



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:44 PM GMT

PDB ID : 1IOK  
Title : CRYSTAL STRUCTURE OF CHAPERONIN-60 FROM PARACOCCLUS  
DENITRIFICANS  
Authors : Fukami, T.A.; Yohda, M.; Taguchi, H.; Yoshida, M.; Miki, K.  
Deposited on : 2001-03-16  
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

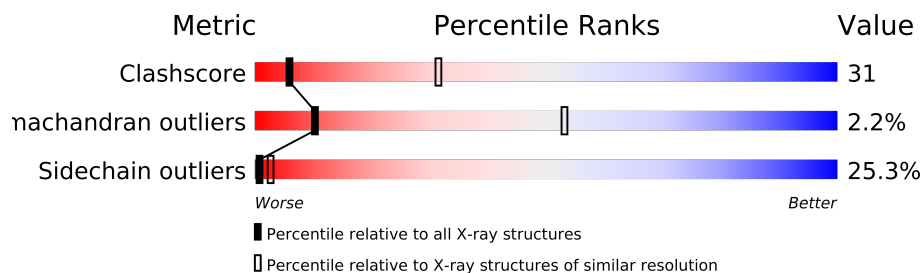
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 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	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	545	
1	B	545	
1	C	545	
1	D	545	
1	E	545	
1	F	545	
1	G	545	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25095 atoms, of which 0 are hydrogen and 0 are deuterium.

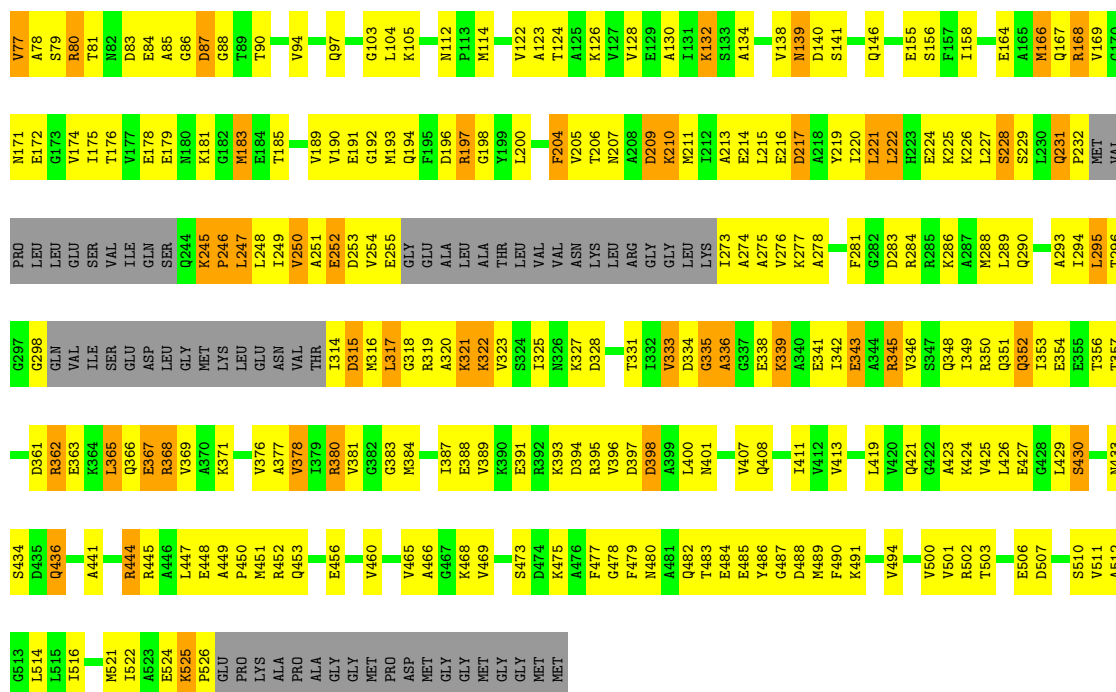
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CHAPERONIN 60.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	B	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	C	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	D	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	E	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	F	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			
1	G	482	Total	C	N	O	S	0	0	0
			3585	2218	635	717	15			

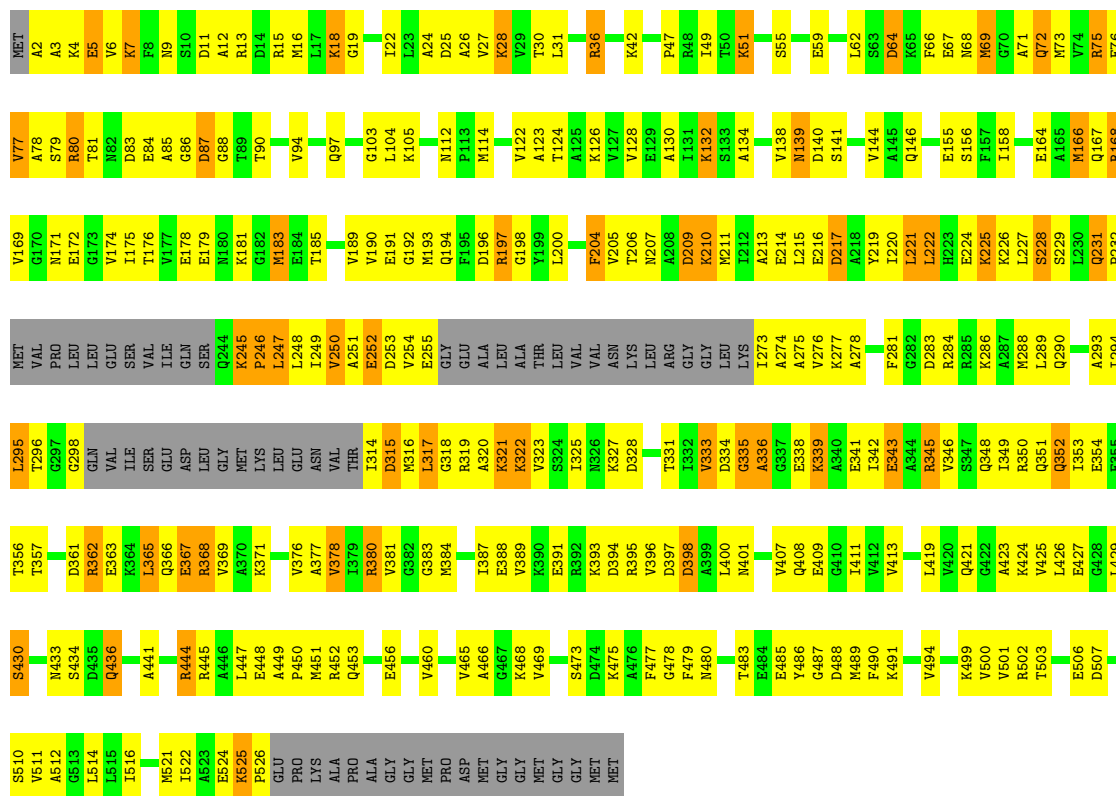






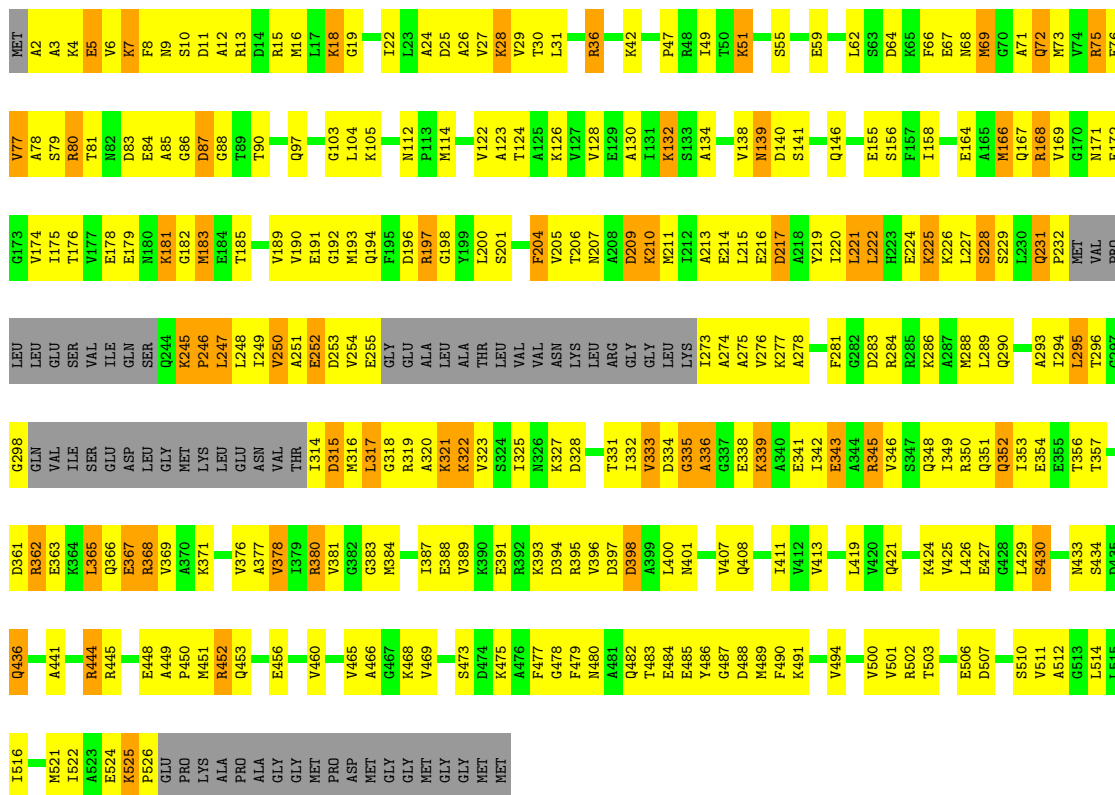
### • Molecule 1: CHAPERONIN 60

Chain E:



### • Molecule 1: CHAPERONIN 60

Chain F:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.36Å 286.36Å 153.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.204 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25095	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	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	0.32	0/3609	0.48	0/4855
1	B	0.33	0/3609	0.48	0/4855
1	C	0.32	0/3609	0.49	0/4855
1	D	0.34	0/3609	0.48	0/4855
1	E	0.33	0/3609	0.48	0/4855
1	F	0.32	0/3609	0.49	0/4855
1	G	0.33	0/3609	0.48	0/4855
All	All	0.33	0/25263	0.48	0/33985

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3585	0	3657	233	0
1	B	3585	0	3657	231	0
1	C	3585	0	3657	229	0
1	D	3585	0	3657	228	0
1	E	3585	0	3657	231	0
1	F	3585	0	3657	235	0
1	G	3585	0	3657	231	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25095	0	25599	1574	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (1574) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:139:ASN:HD22	1:D:140:ASP:H	1.17	0.93
1:G:139:ASN:HD22	1:G:140:ASP:H	1.16	0.92
1:C:139:ASN:HD22	1:C:140:ASP:H	1.17	0.92
1:C:36:ARG:HG2	1:C:36:ARG:HH11	1.35	0.92
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.35	0.91
1:F:139:ASN:HD22	1:F:140:ASP:H	1.17	0.91
1:E:139:ASN:HD22	1:E:140:ASP:H	1.17	0.91
1:F:36:ARG:HH11	1:F:36:ARG:HG2	1.34	0.91
1:A:139:ASN:HD22	1:A:140:ASP:H	1.18	0.90
1:B:36:ARG:HH11	1:B:36:ARG:HG2	1.35	0.90
1:E:36:ARG:HG2	1:E:36:ARG:HH11	1.36	0.90
1:F:227:LEU:HB2	1:F:254:VAL:HA	1.54	0.89
1:C:227:LEU:HB2	1:C:254:VAL:HA	1.54	0.89
1:G:227:LEU:HB2	1:G:254:VAL:HA	1.55	0.89
1:A:227:LEU:HB2	1:A:254:VAL:HA	1.55	0.89
1:B:227:LEU:HB2	1:B:254:VAL:HA	1.55	0.89
1:B:139:ASN:HD22	1:B:140:ASP:H	1.18	0.88
1:D:227:LEU:HB2	1:D:254:VAL:HA	1.55	0.88
1:E:227:LEU:HB2	1:E:254:VAL:HA	1.55	0.88
1:D:36:ARG:HH11	1:D:36:ARG:HG2	1.36	0.88
1:G:36:ARG:HH11	1:G:36:ARG:HG2	1.40	0.86
1:A:228:SER:HA	1:A:255:GLU:HB2	1.58	0.85
1:G:228:SER:HA	1:G:255:GLU:HB2	1.59	0.85
1:B:228:SER:HA	1:B:255:GLU:HB2	1.59	0.84
1:C:228:SER:HA	1:C:255:GLU:HB2	1.59	0.83
1:A:449:ALA:HB3	1:A:450:PRO:HD3	1.60	0.83
1:E:228:SER:HA	1:E:255:GLU:HB2	1.59	0.83
1:F:514:LEU:HD13	1:G:49:ILE:HD12	1.61	0.82
1:D:228:SER:HA	1:D:255:GLU:HB2	1.59	0.82
1:F:228:SER:HA	1:F:255:GLU:HB2	1.59	0.82
1:G:449:ALA:HB3	1:G:450:PRO:HD3	1.62	0.82
1:B:514:LEU:HD13	1:C:49:ILE:HD12	1.63	0.81
1:F:449:ALA:HB3	1:F:450:PRO:HD3	1.62	0.81
1:A:322:LYS:HB3	1:A:333:VAL:HG23	1.63	0.81
1:B:449:ALA:HB3	1:B:450:PRO:HD3	1.62	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:322:LYS:HB3	1:F:333:VAL:HG23	1.63	0.81
1:D:322:LYS:HB3	1:D:333:VAL:HG23	1.63	0.81
1:D:449:ALA:HB3	1:D:450:PRO:HD3	1.61	0.80
1:E:322:LYS:HB3	1:E:333:VAL:HG23	1.63	0.80
1:G:322:LYS:HB3	1:G:333:VAL:HG23	1.64	0.80
1:A:49:ILE:HD12	1:G:514:LEU:HD13	1.63	0.80
1:C:514:LEU:HD13	1:D:49:ILE:HD12	1.63	0.80
1:B:322:LYS:HB3	1:B:333:VAL:HG23	1.64	0.80
1:C:322:LYS:HB3	1:C:333:VAL:HG23	1.64	0.80
1:C:449:ALA:HB3	1:C:450:PRO:HD3	1.61	0.79
1:F:250:VAL:HG13	1:F:276:VAL:HG23	1.65	0.78
1:A:197:ARG:HH11	1:A:277:LYS:HG2	1.49	0.78
1:E:449:ALA:HB3	1:E:450:PRO:HD3	1.64	0.78
1:G:250:VAL:HG13	1:G:276:VAL:HG23	1.66	0.78
1:D:197:ARG:HH11	1:D:277:LYS:HG2	1.49	0.77
1:A:250:VAL:HG13	1:A:276:VAL:HG23	1.66	0.77
1:E:197:ARG:HH11	1:E:277:LYS:HG2	1.50	0.77
1:B:380:ARG:HB2	1:B:380:ARG:HH11	1.50	0.77
1:B:197:ARG:HH11	1:B:277:LYS:HG2	1.50	0.77
1:D:250:VAL:HG13	1:D:276:VAL:HG23	1.66	0.77
1:F:197:ARG:HH11	1:F:277:LYS:HG2	1.50	0.77
1:G:197:ARG:HH11	1:G:277:LYS:HG2	1.50	0.77
1:E:380:ARG:HB2	1:E:380:ARG:HH11	1.50	0.77
1:E:250:VAL:HG13	1:E:276:VAL:HG23	1.67	0.77
1:C:250:VAL:HG13	1:C:276:VAL:HG23	1.66	0.77
1:A:380:ARG:HH11	1:A:380:ARG:HB2	1.50	0.76
1:G:380:ARG:HH11	1:G:380:ARG:HB2	1.50	0.76
1:C:197:ARG:HH11	1:C:277:LYS:HG2	1.50	0.76
1:C:380:ARG:HH11	1:C:380:ARG:HB2	1.50	0.76
1:F:380:ARG:HH11	1:F:380:ARG:HB2	1.50	0.76
1:C:413:VAL:HG12	1:C:489:MET:HB3	1.68	0.76
1:B:250:VAL:HG13	1:B:276:VAL:HG23	1.66	0.76
1:D:380:ARG:HH11	1:D:380:ARG:HB2	1.50	0.75
1:B:413:VAL:HG12	1:B:489:MET:HB3	1.69	0.75
1:G:413:VAL:HG12	1:G:489:MET:HB3	1.68	0.74
1:E:413:VAL:HG12	1:E:489:MET:HB3	1.68	0.74
1:A:413:VAL:HG12	1:A:489:MET:HB3	1.69	0.74
1:E:514:LEU:HD13	1:F:49:ILE:HD12	1.70	0.73
1:D:413:VAL:HG12	1:D:489:MET:HB3	1.70	0.73
1:F:413:VAL:HG12	1:F:489:MET:HB3	1.69	0.73
1:A:514:LEU:HD13	1:B:49:ILE:HD12	1.70	0.73
1:E:411:ILE:HD12	1:E:490:PHE:HE1	1.54	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:514:LEU:HD13	1:E:49:ILE:HD12	1.70	0.72
1:C:411:ILE:HD12	1:C:490:PHE:HE1	1.54	0.72
1:B:128:VAL:HG13	1:B:502:ARG:HG3	1.70	0.72
1:F:411:ILE:HD12	1:F:490:PHE:HE1	1.53	0.72
1:E:226:LYS:HG2	1:E:252:GLU:HB2	1.72	0.71
1:D:128:VAL:HG13	1:D:502:ARG:HG3	1.72	0.71
1:B:411:ILE:HD12	1:B:490:PHE:HE1	1.56	0.71
1:D:411:ILE:HD12	1:D:490:PHE:HE1	1.55	0.71
1:A:411:ILE:HD12	1:A:490:PHE:HE1	1.55	0.71
1:C:7:LYS:HD2	1:C:66:PHE:CZ	2.25	0.71
1:D:226:LYS:HG2	1:D:252:GLU:HB2	1.72	0.71
1:F:346:VAL:HG12	1:F:350:ARG:HE	1.56	0.71
1:E:128:VAL:HG13	1:E:502:ARG:HG3	1.73	0.71
1:C:128:VAL:HG13	1:C:502:ARG:HG3	1.72	0.71
1:G:128:VAL:HG13	1:G:502:ARG:HG3	1.72	0.70
1:A:346:VAL:HG12	1:A:350:ARG:HE	1.56	0.70
1:C:226:LYS:HG2	1:C:252:GLU:HB2	1.73	0.70
1:D:139:ASN:HD22	1:D:140:ASP:N	1.90	0.70
1:G:346:VAL:HG12	1:G:350:ARG:HE	1.56	0.70
1:F:7:LYS:HD2	1:F:66:PHE:CZ	2.26	0.70
1:G:7:LYS:HD2	1:G:66:PHE:CZ	2.26	0.70
1:B:36:ARG:NH1	1:B:36:ARG:HG2	2.07	0.70
1:F:128:VAL:HG13	1:F:502:ARG:HG3	1.73	0.70
1:B:346:VAL:HG12	1:B:350:ARG:HE	1.56	0.70
1:G:226:LYS:HG2	1:G:252:GLU:HB2	1.72	0.70
1:D:36:ARG:NH1	1:D:36:ARG:HG2	2.07	0.70
1:F:226:LYS:HG2	1:F:252:GLU:HB2	1.72	0.70
1:A:448:GLU:O	1:A:452:ARG:HD2	1.91	0.70
1:C:346:VAL:HG12	1:C:350:ARG:HE	1.56	0.70
1:D:7:LYS:HD2	1:D:66:PHE:CZ	2.26	0.69
1:A:226:LYS:HG2	1:A:252:GLU:HB2	1.73	0.69
1:G:411:ILE:HD12	1:G:490:PHE:HE1	1.57	0.69
1:F:130:ALA:CB	1:F:425:VAL:HG21	2.22	0.69
1:E:7:LYS:HD2	1:E:66:PHE:CZ	2.26	0.69
1:B:226:LYS:HG2	1:B:252:GLU:HB2	1.72	0.69
1:E:130:ALA:CB	1:E:425:VAL:HG21	2.22	0.69
1:D:346:VAL:HG12	1:D:350:ARG:HE	1.56	0.69
1:G:139:ASN:HD22	1:G:140:ASP:N	1.90	0.69
1:A:130:ALA:CB	1:A:425:VAL:HG21	2.23	0.69
1:G:130:ALA:CB	1:G:425:VAL:HG21	2.23	0.69
1:G:227:LEU:HD22	1:G:254:VAL:HG22	1.75	0.69
1:C:130:ALA:CB	1:C:425:VAL:HG21	2.23	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:166:MET:HG2	1:G:171:ASN:HA	1.74	0.68
1:E:346:VAL:HG12	1:E:350:ARG:HE	1.57	0.68
1:A:73:MET:CE	1:B:49:ILE:HD11	2.23	0.68
1:C:448:GLU:O	1:C:452:ARG:HD2	1.92	0.68
1:B:139:ASN:HD22	1:B:140:ASP:N	1.91	0.68
1:A:128:VAL:HG13	1:A:502:ARG:HG3	1.74	0.68
1:A:366:GLN:O	1:A:369:VAL:HG12	1.94	0.68
1:F:166:MET:HG2	1:F:171:ASN:HA	1.76	0.68
1:B:7:LYS:HD2	1:B:66:PHE:CZ	2.29	0.68
1:D:166:MET:HG2	1:D:171:ASN:HA	1.75	0.68
1:B:130:ALA:CB	1:B:425:VAL:HG21	2.23	0.68
1:F:448:GLU:O	1:F:452:ARG:HD2	1.94	0.68
1:C:366:GLN:O	1:C:369:VAL:HG12	1.94	0.68
1:E:139:ASN:HD22	1:E:140:ASP:N	1.90	0.68
1:B:227:LEU:HD22	1:B:254:VAL:HG22	1.76	0.68
1:E:166:MET:HG2	1:E:171:ASN:HA	1.76	0.68
1:A:227:LEU:HD22	1:A:254:VAL:HG22	1.76	0.67
1:C:321:LYS:HB3	1:C:334:ASP:HB3	1.76	0.67
1:D:130:ALA:CB	1:D:425:VAL:HG21	2.23	0.67
1:C:227:LEU:HD22	1:C:254:VAL:HG22	1.77	0.67
1:C:139:ASN:HD22	1:C:140:ASP:N	1.91	0.67
1:F:227:LEU:HD22	1:F:254:VAL:HG22	1.76	0.67
1:G:448:GLU:O	1:G:452:ARG:HD2	1.93	0.67
1:E:227:LEU:HD22	1:E:254:VAL:HG22	1.76	0.67
1:F:366:GLN:O	1:F:369:VAL:HG12	1.93	0.67
1:D:321:LYS:HB3	1:D:334:ASP:HB3	1.77	0.67
1:D:366:GLN:O	1:D:369:VAL:HG12	1.94	0.67
1:D:227:LEU:HD22	1:D:254:VAL:HG22	1.77	0.67
1:A:132:LYS:HD3	1:A:502:ARG:HD3	1.76	0.67
1:E:130:ALA:HB2	1:E:425:VAL:HG21	1.77	0.67
1:G:366:GLN:O	1:G:369:VAL:HG12	1.93	0.66
1:B:166:MET:HG2	1:B:171:ASN:HA	1.76	0.66
1:A:7:LYS:HD2	1:A:66:PHE:CZ	2.29	0.66
1:G:132:LYS:HD3	1:G:502:ARG:HD3	1.77	0.66
1:A:166:MET:HG2	1:A:171:ASN:HA	1.76	0.66
1:C:166:MET:HG2	1:C:171:ASN:HA	1.75	0.66
1:E:366:GLN:O	1:E:369:VAL:HG12	1.94	0.66
1:C:183:MET:HG2	1:C:384:MET:SD	2.35	0.66
1:A:183:MET:HG2	1:A:384:MET:SD	2.36	0.66
1:F:231:GLN:H	1:F:231:GLN:NE2	1.94	0.66
1:B:366:GLN:O	1:B:369:VAL:HG12	1.95	0.66
1:G:321:LYS:HB3	1:G:334:ASP:HB3	1.76	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:130:ALA:HB2	1:F:425:VAL:HG21	1.77	0.66
1:B:321:LYS:HB3	1:B:334:ASP:HB3	1.78	0.66
1:B:448:GLU:O	1:B:452:ARG:HD2	1.96	0.66
1:D:183:MET:HG2	1:D:384:MET:SD	2.36	0.66
1:E:226:LYS:NZ	1:E:252:GLU:HB3	2.11	0.65
1:A:321:LYS:HB3	1:A:334:ASP:HB3	1.76	0.65
1:F:321:LYS:HB3	1:F:334:ASP:HB3	1.77	0.65
1:E:321:LYS:HB3	1:E:334:ASP:HB3	1.77	0.65
1:D:226:LYS:NZ	1:D:252:GLU:HB3	2.12	0.65
1:F:219:TYR:HB2	1:F:247:LEU:HA	1.79	0.65
1:B:183:MET:HG2	1:B:384:MET:SD	2.37	0.65
1:D:130:ALA:HB2	1:D:425:VAL:HG21	1.79	0.65
1:A:219:TYR:HB2	1:A:247:LEU:HA	1.78	0.65
1:D:231:GLN:H	1:D:231:GLN:NE2	1.94	0.65
1:B:130:ALA:HB2	1:B:425:VAL:HG21	1.78	0.65
1:G:231:GLN:H	1:G:231:GLN:NE2	1.94	0.65
1:B:231:GLN:H	1:B:231:GLN:NE2	1.95	0.65
1:C:226:LYS:NZ	1:C:252:GLU:HB3	2.12	0.65
1:E:448:GLU:O	1:E:452:ARG:HD2	1.97	0.65
1:F:132:LYS:HD3	1:F:502:ARG:HD3	1.78	0.65
1:C:130:ALA:HB2	1:C:425:VAL:HG21	1.78	0.65
1:E:231:GLN:H	1:E:231:GLN:NE2	1.95	0.65
1:C:231:GLN:NE2	1:C:231:GLN:H	1.95	0.65
1:G:36:ARG:HG2	1:G:36:ARG:NH1	2.10	0.65
1:B:128:VAL:HG13	1:B:502:ARG:CG	2.27	0.64
1:A:231:GLN:H	1:A:231:GLN:NE2	1.95	0.64
1:E:209:ASP:HB3	1:E:210:LYS:NZ	2.12	0.64
1:B:72:GLN:HE22	1:B:75:ARG:NH1	1.95	0.64
1:C:36:ARG:HG2	1:C:36:ARG:NH1	2.07	0.64
1:D:73:MET:CE	1:E:49:ILE:HD11	2.27	0.64
1:A:226:LYS:NZ	1:A:252:GLU:HB3	2.12	0.64
1:F:429:LEU:HD12	1:F:430:SER:H	1.62	0.64
1:C:209:ASP:HB3	1:C:210:LYS:NZ	2.12	0.64
1:D:448:GLU:O	1:D:452:ARG:HD2	1.97	0.64
1:G:77:VAL:HA	1:G:80:ARG:HD3	1.79	0.64
1:F:226:LYS:NZ	1:F:252:GLU:HB3	2.12	0.64
1:E:183:MET:HG2	1:E:384:MET:SD	2.37	0.64
1:G:183:MET:HG2	1:G:384:MET:SD	2.36	0.64
1:D:429:LEU:HD12	1:D:430:SER:H	1.63	0.64
1:B:209:ASP:HB3	1:B:210:LYS:NZ	2.13	0.64
1:A:77:VAL:HA	1:A:80:ARG:HD3	1.79	0.64
1:A:130:ALA:HB2	1:A:425:VAL:HG21	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:219:TYR:HB2	1:E:247:LEU:HA	1.78	0.64
1:D:132:LYS:HD3	1:D:502:ARG:HD3	1.78	0.64
1:B:226:LYS:NZ	1:B:252:GLU:HB3	2.12	0.64
1:G:130:ALA:HB2	1:G:425:VAL:HG21	1.79	0.64
1:G:209:ASP:HB3	1:G:210:LYS:NZ	2.13	0.64
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.05	0.64
1:G:250:VAL:HA	1:G:276:VAL:O	1.98	0.64
1:B:219:TYR:HB2	1:B:247:LEU:HA	1.78	0.64
1:F:183:MET:HG2	1:F:384:MET:SD	2.38	0.64
1:D:209:ASP:HB3	1:D:210:LYS:NZ	2.13	0.64
1:C:132:LYS:HD3	1:C:502:ARG:HD3	1.79	0.64
1:G:226:LYS:NZ	1:G:252:GLU:HB3	2.13	0.64
1:D:190:VAL:HG12	1:D:191:GLU:H	1.62	0.64
1:G:219:TYR:HB2	1:G:247:LEU:HA	1.78	0.64
1:D:77:VAL:HA	1:D:80:ARG:HD3	1.78	0.64
1:F:250:VAL:HA	1:F:276:VAL:O	1.98	0.63
1:A:429:LEU:HD12	1:A:430:SER:H	1.64	0.63
1:D:219:TYR:HB2	1:D:247:LEU:HA	1.79	0.63
1:F:77:VAL:HA	1:F:80:ARG:HD3	1.80	0.63
1:A:209:ASP:HB3	1:A:210:LYS:NZ	2.13	0.63
1:F:72:GLN:HE22	1:F:75:ARG:NH1	1.96	0.63
1:F:209:ASP:HB3	1:F:210:LYS:NZ	2.13	0.63
1:F:139:ASN:HD22	1:F:140:ASP:N	1.91	0.63
1:C:219:TYR:HB2	1:C:247:LEU:HA	1.79	0.63
1:E:77:VAL:HA	1:E:80:ARG:HD3	1.80	0.63
1:E:84:GLU:HG3	1:E:500:VAL:HG22	1.81	0.63
1:E:72:GLN:HE22	1:E:75:ARG:NH1	1.96	0.63
1:G:72:GLN:HE22	1:G:75:ARG:NH1	1.97	0.63
1:C:250:VAL:HA	1:C:276:VAL:O	1.98	0.63
1:G:128:VAL:HG13	1:G:502:ARG:CG	2.28	0.63
1:E:248:LEU:HA	1:E:274:ALA:HB3	1.81	0.63
1:A:250:VAL:HA	1:A:276:VAL:O	1.99	0.62
1:D:250:VAL:HA	1:D:276:VAL:O	1.99	0.62
1:B:250:VAL:HA	1:B:276:VAL:O	1.98	0.62
1:E:250:VAL:HA	1:E:276:VAL:O	1.98	0.62
1:B:77:VAL:HA	1:B:80:ARG:HD3	1.79	0.62
1:C:429:LEU:HD12	1:C:430:SER:H	1.63	0.62
1:F:138:VAL:HG12	1:F:407:VAL:HG12	1.81	0.62
1:E:73:MET:CE	1:F:49:ILE:HD11	2.30	0.62
1:E:128:VAL:HG13	1:E:502:ARG:CG	2.29	0.62
1:C:72:GLN:HE22	1:C:75:ARG:NH1	1.97	0.62
1:B:429:LEU:HD12	1:B:430:SER:H	1.64	0.62

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:176:THR:O	1:A:378:VAL:HG23	2.00	0.62
1:B:174:VAL:HG22	1:B:376:VAL:HG13	1.81	0.62
1:A:138:VAL:HG12	1:A:407:VAL:HG12	1.82	0.62
1:C:190:VAL:HG12	1:C:191:GLU:H	1.63	0.62
1:B:176:THR:O	1:B:378:VAL:HG23	1.99	0.62
1:F:248:LEU:HA	1:F:274:ALA:HB3	1.82	0.62
1:E:429:LEU:HD12	1:E:430:SER:H	1.65	0.62
1:C:128:VAL:HG13	1:C:502:ARG:CG	2.28	0.62
1:B:84:GLU:HG3	1:B:500:VAL:HG22	1.81	0.62
1:C:176:THR:O	1:C:378:VAL:HG23	1.99	0.62
1:F:36:ARG:NH1	1:F:36:ARG:HG2	2.07	0.62
1:E:174:VAL:HG22	1:E:376:VAL:HG13	1.82	0.62
1:C:193:MET:HB2	1:C:295:LEU:HD22	1.82	0.62
1:E:132:LYS:HD3	1:E:502:ARG:HD3	1.79	0.62
1:D:174:VAL:HG22	1:D:376:VAL:HG13	1.82	0.62
1:C:73:MET:CE	1:D:49:ILE:HD11	2.30	0.62
1:F:84:GLU:HG3	1:F:500:VAL:HG22	1.82	0.62
1:G:429:LEU:HD12	1:G:430:SER:H	1.63	0.62
1:F:176:THR:O	1:F:378:VAL:HG23	2.00	0.62
1:G:190:VAL:HG12	1:G:191:GLU:H	1.65	0.61
1:A:525:LYS:HD2	1:A:526:PRO:HD2	1.82	0.61
1:D:248:LEU:HA	1:D:274:ALA:HB3	1.82	0.61
1:D:128:VAL:HG13	1:D:502:ARG:CG	2.29	0.61
1:A:128:VAL:HG13	1:A:502:ARG:CG	2.29	0.61
1:B:477:PHE:HA	1:B:487:GLY:O	1.99	0.61
1:B:132:LYS:HD3	1:B:502:ARG:HD3	1.80	0.61
1:B:248:LEU:HA	1:B:274:ALA:HB3	1.82	0.61
1:B:138:VAL:HG12	1:B:407:VAL:HG12	1.83	0.61
1:C:174:VAL:HG22	1:C:376:VAL:HG13	1.83	0.61
1:A:174:VAL:HG22	1:A:376:VAL:HG13	1.82	0.61
1:A:139:ASN:HD22	1:A:140:ASP:N	1.92	0.61
1:A:49:ILE:HD11	1:G:73:MET:CE	2.31	0.61
1:C:221:LEU:HD11	1:C:249:ILE:HG23	1.82	0.61
1:C:77:VAL:HA	1:C:80:ARG:HD3	1.81	0.61
1:C:248:LEU:HA	1:C:274:ALA:HB3	1.82	0.61
1:E:409:GLU:OE2	1:E:499:LYS:HG3	1.99	0.61
1:B:221:LEU:HD11	1:B:249:ILE:HG23	1.82	0.61
1:A:193:MET:HB2	1:A:295:LEU:HD22	1.82	0.61
1:F:73:MET:CE	1:G:49:ILE:HD11	2.30	0.61
1:G:248:LEU:HA	1:G:274:ALA:HB3	1.82	0.61
1:F:525:LYS:HD2	1:F:526:PRO:HD2	1.82	0.61
1:G:221:LEU:HD11	1:G:249:ILE:HG23	1.82	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:367:GLU:HG3	1:E:368:ARG:N	2.16	0.61
1:A:248:LEU:HA	1:A:274:ALA:HB3	1.82	0.61
1:F:73:MET:HE3	1:G:49:ILE:HD11	1.82	0.61
1:F:75:ARG:NH1	1:F:75:ARG:HG2	2.16	0.61
1:E:525:LYS:HD2	1:E:526:PRO:HD2	1.82	0.61
1:B:193:MET:HB2	1:B:295:LEU:HD22	1.82	0.61
1:B:73:MET:HE3	1:C:49:ILE:HD11	1.82	0.61
1:A:49:ILE:HD11	1:G:73:MET:HE3	1.82	0.61
1:D:525:LYS:HD2	1:D:526:PRO:HD2	1.82	0.61
1:A:72:GLN:HE22	1:A:75:ARG:NH1	1.99	0.61
1:G:193:MET:HB2	1:G:295:LEU:HD22	1.82	0.61
1:G:525:LYS:HD2	1:G:526:PRO:HD2	1.83	0.60
1:F:174:VAL:HG22	1:F:376:VAL:HG13	1.84	0.60
1:F:221:LEU:HD11	1:F:249:ILE:HG23	1.82	0.60
1:D:193:MET:HB2	1:D:295:LEU:HD22	1.83	0.60
1:D:176:THR:O	1:D:378:VAL:HG23	2.01	0.60
1:G:174:VAL:HG22	1:G:376:VAL:HG13	1.84	0.60
1:D:84:GLU:HG3	1:D:500:VAL:HG22	1.83	0.60
1:G:477:PHE:HA	1:G:487:GLY:O	2.01	0.60
1:E:221:LEU:HD11	1:E:249:ILE:HG23	1.82	0.60
1:E:75:ARG:HG2	1:E:75:ARG:NH1	2.17	0.60
1:B:367:GLU:HG3	1:B:368:ARG:N	2.16	0.60
1:B:525:LYS:HD2	1:B:526:PRO:HD2	1.83	0.60
1:C:73:MET:HE3	1:D:49:ILE:HD11	1.81	0.60
1:F:128:VAL:HG13	1:F:502:ARG:CG	2.30	0.60
1:F:367:GLU:HG3	1:F:368:ARG:N	2.16	0.60
1:G:367:GLU:HG3	1:G:368:ARG:N	2.16	0.60
1:C:22:ILE:HG21	1:C:62:LEU:HD21	1.84	0.60
1:C:296:THR:O	1:C:336:ALA:HB3	2.02	0.60
1:C:367:GLU:HG3	1:C:368:ARG:N	2.16	0.60
1:E:176:THR:O	1:E:378:VAL:HG23	2.01	0.60
1:C:138:VAL:HG12	1:C:407:VAL:HG12	1.83	0.60
1:A:221:LEU:HD11	1:A:249:ILE:HG23	1.84	0.60
1:D:73:MET:HE3	1:E:49:ILE:HD11	1.84	0.60
1:C:477:PHE:HA	1:C:487:GLY:O	2.02	0.60
1:E:193:MET:HB2	1:E:295:LEU:HD22	1.82	0.60
1:D:72:GLN:HE22	1:D:75:ARG:NH1	2.00	0.60
1:C:84:GLU:HG3	1:C:500:VAL:HG22	1.83	0.60
1:F:477:PHE:HA	1:F:487:GLY:O	2.02	0.60
1:C:525:LYS:HD2	1:C:526:PRO:HD2	1.83	0.60
1:G:84:GLU:HG3	1:G:500:VAL:HG22	1.83	0.59
1:B:73:MET:CE	1:C:49:ILE:HD11	2.32	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:219:TYR:H	1:G:247:LEU:HA	1.66	0.59
1:F:296:THR:O	1:F:336:ALA:HB3	2.02	0.59
1:C:27:VAL:CG1	1:C:90:THR:HG23	2.32	0.59
1:F:193:MET:HB2	1:F:295:LEU:HD22	1.82	0.59
1:A:477:PHE:HA	1:A:487:GLY:O	2.02	0.59
1:C:352:GLN:O	1:C:356:THR:HG23	2.02	0.59
1:D:352:GLN:O	1:D:356:THR:HG23	2.02	0.59
1:D:367:GLU:HG3	1:D:368:ARG:N	2.16	0.59
1:A:84:GLU:HG3	1:A:500:VAL:HG22	1.82	0.59
1:D:296:THR:O	1:D:336:ALA:HB3	2.02	0.59
1:E:73:MET:HE3	1:F:49:ILE:HD11	1.84	0.59
1:A:73:MET:HE3	1:B:49:ILE:HD11	1.83	0.59
1:D:219:TYR:H	1:D:247:LEU:HA	1.67	0.59
1:C:219:TYR:H	1:C:247:LEU:HA	1.66	0.59
1:G:138:VAL:HG12	1:G:407:VAL:HG12	1.85	0.59
1:A:367:GLU:HG3	1:A:368:ARG:N	2.16	0.59
1:F:219:TYR:H	1:F:247:LEU:HA	1.67	0.59
1:D:27:VAL:CG1	1:D:90:THR:HG23	2.33	0.59
1:A:296:THR:O	1:A:336:ALA:HB3	2.02	0.59
1:A:219:TYR:H	1:A:247:LEU:HA	1.67	0.59
1:B:71:ALA:O	1:B:75:ARG:HB3	2.02	0.59
1:F:352:GLN:O	1:F:356:THR:HG23	2.03	0.59
1:C:158:ILE:HG23	1:C:396:VAL:HG22	1.84	0.59
1:G:296:THR:O	1:G:336:ALA:HB3	2.03	0.59
1:B:77:VAL:HG12	1:B:78:ALA:N	2.18	0.59
1:E:352:GLN:O	1:E:356:THR:HG23	2.03	0.59
1:D:221:LEU:HD11	1:D:249:ILE:HG23	1.83	0.59
1:E:27:VAL:CG1	1:E:90:THR:HG23	2.33	0.59
1:B:296:THR:O	1:B:336:ALA:HB3	2.03	0.59
1:F:483:THR:OG1	1:F:485:GLU:HG2	2.03	0.59
1:A:394:ASP:O	1:A:398:ASP:HB2	2.03	0.59
1:E:219:TYR:H	1:E:247:LEU:HA	1.66	0.59
1:E:477:PHE:HA	1:E:487:GLY:O	2.03	0.59
1:F:411:ILE:CD1	1:F:490:PHE:HE1	2.16	0.58
1:D:158:ILE:HG23	1:D:396:VAL:HG22	1.85	0.58
1:G:353:ILE:HG12	1:G:365:LEU:HB3	1.85	0.58
1:B:219:TYR:H	1:B:247:LEU:HA	1.66	0.58
1:E:190:VAL:HG12	1:E:191:GLU:H	1.67	0.58
1:D:77:VAL:HG12	1:D:78:ALA:N	2.17	0.58
1:A:168:ARG:HG2	1:A:189:VAL:HG21	1.86	0.58
1:G:394:ASP:O	1:G:398:ASP:HB2	2.03	0.58
1:D:394:ASP:O	1:D:398:ASP:HB2	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:352:GLN:O	1:G:356:THR:HG23	2.03	0.58
1:C:483:THR:OG1	1:C:485:GLU:HG2	2.03	0.58
1:C:394:ASP:O	1:C:398:ASP:HB2	2.03	0.58
1:E:296:THR:O	1:E:336:ALA:HB3	2.03	0.58
1:G:483:THR:OG1	1:G:485:GLU:HG2	2.04	0.58
1:A:353:ILE:HG12	1:A:365:LEU:HB3	1.86	0.58
1:F:353:ILE:HG12	1:F:365:LEU:HB3	1.85	0.58
1:F:168:ARG:HG2	1:F:189:VAL:HG21	1.86	0.58
1:G:27:VAL:CG1	1:G:90:THR:HG23	2.32	0.58
1:G:71:ALA:O	1:G:75:ARG:HB3	2.04	0.58
1:D:22:ILE:HG21	1:D:62:LEU:HD21	1.86	0.58
1:B:25:ASP:HA	1:B:28:LYS:HD2	1.86	0.58
1:D:477:PHE:HA	1:D:487:GLY:O	2.04	0.58
1:G:365:LEU:O	1:G:368:ARG:HG3	2.04	0.58
1:C:77:VAL:HG12	1:C:78:ALA:N	2.18	0.58
1:G:176:THR:O	1:G:378:VAL:HG23	2.04	0.58
1:E:138:VAL:HG12	1:E:407:VAL:HG12	1.85	0.58
1:A:483:THR:OG1	1:A:485:GLU:HG2	2.04	0.58
1:A:19:GLY:HA3	1:A:67:GLU:O	2.04	0.58
1:A:488:ASP:OD1	1:A:490:PHE:HB2	2.04	0.57
1:B:27:VAL:CG1	1:B:90:THR:HG23	2.33	0.57
1:B:158:ILE:HG23	1:B:396:VAL:HG22	1.84	0.57
1:B:468:LYS:HD3	1:B:486:TYR:CZ	2.39	0.57
1:A:352:GLN:O	1:A:356:THR:HG23	2.03	0.57
1:B:394:ASP:O	1:B:398:ASP:HB2	2.04	0.57
1:B:353:ILE:HG12	1:B:365:LEU:HB3	1.85	0.57
1:B:75:ARG:HG2	1:B:75:ARG:NH1	2.19	0.57
1:F:77:VAL:HG12	1:F:78:ALA:N	2.19	0.57
1:G:158:ILE:HG23	1:G:396:VAL:HG22	1.85	0.57
1:G:25:ASP:HA	1:G:28:LYS:HD2	1.86	0.57
1:D:138:VAL:HG12	1:D:407:VAL:HG12	1.86	0.57
1:B:352:GLN:O	1:B:356:THR:HG23	2.03	0.57
1:B:168:ARG:HG2	1:B:189:VAL:HG21	1.87	0.57
1:E:36:ARG:HG2	1:E:36:ARG:NH1	2.08	0.57
1:F:488:ASP:OD1	1:F:490:PHE:HB2	2.04	0.57
1:G:75:ARG:NH1	1:G:75:ARG:HG2	2.18	0.57
1:F:158:ILE:HG23	1:F:396:VAL:HG22	1.85	0.57
1:C:411:ILE:CD1	1:C:490:PHE:HE1	2.16	0.57
1:D:502:ARG:O	1:D:506:GLU:HG3	2.04	0.57
1:F:75:ARG:HH11	1:F:75:ARG:HG2	1.68	0.57
1:C:168:ARG:HG2	1:C:189:VAL:HG21	1.86	0.57
1:A:365:LEU:O	1:A:368:ARG:HG3	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:353:ILE:HG12	1:E:365:LEU:HB3	1.86	0.57
1:F:468:LYS:HD3	1:F:486:TYR:CZ	2.40	0.57
1:C:226:LYS:HZ1	1:C:252:GLU:HB3	1.69	0.57
1:B:409:GLU:OE2	1:B:499:LYS:HG3	2.05	0.57
1:F:71:ALA:O	1:F:75:ARG:HB3	2.05	0.57
1:A:75:ARG:HG2	1:A:75:ARG:NH1	2.20	0.57
1:B:483:THR:OG1	1:B:485:GLU:HG2	2.05	0.57
1:E:365:LEU:O	1:E:368:ARG:HG3	2.05	0.57
1:E:75:ARG:HG2	1:E:75:ARG:HH11	1.67	0.57
1:E:168:ARG:HG2	1:E:189:VAL:HG21	1.87	0.57
1:C:245:LYS:NZ	1:C:319:ARG:HH21	2.03	0.57
1:G:168:ARG:HG2	1:G:189:VAL:HG21	1.87	0.57
1:A:59:GLU:O	1:G:4:LYS:HD2	2.05	0.57
1:G:77:VAL:HG12	1:G:78:ALA:N	2.18	0.57
1:B:451:MET:HE1	1:B:466:ALA:HA	1.87	0.57
1:B:190:VAL:HG12	1:B:191:GLU:H	1.68	0.57
1:F:365:LEU:O	1:F:368:ARG:HG3	2.05	0.56
1:A:31:LEU:HD13	1:A:90:THR:CG2	2.35	0.56
1:F:394:ASP:O	1:F:398:ASP:HB2	2.05	0.56
1:C:353:ILE:HG12	1:C:365:LEU:HB3	1.85	0.56
1:A:71:ALA:O	1:A:75:ARG:HB3	2.05	0.56
1:A:27:VAL:CG1	1:A:90:THR:HG23	2.35	0.56
1:D:483:THR:OG1	1:D:485:GLU:HG2	2.04	0.56
1:E:22:ILE:HG21	1:E:62:LEU:HD21	1.87	0.56
1:D:168:ARG:HG2	1:D:189:VAL:HG21	1.87	0.56
1:B:479:PHE:N	1:B:489:MET:HE1	2.20	0.56
1:G:502:ARG:O	1:G:506:GLU:HG3	2.05	0.56
1:D:353:ILE:HG12	1:D:365:LEU:HB3	1.85	0.56
1:B:365:LEU:O	1:B:368:ARG:HG3	2.05	0.56
1:E:71:ALA:O	1:E:75:ARG:HB3	2.05	0.56
1:G:468:LYS:HD3	1:G:486:TYR:CZ	2.41	0.56
1:C:468:LYS:HD3	1:C:486:TYR:CZ	2.40	0.56
1:E:394:ASP:O	1:E:398:ASP:HB2	2.05	0.56
1:B:81:THR:HG23	1:B:503:THR:HG22	1.87	0.56
1:E:245:LYS:NZ	1:E:319:ARG:HH21	2.04	0.56
1:A:158:ILE:HG23	1:A:396:VAL:HG22	1.85	0.56
1:C:31:LEU:HD13	1:C:90:THR:CG2	2.36	0.56
1:D:468:LYS:HD3	1:D:486:TYR:CZ	2.40	0.56
1:A:22:ILE:HG21	1:A:62:LEU:HD21	1.87	0.56
1:G:19:GLY:HA3	1:G:67:GLU:O	2.06	0.56
1:F:245:LYS:NZ	1:F:319:ARG:HH21	2.03	0.56
1:E:411:ILE:CD1	1:E:490:PHE:HE1	2.19	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:VAL:HG12	1:A:78:ALA:N	2.19	0.56
1:C:75:ARG:HG2	1:C:75:ARG:NH1	2.20	0.56
1:D:81:THR:HG23	1:D:503:THR:HG22	1.88	0.56
1:G:13:ARG:HD3	1:G:104:LEU:HD22	1.88	0.56
1:D:411:ILE:CD1	1:D:490:PHE:HE1	2.19	0.56
1:B:226:LYS:HZ1	1:B:252:GLU:HB3	1.69	0.56
1:A:209:ASP:HB3	1:A:210:LYS:HZ1	1.71	0.56
1:F:25:ASP:HA	1:F:28:LYS:HD2	1.88	0.56
1:D:4:LYS:HD2	1:E:59:GLU:O	2.06	0.56
1:B:393:LYS:O	1:B:397:ASP:HB2	2.05	0.56
1:D:488:ASP:OD1	1:D:490:PHE:HB2	2.06	0.56
1:A:411:ILE:CD1	1:A:490:PHE:HE1	2.19	0.56
1:F:28:LYS:HG3	1:F:453:GLN:OE1	2.06	0.56
1:A:245:LYS:NZ	1:A:319:ARG:HH21	2.04	0.56
1:G:400:LEU:HG	1:G:400:LEU:O	2.06	0.56
1:A:81:THR:HG23	1:A:503:THR:HG22	1.88	0.56
1:D:25:ASP:HA	1:D:28:LYS:HD2	1.88	0.56
1:E:483:THR:OG1	1:E:485:GLU:HG2	2.05	0.56
1:A:393:LYS:O	1:A:397:ASP:HB2	2.06	0.56
1:G:245:LYS:NZ	1:G:319:ARG:HH21	2.04	0.56
1:E:209:ASP:HB3	1:E:210:LYS:HZ1	1.70	0.56
1:G:75:ARG:HH11	1:G:75:ARG:HG2	1.69	0.56
1:C:71:ALA:O	1:C:75:ARG:HB3	2.06	0.56
1:A:468:LYS:HD3	1:A:486:TYR:CZ	2.40	0.56
1:B:245:LYS:NZ	1:B:319:ARG:HH21	2.04	0.56
1:C:200:LEU:HD23	1:C:275:ALA:O	2.06	0.56
1:B:488:ASP:OD1	1:B:490:PHE:HB2	2.05	0.56
1:D:71:ALA:O	1:D:75:ARG:HB3	2.06	0.56
1:F:27:VAL:CG1	1:F:90:THR:HG23	2.35	0.56
1:C:393:LYS:O	1:C:397:ASP:HB2	2.06	0.56
1:E:158:ILE:HG23	1:E:396:VAL:HG22	1.87	0.56
1:D:13:ARG:HD3	1:D:104:LEU:HD22	1.88	0.55
1:E:13:ARG:HD3	1:E:104:LEU:HD22	1.88	0.55
1:F:19:GLY:HA3	1:F:67:GLU:O	2.06	0.55
1:B:75:ARG:HG2	1:B:75:ARG:HH11	1.71	0.55
1:C:19:GLY:HA3	1:C:67:GLU:O	2.06	0.55
1:E:25:ASP:HA	1:E:28:LYS:HD2	1.89	0.55
1:C:25:ASP:HA	1:C:28:LYS:HD2	1.88	0.55
1:E:488:ASP:OD1	1:E:490:PHE:HB2	2.05	0.55
1:D:365:LEU:O	1:D:368:ARG:HG3	2.05	0.55
1:A:69:MET:HG2	1:B:47:PRO:HB3	1.88	0.55
1:E:77:VAL:HG12	1:E:78:ALA:N	2.19	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:31:LEU:HD13	1:F:90:THR:CG2	2.36	0.55
1:A:25:ASP:HA	1:A:28:LYS:HD2	1.88	0.55
1:F:393:LYS:O	1:F:397:ASP:HB2	2.06	0.55
1:G:393:LYS:O	1:G:397:ASP:HB2	2.06	0.55
1:C:488:ASP:OD1	1:C:490:PHE:HB2	2.05	0.55
1:F:502:ARG:O	1:F:506:GLU:HG3	2.06	0.55
1:G:488:ASP:OD1	1:G:490:PHE:HB2	2.07	0.55
1:D:393:LYS:O	1:D:397:ASP:HB2	2.07	0.55
1:D:245:LYS:NZ	1:D:319:ARG:HH21	2.04	0.55
1:B:19:GLY:HA3	1:B:67:GLU:O	2.06	0.55
1:B:342:ILE:O	1:B:346:VAL:HG23	2.06	0.55
1:C:349:ILE:HG21	1:C:369:VAL:HB	1.89	0.55
1:B:22:ILE:HG21	1:B:62:LEU:HD21	1.89	0.55
1:A:200:LEU:HD23	1:A:275:ALA:O	2.07	0.55
1:F:227:LEU:HB3	1:F:254:VAL:HG13	1.89	0.55
1:E:226:LYS:HG2	1:E:252:GLU:CB	2.37	0.55
1:G:411:ILE:CD1	1:G:490:PHE:HE1	2.20	0.55
1:E:342:ILE:O	1:E:346:VAL:HG23	2.07	0.55
1:G:200:LEU:HD23	1:G:275:ALA:O	2.07	0.55
1:F:400:LEU:HG	1:F:400:LEU:O	2.07	0.55
1:B:502:ARG:O	1:B:506:GLU:HG3	2.06	0.55
1:E:393:LYS:O	1:E:397:ASP:HB2	2.06	0.55
1:B:200:LEU:HD23	1:B:275:ALA:O	2.07	0.55
1:A:227:LEU:HB3	1:A:254:VAL:HG13	1.88	0.55
1:B:411:ILE:CD1	1:B:490:PHE:HE1	2.20	0.55
1:F:342:ILE:O	1:F:346:VAL:HG23	2.07	0.55
1:C:75:ARG:HG2	1:C:75:ARG:HH11	1.72	0.55
1:C:5:GLU:HG3	1:C:525:LYS:HD3	1.88	0.55
1:E:468:LYS:HD3	1:E:486:TYR:CZ	2.42	0.55
1:G:2:ALA:O	1:G:4:LYS:HG2	2.07	0.55
1:A:13:ARG:HD3	1:A:104:LEU:HD22	1.89	0.55
1:F:30:THR:HB	1:F:51:LYS:O	2.06	0.55
1:G:227:LEU:HB3	1:G:254:VAL:HG13	1.89	0.55
1:F:413:VAL:CG1	1:F:489:MET:HB3	2.37	0.55
1:A:342:ILE:O	1:A:346:VAL:HG23	2.06	0.55
1:D:342:ILE:O	1:D:346:VAL:HG23	2.07	0.55
1:A:28:LYS:HG3	1:A:453:GLN:OE1	2.06	0.55
1:G:460:VAL:HG21	1:G:479:PHE:HZ	1.73	0.54
1:E:413:VAL:CG1	1:E:489:MET:HB3	2.37	0.54
1:A:502:ARG:O	1:A:506:GLU:HG3	2.06	0.54
1:D:349:ILE:HG21	1:D:369:VAL:HB	1.89	0.54
1:G:31:LEU:HD13	1:G:90:THR:HG21	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:31:LEU:HD13	1:B:90:THR:CG2	2.37	0.54
1:A:31:LEU:HD13	1:A:90:THR:HG21	1.88	0.54
1:E:4:LYS:HD2	1:F:59:GLU:O	2.07	0.54
1:B:441:ALA:O	1:B:445:ARG:HD3	2.07	0.54
1:E:81:THR:HG23	1:E:503:THR:HG22	1.90	0.54
1:G:342:ILE:O	1:G:346:VAL:HG23	2.07	0.54
1:C:365:LEU:O	1:C:368:ARG:HG3	2.06	0.54
1:A:5:GLU:HG3	1:A:525:LYS:HD3	1.88	0.54
1:A:24:ALA:HB3	1:A:97:GLN:NE2	2.23	0.54
1:C:179:GLU:HA	1:C:381:VAL:HG23	1.90	0.54
1:G:31:LEU:HD13	1:G:90:THR:CG2	2.37	0.54
1:F:22:ILE:HG21	1:F:62:LEU:HD21	1.89	0.54
1:E:200:LEU:HD23	1:E:275:ALA:O	2.07	0.54
1:G:192:GLY:HA2	1:G:295:LEU:HD21	1.90	0.54
1:F:31:LEU:HD13	1:F:90:THR:HG21	1.89	0.54
1:D:179:GLU:HA	1:D:381:VAL:HG23	1.90	0.54
1:C:502:ARG:O	1:C:506:GLU:HG3	2.06	0.54
1:A:226:LYS:HG2	1:A:252:GLU:CB	2.38	0.54
1:B:349:ILE:HG21	1:B:369:VAL:HB	1.90	0.54
1:D:200:LEU:HD23	1:D:275:ALA:O	2.08	0.54
1:C:460:VAL:HG21	1:C:479:PHE:HZ	1.72	0.54
1:G:413:VAL:CG1	1:G:489:MET:HB3	2.38	0.54
1:C:226:LYS:HG2	1:C:252:GLU:CB	2.38	0.54
1:F:452:ARG:O	1:F:456:GLU:HG2	2.08	0.54
1:E:5:GLU:HG3	1:E:525:LYS:HD3	1.88	0.54
1:D:5:GLU:HG3	1:D:525:LYS:HD3	1.89	0.54
1:B:5:GLU:HG3	1:B:525:LYS:HD3	1.88	0.54
1:C:31:LEU:HD13	1:C:90:THR:HG21	1.89	0.54
1:F:179:GLU:HA	1:F:381:VAL:HG23	1.90	0.54
1:C:451:MET:HE1	1:C:466:ALA:HA	1.90	0.54
1:E:227:LEU:HB3	1:E:254:VAL:HG13	1.89	0.54
1:F:226:LYS:HG2	1:F:252:GLU:CB	2.38	0.54
1:C:28:LYS:HG3	1:C:453:GLN:OE1	2.07	0.54
1:F:2:ALA:O	1:F:4:LYS:HG2	2.08	0.54
1:B:383:GLY:N	1:B:389:VAL:HG22	2.23	0.54
1:C:342:ILE:O	1:C:346:VAL:HG23	2.07	0.54
1:G:349:ILE:HG21	1:G:369:VAL:HB	1.90	0.54
1:E:349:ILE:HG21	1:E:369:VAL:HB	1.90	0.54
1:F:200:LEU:HD23	1:F:275:ALA:O	2.08	0.54
1:A:383:GLY:N	1:A:389:VAL:HG22	2.23	0.54
1:G:5:GLU:HG3	1:G:525:LYS:HD3	1.89	0.54
1:E:2:ALA:O	1:E:4:LYS:HG2	2.07	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:383:GLY:N	1:F:389:VAL:HG22	2.23	0.54
1:F:81:THR:HG23	1:F:503:THR:HG22	1.90	0.54
1:E:400:LEU:O	1:E:400:LEU:HG	2.07	0.54
1:D:31:LEU:HD13	1:D:90:THR:CG2	2.38	0.54
1:C:250:VAL:HG12	1:C:278:ALA:HA	1.90	0.53
1:G:479:PHE:N	1:G:489:MET:HE1	2.23	0.53
1:E:460:VAL:HG21	1:E:479:PHE:HZ	1.73	0.53
1:D:75:ARG:HG2	1:D:75:ARG:NH1	2.23	0.53
1:G:441:ALA:O	1:G:445:ARG:HD3	2.07	0.53
1:B:13:ARG:HD3	1:B:104:LEU:HD22	1.90	0.53
1:G:179:GLU:HA	1:G:381:VAL:HG23	1.90	0.53
1:B:179:GLU:HA	1:B:381:VAL:HG23	1.90	0.53
1:D:250:VAL:HG12	1:D:278:ALA:HA	1.90	0.53
1:F:349:ILE:HG21	1:F:369:VAL:HB	1.90	0.53
1:F:5:GLU:HG3	1:F:525:LYS:HD3	1.89	0.53
1:F:190:VAL:HG12	1:F:191:GLU:H	1.72	0.53
1:C:178:GLU:O	1:C:381:VAL:HG22	2.08	0.53
1:C:81:THR:HG23	1:C:503:THR:HG22	1.90	0.53
1:E:179:GLU:HA	1:E:381:VAL:HG23	1.90	0.53
1:C:400:LEU:HG	1:C:400:LEU:O	2.07	0.53
1:C:383:GLY:N	1:C:389:VAL:HG22	2.23	0.53
1:B:250:VAL:HG12	1:B:278:ALA:HA	1.90	0.53
1:A:413:VAL:CG1	1:A:489:MET:HB3	2.38	0.53
1:A:349:ILE:HG21	1:A:369:VAL:HB	1.89	0.53
1:B:226:LYS:HG2	1:B:252:GLU:CB	2.38	0.53
1:G:183:MET:HB3	1:G:384:MET:HE1	1.90	0.53
1:A:75:ARG:HH11	1:A:75:ARG:HG2	1.73	0.53
1:B:227:LEU:HB3	1:B:254:VAL:HG13	1.89	0.53
1:C:66:PHE:HA	1:C:69:MET:HE2	1.91	0.53
1:D:226:LYS:HG2	1:D:252:GLU:CB	2.38	0.53
1:C:192:GLY:HA2	1:C:295:LEU:HD21	1.90	0.53
1:A:192:GLY:HA2	1:A:295:LEU:HD21	1.91	0.53
1:E:24:ALA:HB3	1:E:97:GLN:NE2	2.23	0.53
1:G:81:THR:HG23	1:G:503:THR:HG22	1.91	0.53
1:E:451:MET:HE1	1:E:466:ALA:HA	1.90	0.53
1:C:222:LEU:HB2	1:C:289:LEU:HD22	1.91	0.53
1:A:197:ARG:NH1	1:A:277:LYS:HG2	2.23	0.53
1:C:413:VAL:CG1	1:C:489:MET:HB3	2.37	0.53
1:F:192:GLY:HA2	1:F:295:LEU:HD21	1.90	0.53
1:B:222:LEU:HB2	1:B:289:LEU:HD22	1.91	0.53
1:C:227:LEU:HB3	1:C:254:VAL:HG13	1.89	0.53
1:B:139:ASN:ND2	1:B:139:ASN:H	2.07	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:209:ASP:HB3	1:F:210:LYS:HZ1	1.73	0.53
1:A:2:ALA:O	1:A:4:LYS:HG2	2.09	0.53
1:B:400:LEU:O	1:B:400:LEU:HG	2.07	0.53
1:D:400:LEU:O	1:D:400:LEU:HG	2.07	0.53
1:D:227:LEU:HB3	1:D:254:VAL:HG13	1.89	0.53
1:E:502:ARG:O	1:E:506:GLU:HG3	2.09	0.53
1:A:66:PHE:HA	1:A:69:MET:HE2	1.91	0.53
1:G:24:ALA:HB3	1:G:97:GLN:NE2	2.24	0.53
1:F:24:ALA:HB3	1:F:97:GLN:NE2	2.24	0.53
1:D:178:GLU:O	1:D:381:VAL:HG22	2.09	0.53
1:G:178:GLU:O	1:G:381:VAL:HG22	2.09	0.53
1:F:103:GLY:HA3	1:F:516:ILE:HD11	1.91	0.53
1:B:460:VAL:HG21	1:B:479:PHE:HZ	1.74	0.53
1:D:452:ARG:O	1:D:456:GLU:HG2	2.09	0.53
1:F:178:GLU:O	1:F:381:VAL:HG22	2.09	0.53
1:B:178:GLU:O	1:B:381:VAL:HG22	2.09	0.53
1:D:441:ALA:O	1:D:445:ARG:HD3	2.09	0.53
1:G:30:THR:HB	1:G:51:LYS:O	2.09	0.53
1:A:179:GLU:HA	1:A:381:VAL:HG23	1.91	0.53
1:C:139:ASN:H	1:C:139:ASN:ND2	2.08	0.52
1:E:479:PHE:N	1:E:489:MET:HE1	2.24	0.52
1:A:479:PHE:N	1:A:489:MET:HE1	2.24	0.52
1:C:452:ARG:O	1:C:456:GLU:HG2	2.09	0.52
1:A:190:VAL:HG12	1:A:191:GLU:H	1.73	0.52
1:G:139:ASN:ND2	1:G:139:ASN:H	2.06	0.52
1:A:250:VAL:HG12	1:A:278:ALA:HA	1.90	0.52
1:C:460:VAL:HG21	1:C:479:PHE:CZ	2.45	0.52
1:B:192:GLY:HA2	1:B:295:LEU:HD21	1.91	0.52
1:D:2:ALA:O	1:D:4:LYS:HG2	2.08	0.52
1:E:383:GLY:N	1:E:389:VAL:HG22	2.23	0.52
1:G:383:GLY:N	1:G:389:VAL:HG22	2.25	0.52
1:F:317:LEU:HG	1:F:318:GLY:N	2.24	0.52
1:E:250:VAL:HG12	1:E:278:ALA:HA	1.89	0.52
1:A:460:VAL:HG21	1:A:479:PHE:HZ	1.73	0.52
1:B:66:PHE:HA	1:B:69:MET:HE2	1.92	0.52
1:E:19:GLY:HA3	1:E:67:GLU:O	2.09	0.52
1:F:13:ARG:HD3	1:F:104:LEU:HD22	1.91	0.52
1:A:421:GLN:O	1:A:424:LYS:HB2	2.09	0.52
1:F:426:LEU:HB2	1:F:444:ARG:HD2	1.91	0.52
1:E:139:ASN:H	1:E:139:ASN:ND2	2.07	0.52
1:D:413:VAL:CG1	1:D:489:MET:HB3	2.38	0.52
1:F:460:VAL:HG21	1:F:479:PHE:HZ	1.73	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:PRO:HB3	1:G:69:MET:HG2	1.91	0.52
1:D:31:LEU:HD13	1:D:90:THR:HG21	1.91	0.52
1:A:18:LYS:HB3	1:A:67:GLU:HG2	1.92	0.52
1:D:86:GLY:C	1:D:88:GLY:H	2.13	0.52
1:C:426:LEU:HB2	1:C:444:ARG:HD2	1.91	0.52
1:E:317:LEU:HG	1:E:318:GLY:N	2.25	0.52
1:D:30:THR:HB	1:D:51:LYS:O	2.09	0.52
1:D:139:ASN:H	1:D:139:ASN:ND2	2.08	0.52
1:E:197:ARG:NH1	1:E:277:LYS:HG2	2.24	0.52
1:B:413:VAL:CG1	1:B:489:MET:HB3	2.38	0.52
1:G:66:PHE:HA	1:G:69:MET:CE	2.40	0.52
1:D:7:LYS:HD2	1:D:66:PHE:CE1	2.45	0.52
1:G:365:LEU:HD11	1:G:368:ARG:HH21	1.75	0.52
1:E:365:LEU:HD11	1:E:368:ARG:HH21	1.75	0.52
1:B:317:LEU:HG	1:B:318:GLY:N	2.25	0.52
1:A:441:ALA:O	1:A:445:ARG:HD3	2.09	0.52
1:A:30:THR:HB	1:A:51:LYS:O	2.10	0.52
1:F:222:LEU:HB2	1:F:289:LEU:HD22	1.91	0.52
1:A:222:LEU:HB2	1:A:289:LEU:HD22	1.91	0.52
1:C:4:LYS:HD2	1:D:59:GLU:O	2.08	0.52
1:G:250:VAL:HG12	1:G:278:ALA:HA	1.90	0.52
1:D:185:THR:HA	1:D:380:ARG:O	2.10	0.52
1:D:192:GLY:HA2	1:D:295:LEU:HD21	1.91	0.52
1:E:31:LEU:HD13	1:E:90:THR:CG2	2.40	0.52
1:D:383:GLY:N	1:D:389:VAL:HG22	2.24	0.52
1:E:433:ASN:N	1:E:433:ASN:OD1	2.42	0.52
1:B:2:ALA:O	1:B:4:LYS:HG2	2.09	0.52
1:D:460:VAL:HG21	1:D:479:PHE:HZ	1.74	0.52
1:D:69:MET:HG2	1:E:47:PRO:HB3	1.91	0.52
1:E:192:GLY:HA2	1:E:295:LEU:HD21	1.91	0.52
1:F:477:PHE:CE1	1:F:486:TYR:HB3	2.45	0.52
1:C:441:ALA:O	1:C:445:ARG:HD3	2.10	0.52
1:G:86:GLY:C	1:G:88:GLY:H	2.14	0.52
1:E:421:GLN:O	1:E:424:LYS:HB2	2.10	0.52
1:B:30:THR:HB	1:B:51:LYS:O	2.09	0.52
1:G:7:LYS:HD2	1:G:66:PHE:CE1	2.44	0.52
1:D:66:PHE:HA	1:D:69:MET:HE2	1.92	0.52
1:A:66:PHE:HA	1:A:69:MET:CE	2.40	0.52
1:E:452:ARG:O	1:E:456:GLU:HG2	2.10	0.52
1:B:86:GLY:C	1:B:88:GLY:H	2.13	0.52
1:E:185:THR:HA	1:E:380:ARG:O	2.10	0.52
1:E:365:LEU:HG	1:E:368:ARG:HE	1.75	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:365:LEU:HD11	1:B:368:ARG:HH21	1.75	0.52
1:E:31:LEU:HD13	1:E:90:THR:HG21	1.91	0.52
1:D:222:LEU:HB2	1:D:289:LEU:HD22	1.91	0.52
1:F:185:THR:HA	1:F:380:ARG:O	2.10	0.51
1:G:452:ARG:O	1:G:456:GLU:HG2	2.10	0.51
1:F:365:LEU:HG	1:F:368:ARG:HE	1.76	0.51
1:E:138:VAL:O	1:E:138:VAL:HG12	2.09	0.51
1:B:31:LEU:HD13	1:B:90:THR:HG21	1.90	0.51
1:G:22:ILE:HG21	1:G:62:LEU:HD21	1.91	0.51
1:F:4:LYS:HD2	1:G:59:GLU:O	2.10	0.51
1:B:103:GLY:HA3	1:B:516:ILE:HD11	1.91	0.51
1:C:30:THR:HB	1:C:51:LYS:O	2.09	0.51
1:E:169:VAL:CG2	1:E:377:ALA:HB2	2.41	0.51
1:G:322:LYS:HB3	1:G:333:VAL:CG2	2.39	0.51
1:G:197:ARG:NH1	1:G:277:LYS:HG2	2.24	0.51
1:E:460:VAL:HG21	1:E:479:PHE:CZ	2.45	0.51
1:A:365:LEU:HG	1:A:368:ARG:HE	1.76	0.51
1:G:220:ILE:HG23	1:G:248:LEU:HD22	1.92	0.51
1:C:13:ARG:HD3	1:C:104:LEU:HD22	1.93	0.51
1:C:421:GLN:O	1:C:424:LYS:HB2	2.10	0.51
1:F:197:ARG:NH1	1:F:277:LYS:HG2	2.24	0.51
1:A:185:THR:HA	1:A:380:ARG:O	2.10	0.51
1:A:460:VAL:HG21	1:A:479:PHE:CZ	2.45	0.51
1:C:7:LYS:HD2	1:C:66:PHE:CE1	2.45	0.51
1:G:226:LYS:HG2	1:G:252:GLU:CB	2.38	0.51
1:E:66:PHE:HA	1:E:69:MET:CE	2.41	0.51
1:E:220:ILE:HG23	1:E:248:LEU:HD22	1.93	0.51
1:D:220:ILE:HG23	1:D:248:LEU:HD22	1.93	0.51
1:E:28:LYS:HG3	1:E:453:GLN:OE1	2.11	0.51
1:E:222:LEU:HB2	1:E:289:LEU:HD22	1.91	0.51
1:C:317:LEU:HG	1:C:318:GLY:N	2.25	0.51
1:G:222:LEU:HB2	1:G:289:LEU:HD22	1.91	0.51
1:G:317:LEU:HG	1:G:318:GLY:N	2.25	0.51
1:F:322:LYS:HB3	1:F:333:VAL:CG2	2.38	0.51
1:F:479:PHE:N	1:F:489:MET:HE1	2.25	0.51
1:B:24:ALA:HB3	1:B:97:GLN:NE2	2.26	0.51
1:D:28:LYS:HG3	1:D:453:GLN:OE1	2.11	0.51
1:C:86:GLY:C	1:C:88:GLY:H	2.14	0.51
1:D:479:PHE:N	1:D:489:MET:HE1	2.26	0.51
1:F:460:VAL:HG21	1:F:479:PHE:CZ	2.45	0.51
1:F:7:LYS:HD2	1:F:66:PHE:CE1	2.44	0.51
1:B:452:ARG:O	1:B:456:GLU:HG2	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:468:LYS:HD3	1:B:486:TYR:CE1	2.46	0.51
1:D:468:LYS:HD3	1:D:486:TYR:CE1	2.45	0.51
1:D:451:MET:HE1	1:D:466:ALA:HA	1.92	0.51
1:C:6:VAL:HG22	1:C:522:ILE:HG12	1.92	0.51
1:C:185:THR:HA	1:C:380:ARG:O	2.10	0.51
1:A:26:ALA:HA	1:G:8:PHE:HE1	1.76	0.51
1:D:365:LEU:HD11	1:D:368:ARG:HH21	1.76	0.51
1:G:365:LEU:HG	1:G:368:ARG:HE	1.76	0.51
1:E:178:GLU:O	1:E:381:VAL:HG22	2.10	0.51
1:G:421:GLN:O	1:G:424:LYS:HB2	2.11	0.51
1:G:426:LEU:HB2	1:G:444:ARG:HD2	1.92	0.51
1:A:400:LEU:HG	1:A:400:LEU:O	2.10	0.51
1:F:284:ARG:HH11	1:F:284:ARG:HA	1.76	0.51
1:A:317:LEU:HG	1:A:318:GLY:N	2.25	0.51
1:A:139:ASN:H	1:A:139:ASN:ND2	2.07	0.51
1:F:250:VAL:HG12	1:F:278:ALA:HA	1.91	0.51
1:G:185:THR:HA	1:G:380:ARG:O	2.10	0.51
1:G:460:VAL:HG21	1:G:479:PHE:CZ	2.45	0.51
1:C:66:PHE:HA	1:C:69:MET:CE	2.41	0.51
1:A:452:ARG:O	1:A:456:GLU:HG2	2.11	0.51
1:F:220:ILE:HG23	1:F:248:LEU:HD22	1.93	0.51
1:D:433:ASN:OD1	1:D:433:ASN:N	2.44	0.51
1:B:185:THR:HA	1:B:380:ARG:O	2.10	0.51
1:A:489:MET:HG3	1:A:494:VAL:HB	1.93	0.51
1:E:7:LYS:HD2	1:E:66:PHE:CE1	2.45	0.51
1:C:24:ALA:HB3	1:C:97:GLN:NE2	2.26	0.51
1:B:64:ASP:OD1	1:B:64:ASP:C	2.50	0.51
1:A:284:ARG:HH11	1:A:284:ARG:HA	1.76	0.51
1:F:421:GLN:O	1:F:424:LYS:HB2	2.10	0.51
1:D:19:GLY:HA3	1:D:67:GLU:O	2.10	0.51
1:G:18:LYS:HB3	1:G:67:GLU:HG2	1.93	0.51
1:E:24:ALA:O	1:E:28:LYS:HD2	2.11	0.51
1:A:178:GLU:O	1:A:381:VAL:HG22	2.11	0.51
1:C:103:GLY:HA3	1:C:516:ILE:HD11	1.92	0.51
1:D:421:GLN:O	1:D:424:LYS:HB2	2.11	0.51
1:G:103:GLY:HA3	1:G:516:ILE:HD11	1.93	0.51
1:E:441:ALA:O	1:E:445:ARG:HD3	2.11	0.51
1:F:139:ASN:H	1:F:139:ASN:ND2	2.07	0.50
1:D:460:VAL:HG21	1:D:479:PHE:CZ	2.46	0.50
1:E:226:LYS:HZ1	1:E:252:GLU:HB3	1.76	0.50
1:B:314:ILE:HD12	1:B:315:ASP:N	2.26	0.50
1:C:314:ILE:HD12	1:C:315:ASP:N	2.26	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:479:PHE:N	1:C:489:MET:HE1	2.26	0.50
1:D:66:PHE:HA	1:D:69:MET:CE	2.41	0.50
1:C:365:LEU:HG	1:C:368:ARG:HE	1.76	0.50
1:G:477:PHE:CE1	1:G:486:TYR:HB3	2.46	0.50
1:F:433:ASN:N	1:F:433:ASN:OD1	2.43	0.50
1:G:433:ASN:OD1	1:G:436:GLN:HB2	2.12	0.50
1:B:433:ASN:OD1	1:B:433:ASN:N	2.42	0.50
1:E:6:VAL:HG22	1:E:522:ILE:HG12	1.94	0.50
1:F:86:GLY:C	1:F:88:GLY:H	2.14	0.50
1:A:86:GLY:C	1:A:88:GLY:H	2.14	0.50
1:A:314:ILE:HD12	1:A:315:ASP:N	2.26	0.50
1:E:426:LEU:HB2	1:E:444:ARG:HD2	1.93	0.50
1:B:460:VAL:HG21	1:B:479:PHE:CZ	2.47	0.50
1:D:365:LEU:HG	1:D:368:ARG:HE	1.76	0.50
1:D:231:GLN:N	1:D:232:PRO:HD2	2.27	0.50
1:E:231:GLN:N	1:E:232:PRO:HD2	2.26	0.50
1:C:18:LYS:HB3	1:C:67:GLU:HG2	1.93	0.50
1:C:220:ILE:HG23	1:C:248:LEU:HD22	1.93	0.50
1:G:28:LYS:HG3	1:G:453:GLN:OE1	2.12	0.50
1:A:4:LYS:HD2	1:B:59:GLU:O	2.10	0.50
1:G:433:ASN:OD1	1:G:433:ASN:N	2.44	0.50
1:B:362:ARG:HE	1:B:363:GLU:N	2.09	0.50
1:B:66:PHE:HA	1:B:69:MET:CE	2.42	0.50
1:C:231:GLN:N	1:C:232:PRO:HD2	2.27	0.50
1:A:220:ILE:HG23	1:A:248:LEU:HD22	1.93	0.50
1:D:317:LEU:HG	1:D:318:GLY:N	2.25	0.50
1:F:362:ARG:HE	1:F:363:GLU:N	2.09	0.50
1:G:362:ARG:HE	1:G:363:GLU:N	2.09	0.50
1:D:426:LEU:HB2	1:D:444:ARG:HD2	1.92	0.50
1:D:169:VAL:CG2	1:D:377:ALA:HB2	2.42	0.50
1:C:365:LEU:HD11	1:C:368:ARG:HH21	1.76	0.50
1:B:231:GLN:N	1:B:232:PRO:HD2	2.27	0.50
1:D:477:PHE:CE1	1:D:486:TYR:HB3	2.46	0.50
1:E:18:LYS:HB3	1:E:67:GLU:HG2	1.93	0.50
1:E:103:GLY:HA3	1:E:516:ILE:HD11	1.93	0.50
1:G:451:MET:HE1	1:G:466:ALA:HA	1.94	0.50
1:A:169:VAL:CG2	1:A:377:ALA:HB2	2.41	0.50
1:E:284:ARG:HA	1:E:284:ARG:HH11	1.76	0.50
1:F:66:PHE:HA	1:F:69:MET:CE	2.41	0.50
1:E:30:THR:HB	1:E:51:LYS:O	2.11	0.50
1:F:441:ALA:O	1:F:445:ARG:HD3	2.11	0.50
1:A:426:LEU:HB2	1:A:444:ARG:HD2	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:169:VAL:CG2	1:F:377:ALA:HB2	2.42	0.50
1:A:409:GLU:OE2	1:A:499:LYS:HG3	2.11	0.50
1:C:433:ASN:OD1	1:C:433:ASN:N	2.45	0.50
1:C:433:ASN:OD1	1:C:436:GLN:HB2	2.12	0.50
1:C:362:ARG:HE	1:C:363:GLU:N	2.10	0.50
1:D:284:ARG:HA	1:D:284:ARG:HH11	1.76	0.50
1:D:64:ASP:OD1	1:D:64:ASP:C	2.50	0.50
1:D:221:LEU:HD21	1:D:249:ILE:HG12	1.94	0.50
1:F:138:VAL:HG12	1:F:138:VAL:O	2.11	0.50
1:C:24:ALA:O	1:C:28:LYS:HD2	2.12	0.50
1:B:4:LYS:HD2	1:C:59:GLU:O	2.11	0.50
1:D:222:LEU:HD13	1:D:289:LEU:HB3	1.94	0.50
1:G:339:LYS:HB3	1:G:343:GLU:OE2	2.12	0.50
1:B:224:GLU:HG3	1:B:286:LYS:NZ	2.27	0.50
1:G:314:ILE:HD12	1:G:315:ASP:N	2.26	0.50
1:B:284:ARG:HA	1:B:284:ARG:HH11	1.76	0.50
1:D:226:LYS:HZ3	1:D:252:GLU:HB3	1.77	0.50
1:B:365:LEU:HG	1:B:368:ARG:HE	1.76	0.50
1:C:138:VAL:O	1:C:138:VAL:HG12	2.10	0.50
1:C:468:LYS:HD3	1:C:486:TYR:CE1	2.47	0.50
1:B:28:LYS:HG3	1:B:453:GLN:OE1	2.12	0.50
1:A:433:ASN:OD1	1:A:433:ASN:N	2.43	0.50
1:D:314:ILE:HD12	1:D:315:ASP:N	2.26	0.50
1:A:477:PHE:CE1	1:A:486:TYR:HB3	2.46	0.50
1:G:169:VAL:CG2	1:G:377:ALA:HB2	2.42	0.50
1:E:86:GLY:C	1:E:88:GLY:H	2.14	0.50
1:F:314:ILE:HD12	1:F:315:ASP:N	2.26	0.50
1:D:322:LYS:HB3	1:D:333:VAL:CG2	2.39	0.49
1:F:365:LEU:HD11	1:F:368:ARG:HH21	1.76	0.49
1:A:138:VAL:O	1:A:138:VAL:HG12	2.11	0.49
1:D:75:ARG:HH11	1:D:75:ARG:HG2	1.76	0.49
1:E:224:GLU:HG3	1:E:286:LYS:NZ	2.27	0.49
1:D:224:GLU:HG3	1:D:286:LYS:NZ	2.27	0.49
1:B:169:VAL:CG2	1:B:377:ALA:HB2	2.41	0.49
1:B:322:LYS:HB3	1:B:333:VAL:CG2	2.39	0.49
1:B:220:ILE:HG23	1:B:248:LEU:HD22	1.93	0.49
1:C:222:LEU:HD13	1:C:289:LEU:HB3	1.94	0.49
1:B:222:LEU:HD13	1:B:289:LEU:HB3	1.94	0.49
1:A:362:ARG:HE	1:A:363:GLU:N	2.10	0.49
1:F:224:GLU:HG3	1:F:286:LYS:NZ	2.27	0.49
1:A:365:LEU:HD11	1:A:368:ARG:HH21	1.76	0.49
1:A:248:LEU:HD13	1:A:323:VAL:HG11	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2:ALA:O	1:C:4:LYS:HG2	2.11	0.49
1:C:169:VAL:CG2	1:C:377:ALA:HB2	2.42	0.49
1:A:322:LYS:HB3	1:A:333:VAL:CG2	2.38	0.49
1:A:361:ASP:OD1	1:A:365:LEU:HD13	2.13	0.49
1:C:361:ASP:OD1	1:C:365:LEU:HD13	2.13	0.49
1:A:231:GLN:N	1:A:232:PRO:HD2	2.27	0.49
1:B:248:LEU:HD13	1:B:323:VAL:HG11	1.95	0.49
1:F:11:ASP:CG	1:F:15:ARG:HH12	2.16	0.49
1:F:451:MET:CE	1:F:465:VAL:HG12	2.42	0.49
1:F:451:MET:HE1	1:F:466:ALA:HA	1.94	0.49
1:C:224:GLU:HG3	1:C:286:LYS:NZ	2.28	0.49
1:B:339:LYS:HB3	1:B:343:GLU:OE2	2.13	0.49
1:E:314:ILE:HD12	1:E:315:ASP:N	2.26	0.49
1:C:227:LEU:HD13	1:C:254:VAL:HG22	1.95	0.49
1:B:433:ASN:OD1	1:B:436:GLN:HB2	2.13	0.49
1:A:339:LYS:HB3	1:A:343:GLU:OE2	2.13	0.49
1:A:221:LEU:HD21	1:A:249:ILE:HG12	1.94	0.49
1:G:66:PHE:HA	1:G:69:MET:HE2	1.94	0.49
1:F:231:GLN:N	1:F:232:PRO:HD2	2.27	0.49
1:B:361:ASP:OD1	1:B:365:LEU:HD13	2.13	0.49
1:E:248:LEU:HD13	1:E:323:VAL:HG11	1.95	0.49
1:B:138:VAL:HG12	1:B:138:VAL:O	2.11	0.49
1:E:169:VAL:HG21	1:E:377:ALA:HB2	1.94	0.49
1:A:224:GLU:HG3	1:A:286:LYS:NZ	2.27	0.49
1:D:362:ARG:HE	1:D:363:GLU:N	2.09	0.49
1:G:284:ARG:HA	1:G:284:ARG:HH11	1.76	0.49
1:F:64:ASP:C	1:F:64:ASP:OD1	2.51	0.49
1:D:248:LEU:HD13	1:D:323:VAL:HG11	1.95	0.49
1:G:248:LEU:HD13	1:G:323:VAL:HG11	1.95	0.49
1:G:227:LEU:HD13	1:G:254:VAL:HG22	1.94	0.49
1:D:227:LEU:HD13	1:D:254:VAL:HG22	1.95	0.49
1:G:469:VAL:HG22	1:G:478:GLY:HA2	1.94	0.49
1:G:231:GLN:N	1:G:232:PRO:HD2	2.27	0.49
1:E:477:PHE:CE1	1:E:486:TYR:HB3	2.47	0.49
1:D:18:LYS:HB3	1:D:67:GLU:HG2	1.93	0.49
1:B:122:VAL:HG12	1:B:123:ALA:N	2.28	0.49
1:E:339:LYS:HB3	1:E:343:GLU:OE2	2.12	0.49
1:C:284:ARG:HA	1:C:284:ARG:HH11	1.76	0.49
1:G:501:VAL:HG12	1:G:501:VAL:O	2.13	0.49
1:F:489:MET:HG3	1:F:494:VAL:HB	1.95	0.49
1:A:69:MET:HG2	1:B:47:PRO:HG3	1.95	0.49
1:G:138:VAL:HG12	1:G:138:VAL:O	2.13	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:222:LEU:HD13	1:A:289:LEU:HB3	1.94	0.49
1:F:6:VAL:HG22	1:F:522:ILE:HG12	1.95	0.49
1:C:339:LYS:HB3	1:C:343:GLU:OE2	2.13	0.49
1:E:213:ALA:HB3	1:E:325:ILE:HB	1.95	0.49
1:B:227:LEU:HD13	1:B:254:VAL:HG22	1.95	0.49
1:G:468:LYS:HD3	1:G:486:TYR:CE1	2.47	0.49
1:C:477:PHE:CE1	1:C:486:TYR:HB3	2.47	0.49
1:G:222:LEU:HD13	1:G:289:LEU:HB3	1.94	0.49
1:E:362:ARG:HE	1:E:363:GLU:N	2.09	0.49
1:B:469:VAL:HG22	1:B:478:GLY:HA2	1.95	0.49
1:G:64:ASP:OD1	1:G:64:ASP:C	2.51	0.49
1:E:221:LEU:HD21	1:E:249:ILE:HG12	1.95	0.48
1:D:469:VAL:HG22	1:D:478:GLY:HA2	1.95	0.48
1:E:361:ASP:OD1	1:E:365:LEU:HD13	2.13	0.48
1:B:477:PHE:CE1	1:B:486:TYR:HB3	2.47	0.48
1:F:122:VAL:HG12	1:F:123:ALA:N	2.27	0.48
1:E:433:ASN:OD1	1:E:436:GLN:HB2	2.13	0.48
1:B:421:GLN:O	1:B:424:LYS:HB2	2.12	0.48
1:D:339:LYS:HB3	1:D:343:GLU:OE2	2.13	0.48
1:A:64:ASP:OD1	1:A:64:ASP:C	2.51	0.48
1:G:221:LEU:HD21	1:G:249:ILE:HG12	1.94	0.48
1:F:248:LEU:HD13	1:F:323:VAL:HG11	1.95	0.48
1:E:468:LYS:HD3	1:E:486:TYR:CE1	2.48	0.48
1:D:24:ALA:HB3	1:D:97:GLN:NE2	2.27	0.48
1:E:222:LEU:HD13	1:E:289:LEU:HB3	1.94	0.48
1:G:341:GLU:O	1:G:345:ARG:HG2	2.14	0.48
1:A:341:GLU:O	1:A:345:ARG:HG2	2.13	0.48
1:E:227:LEU:HD13	1:E:254:VAL:HG22	1.95	0.48
1:C:322:LYS:HB3	1:C:333:VAL:CG2	2.39	0.48
1:C:248:LEU:HD13	1:C:323:VAL:HG11	1.95	0.48
1:B:18:LYS:HB3	1:B:67:GLU:HG2	1.95	0.48
1:A:451:MET:HE1	1:A:466:ALA:HA	1.95	0.48
1:F:69:MET:HG2	1:G:47:PRO:HB3	1.95	0.48
1:F:361:ASP:OD1	1:F:365:LEU:HD13	2.13	0.48
1:F:468:LYS:HD3	1:F:486:TYR:CE1	2.47	0.48
1:F:222:LEU:HD13	1:F:289:LEU:HB3	1.94	0.48
1:G:451:MET:CE	1:G:465:VAL:HG12	2.44	0.48
1:C:341:GLU:O	1:C:345:ARG:HG2	2.13	0.48
1:F:213:ALA:HB3	1:F:325:ILE:HB	1.96	0.48
1:B:7:LYS:HD2	1:B:66:PHE:CE1	2.48	0.48
1:F:24:ALA:O	1:F:28:LYS:HD2	2.14	0.48
1:F:433:ASN:OD1	1:F:436:GLN:HB2	2.14	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:213:ALA:HB3	1:G:325:ILE:HB	1.95	0.48
1:D:501:VAL:O	1:D:501:VAL:HG12	2.13	0.48
1:G:224:GLU:HG3	1:G:286:LYS:NZ	2.28	0.48
1:C:221:LEU:HD21	1:C:249:ILE:HG12	1.95	0.48
1:B:426:LEU:HB2	1:B:444:ARG:HD2	1.94	0.48
1:B:501:VAL:O	1:B:501:VAL:HG12	2.14	0.48
1:C:469:VAL:HG22	1:C:478:GLY:HA2	1.94	0.48
1:A:469:VAL:HG22	1:A:478:GLY:HA2	1.95	0.48
1:D:433:ASN:OD1	1:D:436:GLN:HB2	2.14	0.48
1:A:433:ASN:OD1	1:A:436:GLN:HB2	2.14	0.48
1:C:122:VAL:HG12	1:C:123:ALA:N	2.29	0.48
1:F:501:VAL:HG12	1:F:501:VAL:O	2.13	0.48
1:E:12:ALA:HB1	1:E:521:MET:HG3	1.96	0.48
1:G:190:VAL:HG11	1:G:334:ASP:CG	2.34	0.48
1:A:468:LYS:HD3	1:A:486:TYR:CE1	2.48	0.48
1:D:8:PHE:HE1	1:E:26:ALA:HA	1.78	0.48
1:G:122:VAL:HG12	1:G:123:ALA:N	2.27	0.48
1:D:11:ASP:CG	1:D:15:ARG:HH12	2.17	0.48
1:C:64:ASP:C	1:C:64:ASP:OD1	2.52	0.48
1:C:489:MET:HG3	1:C:494:VAL:HB	1.95	0.48
1:D:361:ASP:OD1	1:D:365:LEU:HD13	2.13	0.48
1:F:190:VAL:HG11	1:F:334:ASP:CB	2.43	0.48
1:F:183:MET:HB3	1:F:384:MET:HE1	1.95	0.48
1:F:339:LYS:HB3	1:F:343:GLU:OE2	2.13	0.48
1:B:169:VAL:HG21	1:B:377:ALA:HB2	1.95	0.48
1:F:341:GLU:O	1:F:345:ARG:HG2	2.14	0.48
1:G:6:VAL:HG22	1:G:522:ILE:HG12	1.95	0.48
1:D:122:VAL:HG12	1:D:123:ALA:N	2.29	0.48
1:B:227:LEU:CB	1:B:254:VAL:HG13	2.44	0.47
1:E:322:LYS:HB3	1:E:333:VAL:CG2	2.39	0.47
1:E:469:VAL:HG22	1:E:478:GLY:HA2	1.96	0.47
1:G:124:THR:O	1:G:128:VAL:HG23	2.14	0.47
1:D:220:ILE:HD12	1:D:248:LEU:HD22	1.96	0.47
1:B:341:GLU:O	1:B:345:ARG:HG2	2.14	0.47
1:C:227:LEU:CB	1:C:254:VAL:HG13	2.44	0.47
1:F:221:LEU:HD21	1:F:249:ILE:HG12	1.94	0.47
1:D:138:VAL:HG12	1:D:138:VAL:O	2.12	0.47
1:E:341:GLU:O	1:E:345:ARG:HG2	2.14	0.47
1:A:501:VAL:HG12	1:A:501:VAL:O	2.14	0.47
1:C:501:VAL:O	1:C:501:VAL:HG12	2.13	0.47
1:B:205:VAL:HG12	1:B:207:ASN:H	1.79	0.47
1:F:227:LEU:HD13	1:F:254:VAL:HG22	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:221:LEU:HD21	1:B:249:ILE:HG12	1.95	0.47
1:D:489:MET:HG3	1:D:494:VAL:HB	1.96	0.47
1:C:183:MET:HB3	1:C:384:MET:HE1	1.96	0.47
1:B:205:VAL:HG12	1:B:207:ASN:N	2.30	0.47
1:A:213:ALA:HB3	1:A:325:ILE:HB	1.96	0.47
1:E:64:ASP:C	1:E:64:ASP:OD1	2.52	0.47
1:A:227:LEU:HD13	1:A:254:VAL:HG22	1.96	0.47
1:F:469:VAL:HG22	1:F:478:GLY:HA2	1.95	0.47
1:F:226:LYS:HZ3	1:F:252:GLU:HB3	1.79	0.47
1:D:169:VAL:HG21	1:D:377:ALA:HB2	1.96	0.47
1:A:7:LYS:HD2	1:A:66:PHE:CE1	2.49	0.47
1:D:219:TYR:CD1	1:D:247:LEU:HD12	2.50	0.47
1:F:220:ILE:HD12	1:F:248:LEU:HD22	1.95	0.47
1:A:362:ARG:HE	1:A:363:GLU:HB2	1.79	0.47
1:D:341:GLU:O	1:D:345:ARG:HG2	2.14	0.47
1:B:220:ILE:HD12	1:B:248:LEU:HD22	1.96	0.47
1:C:220:ILE:HD12	1:C:248:LEU:HD22	1.96	0.47
1:G:227:LEU:CB	1:G:254:VAL:HG13	2.44	0.47
1:D:227:LEU:CB	1:D:254:VAL:HG13	2.44	0.47
1:D:197:ARG:NH1	1:D:277:LYS:HG2	2.23	0.47
1:A:221:LEU:HD21	1:A:249:ILE:CG1	2.45	0.47
1:D:321:LYS:CB	1:D:334:ASP:HB3	2.45	0.47
1:G:361:ASP:OD1	1:G:365:LEU:HD13	2.13	0.47
1:F:77:VAL:HG21	1:F:511:VAL:HG13	1.97	0.47
1:B:174:VAL:O	1:B:174:VAL:HG22	2.14	0.47
1:A:220:ILE:HD12	1:A:248:LEU:HD22	1.95	0.47
1:G:362:ARG:HE	1:G:363:GLU:HB2	1.79	0.47
1:F:169:VAL:HG21	1:F:377:ALA:HB2	1.96	0.47
1:E:227:LEU:CB	1:E:254:VAL:HG13	2.45	0.47
1:A:226:LYS:HZ1	1:A:252:GLU:HB3	1.78	0.47
1:B:183:MET:HB3	1:B:384:MET:HE1	1.97	0.47
1:B:219:TYR:CD1	1:B:247:LEU:HD12	2.50	0.47
1:G:429:LEU:HD12	1:G:430:SER:N	2.30	0.47
1:G:220:ILE:HD12	1:G:248:LEU:HD22	1.96	0.47
1:F:18:LYS:HB3	1:F:67:GLU:HG2	1.96	0.47
1:A:289:LEU:O	1:A:293:ALA:HB2	2.15	0.47
1:D:124:THR:O	1:D:128:VAL:HG23	2.15	0.47
1:E:220:ILE:HD12	1:E:248:LEU:HD22	1.96	0.47
1:C:511:VAL:HG23	1:C:512:ALA:N	2.29	0.47
1:B:158:ILE:CG2	1:B:396:VAL:HG22	2.45	0.47
1:B:362:ARG:HE	1:B:363:GLU:HB2	1.79	0.47
1:C:362:ARG:HE	1:C:363:GLU:HB2	1.80	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:213:ALA:HB3	1:C:325:ILE:HB	1.96	0.47
1:C:11:ASP:CG	1:C:15:ARG:HH12	2.18	0.47
1:F:227:LEU:CB	1:F:254:VAL:HG13	2.44	0.47
1:A:227:LEU:CB	1:A:254:VAL:HG13	2.44	0.47
1:C:197:ARG:NH1	1:C:277:LYS:HG2	2.24	0.47
1:G:219:TYR:CD1	1:G:247:LEU:HD12	2.50	0.47
1:D:174:VAL:O	1:D:174:VAL:HG22	2.14	0.47
1:A:174:VAL:O	1:A:174:VAL:HG22	2.14	0.47
1:C:158:ILE:CG2	1:C:396:VAL:HG22	2.45	0.47
1:C:451:MET:CE	1:C:465:VAL:HG12	2.45	0.47
1:A:169:VAL:HG21	1:A:377:ALA:HB2	1.96	0.47
1:B:213:ALA:HB3	1:B:325:ILE:HB	1.96	0.47
1:G:11:ASP:CG	1:G:15:ARG:HH12	2.18	0.47
1:D:213:ALA:HB3	1:D:325:ILE:HB	1.96	0.47
1:F:221:LEU:HD21	1:F:249:ILE:CG1	2.45	0.46
1:C:321:LYS:CB	1:C:334:ASP:HB3	2.45	0.46
1:A:69:MET:HG2	1:B:47:PRO:CB	2.45	0.46
1:G:24:ALA:O	1:G:28:LYS:HD2	2.14	0.46
1:C:112:ASN:OD1	1:C:114:MET:N	2.49	0.46
1:G:221:LEU:HD21	1:G:249:ILE:CG1	2.46	0.46
1:D:198:GLY:O	1:D:276:VAL:HG12	2.15	0.46
1:E:489:MET:HG3	1:E:494:VAL:HB	1.97	0.46
1:G:226:LYS:HZ1	1:G:252:GLU:HB3	1.79	0.46
1:C:429:LEU:HD12	1:C:430:SER:N	2.30	0.46
1:A:19:GLY:HA2	1:A:62:LEU:CD1	2.45	0.46
1:A:24:ALA:O	1:A:28:LYS:HD2	2.15	0.46
1:G:169:VAL:HG21	1:G:377:ALA:HB2	1.97	0.46
1:D:362:ARG:HE	1:D:363:GLU:HB2	1.79	0.46
1:E:205:VAL:HG12	1:E:207:ASN:H	1.79	0.46
1:A:205:VAL:HG12	1:A:207:ASN:N	2.30	0.46
1:B:36:ARG:NH1	1:B:36:ARG:CG	2.76	0.46
1:B:489:MET:HG3	1:B:494:VAL:HB	1.97	0.46
1:F:219:TYR:CD1	1:F:247:LEU:HD12	2.50	0.46
1:A:219:TYR:CD1	1:A:247:LEU:HD12	2.50	0.46
1:G:209:ASP:HB3	1:G:210:LYS:HZ2	1.80	0.46
1:E:511:VAL:HG23	1:E:512:ALA:N	2.30	0.46
1:D:158:ILE:CG2	1:D:396:VAL:HG22	2.46	0.46
1:A:205:VAL:HG12	1:A:207:ASN:H	1.80	0.46
1:E:221:LEU:O	1:E:250:VAL:HG23	2.16	0.46
1:C:77:VAL:HG21	1:C:511:VAL:HG13	1.98	0.46
1:B:24:ALA:O	1:B:28:LYS:HD2	2.16	0.46
1:F:158:ILE:CG2	1:F:396:VAL:HG22	2.46	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:383:GLY:H	1:F:389:VAL:HG22	1.81	0.46
1:C:205:VAL:HG12	1:C:207:ASN:N	2.31	0.46
1:A:11:ASP:CG	1:A:15:ARG:HH12	2.19	0.46
1:G:489:MET:HG3	1:G:494:VAL:HB	1.98	0.46
1:E:66:PHE:HA	1:E:69:MET:HE2	1.96	0.46
1:D:289:LEU:O	1:D:293:ALA:HB2	2.16	0.46
1:C:205:VAL:HG12	1:C:207:ASN:H	1.80	0.46
1:F:227:LEU:HB2	1:F:254:VAL:CA	2.37	0.46
1:D:429:LEU:HD12	1:D:430:SER:N	2.29	0.46
1:E:219:TYR:CD1	1:E:247:LEU:HD12	2.51	0.46
1:C:219:TYR:CD1	1:C:247:LEU:HD12	2.51	0.46
1:B:429:LEU:HD12	1:B:430:SER:N	2.31	0.46
1:A:158:ILE:CG2	1:A:396:VAL:HG22	2.46	0.46
1:C:169:VAL:HG21	1:C:377:ALA:HB2	1.96	0.46
1:A:122:VAL:HG12	1:A:123:ALA:N	2.31	0.46
1:E:11:ASP:CG	1:E:15:ARG:HH12	2.18	0.46
1:E:205:VAL:HG12	1:E:207:ASN:N	2.30	0.46
1:D:103:GLY:HA3	1:D:516:ILE:HD11	1.96	0.46
1:D:205:VAL:HG12	1:D:207:ASN:H	1.80	0.46
1:G:351:GLN:HA	1:G:354:GLU:HB2	1.98	0.46
1:E:122:VAL:HG12	1:E:123:ALA:N	2.29	0.46
1:G:205:VAL:HG12	1:G:207:ASN:H	1.80	0.46
1:B:197:ARG:NH1	1:B:277:LYS:HG2	2.23	0.46
1:E:198:GLY:O	1:E:276:VAL:HG12	2.16	0.46
1:C:69:MET:HG2	1:D:47:PRO:HB3	1.98	0.46
1:G:69:MET:HB2	1:G:69:MET:HE3	1.53	0.46
1:F:80:ARG:HB2	1:F:80:ARG:HH11	1.81	0.46
1:E:174:VAL:HG22	1:E:174:VAL:O	2.15	0.46
1:E:383:GLY:H	1:E:389:VAL:HG22	1.81	0.46
1:F:362:ARG:HE	1:F:363:GLU:HB2	1.79	0.46
1:D:205:VAL:HG12	1:D:207:ASN:N	2.31	0.46
1:F:351:GLN:HA	1:F:354:GLU:HB2	1.98	0.46
1:D:351:GLN:HA	1:D:354:GLU:HB2	1.98	0.46
1:D:221:LEU:HD21	1:D:249:ILE:CG1	2.45	0.46
1:B:221:LEU:HD21	1:B:249:ILE:CG1	2.46	0.46
1:A:217:ASP:O	1:A:246:PRO:HD2	2.16	0.46
1:E:77:VAL:HG21	1:E:511:VAL:HG13	1.98	0.46
1:D:62:LEU:H	1:D:68:ASN:HD22	1.64	0.46
1:A:90:THR:O	1:A:94:VAL:HG23	2.16	0.46
1:C:289:LEU:O	1:C:293:ALA:HB2	2.16	0.46
1:E:289:LEU:O	1:E:293:ALA:HB2	2.15	0.46
1:A:128:VAL:HG11	1:A:506:GLU:OE2	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:217:ASP:O	1:D:246:PRO:HD2	2.16	0.46
1:B:451:MET:CE	1:B:465:VAL:HG12	2.46	0.46
1:G:62:LEU:H	1:G:68:ASN:HD22	1.63	0.46
1:C:294:ILE:HD11	1:C:345:ARG:NH1	2.31	0.46
1:E:194:GLN:HG3	1:E:331:THR:OG1	2.16	0.46
1:A:6:VAL:HG22	1:A:522:ILE:HG12	1.98	0.46
1:G:80:ARG:HB2	1:G:80:ARG:HH11	1.81	0.45
1:C:217:ASP:O	1:C:246:PRO:HD2	2.16	0.45
1:D:36:ARG:CG	1:D:36:ARG:NH1	2.75	0.45
1:G:198:GLY:O	1:G:276:VAL:HG12	2.16	0.45
1:E:221:LEU:HD21	1:E:249:ILE:CG1	2.46	0.45
1:D:69:MET:HE3	1:D:69:MET:HB2	1.53	0.45
1:F:217:ASP:O	1:F:246:PRO:HD2	2.17	0.45
1:G:217:ASP:O	1:G:246:PRO:HD2	2.16	0.45
1:A:175:ILE:HG22	1:A:176:THR:N	2.31	0.45
1:B:19:GLY:HA2	1:B:62:LEU:CD1	2.46	0.45
1:A:451:MET:CE	1:A:465:VAL:HG12	2.47	0.45
1:F:194:GLN:HG3	1:F:331:THR:OG1	2.17	0.45
1:E:351:GLN:HA	1:E:354:GLU:HB2	1.99	0.45
1:C:478:GLY:HA3	1:C:489:MET:HE3	1.97	0.45
1:E:225:LYS:HB2	1:E:226:LYS:H	1.62	0.45
1:B:12:ALA:HB1	1:B:521:MET:SD	2.57	0.45
1:C:19:GLY:HA2	1:C:62:LEU:CD1	2.46	0.45
1:G:378:VAL:HG22	1:G:378:VAL:O	2.16	0.45
1:G:19:GLY:HA2	1:G:62:LEU:CD1	2.47	0.45
1:B:289:LEU:O	1:B:293:ALA:HB2	2.15	0.45
1:E:362:ARG:HE	1:E:363:GLU:HB2	1.80	0.45
1:D:112:ASN:OD1	1:D:114:MET:N	2.49	0.45
1:A:351:GLN:HA	1:A:354:GLU:HB2	1.99	0.45
1:B:11:ASP:CG	1:B:15:ARG:HH12	2.19	0.45
1:C:351:GLN:HA	1:C:354:GLU:HB2	1.98	0.45
1:A:103:GLY:HA3	1:A:516:ILE:HD11	1.97	0.45
1:G:112:ASN:OD1	1:G:114:MET:N	2.49	0.45
1:B:321:LYS:CB	1:B:334:ASP:HB3	2.46	0.45
1:D:378:VAL:O	1:D:378:VAL:HG22	2.17	0.45
1:D:348:GLN:O	1:D:352:GLN:HB2	2.17	0.45
1:D:320:ALA:HA	1:D:335:GLY:O	2.17	0.45
1:F:112:ASN:OD1	1:F:114:MET:N	2.49	0.45
1:F:507:ASP:O	1:F:510:SER:HB3	2.17	0.45
1:F:221:LEU:O	1:F:250:VAL:HG23	2.16	0.45
1:B:80:ARG:HH11	1:B:80:ARG:HB2	1.82	0.45
1:B:348:GLN:O	1:B:352:GLN:HB2	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:383:GLY:H	1:C:389:VAL:HG22	1.82	0.45
1:F:289:LEU:O	1:F:293:ALA:HB2	2.15	0.45
1:G:289:LEU:O	1:G:293:ALA:HB2	2.16	0.45
1:E:112:ASN:OD1	1:E:114:MET:N	2.50	0.45
1:G:221:LEU:O	1:G:250:VAL:HG23	2.16	0.45
1:C:221:LEU:O	1:C:250:VAL:HG23	2.16	0.45
1:F:66:PHE:HA	1:F:69:MET:HE2	1.97	0.45
1:F:128:VAL:HG11	1:F:506:GLU:OE2	2.17	0.45
1:A:69:MET:HB2	1:A:69:MET:HE3	1.55	0.45
1:A:247:LEU:HB3	1:A:273:ILE:HD12	1.99	0.45
1:A:77:VAL:HG21	1:A:511:VAL:HG13	1.99	0.45
1:B:351:GLN:HA	1:B:354:GLU:HB2	1.98	0.45
1:G:194:GLN:HG3	1:G:331:THR:OG1	2.17	0.45
1:C:198:GLY:O	1:C:276:VAL:HG12	2.17	0.45
1:F:478:GLY:HA3	1:F:489:MET:HE3	1.99	0.45
1:C:124:THR:O	1:C:128:VAL:HG23	2.16	0.45
1:E:69:MET:HG2	1:F:47:PRO:HB3	1.99	0.45
1:B:247:LEU:HB3	1:B:273:ILE:HD12	1.99	0.45
1:G:204:PHE:CE1	1:G:273:ILE:HG23	2.52	0.45
1:C:320:ALA:HA	1:C:335:GLY:O	2.17	0.45
1:F:19:GLY:HA2	1:F:62:LEU:CD1	2.46	0.45
1:G:205:VAL:HG12	1:G:207:ASN:N	2.30	0.45
1:E:501:VAL:O	1:E:501:VAL:HG12	2.16	0.45
1:A:221:LEU:O	1:A:250:VAL:HG23	2.16	0.45
1:E:69:MET:HE3	1:E:69:MET:HB2	1.50	0.45
1:A:12:ALA:HB1	1:A:521:MET:HG3	1.99	0.45
1:E:80:ARG:HB2	1:E:80:ARG:HH11	1.82	0.45
1:C:348:GLN:O	1:C:352:GLN:HB2	2.17	0.45
1:E:348:GLN:O	1:E:352:GLN:HB2	2.17	0.45
1:D:221:LEU:O	1:D:250:VAL:HG23	2.16	0.45
1:F:204:PHE:CE1	1:F:273:ILE:HG23	2.52	0.45
1:E:217:ASP:O	1:E:246:PRO:HD2	2.17	0.45
1:B:217:ASP:O	1:B:246:PRO:HD2	2.17	0.45
1:F:511:VAL:HG23	1:F:512:ALA:N	2.32	0.45
1:G:478:GLY:HA3	1:G:489:MET:HE3	1.99	0.45
1:A:124:THR:O	1:A:128:VAL:HG23	2.17	0.45
1:A:429:LEU:HD12	1:A:430:SER:N	2.29	0.45
1:C:62:LEU:H	1:C:68:ASN:HD22	1.64	0.45
1:C:72:GLN:HE22	1:C:75:ARG:CZ	2.30	0.45
1:D:175:ILE:HG22	1:D:176:THR:N	2.32	0.45
1:C:480:ASN:O	1:C:484:GLU:N	2.45	0.45
1:A:383:GLY:H	1:A:389:VAL:HG22	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:GLN:HG3	1:B:331:THR:OG1	2.17	0.45
1:B:112:ASN:OD1	1:B:114:MET:N	2.50	0.45
1:C:221:LEU:HD21	1:C:249:ILE:CG1	2.47	0.44
1:B:225:LYS:HB2	1:B:226:LYS:H	1.62	0.44
1:D:511:VAL:HG23	1:D:512:ALA:N	2.33	0.44
1:C:174:VAL:HG22	1:C:174:VAL:O	2.16	0.44
1:C:80:ARG:HH11	1:C:80:ARG:HB2	1.82	0.44
1:D:19:GLY:HA2	1:D:62:LEU:CD1	2.47	0.44
1:G:158:ILE:CG2	1:G:396:VAL:HG22	2.46	0.44
1:B:383:GLY:H	1:B:389:VAL:HG22	1.81	0.44
1:D:383:GLY:H	1:D:389:VAL:HG22	1.82	0.44
1:D:6:VAL:HG22	1:D:522:ILE:HG12	1.98	0.44
1:B:198:GLY:O	1:B:276:VAL:HG12	2.18	0.44
1:E:320:ALA:HA	1:E:335:GLY:O	2.18	0.44
1:C:204:PHE:CE1	1:C:273:ILE:HG23	2.52	0.44
1:D:90:THR:O	1:D:94:VAL:HG23	2.17	0.44
1:F:294:ILE:HD11	1:F:345:ARG:NH1	2.33	0.44
1:E:294:ILE:HD11	1:E:345:ARG:NH1	2.32	0.44
1:A:194:GLN:HG3	1:A:331:THR:OG1	2.17	0.44
1:E:423:ALA:HB2	1:E:447:LEU:HD13	1.98	0.44
1:A:198:GLY:O	1:A:276:VAL:HG12	2.17	0.44
1:B:221:LEU:O	1:B:250:VAL:HG23	2.16	0.44
1:B:12:ALA:HB1	1:B:521:MET:HG3	1.98	0.44
1:F:247:LEU:HB3	1:F:273:ILE:HD12	1.99	0.44
1:C:247:LEU:HB3	1:C:273:ILE:HD12	1.99	0.44
1:G:174:VAL:HG22	1:G:174:VAL:O	2.16	0.44
1:G:348:GLN:O	1:G:352:GLN:HB2	2.17	0.44
1:E:451:MET:CE	1:E:466:ALA:HA	2.48	0.44
1:G:294:ILE:HD11	1:G:345:ARG:NH1	2.32	0.44
1:D:507:ASP:O	1:D:510:SER:HB3	2.17	0.44
1:B:6:VAL:HG22	1:B:522:ILE:HG12	1.99	0.44
1:C:128:VAL:HG11	1:C:506:GLU:OE2	2.18	0.44
1:B:69:MET:HB2	1:B:69:MET:HE3	1.55	0.44
1:F:320:ALA:HA	1:F:335:GLY:O	2.18	0.44
1:G:320:ALA:HA	1:G:335:GLY:O	2.17	0.44
1:E:158:ILE:CG2	1:E:396:VAL:HG22	2.48	0.44
1:F:429:LEU:HD12	1:F:430:SER:N	2.29	0.44
1:A:80:ARG:HB2	1:A:80:ARG:HH11	1.82	0.44
1:E:204:PHE:CE1	1:E:273:ILE:HG23	2.53	0.44
1:G:219:TYR:N	1:G:246:PRO:O	2.51	0.44
1:C:90:THR:O	1:C:94:VAL:HG23	2.17	0.44
1:F:245:LYS:HZ1	1:F:319:ARG:HH21	1.64	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:13:ARG:CD	1:D:104:LEU:HD22	2.47	0.44
1:D:423:ALA:HB2	1:D:447:LEU:HD13	1.99	0.44
1:G:488:ASP:HB3	1:G:491:LYS:HG3	1.99	0.44
1:A:183:MET:HB3	1:A:384:MET:HE1	1.99	0.44
1:F:231:GLN:N	1:F:231:GLN:NE2	2.65	0.44
1:D:183:MET:HB3	1:D:384:MET:HE1	2.00	0.44
1:F:219:TYR:N	1:F:246:PRO:O	2.51	0.44
1:D:231:GLN:N	1:D:231:GLN:NE2	2.65	0.44
1:G:511:VAL:HG23	1:G:512:ALA:N	2.33	0.44
1:D:80:ARG:HH11	1:D:80:ARG:HB2	1.82	0.44
1:E:429:LEU:HD12	1:E:430:SER:N	2.31	0.44
1:A:480:ASN:HD21	1:A:483:THR:HG23	1.83	0.44
1:C:245:LYS:HZ1	1:C:319:ARG:HH21	1.65	0.44
1:E:62:LEU:H	1:E:68:ASN:HD22	1.66	0.44
1:G:13:ARG:CD	1:G:104:LEU:HD22	2.48	0.44
1:F:205:VAL:HG12	1:F:207:ASN:H	1.81	0.44
1:F:205:VAL:HG12	1:F:207:ASN:N	2.31	0.44
1:B:72:GLN:HE22	1:B:75:ARG:CZ	2.31	0.44
1:A:511:VAL:HG23	1:A:512:ALA:N	2.32	0.44
1:E:75:ARG:HH11	1:E:75:ARG:CG	2.30	0.44
1:G:72:GLN:HE22	1:G:75:ARG:CZ	2.31	0.44
1:C:126:LYS:HG3	1:C:429:LEU:CD2	2.48	0.44
1:F:175:ILE:HG22	1:F:176:THR:N	2.32	0.44
1:F:348:GLN:O	1:F:352:GLN:HB2	2.17	0.44
1:D:194:GLN:HG3	1:D:331:THR:OG1	2.18	0.44
1:C:69:MET:HE3	1:C:69:MET:HB2	1.59	0.44
1:G:77:VAL:HG21	1:G:511:VAL:HG13	2.00	0.44
1:B:77:VAL:HG21	1:B:511:VAL:HG13	2.00	0.44
1:C:190:VAL:HG12	1:C:191:GLU:N	2.32	0.44
1:F:174:VAL:HG22	1:F:174:VAL:O	2.17	0.44
1:E:175:ILE:HG22	1:E:176:THR:N	2.33	0.44
1:D:423:ALA:HB2	1:D:447:LEU:CD1	2.47	0.44
1:G:507:ASP:O	1:G:510:SER:HB3	2.18	0.44
1:C:225:LYS:HG3	1:C:225:LYS:H	1.61	0.44
1:F:198:GLY:O	1:F:276:VAL:HG12	2.17	0.44
1:A:320:ALA:HA	1:A:335:GLY:O	2.17	0.44
1:E:219:TYR:N	1:E:246:PRO:O	2.51	0.44
1:E:247:LEU:HB3	1:E:273:ILE:HD12	1.99	0.44
1:B:320:ALA:HA	1:B:335:GLY:O	2.17	0.44
1:A:348:GLN:O	1:A:352:GLN:HB2	2.18	0.44
1:D:24:ALA:O	1:D:28:LYS:HD2	2.17	0.44
1:A:13:ARG:CD	1:A:104:LEU:HD22	2.48	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:349:ILE:HG22	1:C:353:ILE:HD11	2.00	0.43
1:A:219:TYR:N	1:A:246:PRO:O	2.51	0.43
1:F:126:LYS:HG3	1:F:429:LEU:CD2	2.48	0.43
1:E:72:GLN:HE22	1:E:75:ARG:CZ	2.30	0.43
1:C:175:ILE:HG22	1:C:176:THR:N	2.33	0.43
1:B:451:MET:CE	1:B:466:ALA:HA	2.48	0.43
1:D:139:ASN:N	1:D:139:ASN:ND2	2.66	0.43
1:C:227:LEU:CD1	1:C:251:ALA:HB3	2.48	0.43
1:D:349:ILE:HG22	1:D:353:ILE:HD11	2.00	0.43
1:E:365:LEU:HA	1:E:368:ARG:HG2	2.00	0.43
1:A:204:PHE:CE1	1:A:273:ILE:HG23	2.54	0.43
1:D:72:GLN:HE22	1:D:75:ARG:CZ	2.31	0.43
1:F:480:ASN:HD21	1:F:483:THR:HG23	1.84	0.43
1:B:294:ILE:HD11	1:B:345:ARG:NH1	2.33	0.43
1:A:8:PHE:HE1	1:B:26:ALA:HA	1.83	0.43
1:C:12:ALA:HB1	1:C:521:MET:HG3	1.99	0.43
1:A:488:ASP:HB3	1:A:491:LYS:HG3	2.00	0.43
1:G:128:VAL:HG11	1:G:506:GLU:OE2	2.19	0.43
1:G:225:LYS:HG3	1:G:225:LYS:H	1.62	0.43
1:G:174:VAL:HG13	1:G:376:VAL:HA	2.00	0.43
1:E:19:GLY:HA2	1:E:62:LEU:CD1	2.48	0.43
1:A:112:ASN:OD1	1:A:114:MET:N	2.51	0.43
1:F:488:ASP:HB3	1:F:491:LYS:HG3	1.99	0.43
1:B:488:ASP:HB3	1:B:491:LYS:HG3	1.99	0.43
1:D:247:LEU:HB3	1:D:273:ILE:HD12	1.99	0.43
1:F:62:LEU:H	1:F:68:ASN:HD22	1.66	0.43
1:E:423:ALA:HB2	1:E:447:LEU:CD1	2.48	0.43
1:C:139:ASN:N	1:C:139:ASN:ND2	2.67	0.43
1:F:227:LEU:CD1	1:F:251:ALA:HB3	2.48	0.43
1:D:227:LEU:CD1	1:D:251:ALA:HB3	2.48	0.43
1:F:225:LYS:HB2	1:F:226:LYS:H	1.62	0.43
1:G:247:LEU:HB3	1:G:273:ILE:HD12	2.00	0.43
1:G:175:ILE:HG22	1:G:176:THR:N	2.33	0.43
1:E:13:ARG:CD	1:E:104:LEU:HD22	2.48	0.43
1:B:103:GLY:HA3	1:B:516:ILE:CD1	2.49	0.43
1:D:294:ILE:HD11	1:D:345:ARG:NH1	2.32	0.43
1:C:8:PHE:HE1	1:D:26:ALA:HA	1.84	0.43
1:G:12:ALA:HB1	1:G:521:MET:SD	2.58	0.43
1:E:12:ALA:HB1	1:E:521:MET:SD	2.59	0.43
1:B:69:MET:HG2	1:C:47:PRO:HB3	2.01	0.43
1:F:365:LEU:HA	1:F:368:ARG:HG2	2.00	0.43
1:B:204:PHE:CE1	1:B:273:ILE:HG23	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:204:PHE:CE1	1:D:273:ILE:HG23	2.53	0.43
1:G:75:ARG:HH11	1:G:75:ARG:CG	2.31	0.43
1:B:511:VAL:HG23	1:B:512:ALA:N	2.34	0.43
1:D:480:ASN:HD21	1:D:483:THR:HG23	1.84	0.43
1:E:451:MET:CE	1:E:465:VAL:HG12	2.49	0.43
1:A:478:GLY:HA3	1:A:489:MET:HE3	1.99	0.43
1:F:124:THR:O	1:F:128:VAL:HG23	2.18	0.43
1:D:365:LEU:HA	1:D:368:ARG:HG2	2.00	0.43
1:B:349:ILE:HG22	1:B:353:ILE:HD11	2.00	0.43
1:F:103:GLY:HA3	1:F:516:ILE:CD1	2.49	0.43
1:D:451:MET:CE	1:D:465:VAL:HG12	2.49	0.43
1:E:224:GLU:HG3	1:E:286:LYS:CE	2.49	0.43
1:B:227:LEU:CD1	1:B:251:ALA:HB3	2.49	0.43
1:D:478:GLY:HA3	1:D:489:MET:HE3	2.00	0.43
1:C:488:ASP:HB3	1:C:491:LYS:HG3	1.99	0.43
1:F:349:ILE:HG22	1:F:353:ILE:HD11	2.00	0.43
1:B:365:LEU:HA	1:B:368:ARG:HG2	2.00	0.43
1:A:480:ASN:O	1:A:484:GLU:N	2.47	0.43
1:C:103:GLY:HA3	1:C:516:ILE:CD1	2.49	0.43
1:D:224:GLU:HG3	1:D:286:LYS:CE	2.49	0.43
1:F:451:MET:CE	1:F:466:ALA:HA	2.49	0.43
1:A:294:ILE:HD11	1:A:345:ARG:NH1	2.33	0.43
1:G:227:LEU:CD1	1:G:251:ALA:HB3	2.49	0.43
1:E:128:VAL:HG11	1:E:506:GLU:OE2	2.18	0.43
1:C:365:LEU:HA	1:C:368:ARG:HG2	2.01	0.43
1:G:365:LEU:HA	1:G:368:ARG:HG2	2.00	0.43
1:A:321:LYS:CB	1:A:334:ASP:HB3	2.45	0.43
1:B:175:ILE:HG22	1:B:176:THR:N	2.33	0.43
1:B:224:GLU:HG3	1:B:286:LYS:CE	2.49	0.43
1:C:224:GLU:HG3	1:C:286:LYS:CE	2.49	0.43
1:B:507:ASP:O	1:B:510:SER:HB3	2.18	0.43
1:C:507:ASP:O	1:C:510:SER:HB3	2.19	0.43
1:C:194:GLN:HG3	1:C:331:THR:OG1	2.17	0.43
1:D:12:ALA:HB1	1:D:521:MET:HG3	2.00	0.43
1:A:227:LEU:CD1	1:A:251:ALA:HB3	2.48	0.43
1:E:478:GLY:HA3	1:E:489:MET:HE3	2.01	0.43
1:D:488:ASP:HB3	1:D:491:LYS:HG3	2.00	0.43
1:E:124:THR:O	1:E:128:VAL:HG23	2.19	0.43
1:A:225:LYS:HB2	1:A:226:LYS:H	1.62	0.43
1:B:126:LYS:HG3	1:B:429:LEU:CD2	2.49	0.43
1:B:62:LEU:H	1:B:68:ASN:HD22	1.65	0.43
1:G:383:GLY:H	1:G:389:VAL:HG22	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:227:LEU:CD1	1:E:251:ALA:HB3	2.48	0.42
1:D:69:MET:HG2	1:E:47:PRO:HG3	2.00	0.42
1:F:75:ARG:HH11	1:F:75:ARG:CG	2.30	0.42
1:E:248:LEU:CA	1:E:274:ALA:HB3	2.49	0.42
1:D:480:ASN:O	1:D:484:GLU:N	2.48	0.42
1:A:24:ALA:O	1:A:28:LYS:HB3	2.18	0.42
1:F:13:ARG:CD	1:F:104:LEU:HD22	2.49	0.42
1:A:451:MET:HE1	1:A:465:VAL:HG12	2.01	0.42
1:B:449:ALA:CB	1:B:450:PRO:HD3	2.43	0.42
1:D:128:VAL:O	1:D:128:VAL:HG12	2.18	0.42
1:F:226:LYS:HZ1	1:F:252:GLU:HB3	1.84	0.42
1:A:365:LEU:HA	1:A:368:ARG:HG2	2.00	0.42
1:F:321:LYS:CB	1:F:334:ASP:HB3	2.45	0.42
1:B:231:GLN:N	1:B:231:GLN:NE2	2.65	0.42
1:C:217:ASP:HA	1:C:320:ALA:O	2.19	0.42
1:F:26:ALA:O	1:F:29:VAL:HG22	2.18	0.42
1:B:378:VAL:HG22	1:B:378:VAL:O	2.19	0.42
1:A:507:ASP:O	1:A:510:SER:HB3	2.19	0.42
1:C:227:LEU:HD11	1:C:251:ALA:HB3	2.02	0.42
1:E:488:ASP:HB3	1:E:491:LYS:HG3	2.00	0.42
1:D:69:MET:HG2	1:E:47:PRO:CB	2.49	0.42
1:A:126:LYS:HG3	1:A:429:LEU:CD2	2.49	0.42
1:D:219:TYR:N	1:D:246:PRO:O	2.52	0.42
1:F:220:ILE:CD1	1:F:248:LEU:HD22	2.49	0.42
1:G:248:LEU:CA	1:G:274:ALA:HB3	2.49	0.42
1:E:378:VAL:O	1:E:378:VAL:HG22	2.19	0.42
1:A:62:LEU:H	1:A:68:ASN:HD22	1.65	0.42
1:C:451:MET:CE	1:C:466:ALA:HA	2.48	0.42
1:B:124:THR:O	1:B:128:VAL:HG23	2.19	0.42
1:A:349:ILE:HG22	1:A:353:ILE:HD11	2.01	0.42
1:G:321:LYS:CB	1:G:334:ASP:HB3	2.45	0.42
1:F:126:LYS:HG3	1:F:429:LEU:HD22	2.00	0.42
1:C:19:GLY:O	1:C:71:ALA:HB2	2.20	0.42
1:B:174:VAL:HG13	1:B:376:VAL:HA	2.02	0.42
1:C:174:VAL:HG13	1:C:376:VAL:HA	2.01	0.42
1:G:480:ASN:HD21	1:G:483:THR:HG23	1.84	0.42
1:B:90:THR:O	1:B:94:VAL:HG23	2.20	0.42
1:A:224:GLU:HG3	1:A:286:LYS:CE	2.49	0.42
1:A:423:ALA:HB2	1:A:447:LEU:HD13	2.01	0.42
1:F:36:ARG:CG	1:F:36:ARG:NH1	2.75	0.42
1:G:380:ARG:CB	1:G:380:ARG:HH11	2.28	0.42
1:F:12:ALA:HB1	1:F:521:MET:HG3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:126:LYS:HG3	1:E:429:LEU:CD2	2.49	0.42
1:A:174:VAL:HG13	1:A:376:VAL:HA	2.02	0.42
1:A:220:ILE:CD1	1:A:248:LEU:HD22	2.50	0.42
1:E:221:LEU:HG	1:E:249:ILE:HA	2.02	0.42
1:F:72:GLN:HE22	1:F:75:ARG:CZ	2.31	0.42
1:C:112:ASN:OD1	1:C:112:ASN:C	2.58	0.42
1:D:112:ASN:C	1:D:112:ASN:OD1	2.58	0.42
1:E:139:ASN:ND2	1:E:139:ASN:N	2.66	0.42
1:D:227:LEU:HD11	1:D:251:ALA:HB3	2.02	0.42
1:E:321:LYS:CB	1:E:334:ASP:HB3	2.45	0.42
1:D:126:LYS:HG3	1:D:429:LEU:CD2	2.49	0.42
1:D:174:VAL:HG13	1:D:376:VAL:HA	2.01	0.42
1:C:220:ILE:CD1	1:C:248:LEU:HD22	2.50	0.42
1:F:2:ALA:O	1:F:3:ALA:C	2.57	0.42
1:A:2:ALA:O	1:A:3:ALA:C	2.57	0.42
1:D:298:GLY:HA2	1:D:317:LEU:C	2.40	0.42
1:A:112:ASN:OD1	1:A:112:ASN:C	2.58	0.42
1:E:507:ASP:O	1:E:510:SER:HB3	2.20	0.42
1:B:227:LEU:HD11	1:B:251:ALA:HB3	2.02	0.42
1:B:128:VAL:HG11	1:B:506:GLU:OE2	2.20	0.42
1:D:128:VAL:HG11	1:D:506:GLU:OE2	2.19	0.42
1:E:220:ILE:CD1	1:E:248:LEU:HD22	2.50	0.42
1:B:13:ARG:CD	1:B:104:LEU:HD22	2.49	0.42
1:F:123:ALA:HB1	1:F:426:LEU:HD22	2.02	0.42
1:D:451:MET:CE	1:D:466:ALA:HA	2.49	0.42
1:G:224:GLU:HG3	1:G:286:LYS:CE	2.50	0.42
1:B:112:ASN:C	1:B:112:ASN:OD1	2.59	0.42
1:B:423:ALA:HB2	1:B:447:LEU:HD13	2.01	0.42
1:A:139:ASN:N	1:A:139:ASN:ND2	2.66	0.42
1:B:221:LEU:HG	1:B:249:ILE:HA	2.02	0.42
1:G:225:LYS:HB2	1:G:226:LYS:H	1.62	0.42
1:G:349:ILE:HG22	1:G:353:ILE:HD11	2.01	0.42
1:A:217:ASP:HA	1:A:320:ALA:O	2.20	0.42
1:B:219:TYR:N	1:B:246:PRO:O	2.52	0.42
1:D:77:VAL:HG21	1:D:511:VAL:HG13	2.02	0.42
1:F:215:LEU:HD22	1:F:274:ALA:HB2	2.02	0.42
1:G:126:LYS:HG3	1:G:429:LEU:CD2	2.50	0.42
1:D:215:LEU:HD22	1:D:274:ALA:HB2	2.02	0.42
1:D:220:ILE:CD1	1:D:248:LEU:HD22	2.50	0.42
1:G:215:LEU:HD22	1:G:274:ALA:HB2	2.02	0.42
1:C:219:TYR:N	1:C:246:PRO:O	2.52	0.41
1:A:378:VAL:O	1:A:378:VAL:HG22	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:90:THR:O	1:E:94:VAL:HG23	2.20	0.41
1:C:298:GLY:HA2	1:C:317:LEU:C	2.40	0.41
1:F:224:GLU:HG3	1:F:286:LYS:CE	2.49	0.41
1:B:139:ASN:N	1:B:139:ASN:ND2	2.66	0.41
1:E:7:LYS:HB3	1:E:12:ALA:HB2	2.03	0.41
1:F:323:VAL:HG13	1:F:332:ILE:HG12	2.02	0.41
1:A:215:LEU:HD22	1:A:274:ALA:HB2	2.02	0.41
1:E:298:GLY:HA2	1:E:317:LEU:C	2.41	0.41
1:A:423:ALA:HB2	1:A:447:LEU:CD1	2.50	0.41
1:C:221:LEU:HG	1:C:249:ILE:HA	2.03	0.41
1:F:69:MET:HE3	1:F:69:MET:HB2	1.53	0.41
1:A:7:LYS:HB3	1:A:12:ALA:HB2	2.03	0.41
1:B:75:ARG:HH11	1:B:75:ARG:CG	2.32	0.41
1:D:220:ILE:HG23	1:D:248:LEU:CD2	2.50	0.41
1:C:480:ASN:HD21	1:C:483:THR:HG23	1.85	0.41
1:G:112:ASN:C	1:G:112:ASN:OD1	2.58	0.41
1:F:423:ALA:HB2	1:F:447:LEU:HD13	2.01	0.41
1:A:227:LEU:HD11	1:A:251:ALA:HB3	2.02	0.41
1:E:227:LEU:HB2	1:E:254:VAL:CA	2.38	0.41
1:F:221:LEU:HG	1:F:249:ILE:HA	2.03	0.41
1:F:217:ASP:HA	1:F:320:ALA:O	2.21	0.41
1:E:217:ASP:HA	1:E:320:ALA:O	2.21	0.41
1:C:126:LYS:HG3	1:C:429:LEU:HD22	2.02	0.41
1:C:220:ILE:HG23	1:C:248:LEU:CD2	2.51	0.41
1:G:220:ILE:CD1	1:G:248:LEU:HD22	2.50	0.41
1:G:12:ALA:HB1	1:G:521:MET:HG3	2.03	0.41
1:C:423:ALA:HB2	1:C:447:LEU:CD1	2.50	0.41
1:E:36:ARG:CG	1:E:36:ARG:NH1	2.76	0.41
1:A:12:ALA:HB1	1:A:521:MET:SD	2.60	0.41
1:E:349:ILE:HG22	1:E:353:ILE:HD11	2.01	0.41
1:B:80:ARG:HB2	1:B:80:ARG:NH1	2.36	0.41
1:B:215:LEU:HD22	1:B:274:ALA:HB2	2.02	0.41
1:B:220:ILE:CD1	1:B:248:LEU:HD22	2.50	0.41
1:E:2:ALA:O	1:E:3:ALA:C	2.58	0.41
1:A:451:MET:CE	1:A:466:ALA:HA	2.50	0.41
1:D:221:LEU:HG	1:D:249:ILE:HA	2.03	0.41
1:F:220:ILE:HG23	1:F:248:LEU:CD2	2.50	0.41
1:E:174:VAL:HG13	1:E:376:VAL:HA	2.01	0.41
1:C:215:LEU:HD22	1:C:274:ALA:HB2	2.03	0.41
1:F:174:VAL:HG13	1:F:376:VAL:HA	2.02	0.41
1:G:24:ALA:O	1:G:28:LYS:HB3	2.20	0.41
1:F:298:GLY:HA2	1:F:317:LEU:C	2.41	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2:ALA:O	1:B:3:ALA:C	2.59	0.41
1:G:298:GLY:HA2	1:G:317:LEU:C	2.41	0.41
1:B:423:ALA:HB2	1:B:447:LEU:CD1	2.51	0.41
1:F:8:PHE:HE1	1:G:26:ALA:HA	1.86	0.41
1:F:227:LEU:HD11	1:F:251:ALA:HB3	2.02	0.41
1:G:231:GLN:N	1:G:231:GLN:NE2	2.65	0.41
1:E:245:LYS:HZ1	1:E:319:ARG:HH21	1.66	0.41
1:E:480:ASN:HD21	1:E:483:THR:HG23	1.85	0.41
1:C:24:ALA:O	1:C:28:LYS:HB3	2.21	0.41
1:E:103:GLY:HA3	1:E:516:ILE:CD1	2.50	0.41
1:D:227:LEU:HB2	1:D:254:VAL:CA	2.38	0.41
1:D:126:LYS:HG3	1:D:429:LEU:HD22	2.02	0.41
1:C:378:VAL:HG22	1:C:378:VAL:O	2.21	0.41
1:D:248:LEU:CA	1:D:274:ALA:HB3	2.49	0.41
1:B:220:ILE:HG23	1:B:248:LEU:CD2	2.51	0.41
1:B:248:LEU:CB	1:B:274:ALA:HB3	2.51	0.41
1:A:248:LEU:CB	1:A:274:ALA:HB3	2.51	0.41
1:D:2:ALA:O	1:D:3:ALA:C	2.59	0.41
1:G:181:LYS:HB2	1:G:182:GLY:H	1.78	0.41
1:C:26:ALA:O	1:C:29:VAL:HG22	2.21	0.41
1:D:482:GLN:HA	1:D:482:GLN:NE2	2.36	0.41
1:E:227:LEU:HD11	1:E:251:ALA:HB3	2.02	0.41
1:G:36:ARG:CG	1:G:36:ARG:NH1	2.79	0.41
1:A:190:VAL:HG11	1:A:334:ASP:CB	2.51	0.41
1:A:231:GLN:N	1:A:231:GLN:NE2	2.65	0.41
1:E:220:ILE:HG23	1:E:248:LEU:CD2	2.50	0.41
1:E:215:LEU:HD22	1:E:274:ALA:HB2	2.03	0.41
1:A:220:ILE:HG23	1:A:248:LEU:CD2	2.51	0.41
1:G:2:ALA:O	1:G:3:ALA:C	2.58	0.41
1:F:90:THR:O	1:F:94:VAL:HG23	2.21	0.41
1:C:13:ARG:CD	1:C:104:LEU:HD22	2.50	0.41
1:A:298:GLY:HA2	1:A:317:LEU:C	2.41	0.41
1:F:451:MET:HE1	1:F:465:VAL:HG12	2.02	0.41
1:F:423:ALA:HB2	1:F:447:LEU:CD1	2.51	0.41
1:C:423:ALA:HB2	1:C:447:LEU:HD13	2.02	0.41
1:C:482:GLN:HA	1:C:482:GLN:NE2	2.36	0.41
1:A:221:LEU:HG	1:A:249:ILE:HA	2.03	0.41
1:F:380:ARG:HH11	1:F:380:ARG:CB	2.29	0.41
1:A:72:GLN:HE22	1:A:75:ARG:CZ	2.34	0.41
1:B:298:GLY:HA2	1:B:317:LEU:C	2.41	0.41
1:C:55:SER:O	1:C:59:GLU:HG2	2.20	0.41
1:F:489:MET:HG3	1:F:494:VAL:O	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:7:LYS:HB3	1:F:12:ALA:HB2	2.03	0.40
1:G:220:ILE:HG23	1:G:248:LEU:CD2	2.50	0.40
1:G:248:LEU:CB	1:G:274:ALA:HB3	2.51	0.40
1:G:323:VAL:HG13	1:G:332:ILE:HG12	2.03	0.40
1:G:26:ALA:O	1:G:29:VAL:HG22	2.21	0.40
1:G:227:LEU:HD11	1:G:251:ALA:HB3	2.03	0.40
1:B:201:SER:O	1:B:204:PHE:HB2	2.21	0.40
1:C:80:ARG:HB2	1:C:80:ARG:NH1	2.36	0.40
1:D:19:GLY:HA2	1:D:62:LEU:HD11	2.03	0.40
1:B:480:ASN:HD21	1:B:483:THR:HG23	1.85	0.40
1:G:103:GLY:HA3	1:G:516:ILE:CD1	2.50	0.40
1:E:112:ASN:C	1:E:112:ASN:OD1	2.58	0.40
1:B:7:LYS:HB3	1:B:12:ALA:HB2	2.04	0.40
1:F:190:VAL:HG12	1:F:191:GLU:N	2.36	0.40
1:G:217:ASP:HA	1:G:320:ALA:O	2.22	0.40
1:F:80:ARG:HB2	1:F:80:ARG:NH1	2.35	0.40
1:E:126:LYS:HG3	1:E:429:LEU:HD22	2.02	0.40
1:A:323:VAL:HG13	1:A:332:ILE:HG12	2.03	0.40
1:G:480:ASN:O	1:G:484:GLU:N	2.48	0.40
1:B:217:ASP:HA	1:B:320:ALA:O	2.22	0.40
1:F:378:VAL:HG22	1:F:378:VAL:O	2.21	0.40
1:B:323:VAL:HG13	1:B:332:ILE:HG12	2.03	0.40
1:A:80:ARG:NH1	1:A:80:ARG:HB2	2.36	0.40
1:G:201:SER:O	1:G:204:PHE:HB2	2.21	0.40
1:C:2:ALA:O	1:C:3:ALA:C	2.60	0.40
1:G:482:GLN:NE2	1:G:482:GLN:HA	2.37	0.40
1:E:144:VAL:O	1:E:144:VAL:CG1	2.70	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	474/545 (87%)	404 (85%)	59 (12%)	11 (2%)	10 52

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	474/545 (87%)	405 (85%)	59 (12%)	10 (2%)	11	55
1	C	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	11	55
1	D	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	11	55
1	E	474/545 (87%)	404 (85%)	60 (13%)	10 (2%)	11	55
1	F	474/545 (87%)	404 (85%)	58 (12%)	12 (2%)	9	49
1	G	474/545 (87%)	405 (85%)	59 (12%)	10 (2%)	11	55
All	All	3318/3815 (87%)	2830 (85%)	415 (12%)	73 (2%)	10	53

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	85	ALA
1	A	228	SER
1	A	378	VAL
1	B	9	ASN
1	B	85	ALA
1	B	134	ALA
1	B	228	SER
1	B	378	VAL
1	C	9	ASN
1	C	85	ALA
1	C	134	ALA
1	C	228	SER
1	C	378	VAL
1	D	9	ASN
1	D	85	ALA
1	D	228	SER
1	D	378	VAL
1	E	9	ASN
1	E	85	ALA
1	E	134	ALA
1	E	228	SER
1	E	378	VAL
1	F	9	ASN
1	F	85	ALA
1	F	228	SER
1	F	378	VAL
1	G	9	ASN
1	G	85	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	228	SER
1	G	378	VAL
1	A	134	ALA
1	A	335	GLY
1	B	335	GLY
1	C	335	GLY
1	D	134	ALA
1	D	335	GLY
1	E	335	GLY
1	F	134	ALA
1	F	335	GLY
1	G	134	ALA
1	G	335	GLY
1	A	87	ASP
1	A	336	ALA
1	A	475	LYS
1	B	87	ASP
1	B	336	ALA
1	B	475	LYS
1	C	87	ASP
1	C	336	ALA
1	C	475	LYS
1	D	87	ASP
1	D	336	ALA
1	D	475	LYS
1	E	87	ASP
1	E	336	ALA
1	E	475	LYS
1	F	87	ASP
1	F	336	ALA
1	F	475	LYS
1	G	87	ASP
1	G	336	ALA
1	G	475	LYS
1	F	3	ALA
1	A	246	PRO
1	B	246	PRO
1	C	246	PRO
1	D	246	PRO
1	F	246	PRO
1	E	246	PRO
1	G	246	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	374	GLY
1	A	374	GLY

### 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	372/421 (88%)	278 (75%)	94 (25%)	1	3
1	B	372/421 (88%)	279 (75%)	93 (25%)	1	3
1	C	372/421 (88%)	277 (74%)	95 (26%)	1	3
1	D	372/421 (88%)	279 (75%)	93 (25%)	1	3
1	E	372/421 (88%)	278 (75%)	94 (25%)	1	3
1	F	372/421 (88%)	278 (75%)	94 (25%)	1	3
1	G	372/421 (88%)	277 (74%)	95 (26%)	1	3
All	All	2604/2947 (88%)	1946 (75%)	658 (25%)	1	3

All (658) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	LYS
1	A	16	MET
1	A	18	LYS
1	A	28	LYS
1	A	36	ARG
1	A	42	LYS
1	A	51	LYS
1	A	55	SER
1	A	69	MET
1	A	72	GLN
1	A	75	ARG
1	A	76	GLU
1	A	77	VAL
1	A	79	SER
1	A	80	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	83	ASP
1	A	87	ASP
1	A	105	LYS
1	A	132	LYS
1	A	139	ASN
1	A	141	SER
1	A	146	GLN
1	A	155	GLU
1	A	156	SER
1	A	164	GLU
1	A	166	MET
1	A	167	GLN
1	A	168	ARG
1	A	172	GLU
1	A	181	LYS
1	A	183	MET
1	A	196	ASP
1	A	197	ARG
1	A	204	PHE
1	A	206	THR
1	A	209	ASP
1	A	210	LYS
1	A	211	MET
1	A	214	GLU
1	A	216	GLU
1	A	217	ASP
1	A	221	LEU
1	A	222	LEU
1	A	225	LYS
1	A	229	SER
1	A	231	GLN
1	A	245	LYS
1	A	247	LEU
1	A	250	VAL
1	A	252	GLU
1	A	253	ASP
1	A	281	PHE
1	A	283	ASP
1	A	288	MET
1	A	290	GLN
1	A	295	LEU
1	A	315	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	316	MET
1	A	317	LEU
1	A	321	LYS
1	A	322	LYS
1	A	327	LYS
1	A	328	ASP
1	A	333	VAL
1	A	338	GLU
1	A	339	LYS
1	A	343	GLU
1	A	345	ARG
1	A	352	GLN
1	A	357	THR
1	A	362	ARG
1	A	365	LEU
1	A	367	GLU
1	A	368	ARG
1	A	371	LYS
1	A	380	ARG
1	A	387	ILE
1	A	388	GLU
1	A	391	GLU
1	A	395	ARG
1	A	398	ASP
1	A	401	ASN
1	A	408	GLN
1	A	419	LEU
1	A	427	GLU
1	A	430	SER
1	A	434	SER
1	A	436	GLN
1	A	444	ARG
1	A	452	ARG
1	A	473	SER
1	A	524	GLU
1	A	525	LYS
1	B	5	GLU
1	B	7	LYS
1	B	16	MET
1	B	18	LYS
1	B	28	LYS
1	B	36	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	42	LYS
1	B	51	LYS
1	B	55	SER
1	B	69	MET
1	B	72	GLN
1	B	75	ARG
1	B	76	GLU
1	B	77	VAL
1	B	79	SER
1	B	80	ARG
1	B	83	ASP
1	B	87	ASP
1	B	105	LYS
1	B	132	LYS
1	B	139	ASN
1	B	141	SER
1	B	146	GLN
1	B	155	GLU
1	B	156	SER
1	B	164	GLU
1	B	166	MET
1	B	167	GLN
1	B	168	ARG
1	B	172	GLU
1	B	181	LYS
1	B	183	MET
1	B	196	ASP
1	B	197	ARG
1	B	204	PHE
1	B	206	THR
1	B	209	ASP
1	B	210	LYS
1	B	211	MET
1	B	214	GLU
1	B	216	GLU
1	B	217	ASP
1	B	221	LEU
1	B	222	LEU
1	B	225	LYS
1	B	229	SER
1	B	231	GLN
1	B	245	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	247	LEU
1	B	250	VAL
1	B	252	GLU
1	B	253	ASP
1	B	281	PHE
1	B	283	ASP
1	B	288	MET
1	B	290	GLN
1	B	295	LEU
1	B	315	ASP
1	B	316	MET
1	B	317	LEU
1	B	321	LYS
1	B	322	LYS
1	B	327	LYS
1	B	328	ASP
1	B	333	VAL
1	B	338	GLU
1	B	339	LYS
1	B	343	GLU
1	B	345	ARG
1	B	352	GLN
1	B	357	THR
1	B	362	ARG
1	B	365	LEU
1	B	367	GLU
1	B	368	ARG
1	B	371	LYS
1	B	380	ARG
1	B	387	ILE
1	B	388	GLU
1	B	391	GLU
1	B	395	ARG
1	B	398	ASP
1	B	401	ASN
1	B	408	GLN
1	B	419	LEU
1	B	427	GLU
1	B	430	SER
1	B	434	SER
1	B	436	GLN
1	B	444	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	473	SER
1	B	524	GLU
1	B	525	LYS
1	C	5	GLU
1	C	7	LYS
1	C	16	MET
1	C	18	LYS
1	C	28	LYS
1	C	36	ARG
1	C	42	LYS
1	C	51	LYS
1	C	55	SER
1	C	69	MET
1	C	72	GLN
1	C	75	ARG
1	C	76	GLU
1	C	77	VAL
1	C	79	SER
1	C	80	ARG
1	C	83	ASP
1	C	87	ASP
1	C	105	LYS
1	C	132	LYS
1	C	139	ASN
1	C	141	SER
1	C	146	GLN
1	C	155	GLU
1	C	156	SER
1	C	164	GLU
1	C	166	MET
1	C	167	GLN
1	C	168	ARG
1	C	172	GLU
1	C	181	LYS
1	C	183	MET
1	C	196	ASP
1	C	197	ARG
1	C	204	PHE
1	C	206	THR
1	C	209	ASP
1	C	210	LYS
1	C	211	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	214	GLU
1	C	216	GLU
1	C	217	ASP
1	C	221	LEU
1	C	222	LEU
1	C	225	LYS
1	C	229	SER
1	C	231	GLN
1	C	245	LYS
1	C	247	LEU
1	C	250	VAL
1	C	252	GLU
1	C	253	ASP
1	C	281	PHE
1	C	283	ASP
1	C	288	MET
1	C	290	GLN
1	C	295	LEU
1	C	315	ASP
1	C	316	MET
1	C	317	LEU
1	C	321	LYS
1	C	322	LYS
1	C	327	LYS
1	C	328	ASP
1	C	333	VAL
1	C	338	GLU
1	C	339	LYS
1	C	343	GLU
1	C	345	ARG
1	C	352	GLN
1	C	357	THR
1	C	362	ARG
1	C	365	LEU
1	C	367	GLU
1	C	368	ARG
1	C	371	LYS
1	C	380	ARG
1	C	387	ILE
1	C	388	GLU
1	C	391	GLU
1	C	392	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	395	ARG
1	C	398	ASP
1	C	401	ASN
1	C	408	GLN
1	C	419	LEU
1	C	427	GLU
1	C	430	SER
1	C	434	SER
1	C	436	GLN
1	C	444	ARG
1	C	452	ARG
1	C	473	SER
1	C	524	GLU
1	C	525	LYS
1	D	5	GLU
1	D	7	LYS
1	D	16	MET
1	D	18	LYS
1	D	28	LYS
1	D	36	ARG
1	D	42	LYS
1	D	51	LYS
1	D	55	SER
1	D	69	MET
1	D	72	GLN
1	D	75	ARG
1	D	76	GLU
1	D	77	VAL
1	D	79	SER
1	D	80	ARG
1	D	83	ASP
1	D	87	ASP
1	D	105	LYS
1	D	132	LYS
1	D	139	ASN
1	D	141	SER
1	D	146	GLN
1	D	155	GLU
1	D	156	SER
1	D	164	GLU
1	D	166	MET
1	D	167	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	168	ARG
1	D	172	GLU
1	D	181	LYS
1	D	183	MET
1	D	196	ASP
1	D	197	ARG
1	D	204	PHE
1	D	206	THR
1	D	209	ASP
1	D	210	LYS
1	D	211	MET
1	D	214	GLU
1	D	216	GLU
1	D	217	ASP
1	D	221	LEU
1	D	222	LEU
1	D	225	LYS
1	D	229	SER
1	D	231	GLN
1	D	245	LYS
1	D	247	LEU
1	D	250	VAL
1	D	252	GLU
1	D	253	ASP
1	D	281	PHE
1	D	283	ASP
1	D	288	MET
1	D	290	GLN
1	D	295	LEU
1	D	315	ASP
1	D	316	MET
1	D	317	LEU
1	D	321	LYS
1	D	322	LYS
1	D	327	LYS
1	D	328	ASP
1	D	333	VAL
1	D	338	GLU
1	D	339	LYS
1	D	343	GLU
1	D	345	ARG
1	D	352	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	357	THR
1	D	362	ARG
1	D	365	LEU
1	D	367	GLU
1	D	368	ARG
1	D	371	LYS
1	D	380	ARG
1	D	387	ILE
1	D	388	GLU
1	D	391	GLU
1	D	395	ARG
1	D	398	ASP
1	D	401	ASN
1	D	408	GLN
1	D	419	LEU
1	D	427	GLU
1	D	430	SER
1	D	434	SER
1	D	436	GLN
1	D	444	ARG
1	D	473	SER
1	D	524	GLU
1	D	525	LYS
1	E	5	GLU
1	E	7	LYS
1	E	16	MET
1	E	18	LYS
1	E	28	LYS
1	E	36	ARG
1	E	42	LYS
1	E	51	LYS
1	E	55	SER
1	E	64	ASP
1	E	69	MET
1	E	72	GLN
1	E	75	ARG
1	E	76	GLU
1	E	77	VAL
1	E	79	SER
1	E	80	ARG
1	E	83	ASP
1	E	87	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	105	LYS
1	E	132	LYS
1	E	139	ASN
1	E	141	SER
1	E	146	GLN
1	E	155	GLU
1	E	156	SER
1	E	164	GLU
1	E	166	MET
1	E	167	GLN
1	E	168	ARG
1	E	172	GLU
1	E	181	LYS
1	E	183	MET
1	E	196	ASP
1	E	197	ARG
1	E	204	PHE
1	E	206	THR
1	E	209	ASP
1	E	210	LYS
1	E	211	MET
1	E	214	GLU
1	E	216	GLU
1	E	217	ASP
1	E	221	LEU
1	E	222	LEU
1	E	225	LYS
1	E	229	SER
1	E	231	GLN
1	E	245	LYS
1	E	247	LEU
1	E	250	VAL
1	E	252	GLU
1	E	253	ASP
1	E	281	PHE
1	E	283	ASP
1	E	288	MET
1	E	290	GLN
1	E	295	LEU
1	E	315	ASP
1	E	316	MET
1	E	317	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	321	LYS
1	E	322	LYS
1	E	327	LYS
1	E	328	ASP
1	E	333	VAL
1	E	338	GLU
1	E	339	LYS
1	E	343	GLU
1	E	345	ARG
1	E	352	GLN
1	E	357	THR
1	E	362	ARG
1	E	365	LEU
1	E	367	GLU
1	E	368	ARG
1	E	371	LYS
1	E	380	ARG
1	E	387	ILE
1	E	388	GLU
1	E	391	GLU
1	E	395	ARG
1	E	398	ASP
1	E	401	ASN
1	E	408	GLN
1	E	419	LEU
1	E	427	GLU
1	E	430	SER
1	E	434	SER
1	E	436	GLN
1	E	444	ARG
1	E	473	SER
1	E	524	GLU
1	E	525	LYS
1	F	5	GLU
1	F	7	LYS
1	F	16	MET
1	F	18	LYS
1	F	28	LYS
1	F	36	ARG
1	F	42	LYS
1	F	51	LYS
1	F	55	SER

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	69	MET
1	F	72	GLN
1	F	75	ARG
1	F	76	GLU
1	F	77	VAL
1	F	79	SER
1	F	80	ARG
1	F	83	ASP
1	F	87	ASP
1	F	105	LYS
1	F	132	LYS
1	F	139	ASN
1	F	141	SER
1	F	146	GLN
1	F	155	GLU
1	F	156	SER
1	F	164	GLU
1	F	166	MET
1	F	167	GLN
1	F	168	ARG
1	F	172	GLU
1	F	181	LYS
1	F	183	MET
1	F	196	ASP
1	F	197	ARG
1	F	204	PHE
1	F	206	THR
1	F	209	ASP
1	F	210	LYS
1	F	211	MET
1	F	214	GLU
1	F	216	GLU
1	F	217	ASP
1	F	221	LEU
1	F	222	LEU
1	F	225	LYS
1	F	229	SER
1	F	231	GLN
1	F	245	LYS
1	F	247	LEU
1	F	250	VAL
1	F	252	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	253	ASP
1	F	281	PHE
1	F	283	ASP
1	F	288	MET
1	F	290	GLN
1	F	295	LEU
1	F	315	ASP
1	F	316	MET
1	F	317	LEU
1	F	321	LYS
1	F	322	LYS
1	F	327	LYS
1	F	328	ASP
1	F	333	VAL
1	F	338	GLU
1	F	339	LYS
1	F	343	GLU
1	F	345	ARG
1	F	352	GLN
1	F	357	THR
1	F	362	ARG
1	F	365	LEU
1	F	367	GLU
1	F	368	ARG
1	F	371	LYS
1	F	380	ARG
1	F	387	ILE
1	F	388	GLU
1	F	391	GLU
1	F	395	ARG
1	F	398	ASP
1	F	401	ASN
1	F	408	GLN
1	F	419	LEU
1	F	427	GLU
1	F	430	SER
1	F	434	SER
1	F	436	GLN
1	F	444	ARG
1	F	452	ARG
1	F	473	SER
1	F	524	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	525	LYS
1	G	5	GLU
1	G	7	LYS
1	G	10	SER
1	G	16	MET
1	G	18	LYS
1	G	28	LYS
1	G	36	ARG
1	G	42	LYS
1	G	51	LYS
1	G	55	SER
1	G	69	MET
1	G	72	GLN
1	G	75	ARG
1	G	76	GLU
1	G	77	VAL
1	G	79	SER
1	G	80	ARG
1	G	83	ASP
1	G	87	ASP
1	G	105	LYS
1	G	132	LYS
1	G	139	ASN
1	G	141	SER
1	G	146	GLN
1	G	155	GLU
1	G	156	SER
1	G	164	GLU
1	G	166	MET
1	G	167	GLN
1	G	168	ARG
1	G	172	GLU
1	G	181	LYS
1	G	183	MET
1	G	196	ASP
1	G	197	ARG
1	G	204	PHE
1	G	206	THR
1	G	209	ASP
1	G	210	LYS
1	G	211	MET
1	G	214	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	216	GLU
1	G	217	ASP
1	G	221	LEU
1	G	222	LEU
1	G	225	LYS
1	G	229	SER
1	G	231	GLN
1	G	245	LYS
1	G	247	LEU
1	G	250	VAL
1	G	252	GLU
1	G	253	ASP
1	G	281	PHE
1	G	283	ASP
1	G	288	MET
1	G	290	GLN
1	G	295	LEU
1	G	315	ASP
1	G	316	MET
1	G	317	LEU
1	G	321	LYS
1	G	322	LYS
1	G	327	LYS
1	G	328	ASP
1	G	333	VAL
1	G	338	GLU
1	G	339	LYS
1	G	343	GLU
1	G	345	ARG
1	G	352	GLN
1	G	357	THR
1	G	362	ARG
1	G	365	LEU
1	G	367	GLU
1	G	368	ARG
1	G	371	LYS
1	G	380	ARG
1	G	387	ILE
1	G	388	GLU
1	G	391	GLU
1	G	395	ARG
1	G	398	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	401	ASN
1	G	408	GLN
1	G	419	LEU
1	G	427	GLU
1	G	430	SER
1	G	434	SER
1	G	436	GLN
1	G	444	ARG
1	G	452	ARG
1	G	473	SER
1	G	524	GLU
1	G	525	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	72	GLN
1	A	97	GLN
1	A	139	ASN
1	A	153	ASN
1	A	194	GLN
1	A	231	GLN
1	A	348	GLN
1	A	352	GLN
1	A	480	ASN
1	B	68	ASN
1	B	72	GLN
1	B	97	GLN
1	B	139	ASN
1	B	153	ASN
1	B	194	GLN
1	B	231	GLN
1	B	348	GLN
1	B	352	GLN
1	B	480	ASN
1	C	37	ASN
1	C	68	ASN
1	C	72	GLN
1	C	97	GLN
1	C	139	ASN
1	C	153	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	194	GLN
1	C	231	GLN
1	C	348	GLN
1	C	352	GLN
1	C	480	ASN
1	D	68	ASN
1	D	72	GLN
1	D	139	ASN
1	D	153	ASN
1	D	194	GLN
1	D	231	GLN
1	D	348	GLN
1	D	352	GLN
1	D	480	ASN
1	E	68	ASN
1	E	72	GLN
1	E	97	GLN
1	E	139	ASN
1	E	153	ASN
1	E	231	GLN
1	E	348	GLN
1	E	352	GLN
1	E	480	ASN
1	F	68	ASN
1	F	72	GLN
1	F	97	GLN
1	F	139	ASN
1	F	153	ASN
1	F	194	GLN
1	F	231	GLN
1	F	348	GLN
1	F	352	GLN
1	F	480	ASN
1	G	68	ASN
1	G	72	GLN
1	G	97	GLN
1	G	139	ASN
1	G	153	ASN
1	G	194	GLN
1	G	231	GLN
1	G	348	GLN
1	G	352	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	480	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.