PRO:HG2	1.98	0.45
1:A:162:ILE:HG23	1:A:162:ILE:O	2.16	0.45
1:A:427:LYS:HG2	1:A:430:GLY:H	1.80	0.45
1:A:421:LEU:HD21	1:B:421:LEU:HD21	1.97	0.45
1:C:256:PHE:CZ	1:C:295:LEU:HD23	2.52	0.45
1:C:505:THR:C	1:D:150:ARG:HH22	2.19	0.45
1:F:104:SER:HG	1:F:107:GLU:H	1.61	0.45
1:A:402:THR:O	1:A:405:TYR:N	2.49	0.45
1:A:484:ALA:O	1:A:487:VAL:HB	2.16	0.45
1:A:54:ARG:O	1:A:58:PRO:CD	2.57	0.45
1:B:13:PHE:CE1	1:B:107:GLU:HA	2.51	0.45
1:B:256:PHE:HB3	1:B:279:GLU:OE1	2.17	0.45
1:D:460:THR:O	1:D:461:MET:C	2.55	0.45
1:D:56:ILE:O	1:D:86:HIS:CE1	2.70	0.45
1:E:482:ARG:O	1:E:485:ALA:HB3	2.16	0.45
1:E:52:ILE:O	1:E:55:ILE:HB	2.15	0.45
1:E:61:HIS:CD2	1:E:88:GLN:NE2	2.81	0.45
1:F:306:LEU:H	1:F:306:LEU:HD12	1.82	0.45
1:F:314:TYR:CE2	1:F:318:ILE:HA	2.44	0.45
1:A:253:VAL:HA	1:A:327:ILE:HG12	1.97	0.45
1:A:350:GLU:OE2	1:A:482:ARG:NH2	2.40	0.45
1:B:336:THR:HG22	1:B:357:THR:HG21	1.99	0.45
1:C:108:VAL:HG23	1:C:109:LYS:N	2.32	0.45
1:C:334:GLN:HA	1:C:334:GLN:NE2	2.31	0.45
1:C:462:GLU:O	1:C:463:ALA:C	2.52	0.45
1:C:77:GLU:CA	1:F:54:ARG:HH12	2.30	0.45
1:E:150:ARG:O	1:E:154:MET:HG2	2.16	0.45
1:A:227:ILE:CD1	1:A:349:ALA:HB2	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:LYS:CG	1:A:428:HIS:N	2.78	0.45
1:B:146:GLU:HG3	1:B:182:TRP:CD2	2.51	0.45
1:C:190:THR:CG2	1:C:191:ILE:H	2.16	0.45
1:C:477:LEU:HD12	1:C:484:ALA:CB	2.46	0.45
1:D:31:LYS:HD3	1:D:35:ASP:OD2	2.15	0.45
1:D:320:GLU:O	1:D:321:ALA:C	2.54	0.45
1:D:488:ASN:O	1:D:492:LYS:HG2	2.17	0.45
1:E:169:PRO:O	1:E:202:VAL:HG23	2.16	0.45
1:E:183:ILE:O	1:E:184:ALA:C	2.52	0.45
1:A:253:VAL:HG22	1:A:253:VAL:O	2.17	0.45
1:A:33:VAL:O	1:A:34:GLU:O	2.34	0.45
1:B:248:ASP:CG	1:B:249:LYS:N	2.69	0.45
1:B:320:GLU:HG2	1:B:342:ARG:HG2	1.98	0.45
1:C:284:ILE:HD12	1:C:284:ILE:HA	1.70	0.45
1:C:293:LYS:O	1:C:293:LYS:HE2	2.16	0.45
1:C:433:PRO:HA	1:D:420:SER:OG	2.17	0.45
1:D:207:ILE:HD11	1:D:212:ILE:O	2.16	0.45
1:E:264:MET:HE3	1:E:292:PRO:CA	2.45	0.45
1:E:281:ASP:HB2	1:E:306:LEU:CD1	2.45	0.45
1:F:318:ILE:O	1:F:321:ALA:N	2.49	0.45
1:A:224:PHE:CE2	1:A:270:PHE:CD2	3.05	0.45
1:A:224:PHE:HD1	1:A:225:HIS:N	2.12	0.45
1:A:390:LEU:O	1:A:394:ASN:ND2	2.49	0.45
1:A:71:ARG:HD2	1:A:77:GLU:OE2	2.16	0.45
1:A:86:HIS:CD2	1:A:116:THR:CG2	2.90	0.45
1:B:264:MET:HE1	1:B:292:PRO:HA	1.98	0.45
1:B:325:ILE:HG22	1:B:347:ILE:CB	2.47	0.45
1:C:13:PHE:CE1	1:C:107:GLU:HA	2.52	0.45
1:D:284:ILE:CG1	1:D:305:ILE:HD12	2.47	0.45
1:D:440:PHE:CE1	1:E:413:LEU:HD22	2.51	0.45
1:E:101:THR:HA	1:E:134:LYS:HG3	1.99	0.45
1:E:135:ILE:HG13	1:E:140:TYR:CE2	2.51	0.45
1:F:243:THR:O	1:F:243:THR:CG2	2.63	0.45
1:F:333:LYS:HA	1:F:355:PRO:O	2.17	0.45
1:F:418:GLN:OE1	1:F:434:ILE:HG12	2.17	0.45
1:A:101:THR:HG22	1:A:101:THR:O	2.17	0.45
1:A:231:ILE:HG22	1:A:232:ASN:OD1	2.17	0.45
1:A:335:LEU:HD13	1:A:348:ILE:HD13	1.98	0.45
1:B:264:MET:HE3	1:B:292:PRO:CB	2.47	0.45
1:B:387:PHE:HD2	1:B:387:PHE:N	2.15	0.45
1:C:339:ASN:C	1:C:339:ASN:HD22	2.18	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:ILE:O	1:C:468:ILE:HG22	2.15	0.45
1:A:143:ASN:ND2	1:C:70:ARG:NH2	2.65	0.45
1:D:23:ARG:HD2	1:D:483:THR:HB	1.98	0.45
1:D:418:GLN:O	1:D:419:GLU:C	2.54	0.45
1:A:62:VAL:CG1	1:E:64:SER:HB2	2.46	0.45
1:C:159:LYS:HD2	1:F:161:PHE:CZ	2.52	0.45
1:F:23:ARG:O	1:F:26:SER:OG	2.35	0.45
1:F:343:VAL:HG11	1:F:364:PHE:CE1	2.52	0.45
1:A:370:MET:CB	1:A:479:LEU:HD23	2.43	0.45
1:A:489:ALA:O	1:A:493:VAL:HG23	2.16	0.45
1:B:502:VAL:O	1:B:505:THR:HG21	2.17	0.45
1:C:229:ASN:HD21	1:C:462:GLU:CA	2.28	0.45
1:C:266:TYR:O	1:C:267:LEU:C	2.54	0.45
1:C:26:SER:O	1:C:27:ILE:C	2.55	0.45
1:C:308:PHE:C	1:C:309:PRO:O	2.55	0.45
1:C:494:PHE:CD2	1:C:494:PHE:C	2.90	0.45
1:D:104:SER:O	1:D:107:GLU:N	2.49	0.45
1:D:31:LYS:HD2	1:D:36:LEU:HD11	1.98	0.45
1:D:37:ARG:HH11	1:D:37:ARG:CB	2.11	0.45
1:D:381:GLY:C	1:D:383:THR:H	2.20	0.45
1:D:40:GLU:O	1:D:42:GLU:N	2.50	0.45
1:D:51:GLY:HA2	1:D:54:ARG:HG2	1.98	0.45
1:B:254:GLN:HG3	1:B:318:ILE:HD11	2.00	0.45
1:B:51:GLY:O	1:B:55:ILE:HG13	2.18	0.45
1:C:146:GLU:HA	1:C:182:TRP:CE3	2.52	0.45
1:C:264:MET:HE3	1:C:292:PRO:CG	2.47	0.45
1:F:375:LEU:HD23	1:F:485:ALA:HB1	1.99	0.45
1:A:396:VAL:HG22	1:F:390:LEU:HD21	1.98	0.45
1:F:501:GLY:HA3	1:F:504:PHE:O	2.16	0.45
1:A:341:PRO:HA	1:A:367:ARG:NE	2.32	0.44
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.78	0.44
1:B:71:ARG:NE	1:B:77:GLU:OE2	2.49	0.44
1:C:23:ARG:HE	1:C:483:THR:HG21	1.82	0.44
1:C:432:ILE:HG22	1:C:434:ILE:HD11	1.99	0.44
1:D:112:ALA:O	1:D:115:MET:N	2.50	0.44
1:D:390:LEU:HD22	1:E:396:VAL:CG2	2.48	0.44
1:F:220:GLY:O	1:F:223:VAL:HB	2.17	0.44
1:A:144:GLU:O	1:A:147:LYS:HB2	2.17	0.44
1:A:350:GLU:HG2	1:A:355:PRO:CG	2.48	0.44
1:B:407:ARG:NH1	1:B:411:TYR:CD2	2.85	0.44
1:B:431:THR:HG22	1:B:433:PRO:HD3	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:SER:O	1:C:218:ALA:C	2.56	0.44
1:C:259:VAL:HG21	1:C:351:GLY:O	2.17	0.44
1:C:27:ILE:HG22	1:C:475:TYR:CD1	2.52	0.44
1:D:398:TYR:CE2	1:E:401:LEU:HD22	2.52	0.44
1:D:457:LEU:HD22	1:D:461:MET:HG2	1.98	0.44
1:E:28:VAL:CG1	1:E:32:LEU:HD22	2.48	0.44
1:E:71:ARG:HH11	1:E:71:ARG:CB	2.18	0.44
1:F:285:TRP:HE1	1:F:287:PRO:CG	2.29	0.44
1:A:206:PRO:HD2	1:A:209:GLN:HB2	1.99	0.44
1:A:251:PHE:HE1	1:A:272:ALA:CB	2.31	0.44
1:A:348:ILE:O	1:A:371:VAL:HG13	2.17	0.44
1:A:40:GLU:HG3	1:A:40:GLU:O	2.16	0.44
1:A:452:ILE:N	1:A:452:ILE:HD12	2.32	0.44
1:A:55:ILE:HD12	1:A:55:ILE:N	2.32	0.44
1:B:151:ARG:O	1:B:155:GLU:HG2	2.17	0.44
1:B:49:VAL:C	1:B:51:GLY:H	2.18	0.44
1:C:212:ILE:O	1:C:212:ILE:HG23	2.16	0.44
1:D:226:GLY:HA3	1:D:377:LEU:CD1	2.47	0.44
1:D:317:SER:O	1:D:319:LEU:N	2.50	0.44
1:F:449:GLU:O	1:F:450:LYS:C	2.56	0.44
1:F:500:ALA:HA	1:F:505:THR:O	2.16	0.44
1:A:209:GLN:NE2	1:F:496:VAL:O	2.51	0.44
1:B:157:ALA:HA	1:B:162:ILE:HG22	1.99	0.44
1:B:24:GLY:O	1:B:27:ILE:N	2.49	0.44
1:B:293:LYS:NZ	1:B:297:ASP:OD2	2.48	0.44
1:C:418:GLN:O	1:C:419:GLU:C	2.55	0.44
1:D:125:PRO:O	1:D:126:PHE:HD2	2.01	0.44
1:D:435:VAL:HG13	1:D:435:VAL:O	2.16	0.44
1:E:186:THR:O	1:E:190:THR:HB	2.18	0.44
1:E:46:ARG:HA	1:E:46:ARG:HE	1.82	0.44
1:E:62:VAL:O	1:E:62:VAL:HG13	2.16	0.44
1:F:168:VAL:O	1:F:169:PRO:O	2.35	0.44
1:F:55:ILE:HG22	1:F:56:ILE:N	2.32	0.44
1:A:169:PRO:HD2	1:A:202:VAL:HG23	1.99	0.44
1:B:180:MET:N	1:B:180:MET:HE3	2.33	0.44
1:B:292:PRO:O	1:B:293:LYS:C	2.55	0.44
1:D:116:THR:H	1:D:128:GLY:HA3	1.83	0.44
1:D:380:GLY:O	1:D:383:THR:HB	2.17	0.44
1:F:12:ASN:O	1:F:13:PHE:C	2.55	0.44
1:F:170:ALA:CA	1:F:180:MET:CE	2.96	0.44
1:F:266:TYR:O	1:F:267:LEU:C	2.56	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:ASP:HA	1:F:344:LYS:HB2	1.99	0.44
1:F:474:LYS:NZ	1:F:475:TYR:CE2	2.85	0.44
1:A:299:LYS:HB2	1:A:305:ILE:HG22	2.00	0.44
1:A:317:SER:OG	1:A:320:GLU:OE2	2.36	0.44
1:A:388:GLU:O	1:A:391:LYS:HB3	2.17	0.44
1:A:350:GLU:CD	1:A:482:ARG:HH22	2.20	0.44
1:B:298:PHE:CZ	1:B:302:HIS:CE1	3.05	0.44
1:B:418:GLN:OE1	1:B:432:ILE:HA	2.18	0.44
1:C:340:ALA:HB1	1:C:363:ILE:HG21	2.00	0.44
1:C:38:THR:CG2	1:C:38:THR:O	2.65	0.44
1:D:190:THR:HG22	1:D:191:ILE:H	1.79	0.44
1:D:264:MET:HG2	1:D:292:PRO:HG3	2.00	0.44
1:D:265:ARG:HG2	1:D:292:PRO:HB3	1.99	0.44
1:D:79:ILE:HG22	1:D:80:GLU:N	2.31	0.44
1:D:386:TYR:OH	1:E:396:VAL:HG22	2.17	0.44
1:E:480:ASP:CG	1:E:483:THR:CG2	2.86	0.44
1:F:130:LYS:HG3	1:F:131:ALA:N	2.32	0.44
1:F:13:PHE:HD1	1:F:14:PHE:H	1.44	0.44
1:F:141:THR:OG1	1:F:144:GLU:HG3	2.18	0.44
1:F:34:GLU:HA	1:F:38:THR:CB	2.44	0.44
1:F:89:HIS:HD2	1:F:496:VAL:HG21	1.83	0.44
1:B:229:ASN:ND2	1:B:462:GLU:HA	2.33	0.44
1:B:237:MET:O	1:B:242:MET:N	2.50	0.44
1:B:244:PRO:O	1:B:248:ASP:HA	2.18	0.44
1:B:495:LYS:O	1:B:496:VAL:C	2.55	0.44
1:B:51:GLY:CA	1:B:54:ARG:HG3	2.47	0.44
1:C:221:ARG:HE	1:C:225:HIS:HE1	1.65	0.44
1:C:438:ALA:O	1:C:441:GLN:N	2.48	0.44
1:C:47:ASN:O	1:C:50:ARG:CG	2.65	0.44
1:C:72:ASP:OD1	1:C:144:GLU:HG2	2.17	0.44
1:D:72:ASP:OD2	1:D:141:THR:HG21	2.18	0.44
1:D:291:ASP:HA	1:D:292:PRO:HD3	1.80	0.44
1:D:345:ALA:O	1:D:369:ILE:CD1	2.64	0.44
1:D:377:LEU:O	1:D:377:LEU:HG	2.17	0.44
1:D:489:ALA:O	1:D:493:VAL:HG23	2.17	0.44
1:F:285:TRP:NE1	1:F:287:PRO:CD	2.81	0.44
1:B:433:PRO:HA	1:F:420:SER:CB	2.48	0.44
1:B:168:VAL:CG1	1:B:202:VAL:HA	2.47	0.44
1:B:32:LEU:HD21	1:B:494:PHE:CG	2.52	0.44
1:D:339:ASN:HD22	1:D:340:ALA:N	2.16	0.44
1:D:440:PHE:CG	1:E:412:HIS:HB3	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:487:VAL:O	1:D:488:ASN:C	2.56	0.44
1:E:180:MET:HG3	1:E:202:VAL:HG22	1.99	0.44
1:F:383:THR:O	1:F:386:TYR:HB3	2.17	0.44
1:F:418:GLN:HG3	1:F:433:PRO:CD	2.47	0.44
1:B:215:ARG:O	1:B:216:ILE:C	2.57	0.44
1:B:427:LYS:HG2	1:B:430:GLY:CA	2.48	0.44
1:B:91:THR:OG1	1:B:92:PRO:HD3	2.18	0.44
1:C:47:ASN:O	1:C:50:ARG:HG3	2.18	0.44
1:D:135:ILE:HD13	1:D:140:TYR:CE2	2.53	0.44
1:D:326:LEU:O	1:D:328:PRO:HD3	2.18	0.44
1:D:439:GLU:CD	1:D:439:GLU:H	2.21	0.44
1:E:477:LEU:HD13	1:E:483:THR:HG23	2.00	0.44
1:F:146:GLU:HA	1:F:182:TRP:CE3	2.53	0.44
1:F:218:ALA:O	1:F:219:THR:C	2.54	0.44
1:F:228:GLU:O	1:F:231:ILE:HG22	2.18	0.44
1:F:320:GLU:OE1	1:F:342:ARG:HB3	2.18	0.44
1:F:336:THR:O	1:F:337:LYS:C	2.57	0.44
1:F:27:ILE:HG22	1:F:475:TYR:CD1	2.53	0.44
1:A:38:THR:O	1:A:38:THR:HG22	2.17	0.43
1:A:44:GLN:C	1:A:46:ARG:H	2.20	0.43
1:A:494:PHE:CD2	1:A:494:PHE:C	2.91	0.43
1:A:51:GLY:O	1:A:52:ILE:C	2.56	0.43
1:B:183:ILE:N	1:B:183:ILE:HD12	2.33	0.43
1:B:231:ILE:HG23	1:B:231:ILE:O	2.17	0.43
1:C:162:ILE:O	1:C:162:ILE:HG12	2.17	0.43
1:C:71:ARG:CG	1:C:71:ARG:HH11	2.31	0.43
1:C:78:VAL:CG2	1:C:78:VAL:O	2.66	0.43
1:C:57:LYS:O	1:C:86:HIS:HE1	2.01	0.43
1:D:10:ASP:O	1:D:10:ASP:CG	2.56	0.43
1:D:114:LEU:HD12	1:D:114:LEU:HA	1.80	0.43
1:D:256:PHE:HD1	1:D:299:LYS:HG2	1.83	0.43
1:D:317:SER:C	1:D:319:LEU:H	2.21	0.43
1:D:340:ALA:HB3	1:D:341:PRO:HD3	2.00	0.43
1:D:340:ALA:O	1:D:343:VAL:HG22	2.18	0.43
1:D:373:PRO:HD3	1:D:481:LEU:HB2	2.00	0.43
1:D:48:ARG:C	1:D:50:ARG:H	2.21	0.43
1:E:168:VAL:HA	1:E:201:CYS:O	2.18	0.43
1:E:285:TRP:O	1:E:286:ASN:HB2	2.18	0.43
1:F:63:LEU:HD22	1:F:161:PHE:CD2	2.53	0.43
1:F:97:ILE:HD13	1:F:131:ALA:HB3	2.00	0.43
1:B:418:GLN:HG2	1:B:422:GLU:OE2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:THR:CB	1:B:92:PRO:HD3	2.48	0.43
1:C:10:ASP:HA	1:C:11:PRO:HD3	1.76	0.43
1:D:306:LEU:CD1	1:D:306:LEU:H	2.32	0.43
1:E:10:ASP:HA	1:E:11:PRO:HD3	1.75	0.43
1:E:380:GLY:O	1:E:384:VAL:HG23	2.18	0.43
1:E:414:LEU:HB3	1:E:434:ILE:HA	1.99	0.43
1:E:69:ILE:HD13	1:E:148:ILE:CG1	2.48	0.43
1:F:223:VAL:HG11	1:F:263:SER:HG	1.80	0.43
1:F:46:ARG:HE	1:F:46:ARG:CA	2.30	0.43
1:A:32:LEU:HD21	1:A:494:PHE:CG	2.53	0.43
1:A:376:TYR:CD1	1:A:377:LEU:N	2.86	0.43
1:A:43:GLU:C	1:A:45:LYS:N	2.70	0.43
1:A:503:THR:OG1	1:E:151:ARG:CZ	2.66	0.43
1:B:254:GLN:OE1	1:B:319:LEU:HD11	2.19	0.43
1:C:157:ALA:N	1:C:162:ILE:HG22	2.33	0.43
1:C:264:MET:HE3	1:C:292:PRO:CB	2.48	0.43
1:C:372:ILE:HA	1:C:373:PRO:HD3	1.61	0.43
1:C:91:THR:OG1	1:C:92:PRO:HD3	2.18	0.43
1:D:104:SER:O	1:D:105:VAL:C	2.57	0.43
1:D:284:ILE:HD12	1:D:311:ALA:CB	2.48	0.43
1:D:465:ALA:O	1:D:469:MET:HG3	2.18	0.43
1:E:223:VAL:HG12	1:E:224:PHE:N	2.33	0.43
1:E:86:HIS:CD2	1:E:116:THR:CG2	2.90	0.43
1:F:59:CYS:SG	1:F:109:LYS:O	2.63	0.43
1:F:153:THR:HG23	1:F:183:ILE:HG23	1.99	0.43
1:F:256:PHE:CZ	1:F:296:GLU:HA	2.51	0.43
1:F:34:GLU:CA	1:F:38:THR:HB	2.44	0.43
1:A:112:ALA:HB1	1:A:129:ALA:HA	2.00	0.43
1:A:170:ALA:C	1:A:180:MET:CE	2.87	0.43
1:A:334:GLN:N	1:A:355:PRO:O	2.51	0.43
1:A:372:ILE:HG21	1:A:377:LEU:HD13	2.00	0.43
1:B:94:LYS:CB	1:B:126:PHE:CD1	3.01	0.43
1:B:427:LYS:CG	1:B:430:GLY:H	2.31	0.43
1:C:136:ASN:HA	1:C:137:PRO:HD3	1.76	0.43
1:D:135:ILE:HG23	1:D:136:ASN:N	2.33	0.43
1:D:220:GLY:C	1:D:222:GLY:N	2.71	0.43
1:D:231:ILE:O	1:D:237:MET:HG3	2.16	0.43
1:D:387:PHE:HD1	1:D:453:VAL:HG13	1.83	0.43
1:D:484:ALA:O	1:D:487:VAL:HB	2.19	0.43
1:E:231:ILE:CG2	1:E:232:ASN:N	2.82	0.43
1:E:23:ARG:HD3	1:E:23:ARG:C	2.38	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:449:GLU:O	1:E:451:ASP:N	2.51	0.43
1:F:256:PHE:CD1	1:F:299:LYS:HG2	2.53	0.43
1:F:37:ARG:HD3	1:F:37:ARG:C	2.38	0.43
1:A:374:ASP:O	1:A:376:TYR:N	2.52	0.43
1:A:56:ILE:O	1:A:86:HIS:CE1	2.71	0.43
1:B:169:PRO:HB2	1:B:202:VAL:CG2	2.45	0.43
1:B:171:PRO:HB2	1:B:175:THR:O	2.19	0.43
1:B:300:LEU:O	1:B:301:GLN:C	2.56	0.43
1:B:86:HIS:HB3	1:B:116:THR:CG2	2.49	0.43
1:C:116:THR:HG22	1:C:128:GLY:N	2.33	0.43
1:C:162:ILE:HA	1:C:167:ASP:O	2.19	0.43
1:E:320:GLU:OE2	1:E:342:ARG:NE	2.51	0.43
1:F:480:ASP:OD2	1:F:483:THR:HG23	2.18	0.43
1:A:116:THR:HG22	1:A:128:GLY:H	1.81	0.43
1:A:90:ARG:HG2	1:A:125:PRO:HA	2.01	0.43
1:A:176:GLY:O	1:A:178:ARG:N	2.52	0.43
1:B:94:LYS:HB2	1:B:126:PHE:CG	2.52	0.43
1:B:147:LYS:O	1:B:151:ARG:HG3	2.18	0.43
1:C:386:TYR:O	1:C:390:LEU:HG	2.19	0.43
1:C:440:PHE:CD2	1:D:412:HIS:HB3	2.54	0.43
1:C:76:TRP:CD1	1:F:502:VAL:HG11	2.53	0.43
1:D:130:LYS:HG3	1:D:131:ALA:N	2.32	0.43
1:D:383:THR:O	1:D:386:TYR:HB3	2.18	0.43
1:E:136:ASN:OD1	1:E:138:LYS:CB	2.66	0.43
1:E:146:GLU:HA	1:E:182:TRP:CE3	2.53	0.43
1:E:279:GLU:OE1	1:E:299:LYS:NZ	2.44	0.43
1:E:298:PHE:CZ	1:E:302:HIS:HE1	2.37	0.43
1:E:410:ASN:O	1:E:413:LEU:HB2	2.19	0.43
1:F:224:PHE:CE2	1:F:266:TYR:O	2.71	0.43
1:F:286:ASN:ND2	1:F:310:LYS:O	2.50	0.43
1:F:474:LYS:NZ	1:F:475:TYR:CZ	2.85	0.43
1:A:212:ILE:CG1	1:A:449:GLU:OE1	2.67	0.43
1:A:254:GLN:HG2	1:A:254:GLN:O	2.17	0.43
1:B:63:LEU:HD21	1:B:65:LEU:CD2	2.49	0.43
1:C:33:VAL:C	1:C:38:THR:HG1	2.22	0.43
1:C:229:ASN:OD1	1:C:466:ARG:NH1	2.51	0.43
1:D:400:ARG:HB3	1:D:401:LEU:HD12	2.01	0.43
1:D:63:LEU:CD2	1:D:65:LEU:HD21	2.39	0.43
1:E:116:THR:CG2	1:E:128:GLY:CA	2.96	0.43
1:E:319:LEU:N	1:E:319:LEU:CD1	2.81	0.43
1:E:38:THR:O	1:E:38:THR:HG22	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:THR:O	1:E:461:MET:C	2.56	0.43
1:C:503:THR:CG2	1:F:151:ARG:HD3	2.48	0.43
1:F:221:ARG:HD3	1:F:454:HIS:CG	2.53	0.43
1:F:49:VAL:C	1:F:51:GLY:H	2.21	0.43
1:A:17:VAL:HG22	1:A:114:LEU:CD1	2.49	0.43
1:A:229:ASN:ND2	1:A:462:GLU:HA	2.33	0.43
1:B:177:GLU:HB2	1:B:206:PRO:HG3	2.00	0.43
1:B:500:ALA:C	1:B:505:THR:O	2.57	0.43
1:C:334:GLN:HE21	1:C:334:GLN:N	2.16	0.43
1:C:94:LYS:HB3	1:C:115:MET:HE1	2.01	0.43
1:D:136:ASN:C	1:D:138:LYS:N	2.72	0.43
1:D:180:MET:HG2	1:D:203:THR:O	2.18	0.43
1:D:243:THR:O	1:D:243:THR:CG2	2.65	0.43
1:D:268:HIS:ND1	1:D:292:PRO:CD	2.82	0.43
1:D:295:LEU:HD11	1:D:305:ILE:HB	2.00	0.43
1:D:57:LYS:HB3	1:D:58:PRO:HD3	2.00	0.43
1:E:12:ASN:O	1:E:13:PHE:C	2.57	0.43
1:C:151:ARG:NH2	1:F:504:PHE:CE1	2.87	0.43
1:A:179:GLU:CD	1:A:179:GLU:H	2.21	0.43
1:A:436:PRO:HB3	1:A:440:PHE:CD1	2.46	0.43
1:B:122:VAL:O	1:B:124:VAL:HG23	2.19	0.43
1:B:33:VAL:O	1:B:37:ARG:HG3	2.18	0.43
1:B:376:TYR:O	1:B:378:ASN:N	2.50	0.43
1:C:21:PHE:CE2	1:C:57:LYS:HB2	2.54	0.43
1:C:432:ILE:CG2	1:C:434:ILE:HD11	2.48	0.43
1:D:183:ILE:O	1:D:184:ALA:C	2.56	0.43
1:D:248:ASP:C	1:D:249:LYS:HG3	2.38	0.43
1:D:251:PHE:CD2	1:D:327:ILE:HD11	2.52	0.43
1:E:151:ARG:O	1:E:152:PHE:C	2.57	0.43
1:E:168:VAL:HG13	1:E:202:VAL:HA	2.00	0.43
1:C:396:VAL:CG1	1:E:386:TYR:OH	2.55	0.43
1:F:485:ALA:O	1:F:488:ASN:HB3	2.18	0.43
1:F:83:ARG:HD2	1:F:131:ALA:CB	2.40	0.43
1:A:142:ASP:O	1:A:145:LEU:HB2	2.19	0.43
1:A:376:TYR:HD1	1:A:377:LEU:N	2.16	0.43
1:A:37:ARG:O	1:A:37:ARG:NH1	2.52	0.43
1:A:395:HIS:C	1:A:396:VAL:CG2	2.87	0.43
1:B:133:VAL:O	1:B:135:ILE:N	2.52	0.43
1:B:93:CYS:HB3	1:B:167:ASP:OD1	2.19	0.43
1:C:10:ASP:OD1	1:C:10:ASP:N	2.52	0.43
1:C:435:VAL:HA	1:C:436:PRO:HD3	1.78	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:HIS:HB2	1:C:449:GLU:HG2	2.01	0.43
1:D:358:PRO:O	1:D:361:ASP:HB2	2.19	0.43
1:E:69:ILE:HD13	1:E:148:ILE:HG12	2.01	0.43
1:E:34:GLU:O	1:E:35:ASP:C	2.57	0.43
1:F:108:VAL:CG2	1:F:109:LYS:N	2.82	0.43
1:F:406:GLU:O	1:F:407:ARG:C	2.57	0.43
1:C:151:ARG:NH2	1:F:503:THR:OG1	2.52	0.43
1:A:242:MET:HA	1:A:244:PRO:HG3	2.00	0.42
1:A:78:VAL:CG2	1:A:78:VAL:O	2.66	0.42
1:B:198:ALA:C	1:B:200:ALA:H	2.22	0.42
1:A:390:LEU:HD22	1:B:396:VAL:HG22	2.00	0.42
1:C:436:PRO:HA	1:D:416:SER:CB	2.47	0.42
1:D:151:ARG:O	1:D:155:GLU:HG2	2.19	0.42
1:D:347:ILE:HG23	1:D:370:MET:HE3	2.01	0.42
1:D:446:GLY:O	1:D:447:ALA:C	2.57	0.42
1:D:240:LEU:HD21	1:D:479:LEU:CD2	2.48	0.42
1:D:373:PRO:HG3	1:D:482:ARG:HA	2.01	0.42
1:E:223:VAL:HG22	1:E:377:LEU:HG	2.01	0.42
1:E:418:GLN:CG	1:E:433:PRO:HD2	2.49	0.42
1:F:69:ILE:HA	1:F:151:ARG:NH1	2.34	0.42
1:A:53:LEU:HD13	1:A:494:PHE:HD1	1.84	0.42
1:B:113:SER:HG	1:B:117:TYR:HE2	1.62	0.42
1:B:285:TRP:NE1	1:B:287:PRO:HG3	2.34	0.42
1:B:425:PHE:HE1	1:B:427:LYS:HD3	1.84	0.42
1:B:52:ILE:HG22	1:B:53:LEU:N	2.34	0.42
1:C:117:TYR:CE1	1:C:490:ILE:HD13	2.53	0.42
1:C:118:LYS:HG3	1:C:118:LYS:HZ2	1.66	0.42
1:C:327:ILE:O	1:C:327:ILE:HG12	2.19	0.42
1:C:359:GLU:O	1:C:363:ILE:HD13	2.19	0.42
1:C:425:PHE:CD1	1:C:427:LYS:HB2	2.54	0.42
1:D:221:ARG:NH2	1:D:266:TYR:OH	2.52	0.42
1:D:254:GLN:NE2	1:D:334:GLN:HG2	2.34	0.42
1:D:444:ILE:O	1:D:444:ILE:HG22	2.19	0.42
1:D:471:THR:O	1:D:474:LYS:HB3	2.19	0.42
1:E:144:GLU:O	1:E:148:ILE:HG13	2.19	0.42
1:E:168:VAL:CG1	1:E:202:VAL:HA	2.50	0.42
1:E:448:SER:O	1:E:451:ASP:HB2	2.19	0.42
1:E:502:VAL:O	1:E:505:THR:HG21	2.19	0.42
1:A:195:ASP:O	1:A:197:ASN:N	2.52	0.42
1:A:256:PHE:HE2	1:A:264:MET:HE2	1.85	0.42
1:A:230:PHE:CD2	1:A:469:MET:HE2	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:CD2	1:B:87:SER:HB2	2.55	0.42
1:C:124:VAL:HA	1:C:125:PRO:HD2	1.52	0.42
1:C:170:ALA:HB1	1:C:171:PRO:HD3	2.00	0.42
1:C:300:LEU:HD13	1:C:300:LEU:HA	1.92	0.42
1:C:413:LEU:H	1:C:413:LEU:CD2	2.32	0.42
1:C:418:GLN:HB2	1:C:433:PRO:HD2	2.01	0.42
1:C:502:VAL:HG23	1:C:504:PHE:H	1.85	0.42
1:D:376:TYR:OH	1:D:465:ALA:HB2	2.19	0.42
1:E:179:GLU:O	1:E:183:ILE:HG13	2.19	0.42
1:E:71:ARG:NH1	1:E:144:GLU:OE2	2.52	0.42
1:F:462:GLU:HB3	1:F:463:ALA:H	1.71	0.42
1:A:135:ILE:HG23	1:A:136:ASN:N	2.33	0.42
1:A:243:THR:O	1:A:243:THR:CG2	2.64	0.42
1:A:360:ALA:O	1:A:364:PHE:HD2	2.03	0.42
1:A:502:VAL:HG11	1:E:76:TRP:CE2	2.54	0.42
1:B:233:GLU:HG2	1:B:236:TYR:CD1	2.53	0.42
1:C:396:VAL:HG13	1:E:386:TYR:CZ	2.53	0.42
1:C:82:TYR:O	1:C:131:ALA:HB1	2.19	0.42
1:D:337:LYS:HZ2	1:D:337:LYS:HB3	1.79	0.42
1:D:482:ARG:HE	1:D:482:ARG:HB2	1.60	0.42
1:E:105:VAL:O	1:E:109:LYS:HG3	2.19	0.42
1:E:196:ILE:O	1:E:395:HIS:CE1	2.72	0.42
1:E:252:VAL:CG2	1:E:275:ILE:HG22	2.45	0.42
1:F:285:TRP:NE1	1:F:287:PRO:CG	2.82	0.42
1:F:253:VAL:HB	1:F:327:ILE:HD11	2.00	0.42
1:F:433:PRO:C	1:F:435:VAL:N	2.73	0.42
1:F:82:TYR:N	1:F:82:TYR:CD1	2.87	0.42
1:F:83:ARG:HG2	1:F:161:PHE:HB3	2.00	0.42
1:A:143:ASN:HD21	1:C:70:ARG:NH2	2.06	0.42
1:B:449:GLU:O	1:B:450:LYS:C	2.55	0.42
1:B:464:SER:O	1:B:468:ILE:HG12	2.20	0.42
1:C:168:VAL:HG13	1:C:201:CYS:O	2.20	0.42
1:C:435:VAL:O	1:C:435:VAL:CG1	2.63	0.42
1:D:94:LYS:HE3	1:D:385:SER:HB2	2.01	0.42
1:D:387:PHE:CD2	1:D:387:PHE:N	2.86	0.42
1:D:57:LYS:N	1:D:58:PRO:HD2	2.35	0.42
1:E:136:ASN:OD1	1:E:138:LYS:HB2	2.19	0.42
1:E:99:TYR:HB3	1:E:137:PRO:HG3	2.02	0.42
1:E:206:PRO:HD2	1:E:209:GLN:CG	2.48	0.42
1:E:221:ARG:NH1	1:E:221:ARG:HG2	2.34	0.42
1:E:234:ALA:O	1:E:235:SER:C	2.56	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:282:GLY:H	1:E:306:LEU:HD11	1.84	0.42
1:F:223:VAL:CG1	1:F:263:SER:OG	2.62	0.42
1:F:384:VAL:HA	1:F:387:PHE:CD1	2.54	0.42
1:A:187:TYR:CE2	1:A:192:GLY:HA3	2.55	0.42
1:B:157:ALA:HA	1:B:162:ILE:CG2	2.49	0.42
1:B:33:VAL:HG12	1:B:34:GLU:N	2.35	0.42
1:C:504:PHE:CB	1:F:70:ARG:HH22	2.32	0.42
1:D:342:ARG:CB	1:D:342:ARG:NH1	2.82	0.42
1:E:386:TYR:CE2	1:E:390:LEU:HD11	2.54	0.42
1:E:397:SER:O	1:E:400:ARG:HB2	2.19	0.42
1:E:433:PRO:C	1:E:435:VAL:N	2.71	0.42
1:E:477:LEU:HD22	1:E:483:THR:HG21	2.02	0.42
1:E:89:HIS:CE1	1:E:493:VAL:HG22	2.55	0.42
1:F:149:THR:HG21	1:F:182:TRP:HE3	1.84	0.42
1:F:316:GLY:O	1:F:317:SER:O	2.37	0.42
1:A:314:TYR:CE2	1:A:318:ILE:HA	2.52	0.42
1:C:409:SER:OG	1:E:443:ARG:NH2	2.53	0.42
1:C:71:ARG:HD2	1:C:77:GLU:HB2	2.02	0.42
1:C:83:ARG:HD3	1:C:131:ALA:CB	2.33	0.42
1:D:154:MET:O	1:D:158:LYS:HG3	2.20	0.42
1:D:371:VAL:CG1	1:D:482:ARG:HH21	2.31	0.42
1:E:374:ASP:OD2	1:E:375:LEU:N	2.53	0.42
1:F:100:SER:O	1:F:103:VAL:HG13	2.19	0.42
1:F:133:VAL:O	1:F:135:ILE:N	2.53	0.42
1:F:185:ASP:O	1:F:189:SER:OG	2.36	0.42
1:F:283:SER:HB2	1:F:314:TYR:O	2.20	0.42
1:B:285:TRP:CD1	1:B:286:ASN:N	2.87	0.42
1:B:403:PHE:CD2	1:B:447:ALA:HB1	2.54	0.42
1:B:475:TYR:CE2	1:B:487:VAL:HG11	2.55	0.42
1:B:502:VAL:CG2	1:B:503:THR:H	2.23	0.42
1:C:339:ASN:O	1:C:340:ALA:C	2.58	0.42
1:C:413:LEU:HD22	1:C:413:LEU:N	2.34	0.42
1:C:225:HIS:CE1	1:C:458:ALA:HB2	2.55	0.42
1:D:364:PHE:CD1	1:D:369:ILE:HG21	2.55	0.42
1:B:158:LYS:HD3	1:E:193:HIS:CE1	2.55	0.42
1:E:23:ARG:HD3	1:E:23:ARG:O	2.20	0.42
1:E:67:PHE:HE2	1:E:152:PHE:HD1	1.67	0.42
1:F:168:VAL:HG13	1:F:202:VAL:HA	2.02	0.42
1:F:462:GLU:O	1:F:465:ALA:N	2.52	0.42
1:F:480:ASP:OD1	1:F:483:THR:HG23	2.20	0.42
1:A:367:ARG:H	1:A:367:ARG:HG2	1.68	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:CD2	1:A:479:LEU:HD21	2.50	0.42
1:B:33:VAL:O	1:B:34:GLU:O	2.38	0.42
1:D:108:VAL:HG23	1:D:109:LYS:N	2.34	0.42
1:D:335:LEU:HD12	1:D:356:THR:HG22	2.02	0.42
1:D:51:GLY:O	1:D:54:ARG:CG	2.68	0.42
1:E:367:ARG:NH1	1:E:367:ARG:CB	2.82	0.42
1:E:460:THR:HG22	1:E:461:MET:N	2.34	0.42
1:E:49:VAL:C	1:E:51:GLY:H	2.23	0.42
1:F:90:ARG:HD2	1:F:90:ARG:HA	1.93	0.42
1:A:221:ARG:O	1:A:222:GLY:C	2.56	0.42
1:A:250:THR:HB	1:A:324:ASP:OD1	2.20	0.42
1:A:329:ALA:O	1:A:330:ALA:HB2	2.20	0.42
1:A:433:PRO:CD	1:A:434:ILE:N	2.83	0.42
1:A:371:VAL:O	1:A:481:LEU:HD22	2.20	0.42
1:B:398:TYR:HB3	1:B:452:ILE:HD12	2.01	0.42
1:D:340:ALA:N	1:D:341:PRO:CD	2.83	0.42
1:D:343:VAL:HG23	1:D:367:ARG:NH2	2.35	0.42
1:D:94:LYS:NZ	1:D:170:ALA:HB2	2.35	0.42
1:E:224:PHE:CD2	1:E:267:LEU:HD22	2.55	0.42
1:E:29:GLU:O	1:E:30:ASP:C	2.58	0.42
1:E:488:ASN:O	1:E:492:LYS:HG3	2.20	0.42
1:E:502:VAL:HG23	1:E:504:PHE:H	1.85	0.42
1:E:93:CYS:HA	1:E:127:GLY:O	2.20	0.42
1:F:251:PHE:HB2	1:F:325:ILE:O	2.19	0.42
1:F:62:VAL:HG23	1:F:84:ALA:HB2	2.01	0.42
1:A:320:GLU:O	1:A:321:ALA:O	2.37	0.41
1:A:91:THR:HG22	1:A:165:GLY:O	2.20	0.41
1:B:193:HIS:CE1	1:E:158:LYS:HD3	2.55	0.41
1:B:52:ILE:HA	1:B:52:ILE:HD13	1.90	0.41
1:C:242:MET:O	1:C:243:THR:HG22	2.20	0.41
1:C:298:PHE:O	1:C:299:LYS:C	2.57	0.41
1:C:377:LEU:HD12	1:C:377:LEU:O	2.20	0.41
1:C:398:TYR:CZ	1:D:401:LEU:CD2	3.03	0.41
1:C:432:ILE:O	1:D:420:SER:OG	2.38	0.41
1:D:240:LEU:CD2	1:D:479:LEU:HD23	2.50	0.41
1:D:254:GLN:HE22	1:D:334:GLN:CG	2.33	0.41
1:D:73:ASP:C	1:D:73:ASP:OD2	2.57	0.41
1:E:153:THR:O	1:E:154:MET:C	2.58	0.41
1:D:165:GLY:HA3	1:E:196:ILE:HG13	2.02	0.41
1:F:145:LEU:O	1:F:149:THR:HG23	2.19	0.41
1:F:31:LYS:O	1:F:34:GLU:HG2	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:407:ARG:O	1:F:408:ASP:C	2.56	0.41
1:A:356:THR:OG1	1:A:482:ARG:NH2	2.54	0.41
1:B:37:ARG:CB	1:B:37:ARG:HH11	2.12	0.41
1:A:440:PHE:CG	1:B:412:HIS:HB3	2.54	0.41
1:B:59:CYS:HA	1:B:86:HIS:HA	2.02	0.41
1:C:321:ALA:O	1:C:344:LYS:HB2	2.20	0.41
1:C:32:LEU:HD21	1:C:494:PHE:CG	2.55	0.41
1:C:46:ARG:HA	1:C:46:ARG:HE	1.84	0.41
1:C:500:ALA:HA	1:C:505:THR:OXT	2.20	0.41
1:D:336:THR:C	1:D:338:SER:N	2.71	0.41
1:D:505:THR:O	1:E:185:ASP:CG	2.58	0.41
1:E:221:ARG:HG3	1:E:266:TYR:CE2	2.55	0.41
1:E:500:ALA:C	1:E:505:THR:OXT	2.58	0.41
1:E:72:ASP:OD1	1:E:141:THR:CG2	2.68	0.41
1:F:238:SER:C	1:F:240:LEU:N	2.73	0.41
1:F:264:MET:HE1	1:F:292:PRO:HA	2.02	0.41
1:F:333:LYS:HE3	1:F:357:THR:CG2	2.29	0.41
1:F:343:VAL:HG11	1:F:364:PHE:CZ	2.55	0.41
1:F:44:GLN:O	1:F:44:GLN:HG3	2.20	0.41
1:F:229:ASN:OD1	1:F:462:GLU:HG3	2.19	0.41
1:A:116:THR:CG2	1:A:128:GLY:H	2.32	0.41
1:A:170:ALA:HB1	1:A:171:PRO:CD	2.50	0.41
1:B:267:LEU:HA	1:B:267:LEU:HD13	1.81	0.41
1:C:23:ARG:O	1:C:27:ILE:HG13	2.20	0.41
1:C:323:CYS:SG	1:C:345:ALA:HB2	2.60	0.41
1:D:227:ILE:HD11	1:D:349:ALA:HB1	1.97	0.41
1:D:281:ASP:HB2	1:D:282:GLY:H	1.62	0.41
1:D:416:SER:O	1:D:420:SER:CB	2.68	0.41
1:E:78:VAL:C	1:E:79:ILE:HD12	2.41	0.41
1:A:43:GLU:HB3	1:A:45:LYS:HG3	2.02	0.41
1:A:479:LEU:HD12	1:A:479:LEU:N	2.35	0.41
1:A:49:VAL:HG22	1:A:49:VAL:O	2.20	0.41
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.76	0.41
1:B:34:GLU:O	1:B:38:THR:N	2.49	0.41
1:B:435:VAL:HG11	1:F:423:ARG:HH21	1.85	0.41
1:C:168:VAL:HG13	1:C:201:CYS:C	2.39	0.41
1:C:502:VAL:HG11	1:F:76:TRP:CD1	2.55	0.41
1:D:252:VAL:CG1	1:D:276:ALA:HB3	2.47	0.41
1:D:486:TYR:O	1:D:490:ILE:HG13	2.20	0.41
1:E:122:VAL:HG23	1:E:124:VAL:CG2	2.46	0.41
1:E:152:PHE:O	1:E:156:LEU:HD13	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:ALA:O	1:E:369:ILE:CD1	2.68	0.41
1:E:414:LEU:HD23	1:E:414:LEU:HA	1.75	0.41
1:F:180:MET:HE3	1:F:202:VAL:HG22	2.01	0.41
1:A:298:PHE:CD2	1:A:305:ILE:HA	2.56	0.41
1:B:261:LEU:HD12	1:B:261:LEU:O	2.20	0.41
1:C:437:THR:HG23	1:D:416:SER:CA	2.48	0.41
1:D:382:VAL:HA	1:D:385:SER:OG	2.21	0.41
1:D:418:GLN:OE1	1:D:434:ILE:HG23	2.21	0.41
1:D:499:GLU:OE1	1:E:208:SER:OG	2.30	0.41
1:E:169:PRO:C	1:E:202:VAL:HG23	2.41	0.41
1:A:170:ALA:CA	1:A:180:MET:HE2	2.50	0.41
1:B:86:HIS:CG	1:B:116:THR:HG21	2.54	0.41
1:B:290:ILE:HG23	1:B:308:PHE:HE2	1.85	0.41
1:B:298:PHE:CE2	1:B:302:HIS:HE1	2.37	0.41
1:B:319:LEU:HD23	1:B:335:LEU:HD23	2.03	0.41
1:B:400:ARG:HD2	1:B:400:ARG:O	2.20	0.41
1:C:94:LYS:HB3	1:C:115:MET:CE	2.51	0.41
1:C:343:VAL:HG21	1:C:364:PHE:HE1	1.84	0.41
1:D:99:TYR:CZ	1:D:149:THR:HG22	2.46	0.41
1:D:401:LEU:HD12	1:D:401:LEU:N	2.36	0.41
1:E:314:TYR:HE2	1:E:318:ILE:HA	1.85	0.41
1:F:348:ILE:HG22	1:F:371:VAL:HG13	2.02	0.41
1:F:348:ILE:O	1:F:372:ILE:HG13	2.20	0.41
1:F:384:VAL:O	1:F:387:PHE:HB2	2.20	0.41
1:F:55:ILE:O	1:F:58:PRO:CG	2.69	0.41
1:A:169:PRO:O	1:A:202:VAL:CG2	2.69	0.41
1:A:438:ALA:O	1:A:439:GLU:C	2.58	0.41
1:A:473:MET:O	1:A:475:TYR:N	2.53	0.41
1:A:21:PHE:CD2	1:A:57:LYS:HG3	2.55	0.41
1:B:244:PRO:HG2	1:B:248:ASP:H	1.76	0.41
1:B:404:LYS:NZ	1:B:407:ARG:NH2	2.68	0.41
1:B:71:ARG:HH11	1:B:71:ARG:HB3	1.86	0.41
1:C:265:ARG:HG2	1:C:292:PRO:HB3	2.03	0.41
1:C:332:GLU:O	1:C:333:LYS:C	2.59	0.41
1:D:236:TYR:C	1:D:238:SER:H	2.24	0.41
1:D:343:VAL:HG22	1:D:367:ARG:HH21	1.85	0.41
1:D:334:GLN:N	1:D:355:PRO:O	2.54	0.41
1:D:373:PRO:HG3	1:D:482:ARG:N	2.35	0.41
1:D:421:LEU:HD23	1:E:421:LEU:HD11	2.01	0.41
1:E:57:LYS:N	1:E:58:PRO:CD	2.83	0.41
1:F:284:ILE:CG1	1:F:305:ILE:HD12	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:LEU:N	1:F:479:LEU:HD12	2.36	0.41
1:F:52:ILE:HG13	1:F:494:PHE:CE1	2.56	0.41
1:A:418:GLN:OE1	1:A:434:ILE:HG23	2.20	0.41
1:A:52:ILE:O	1:A:55:ILE:HB	2.21	0.41
1:B:180:MET:CE	1:B:180:MET:CA	2.99	0.41
1:B:182:TRP:O	1:B:183:ILE:C	2.58	0.41
1:B:207:ILE:HG12	1:B:213:HIS:CD2	2.56	0.41
1:B:284:ILE:HG13	1:B:311:ALA:HB1	2.03	0.41
1:C:153:THR:O	1:C:154:MET:C	2.59	0.41
1:C:91:THR:HB	1:C:92:PRO:HD3	2.02	0.41
1:D:135:ILE:CG2	1:D:136:ASN:N	2.84	0.41
1:D:396:VAL:HG12	1:D:397:SER:H	1.85	0.41
1:D:402:THR:O	1:D:403:PHE:C	2.58	0.41
1:D:43:GLU:CB	1:D:45:LYS:HG3	2.43	0.41
1:E:293:LYS:NZ	1:E:297:ASP:CG	2.74	0.41
1:E:336:THR:O	1:E:339:ASN:ND2	2.54	0.41
1:E:38:THR:HG23	1:E:41:SER:CB	2.29	0.41
1:F:350:GLU:HB3	1:F:374:ASP:HB3	2.02	0.41
1:F:349:ALA:HB2	1:F:372:ILE:HD12	2.01	0.41
1:F:409:SER:O	1:F:410:ASN:C	2.57	0.41
1:F:37:ARG:HE	1:F:46:ARG:HD3	1.86	0.41
1:A:112:ALA:O	1:A:113:SER:C	2.59	0.41
1:A:373:PRO:O	1:A:374:ASP:C	2.59	0.41
1:C:108:VAL:HG23	1:C:109:LYS:H	1.84	0.41
1:C:206:PRO:O	1:C:207:ILE:C	2.57	0.41
1:C:23:ARG:HG3	1:C:23:ARG:NH1	2.36	0.41
1:C:363:ILE:HG22	1:C:364:PHE:N	2.35	0.41
1:C:432:ILE:HG22	1:C:434:ILE:HG12	2.03	0.41
1:C:77:GLU:HA	1:F:54:ARG:NH1	2.35	0.41
1:D:18:GLU:O	1:D:19:GLY:C	2.59	0.41
1:D:19:GLY:O	1:D:22:ASP:N	2.54	0.41
1:D:256:PHE:HE2	1:D:264:MET:CE	2.33	0.41
1:D:306:LEU:CD1	1:D:306:LEU:N	2.84	0.41
1:F:136:ASN:O	1:F:138:LYS:N	2.54	0.41
1:F:254:GLN:HE22	1:F:334:GLN:HG2	1.86	0.41
1:F:268:HIS:ND1	1:F:268:HIS:C	2.73	0.41
1:F:29:GLU:OE2	1:F:50:ARG:HD2	2.21	0.41
1:F:500:ALA:HB1	1:F:505:THR:O	2.21	0.41
1:F:63:LEU:HG	1:F:65:LEU:HD21	2.02	0.41
1:A:375:LEU:HD22	1:A:486:TYR:CD2	2.55	0.41
1:A:438:ALA:O	1:A:441:GLN:N	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD1	1:A:144:GLU:CG	2.66	0.41
1:B:21:PHE:CD1	1:B:117:TYR:OH	2.68	0.41
1:C:337:LYS:HZ2	1:C:337:LYS:HB2	1.85	0.41
1:C:117:TYR:CE1	1:C:490:ILE:CD1	3.04	0.41
1:C:500:ALA:HB1	1:C:505:THR:C	2.41	0.41
1:D:435:VAL:HA	1:D:436:PRO:HD3	1.84	0.41
1:D:440:PHE:HE1	1:E:413:LEU:HD22	1.85	0.41
1:D:452:ILE:HD13	1:E:405:TYR:CD1	2.56	0.41
1:D:390:LEU:HD21	1:E:396:VAL:HG23	2.03	0.41
1:E:67:PHE:CD1	1:E:67:PHE:C	2.94	0.41
1:A:54:ARG:HH12	1:E:78:VAL:HG13	1.86	0.41
1:F:254:GLN:HB3	1:F:328:PRO:HA	2.02	0.41
1:F:432:ILE:N	1:F:432:ILE:CD1	2.64	0.41
1:C:126:PHE:HZ	1:C:389:TRP:CE3	2.39	0.41
1:C:239:ILE:O	1:C:239:ILE:HG22	2.19	0.41
1:C:252:VAL:HG13	1:C:276:ALA:CB	2.36	0.41
1:C:264:MET:CE	1:C:292:PRO:HG3	2.50	0.41
1:D:211:GLY:O	1:D:391:LYS:HE2	2.21	0.41
1:E:13:PHE:CE1	1:E:107:GLU:HA	2.56	0.41
1:E:220:GLY:O	1:E:221:ARG:C	2.58	0.41
1:E:339:ASN:ND2	1:E:340:ALA:N	2.67	0.41
1:E:340:ALA:O	1:E:343:VAL:HG22	2.21	0.41
1:F:217:SER:HA	1:F:262:HIS:HD2	1.84	0.41
1:F:227:ILE:HD11	1:F:349:ALA:CB	2.50	0.41
1:F:425:PHE:CD1	1:F:427:LYS:HB2	2.56	0.41
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.89	0.40
1:B:143:ASN:HD21	1:E:70:ARG:NH1	2.13	0.40
1:B:211:GLY:HA2	1:B:388:GLU:OE1	2.21	0.40
1:B:268:HIS:O	1:B:270:PHE:N	2.54	0.40
1:B:302:HIS:O	1:B:303:GLY:C	2.59	0.40
1:B:363:ILE:HG22	1:B:367:ARG:HD3	2.04	0.40
1:C:157:ALA:O	1:C:159:LYS:N	2.55	0.40
1:D:12:ASN:O	1:D:13:PHE:C	2.59	0.40
1:D:32:LEU:C	1:D:32:LEU:HD12	2.42	0.40
1:D:449:GLU:O	1:D:453:VAL:HG23	2.21	0.40
1:E:350:GLU:OE1	1:E:374:ASP:N	2.49	0.40
1:E:63:LEU:O	1:E:82:TYR:HA	2.21	0.40
1:E:89:HIS:NE2	1:E:493:VAL:HG22	2.36	0.40
1:F:73:ASP:C	1:F:73:ASP:OD2	2.59	0.40
1:F:79:ILE:HD12	1:F:79:ILE:N	2.36	0.40
1:A:367:ARG:HH11	1:A:367:ARG:HB2	1.87	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASP:HB2	1:B:282:GLY:H	1.55	0.40
1:B:402:THR:O	1:B:403:PHE:C	2.59	0.40
1:B:424:LYS:O	1:B:425:PHE:HB2	2.20	0.40
1:C:87:SER:O	1:C:127:GLY:HA3	2.21	0.40
1:D:124:VAL:HA	1:D:125:PRO:HD2	1.93	0.40
1:D:16:MET:CE	1:D:333:LYS:CE	2.99	0.40
1:D:240:LEU:HD23	1:D:479:LEU:CD2	2.48	0.40
1:E:327:ILE:HA	1:E:328:PRO:HD3	1.86	0.40
1:E:363:ILE:O	1:E:367:ARG:HG3	2.21	0.40
1:F:500:ALA:C	1:F:505:THR:O	2.59	0.40
1:A:227:ILE:CD1	1:A:349:ALA:CB	3.00	0.40
1:A:448:SER:O	1:A:451:ASP:HB2	2.22	0.40
1:A:474:LYS:HD3	1:A:475:TYR:CE2	2.56	0.40
1:B:10:ASP:HA	1:B:11:PRO:HD3	1.76	0.40
1:B:206:PRO:HD2	1:B:209:GLN:HB2	2.03	0.40
1:B:249:LYS:HB2	1:B:272:ALA:HA	2.02	0.40
1:B:318:ILE:CD1	1:B:319:LEU:HD12	2.52	0.40
1:B:32:LEU:HD21	1:B:494:PHE:CD2	2.57	0.40
1:B:342:ARG:HG2	1:B:342:ARG:O	2.21	0.40
1:B:71:ARG:HD2	1:B:77:GLU:OE2	2.21	0.40
1:B:78:VAL:CG2	1:B:78:VAL:O	2.69	0.40
1:C:152:PHE:O	1:C:156:LEU:HD22	2.22	0.40
1:C:177:GLU:HB2	1:C:206:PRO:HG3	2.02	0.40
1:D:97:ILE:CD1	1:D:131:ALA:HB3	2.40	0.40
1:D:13:PHE:HD1	1:D:14:PHE:H	1.69	0.40
1:D:336:THR:N	1:D:339:ASN:HD21	2.17	0.40
1:E:261:LEU:HD12	1:E:261:LEU:C	2.42	0.40
1:E:377:LEU:HD12	1:E:377:LEU:HA	1.83	0.40
1:A:240:LEU:O	1:A:346:LYS:HE3	2.21	0.40
1:A:28:VAL:CG1	1:A:32:LEU:HD22	2.52	0.40
1:A:90:ARG:HD2	1:A:90:ARG:HA	1.74	0.40
1:B:293:LYS:HZ3	1:B:297:ASP:CG	2.24	0.40
1:B:336:THR:C	1:B:338:SER:N	2.74	0.40
1:C:13:PHE:CE2	1:C:107:GLU:HG3	2.53	0.40
1:C:211:GLY:O	1:C:391:LYS:NZ	2.38	0.40
1:C:196:ILE:O	1:C:395:HIS:CE1	2.74	0.40
1:D:90:ARG:HG2	1:D:125:PRO:HA	2.04	0.40
1:D:285:TRP:O	1:D:286:ASN:HB2	2.20	0.40
1:D:373:PRO:HG3	1:D:482:ARG:CA	2.51	0.40
1:C:406:GLU:OE1	1:D:405:TYR:HE2	2.05	0.40
1:C:440:PHE:HB2	1:D:412:HIS:ND1	2.36	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:505:THR:CG2	1:E:185:ASP:OD1	2.58	0.40
1:F:83:ARG:CD	1:F:131:ALA:HB2	2.40	0.40
1:F:308:PHE:O	1:F:311:ALA:HB3	2.21	0.40
1:F:336:THR:HG22	1:F:357:THR:HG23	2.03	0.40
1:F:492:LYS:O	1:F:493:VAL:C	2.60	0.40
1:F:56:ILE:HG12	1:F:497:TYR:CE2	2.56	0.40
1:A:224:PHE:CE2	1:A:270:PHE:HD2	2.40	0.40
1:A:465:ALA:O	1:A:469:MET:HG3	2.21	0.40
1:B:179:GLU:O	1:B:182:TRP:HB2	2.22	0.40
1:B:34:GLU:C	1:B:38:THR:HB	2.41	0.40
1:B:420:SER:O	1:B:423:ARG:HB2	2.21	0.40
1:B:432:ILE:HG22	1:B:434:ILE:HD11	2.02	0.40
1:B:435:VAL:CG1	1:F:423:ARG:HH21	2.34	0.40
1:C:228:GLU:O	1:C:231:ILE:HG22	2.22	0.40
1:E:242:MET:O	1:E:243:THR:HG22	2.22	0.40
1:E:273:LYS:HD3	1:E:288:ASP:O	2.22	0.40
1:E:28:VAL:O	1:E:29:GLU:C	2.59	0.40
1:E:32:LEU:HD21	1:E:494:PHE:CG	2.57	0.40
1:E:218:ALA:HB1	1:E:384:VAL:HG21	2.02	0.40
1:E:483:THR:HG23	1:E:484:ALA:N	2.36	0.40
1:F:263:SER:O	1:F:267:LEU:HD22	2.21	0.40
1:F:350:GLU:OE2	1:F:355:PRO:CD	2.60	0.40
1:F:349:ALA:CB	1:F:372:ILE:HD12	2.52	0.40





There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	494/496 (100%)	350 (71%)	105 (21%)	39 (8%)	 
1	B	494/496 (100%)	366 (74%)	86 (17%)	42 (8%)	 

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	494/496 (100%)	386 (78%)	76 (15%)	32 (6%)	1	13
1	D	494/496 (100%)	374 (76%)	76 (15%)	44 (9%)	1	6
1	E	494/496 (100%)	382 (77%)	87 (18%)	25 (5%)	2	19
1	F	494/496 (100%)	358 (72%)	100 (20%)	36 (7%)	1	10
All	All	2964/2976 (100%)	2216 (75%)	530 (18%)	218 (7%)	1	10

All (218) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	35	ASP
1	A	134	LYS
1	A	173	MET
1	A	248	ASP
1	A	310	LYS
1	A	317	SER
1	A	321	ALA
1	A	331	SER
1	A	425	PHE
1	A	474	LYS
1	A	502	VAL
1	B	29	GLU
1	B	34	GLU
1	B	41	SER
1	B	105	VAL
1	B	173	MET
1	B	310	LYS
1	B	377	LEU
1	B	425	PHE
1	C	34	GLU
1	C	35	ASP
1	C	134	LYS
1	C	162	ILE
1	C	173	MET
1	C	218	ALA
1	C	331	SER
1	C	391	LYS
1	C	409	SER
1	C	410	ASN
1	C	425	PHE
1	C	434	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	500	ALA
1	D	34	GLU
1	D	41	SER
1	D	91	THR
1	D	134	LYS
1	D	173	MET
1	D	269	ARG
1	D	310	LYS
1	D	321	ALA
1	D	425	PHE
1	D	485	ALA
1	E	29	GLU
1	E	34	GLU
1	E	35	ASP
1	E	74	GLY
1	E	173	MET
1	E	317	SER
1	E	331	SER
1	E	425	PHE
1	E	434	ILE
1	F	33	VAL
1	F	34	GLU
1	F	91	THR
1	F	173	MET
1	F	218	ALA
1	F	239	ILE
1	F	248	ASP
1	F	310	LYS
1	F	317	SER
1	F	331	SER
1	F	425	PHE
1	F	434	ILE
1	F	463	ALA
1	F	502	VAL
1	A	162	ILE
1	A	235	SER
1	A	269	ARG
1	A	303	GLY
1	A	333	LYS
1	A	368	ASN
1	A	481	LEU
1	B	33	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	109	LYS
1	B	134	LYS
1	B	151	ARG
1	B	216	ILE
1	B	239	ILE
1	B	269	ARG
1	B	303	GLY
1	B	330	ALA
1	B	333	LYS
1	B	368	ASN
1	B	426	GLY
1	B	430	GLY
1	B	434	ILE
1	C	33	VAL
1	C	91	THR
1	C	281	ASP
1	C	298	PHE
1	C	299	LYS
1	C	333	LYS
1	C	368	ASN
1	C	426	GLY
1	C	430	GLY
1	D	11	PRO
1	D	239	ILE
1	D	302	HIS
1	D	317	SER
1	D	330	ALA
1	D	337	LYS
1	D	350	GLU
1	D	400	ARG
1	D	426	GLY
1	D	434	ILE
1	D	447	ALA
1	D	486	TYR
1	E	33	VAL
1	E	101	THR
1	E	303	GLY
1	E	426	GLY
1	E	502	VAL
1	F	35	ASP
1	F	123	ASP
1	F	134	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	162	ILE
1	F	169	PRO
1	F	321	ALA
1	F	400	ARG
1	F	422	GLU
1	F	426	GLY
1	F	462	GLU
1	A	52	ILE
1	A	218	ALA
1	A	261	LEU
1	A	286	ASN
1	A	375	LEU
1	A	500	ALA
1	B	13	PHE
1	B	72	ASP
1	B	123	ASP
1	B	234	ALA
1	B	248	ASP
1	B	500	ALA
1	C	125	PRO
1	C	158	LYS
1	C	248	ASP
1	C	439	GLU
1	D	101	THR
1	D	137	PRO
1	D	224	PHE
1	D	237	MET
1	D	248	ASP
1	D	313	PRO
1	D	318	ILE
1	E	463	ALA
1	F	38	THR
1	F	41	SER
1	F	305	ILE
1	F	330	ALA
1	A	33	VAL
1	A	177	GLU
1	A	400	ARG
1	A	426	GLY
1	A	462	GLU
1	B	30	ASP
1	B	235	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	242	MET
1	B	281	ASP
1	B	306	LEU
1	B	313	PRO
1	B	403	PHE
1	C	390	LEU
1	C	482	ARG
1	D	235	SER
1	D	279	GLU
1	D	331	SER
1	D	418	GLN
1	E	30	ASP
1	F	258	ASN
1	F	286	ASN
1	A	41	SER
1	A	68	PRO
1	A	330	ALA
1	A	403	PHE
1	A	433	PRO
1	B	177	GLU
1	C	68	PRO
1	C	269	ARG
1	C	338	SER
1	D	234	ALA
1	E	13	PHE
1	E	71	ARG
1	E	91	THR
1	E	130	LYS
1	E	248	ASP
1	F	313	PRO
1	A	268	HIS
1	B	301	GLN
1	B	447	ALA
1	D	123	ASP
1	D	500	ALA
1	F	216	ILE
1	F	433	PRO
1	F	499	GLU
1	A	49	VAL
1	A	313	PRO
1	C	303	GLY
1	D	105	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	286	ASN
1	D	303	GLY
1	B	183	ILE
1	D	33	VAL
1	D	502	VAL
1	B	108	VAL
1	B	169	PRO
1	D	373	PRO
1	D	382	VAL
1	E	68	PRO
1	E	358	PRO
1	E	433	PRO
1	F	68	PRO
1	F	122	VAL
1	A	244	PRO
1	D	316	GLY
1	E	239	ILE
1	B	275	ILE

### 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	412/412 (100%)	356 (86%)	56 (14%)	5	21
1	B	412/412 (100%)	354 (86%)	58 (14%)	4	20
1	C	412/412 (100%)	355 (86%)	57 (14%)	4	20
1	D	412/412 (100%)	357 (87%)	55 (13%)	5	21
1	E	412/412 (100%)	364 (88%)	48 (12%)	7	28
1	F	412/412 (100%)	360 (87%)	52 (13%)	5	24
All	All	2472/2472 (100%)	2146 (87%)	326 (13%)	5	22

All (326) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	31	LYS
1	A	36	LEU
1	A	37	ARG
1	A	43	GLU
1	A	44	GLN
1	A	54	ARG
1	A	59	CYS
1	A	67	PHE
1	A	68	PRO
1	A	71	ARG
1	A	72	ASP
1	A	76	TRP
1	A	82	TYR
1	A	90	ARG
1	A	100	SER
1	A	105	VAL
1	A	116	THR
1	A	124	VAL
1	A	135	ILE
1	A	141	THR
1	A	180	MET
1	A	183	ILE
1	A	212	ILE
1	A	231	ILE
1	A	253	VAL
1	A	261	LEU
1	A	263	SER
1	A	267	LEU
1	A	293	LYS
1	A	300	LEU
1	A	319	LEU
1	A	320	GLU
1	A	326	LEU
1	A	327	ILE
1	A	334	GLN
1	A	338	SER
1	A	339	ASN
1	A	366	GLU
1	A	367	ARG
1	A	376	TYR
1	A	378	ASN
1	A	386	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	396	VAL
1	A	409	SER
1	A	421	LEU
1	A	425	PHE
1	A	427	LYS
1	A	428	HIS
1	A	443	ARG
1	A	457	LEU
1	A	476	ASN
1	A	483	THR
1	A	498	ASN
1	A	499	GLU
1	A	505	THR
1	B	13	PHE
1	B	28	VAL
1	B	37	ARG
1	B	53	LEU
1	B	62	VAL
1	B	65	LEU
1	B	68	PRO
1	B	72	ASP
1	B	83	ARG
1	B	91	THR
1	B	108	VAL
1	B	115	MET
1	B	116	THR
1	B	135	ILE
1	B	141	THR
1	B	156	LEU
1	B	180	MET
1	B	196	ILE
1	B	207	ILE
1	B	219	THR
1	B	231	ILE
1	B	238	SER
1	B	253	VAL
1	B	259	VAL
1	B	263	SER
1	B	267	LEU
1	B	281	ASP
1	B	293	LYS
1	B	302	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	318	ILE
1	B	324	ASP
1	B	325	ILE
1	B	327	ILE
1	B	334	GLN
1	B	337	LYS
1	B	339	ASN
1	B	357	THR
1	B	367	ARG
1	B	371	VAL
1	B	376	TYR
1	B	378	ASN
1	B	396	VAL
1	B	406	GLU
1	B	409	SER
1	B	413	LEU
1	B	415	MET
1	B	420	SER
1	B	421	LEU
1	B	428	HIS
1	B	432	ILE
1	B	440	PHE
1	B	457	LEU
1	B	471	THR
1	B	473	MET
1	B	477	LEU
1	B	479	LEU
1	B	481	LEU
1	B	498	ASN
1	C	13	PHE
1	C	16	MET
1	C	28	VAL
1	C	37	ARG
1	C	46	ARG
1	C	50	ARG
1	C	64	SER
1	C	68	PRO
1	C	70	ARG
1	C	71	ARG
1	C	72	ASP
1	C	87	SER
1	C	90	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	91	THR
1	C	98	ARG
1	C	106	ASP
1	C	116	THR
1	C	135	ILE
1	C	141	THR
1	C	156	LEU
1	C	180	MET
1	C	191	ILE
1	C	221	ARG
1	C	235	SER
1	C	256	PHE
1	C	259	VAL
1	C	263	SER
1	C	265	ARG
1	C	275	ILE
1	C	281	ASP
1	C	284	ILE
1	C	292	PRO
1	C	293	LYS
1	C	312	LYS
1	C	326	LEU
1	C	327	ILE
1	C	334	GLN
1	C	338	SER
1	C	339	ASN
1	C	356	THR
1	C	359	GLU
1	C	362	LYS
1	C	367	ARG
1	C	378	ASN
1	C	396	VAL
1	C	409	SER
1	C	415	MET
1	C	421	LEU
1	C	431	THR
1	C	432	ILE
1	C	435	VAL
1	C	443	ARG
1	C	445	SER
1	C	466	ARG
1	C	473	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	483	THR
1	C	487	VAL
1	D	13	PHE
1	D	23	ARG
1	D	37	ARG
1	D	54	ARG
1	D	64	SER
1	D	68	PRO
1	D	69	ILE
1	D	90	ARG
1	D	91	THR
1	D	101	THR
1	D	105	VAL
1	D	115	MET
1	D	116	THR
1	D	135	ILE
1	D	141	THR
1	D	151	ARG
1	D	156	LEU
1	D	166	ILE
1	D	180	MET
1	D	189	SER
1	D	202	VAL
1	D	203	THR
1	D	219	THR
1	D	231	ILE
1	D	239	ILE
1	D	263	SER
1	D	279	GLU
1	D	293	LYS
1	D	300	LEU
1	D	315	GLU
1	D	320	GLU
1	D	325	ILE
1	D	326	LEU
1	D	327	ILE
1	D	331	SER
1	D	334	GLN
1	D	337	LYS
1	D	339	ASN
1	D	367	ARG
1	D	378	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	396	VAL
1	D	400	ARG
1	D	402	THR
1	D	406	GLU
1	D	409	SER
1	D	421	LEU
1	D	425	PHE
1	D	428	HIS
1	D	443	ARG
1	D	445	SER
1	D	457	LEU
1	D	476	ASN
1	D	481	LEU
1	D	483	THR
1	D	505	THR
1	E	10	ASP
1	E	13	PHE
1	E	23	ARG
1	E	37	ARG
1	E	44	GLN
1	E	68	PRO
1	E	72	ASP
1	E	76	TRP
1	E	83	ARG
1	E	91	THR
1	E	101	THR
1	E	108	VAL
1	E	135	ILE
1	E	141	THR
1	E	180	MET
1	E	189	SER
1	E	231	ILE
1	E	235	SER
1	E	253	VAL
1	E	258	ASN
1	E	259	VAL
1	E	267	LEU
1	E	275	ILE
1	E	293	LYS
1	E	300	LEU
1	E	320	GLU
1	E	325	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	326	LEU
1	E	334	GLN
1	E	337	LYS
1	E	339	ASN
1	E	357	THR
1	E	358	PRO
1	E	363	ILE
1	E	400	ARG
1	E	406	GLU
1	E	413	LEU
1	E	415	MET
1	E	421	LEU
1	E	424	LYS
1	E	428	HIS
1	E	455	SER
1	E	457	LEU
1	E	471	THR
1	E	481	LEU
1	E	498	ASN
1	E	499	GLU
1	E	505	THR
1	F	13	PHE
1	F	23	ARG
1	F	31	LYS
1	F	36	LEU
1	F	37	ARG
1	F	40	GLU
1	F	46	ARG
1	F	49	VAL
1	F	55	ILE
1	F	62	VAL
1	F	64	SER
1	F	68	PRO
1	F	82	TYR
1	F	90	ARG
1	F	91	THR
1	F	116	THR
1	F	149	THR
1	F	155	GLU
1	F	162	ILE
1	F	177	GLU
1	F	189	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	221	ARG
1	F	231	ILE
1	F	261	LEU
1	F	263	SER
1	F	267	LEU
1	F	275	ILE
1	F	288	ASP
1	F	293	LYS
1	F	300	LEU
1	F	312	LYS
1	F	318	ILE
1	F	320	GLU
1	F	334	GLN
1	F	339	ASN
1	F	342	ARG
1	F	355	PRO
1	F	367	ARG
1	F	372	ILE
1	F	378	ASN
1	F	396	VAL
1	F	416	SER
1	F	431	THR
1	F	432	ILE
1	F	443	ARG
1	F	455	SER
1	F	467	GLN
1	F	481	LEU
1	F	483	THR
1	F	498	ASN
1	F	499	GLU
1	F	502	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	61	HIS
1	A	85	GLN
1	A	86	HIS
1	A	139	ASN
1	A	143	ASN
1	A	229	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	268	HIS
1	A	334	GLN
1	A	339	ASN
1	A	368	ASN
1	A	378	ASN
1	A	392	ASN
1	A	394	ASN
1	A	410	ASN
1	A	454	HIS
1	A	498	ASN
1	B	86	HIS
1	B	139	ASN
1	B	143	ASN
1	B	213	HIS
1	B	302	HIS
1	B	334	GLN
1	B	339	ASN
1	B	378	ASN
1	B	392	ASN
1	B	395	HIS
1	B	410	ASN
1	B	454	HIS
1	B	498	ASN
1	C	61	HIS
1	C	86	HIS
1	C	143	ASN
1	C	199	HIS
1	C	225	HIS
1	C	232	ASN
1	C	254	GLN
1	C	262	HIS
1	C	334	GLN
1	C	339	ASN
1	C	378	ASN
1	C	392	ASN
1	C	395	HIS
1	C	410	ASN
1	C	467	GLN
1	C	488	ASN
1	D	61	HIS
1	D	86	HIS
1	D	193	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	232	ASN
1	D	254	GLN
1	D	339	ASN
1	D	368	ASN
1	D	378	ASN
1	D	392	ASN
1	D	395	HIS
1	D	410	ASN
1	D	476	ASN
1	D	498	ASN
1	E	61	HIS
1	E	86	HIS
1	E	193	HIS
1	E	232	ASN
1	E	301	GLN
1	E	302	HIS
1	E	334	GLN
1	E	339	ASN
1	E	392	ASN
1	E	395	HIS
1	E	410	ASN
1	E	412	HIS
1	E	428	HIS
1	E	498	ASN
1	F	61	HIS
1	F	86	HIS
1	F	88	GLN
1	F	209	GLN
1	F	232	ASN
1	F	334	GLN
1	F	339	ASN
1	F	378	ASN
1	F	392	ASN
1	F	395	HIS
1	F	498	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.