



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:31 AM GMT

PDB ID : 3IKO  
Title : Crystal structure of the heterotrimeric Sec13-Nup145C-Nup84 nucleoporin complex  
Authors : Nagy, V.; Hsia, K.-C.; Debler, E.W.; Davenport, A.; Blobel, G.; Hoelz, A.  
Deposited on : 2009-08-06  
Resolution : 3.20 Å(reported)

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

---

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

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

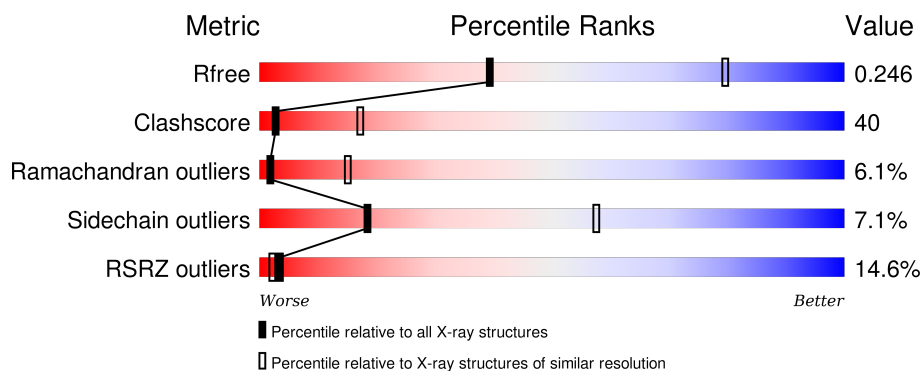
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	297	<div> <div>31%</div> <div>32% 54% 6% 8%</div> </div>
1	D	297	<div> <div>34%</div> <div>34% 52% 7% 8%</div> </div>
1	G	297	<div> <div>39%</div> <div>31% 54% 7% 8%</div> </div>
2	B	442	<div> <div>3%</div> <div>43% 46% 8% . .</div> </div>
2	E	442	<div> <div>8%</div> <div>43% 44% 8% . .</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	442	<div><div></div><div>18%</div><div>42%</div><div>43%</div><div>9%</div><div>5%</div></div>
3	C	460	<div><div></div><div>3%</div><div>45%</div><div>39%</div><div>7%</div><div>9%</div></div>
3	F	460	<div><div></div><div>5%</div><div>45%</div><div>39%</div><div>7%</div><div>9%</div></div>
3	I	460	<div><div></div><div>4%</div><div>44%</div><div>38%</div><div>7%</div><div>10%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27032 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 Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	D	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			
1	G	274	Total	C	N	O	S	0	0	0
			2160	1379	369	409	3			

- Molecule 2 is a protein called Nucleoporin NUP145C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	434	Total	C	N	O	S	9	0	0
			3528	2254	587	675	12			
2	E	423	Total	C	N	O	S	9	0	0
			3438	2201	570	656	11			
2	H	420	Total	C	N	O	S	9	0	0
			3409	2182	566	650	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	111	MET	-	EXPRESSION TAG	UNP P49687
B	112	GLY	-	EXPRESSION TAG	UNP P49687
B	113	SER	-	EXPRESSION TAG	UNP P49687
B	114	SER	-	EXPRESSION TAG	UNP P49687
B	115	HIS	-	EXPRESSION TAG	UNP P49687
B	116	HIS	-	EXPRESSION TAG	UNP P49687
B	117	HIS	-	EXPRESSION TAG	UNP P49687
B	118	HIS	-	EXPRESSION TAG	UNP P49687
B	119	HIS	-	EXPRESSION TAG	UNP P49687
B	120	HIS	-	EXPRESSION TAG	UNP P49687
B	121	SER	-	EXPRESSION TAG	UNP P49687
B	122	GLN	-	EXPRESSION TAG	UNP P49687

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	123	ASP	-	EXPRESSION TAG	UNP P49687
B	124	PRO	-	EXPRESSION TAG	UNP P49687
E	111	MET	-	EXPRESSION TAG	UNP P49687
E	112	GLY	-	EXPRESSION TAG	UNP P49687
E	113	SER	-	EXPRESSION TAG	UNP P49687
E	114	SER	-	EXPRESSION TAG	UNP P49687
E	115	HIS	-	EXPRESSION TAG	UNP P49687
E	116	HIS	-	EXPRESSION TAG	UNP P49687
E	117	HIS	-	EXPRESSION TAG	UNP P49687
E	118	HIS	-	EXPRESSION TAG	UNP P49687
E	119	HIS	-	EXPRESSION TAG	UNP P49687
E	120	HIS	-	EXPRESSION TAG	UNP P49687
E	121	SER	-	EXPRESSION TAG	UNP P49687
E	122	GLN	-	EXPRESSION TAG	UNP P49687
E	123	ASP	-	EXPRESSION TAG	UNP P49687
E	124	PRO	-	EXPRESSION TAG	UNP P49687
H	111	MET	-	EXPRESSION TAG	UNP P49687
H	112	GLY	-	EXPRESSION TAG	UNP P49687
H	113	SER	-	EXPRESSION TAG	UNP P49687
H	114	SER	-	EXPRESSION TAG	UNP P49687
H	115	HIS	-	EXPRESSION TAG	UNP P49687
H	116	HIS	-	EXPRESSION TAG	UNP P49687
H	117	HIS	-	EXPRESSION TAG	UNP P49687
H	118	HIS	-	EXPRESSION TAG	UNP P49687
H	119	HIS	-	EXPRESSION TAG	UNP P49687
H	120	HIS	-	EXPRESSION TAG	UNP P49687
H	121	SER	-	EXPRESSION TAG	UNP P49687
H	122	GLN	-	EXPRESSION TAG	UNP P49687
H	123	ASP	-	EXPRESSION TAG	UNP P49687
H	124	PRO	-	EXPRESSION TAG	UNP P49687

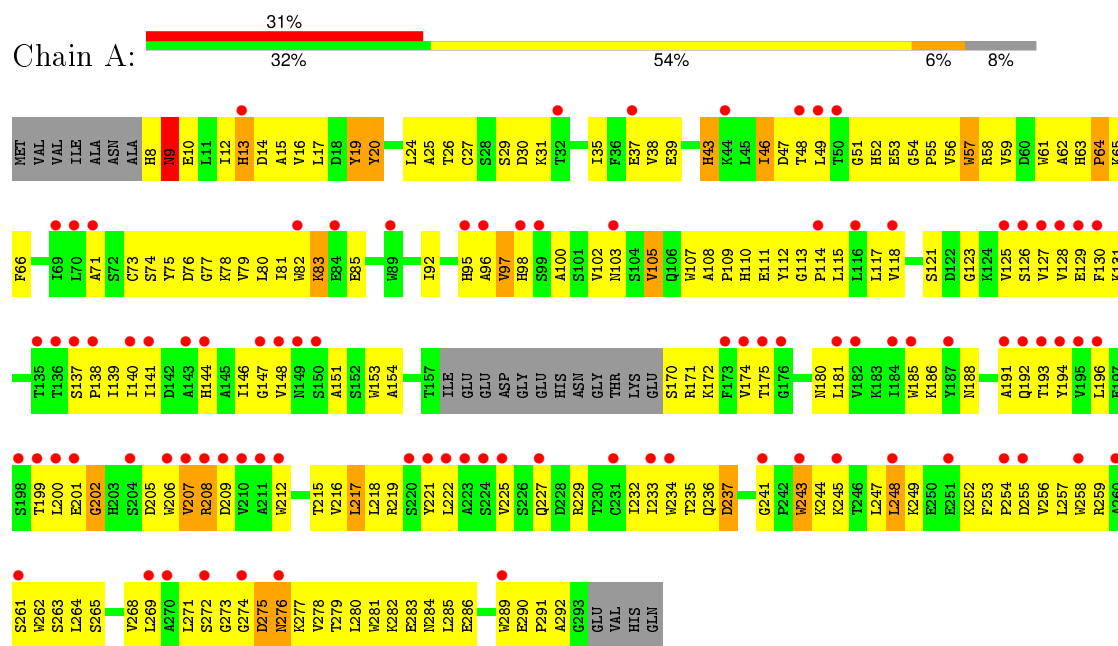
- Molecule 3 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	419	Total	C	N	O	S	0	0	0
			3404	2178	557	657	12			
3	F	419	Total	C	N	O	S	0	0	0
			3404	2178	558	656	12			
3	I	414	Total	C	N	O	S	0	0	0
			3369	2155	554	649	11			

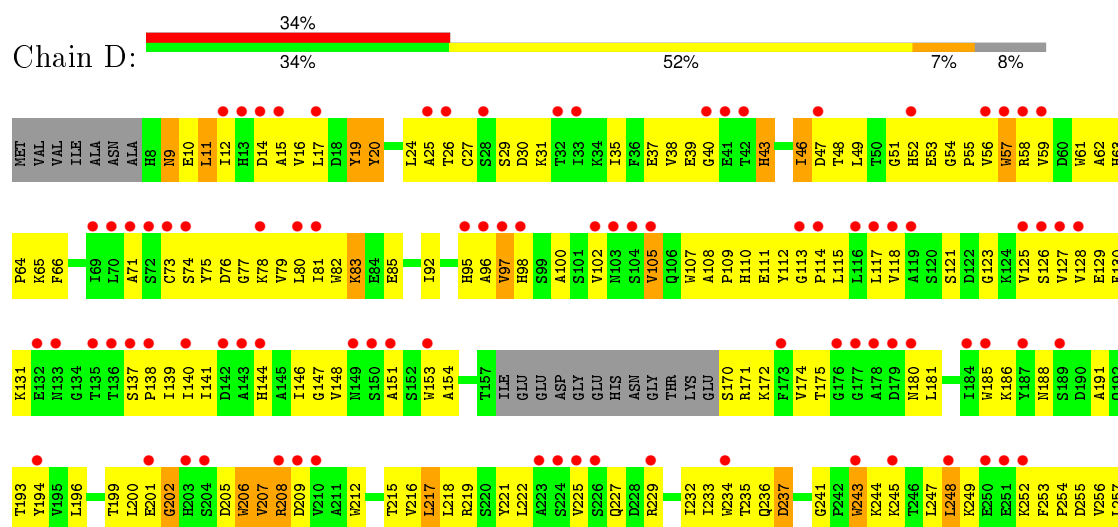
### 3 Residue-property plots

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

#### • Molecule 1: Protein transport protein SEC13

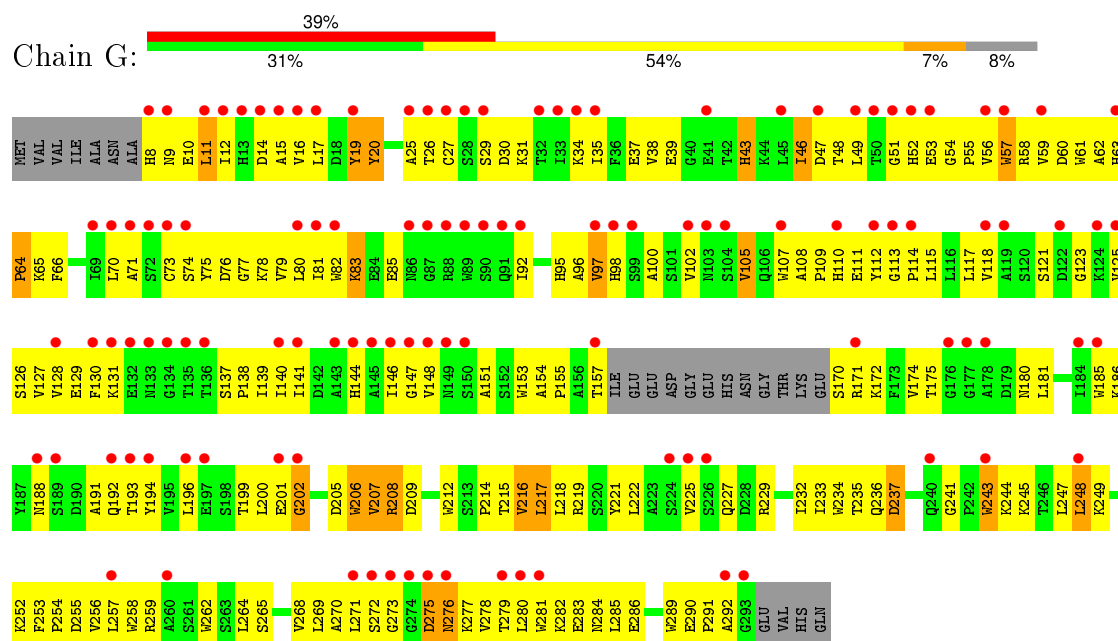


#### • Molecule 1: Protein transport protein SEC13

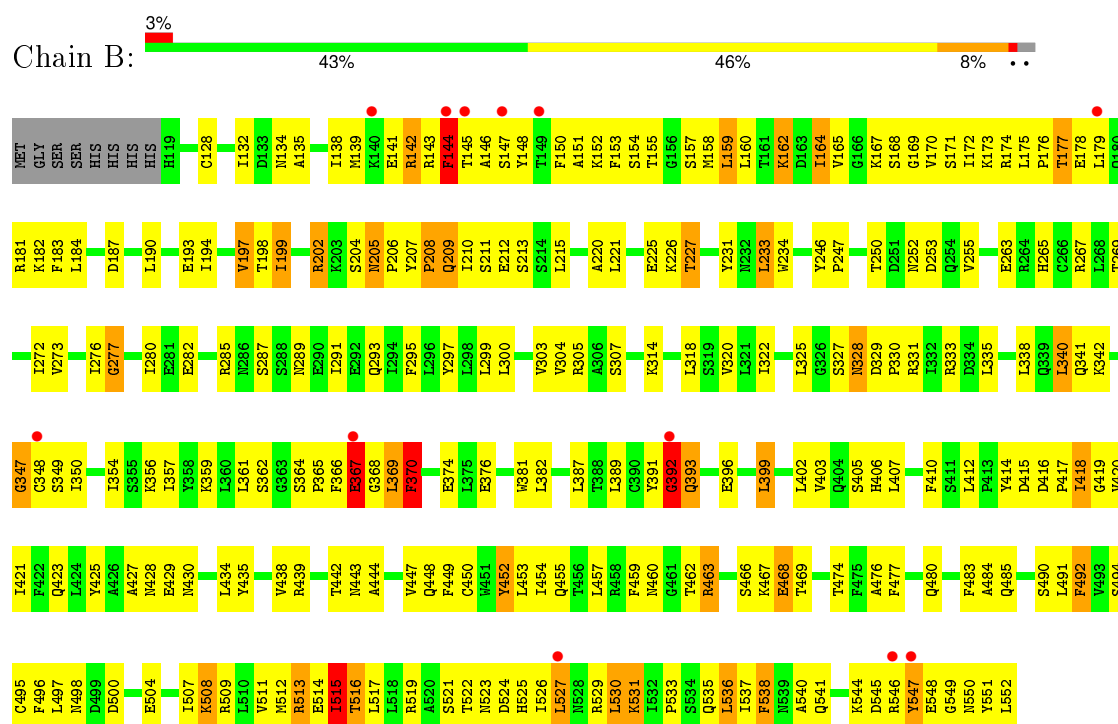




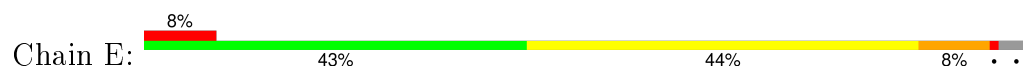
• Molecule 1: Protein transport protein SEC13

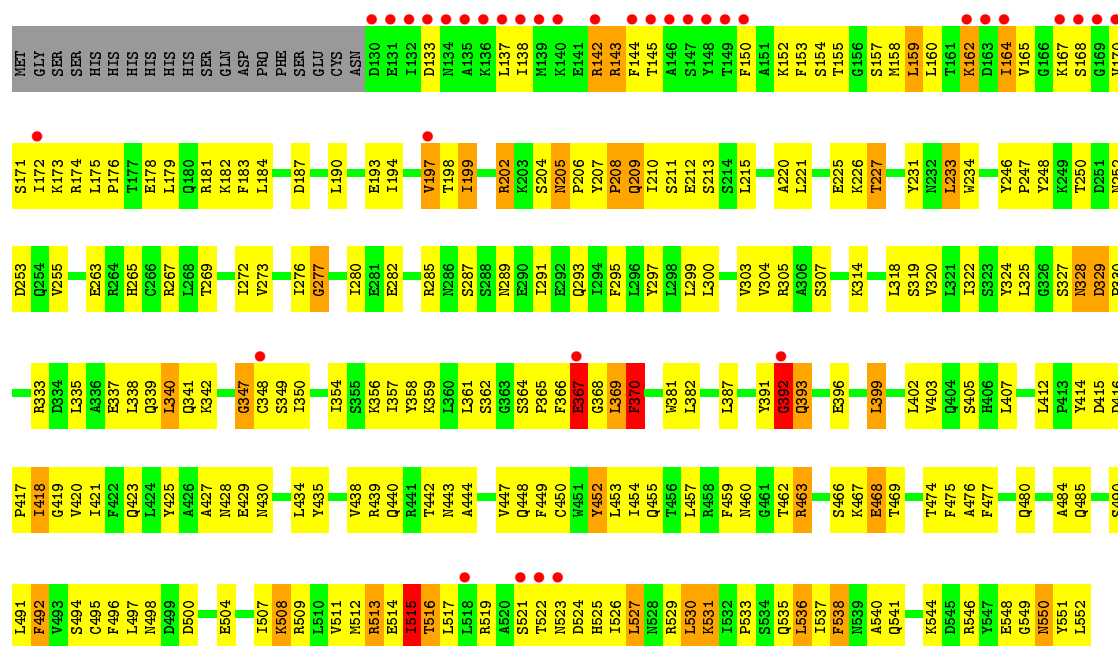


• Molecule 2: Nucleoporin NUP145C

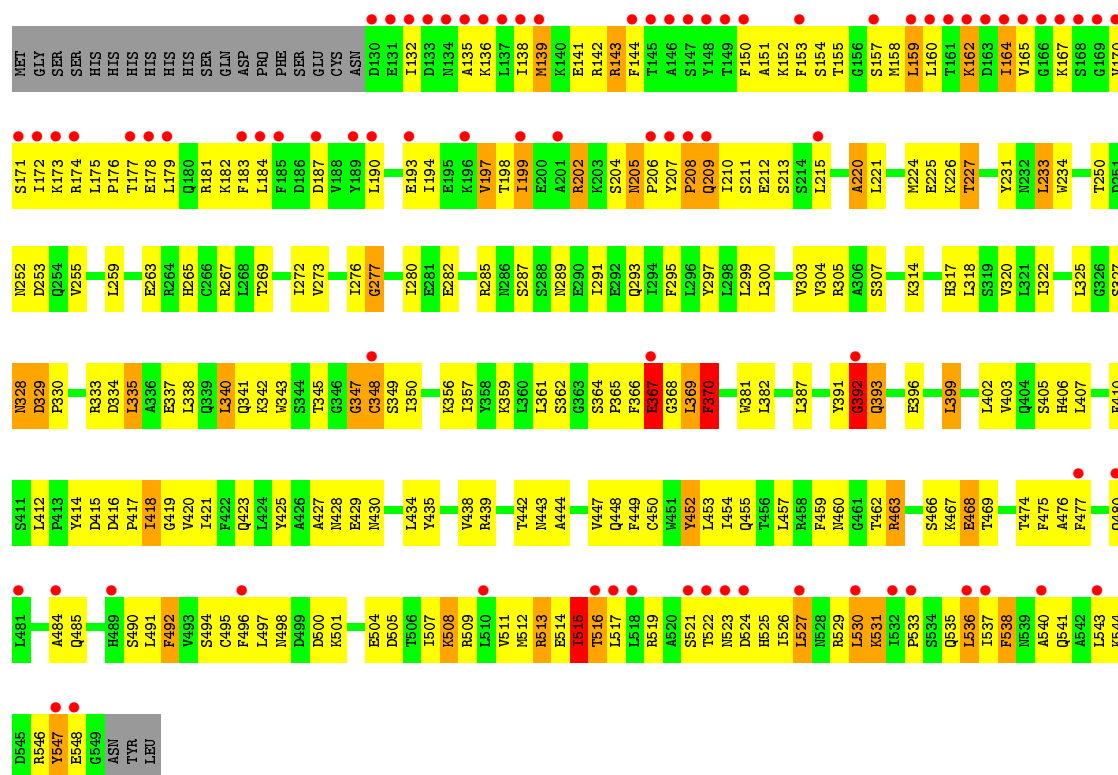


• Molecule 2: Nucleoporin NUP145C

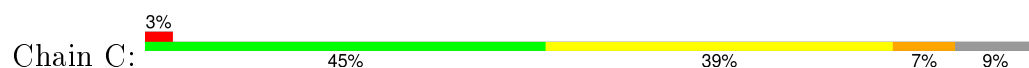




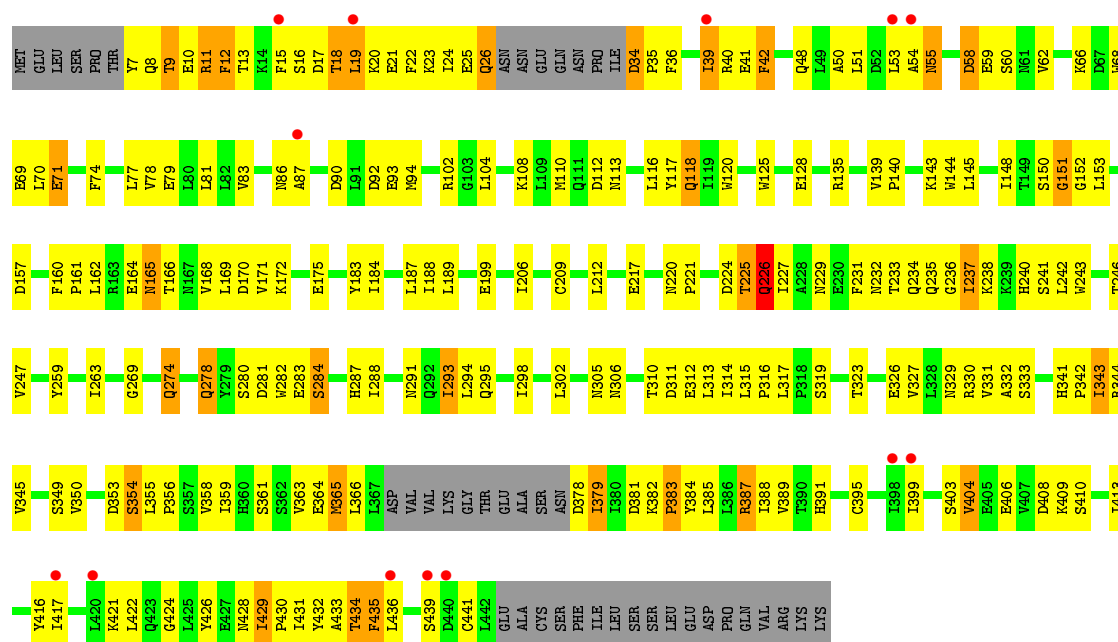
• Molecule 2: Nucleoporin NUP145C



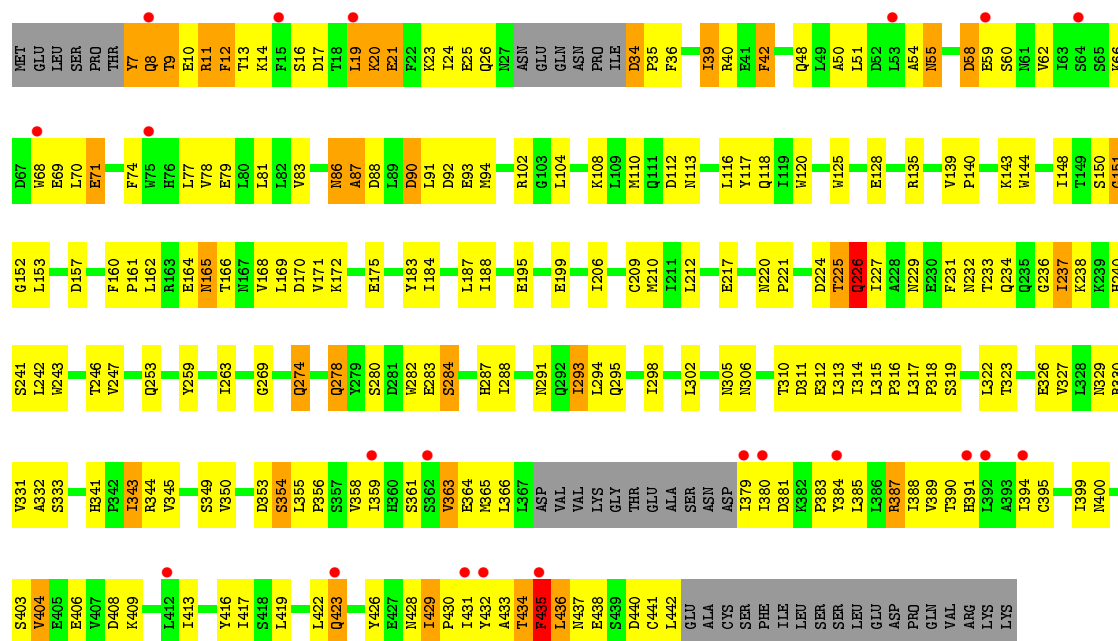
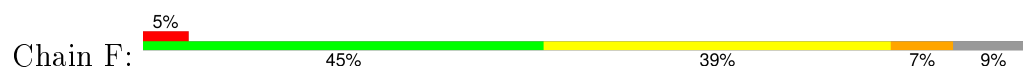
• Molecule 3: Nucleoporin NUP84



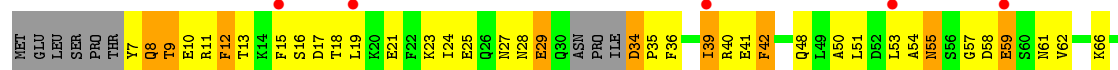
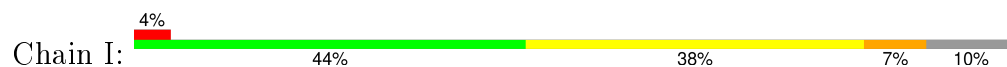




• Molecule 3: Nucleoporin NUP84



• Molecule 3: Nucleoporin NUP84



D408	K409	H341	H243	G151	L70
L412	L413	I343	T246	G152	E71
I413	V344	R344	V247	L153	F74
Y416	V345	S251	S251	D159	L77
I417	S349	Y259	Y259	F160	V78
S418	V350	E260	E260	P161	E79
L419	D353	R261	R261	L162	L80
L420	L421	A262	A262	E164	L81
K421	S354	L263	L263	N165	L82
L422	L355	T166	T166	T166	V83
Q423	P356	G269	G269	N167	N86
G424	S357	Q274	Q274	V168	L89
L425	V358	Q274	Q274	L169	D90
Y426	I359	Q278	Q278	V171	V91
E427	H360	Y279	Y279	K172	L91
N428	S361	S280	S280	D92	D92
I429	S362	D281	D281	E175	E93
P430	V363	E282	E282	Y183	N94
I431	E364	E283	E283	I184	E95
Y432	N365	S284	S284	Y184	L96
A433	L366	H287	H287	I188	Y99
T434	L367	I289	I289	L189	Y99
F435	ASP	N291	N291	E199	R102
L436	VAL	GLY	GLY	G103	G103
ASN	LYS	THR	THR	L104	L104
GLU	GLY	I292	I292	K108	K108
SER	ASP	L293	L293	L109	L109
ASP	CYS	L294	L294	M110	M110
CYS	LEU	Q295	Q295	P210	P210
LEU	GLU	I298	I298	I211	Q111
GLU	ALA	L302	L302	D112	D112
ALA	ASN	L302	L302	N113	N113
ASN	ASP	L302	L302	K114	K114
CYS	ILE	L302	L302	E217	E217
SER	ILE	L302	L302	L116	Q115
PHE	ILE	L302	L302	Y117	Y117
ILE	D381	L302	L302	I223	Q118
LEU	R382	L302	L302	D224	I119
SER	P383	L302	L302	T225	W120
SER	Y384	L302	L302	Q226	W120
LEU	L385	L302	L302	I227	W125
LEU	L386	L302	L302	A228	E128
ASP	R387	L302	L302	E230	R135
PRO	I388	L302	L302	F231	N232
GLN	V389	L302	L302	T233	V139
VAL	T390	L302	L302	Q234	P140
ARG	H391	L302	L302	Q236	K143
LYS	C395	L302	L302	I237	W144
LYS	C395	L302	L302	K238	L145
LYS	C395	L302	L302	E239	I148
LYS	C395	L302	L302	H240	T149
LYS	C395	L302	L302	S241	S150
LYS	C395	L302	L302	L242	S150

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.40Å 194.05Å 327.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 48.79 – 3.18	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-3.20) 96.2 (48.79-3.18)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 3.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.234 , 0.273 0.243 , 0.246	Depositor DCC
$R_{free}$ test set	5204 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	86.0	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 110.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 104908 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	27032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.48	0/2220	0.68	1/3028 (0.0%)
1	D	0.47	0/2220	0.67	0/3028
1	G	0.47	0/2220	0.67	0/3028
2	B	0.55	0/3598	0.74	1/4856 (0.0%)
2	E	0.57	0/3504	0.75	1/4728 (0.0%)
2	H	0.56	0/3474	0.74	1/4688 (0.0%)
3	C	0.63	0/3472	0.76	0/4714
3	F	0.63	0/3472	0.77	3/4714 (0.1%)
3	I	0.62	0/3437	0.76	0/4666
All	All	0.57	0/27617	0.74	7/37450 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
3	F	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	392	GLY	N-CA-C	5.99	128.08	113.10
2	H	392	GLY	N-CA-C	5.98	128.05	113.10
2	B	392	GLY	N-CA-C	5.96	128.01	113.10
3	F	435	PHE	N-CA-C	5.71	126.41	111.00
3	F	436	LEU	N-CA-C	5.29	125.28	111.00
1	A	9	ASN	CA-C-N	-5.09	105.99	117.20
3	F	436	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	435	PHE	Mainchain
3	F	435	PHE	Mainchain

## 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	2160	0	2096	239	0
1	D	2160	0	2096	228	0
1	G	2160	0	2096	226	0
2	B	3528	0	3521	301	0
2	E	3438	0	3452	293	0
2	H	3409	0	3426	313	0
3	C	3404	0	3378	249	0
3	F	3404	0	3380	246	0
3	I	3369	0	3341	243	0
All	All	27032	0	26786	2165	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 40.

All (2165) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:369:LEU:O	2:E:369:LEU:HG	1.36	1.13
2:E:208:PRO:HB3	2:E:531:LYS:HB2	1.32	1.10
1:A:131:LYS:HE3	1:A:137:SER:HB2	1.38	1.06
2:H:208:PRO:HB3	2:H:531:LYS:HB2	1.32	1.06
2:H:139:MET:HG2	2:H:144:PHE:O	1.56	1.05
2:B:208:PRO:HB3	2:B:531:LYS:HB2	1.32	1.05
1:A:126:SER:HB3	1:A:140:ILE:HG13	1.38	1.04
1:D:131:LYS:HE3	1:D:137:SER:HB2	1.38	1.04
3:C:70:LEU:HD22	3:C:343:ILE:HD11	1.35	1.03
1:G:131:LYS:HE3	1:G:137:SER:HB2	1.38	1.03

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:LYS:HA	2:H:139:MET:HB3	1.40	1.02
2:H:202:ARG:HG2	2:H:209:GLN:NE2	1.75	1.02
2:E:202:ARG:HG2	2:E:209:GLN:NE2	1.75	1.02
1:A:13:HIS:CE1	2:B:144:PHE:CZ	2.47	1.01
2:B:202:ARG:HG2	2:B:209:GLN:NE2	1.75	1.01
1:A:259:ARG:NH1	2:B:150:PHE:HB2	1.76	1.00
1:D:126:SER:HB3	1:D:140:ILE:HG13	1.38	1.00
1:G:126:SER:HB3	1:G:140:ILE:HG13	1.38	1.00
3:F:70:LEU:HD22	3:F:343:ILE:HD11	1.44	0.99
3:I:8:GLN:NE2	3:I:53:LEU:HG	1.77	0.99
3:F:13:THR:O	3:F:17:ASP:HB2	1.63	0.99
2:B:198:THR:HB	2:B:212:GLU:HB2	1.44	0.98
1:G:212:TRP:HA	1:G:222:LEU:CD2	1.94	0.98
1:G:229:ARG:HH11	1:G:229:ARG:HB2	1.29	0.98
1:D:212:TRP:HA	1:D:222:LEU:CD2	1.94	0.98
1:D:229:ARG:HB2	1:D:229:ARG:HH11	1.29	0.97
1:A:212:TRP:HA	1:A:222:LEU:CD2	1.94	0.97
2:H:320:VAL:HA	3:I:246:THR:HG21	1.45	0.97
2:H:198:THR:HB	2:H:212:GLU:HB2	1.44	0.96
1:A:229:ARG:HB2	1:A:229:ARG:HH11	1.29	0.96
2:E:198:THR:HB	2:E:212:GLU:HB2	1.45	0.96
3:I:384:TYR:HA	3:I:387:ARG:HH12	1.31	0.95
3:F:341:HIS:HE1	3:F:343:ILE:HG23	1.32	0.95
3:C:341:HIS:HE1	3:C:343:ILE:HG23	1.32	0.94
3:F:384:TYR:HA	3:F:387:ARG:HH12	1.31	0.94
3:I:341:HIS:HE1	3:I:343:ILE:HG23	1.32	0.94
1:G:227:GLN:HA	1:G:256:VAL:HG13	1.50	0.94
3:C:384:TYR:HA	3:C:387:ARG:HH12	1.30	0.93
2:B:524:ASP:HA	2:B:527:LEU:HD12	1.51	0.93
1:D:229:ARG:HH12	1:D:252:LYS:HD3	1.34	0.93
1:A:227:GLN:HA	1:A:256:VAL:HG13	1.50	0.93
1:G:229:ARG:HH12	1:G:252:LYS:HD3	1.34	0.93
1:D:227:GLN:HA	1:D:256:VAL:HG13	1.50	0.92
2:H:524:ASP:HA	2:H:527:LEU:HD12	1.51	0.92
2:E:524:ASP:HA	2:E:527:LEU:HD12	1.50	0.92
1:D:49:LEU:HB3	1:D:82:TRP:CZ3	2.05	0.92
1:G:64:PRO:HB2	2:H:543:LEU:HD11	1.50	0.92
2:E:320:VAL:HA	3:F:246:THR:HG21	1.52	0.92
1:A:49:LEU:HB3	1:A:82:TRP:CZ3	2.06	0.92
3:F:314:ILE:HG22	3:F:315:LEU:HG	1.52	0.91
3:I:8:GLN:HE22	3:I:53:LEU:HG	1.31	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:LEU:HB3	1:G:82:TRP:CZ3	2.05	0.91
1:A:261:SER:HB2	2:B:152:LYS:HG2	1.51	0.91
1:A:20:TYR:CE2	2:B:544:LYS:HD3	2.06	0.90
3:C:314:ILE:HG22	3:C:315:LEU:HG	1.51	0.90
2:H:155:THR:HG22	2:H:513:ARG:HG3	1.52	0.90
1:A:229:ARG:HB2	1:A:229:ARG:NH1	1.87	0.90
1:A:229:ARG:HH12	1:A:252:LYS:HD3	1.34	0.90
3:I:89:LEU:HD13	3:I:114:LYS:HZ3	1.37	0.89
3:C:34:ASP:HB3	3:C:35:PRO:HD3	1.54	0.89
3:C:16:SER:HA	3:C:19:LEU:HD12	1.55	0.89
3:I:314:ILE:HG22	3:I:315:LEU:HG	1.51	0.89
1:G:229:ARG:HB2	1:G:229:ARG:NH1	1.87	0.89
1:D:229:ARG:NH1	1:D:229:ARG:HB2	1.87	0.89
3:I:34:ASP:HB3	3:I:35:PRO:HD3	1.54	0.88
2:E:181:ARG:HD2	2:E:448:GLN:OE1	1.74	0.88
3:F:280:SER:HB2	3:F:284:SER:HB3	1.56	0.88
3:F:34:ASP:HB3	3:F:35:PRO:HD3	1.55	0.88
1:D:229:ARG:NH1	1:D:252:LYS:HD3	1.88	0.87
1:A:229:ARG:NH1	1:A:252:LYS:HD3	1.88	0.87
3:C:280:SER:HB2	3:C:284:SER:HB3	1.56	0.87
1:G:229:ARG:NH1	1:G:252:LYS:HD3	1.88	0.87
3:I:70:LEU:HD22	3:I:343:ILE:HD11	1.56	0.87
2:H:181:ARG:HD2	2:H:448:GLN:OE1	1.74	0.87
1:G:232:ILE:HG12	1:G:247:LEU:HD23	1.56	0.87
1:D:17:LEU:HD12	2:E:154:SER:HA	1.54	0.87
2:H:291:ILE:HD12	2:H:291:ILE:H	1.40	0.87
2:E:524:ASP:O	2:E:527:LEU:HB2	1.75	0.86
2:B:524:ASP:O	2:B:527:LEU:HB2	1.75	0.86
3:I:341:HIS:CE1	3:I:343:ILE:HG23	2.10	0.86
1:A:13:HIS:CE1	2:B:144:PHE:CE1	2.63	0.86
3:F:341:HIS:CE1	3:F:343:ILE:HG23	2.10	0.86
2:H:524:ASP:O	2:H:527:LEU:HB2	1.75	0.86
1:D:232:ILE:HG12	1:D:247:LEU:HD23	1.56	0.86
2:B:181:ARG:HD2	2:B:448:GLN:OE1	1.75	0.85
1:A:64:PRO:HB3	2:B:547:TYR:HB2	1.57	0.85
3:F:437:ASN:O	3:F:440:ASP:HB2	1.77	0.85
3:I:280:SER:HB2	3:I:284:SER:HB3	1.56	0.85
3:C:341:HIS:CE1	3:C:343:ILE:HG23	2.10	0.85
1:A:20:TYR:HE2	2:B:544:LYS:HD3	1.35	0.85
1:A:261:SER:CB	2:B:152:LYS:HA	2.07	0.85
2:E:291:ILE:H	2:E:291:ILE:HD12	1.41	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:HD12	2:B:291:ILE:H	1.41	0.84
1:A:232:ILE:HG12	1:A:247:LEU:HD23	1.56	0.84
2:B:320:VAL:HA	3:C:246:THR:HG21	1.60	0.84
1:D:57:TRP:HE1	2:E:142:ARG:NH2	1.75	0.83
3:C:20:LYS:O	3:C:24:ILE:HG12	1.79	0.83
2:E:434:LEU:O	2:E:438:VAL:HG23	1.78	0.83
2:H:210:ILE:HD12	2:H:210:ILE:H	1.43	0.83
2:B:434:LEU:O	2:B:438:VAL:HG23	1.78	0.83
3:I:416:TYR:HE2	3:I:432:TYR:CE2	1.97	0.83
3:I:8:GLN:C	3:I:10:GLU:H	1.82	0.82
1:G:64:PRO:HB2	2:H:543:LEU:CD1	2.09	0.82
2:B:210:ILE:H	2:B:210:ILE:HD12	1.43	0.82
1:D:25:ALA:O	1:D:59:VAL:HG21	1.79	0.82
3:C:83:VAL:O	3:C:87:ALA:HB3	1.80	0.82
1:G:25:ALA:O	1:G:59:VAL:HG21	1.79	0.82
3:I:13:THR:HG22	3:I:17:ASP:OD2	1.81	0.81
2:H:434:LEU:O	2:H:438:VAL:HG23	1.78	0.81
2:H:175:LEU:HD12	2:H:176:PRO:HD2	1.63	0.81
1:G:212:TRP:HA	1:G:222:LEU:HD23	1.62	0.81
2:E:512:MET:HG2	2:E:540:ALA:HB2	1.62	0.81
1:A:78:LYS:HA	1:A:96:ALA:HB2	1.62	0.81
1:D:78:LYS:HA	1:D:96:ALA:HB2	1.62	0.81
3:C:13:THR:O	3:C:17:ASP:HB2	1.78	0.81
2:E:340:LEU:CD2	2:E:370:PHE:CD1	2.64	0.81
2:B:190:LEU:O	2:B:194:ILE:HG13	1.81	0.81
2:B:175:LEU:HD12	2:B:176:PRO:HD2	1.63	0.81
3:I:89:LEU:HD13	3:I:114:LYS:CE	2.11	0.80
1:G:217:LEU:HD22	1:G:218:LEU:H	1.46	0.80
1:A:25:ALA:O	1:A:59:VAL:HG21	1.79	0.80
1:D:217:LEU:HD22	1:D:218:LEU:H	1.47	0.80
3:I:8:GLN:HE22	3:I:53:LEU:CG	1.93	0.80
1:G:19:TYR:HD2	1:G:20:TYR:CE1	1.99	0.80
3:I:237:ILE:HD12	3:I:237:ILE:C	2.02	0.80
1:A:12:ILE:HD12	2:B:169:GLY:HA3	1.62	0.80
2:H:512:MET:HG2	2:H:540:ALA:HB2	1.61	0.80
2:H:340:LEU:CD2	2:H:370:PHE:CD1	2.64	0.80
1:A:19:TYR:HD2	1:A:20:TYR:CE1	1.98	0.80
2:H:136:LYS:HA	2:H:139:MET:CB	2.11	0.80
2:B:442:THR:HG22	2:B:444:ALA:H	1.46	0.80
2:H:155:THR:O	2:H:513:ARG:HD2	1.80	0.80
2:H:442:THR:HG22	2:H:444:ALA:H	1.46	0.80

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:59:GLU:HA	3:I:62:VAL:HG23	1.62	0.80
1:G:78:LYS:HA	1:G:96:ALA:HB2	1.62	0.80
1:D:19:TYR:HD2	1:D:20:TYR:CE1	1.99	0.80
2:E:175:LEU:HD12	2:E:176:PRO:HD2	1.63	0.79
3:F:237:ILE:C	3:F:237:ILE:HD12	2.03	0.79
2:E:210:ILE:H	2:E:210:ILE:HD12	1.43	0.79
2:B:512:MET:HG2	2:B:540:ALA:HB2	1.61	0.79
3:F:94:MET:HE2	3:F:108:LYS:HB2	1.64	0.79
2:H:190:LEU:O	2:H:194:ILE:HG13	1.81	0.79
2:B:210:ILE:CD1	2:B:495:CYS:HB2	2.12	0.79
3:I:89:LEU:HD13	3:I:114:LYS:NZ	1.96	0.79
2:H:210:ILE:CD1	2:H:495:CYS:HB2	2.12	0.79
3:C:237:ILE:HD12	3:C:237:ILE:C	2.03	0.79
1:G:65:LYS:HA	2:H:546:ARG:NH2	1.97	0.79
2:E:210:ILE:CD1	2:E:495:CYS:HB2	2.12	0.79
2:E:442:THR:HG22	2:E:444:ALA:H	1.46	0.79
1:D:212:TRP:HA	1:D:222:LEU:HD23	1.62	0.79
2:H:265:HIS:HB2	2:H:399:LEU:HD21	1.64	0.79
3:I:416:TYR:CE2	3:I:432:TYR:CE2	2.71	0.78
1:G:278:VAL:HG21	2:H:151:ALA:HB3	1.64	0.78
3:I:419:LEU:HD23	3:I:422:LEU:HD12	1.65	0.78
3:F:416:TYR:CE2	3:F:432:TYR:CE2	2.71	0.78
2:E:190:LEU:O	2:E:194:ILE:HG13	1.81	0.78
2:E:265:HIS:HB2	2:E:399:LEU:HD21	1.65	0.78
2:E:320:VAL:HG22	3:F:246:THR:HG22	1.65	0.78
3:C:20:LYS:HG2	3:C:431:ILE:CG1	2.14	0.78
1:A:217:LEU:HD22	1:A:218:LEU:H	1.47	0.78
1:A:29:SER:HA	1:A:55:PRO:HB3	1.66	0.78
3:F:108:LYS:HE3	3:F:112:ASP:OD2	1.83	0.78
2:H:320:VAL:HG22	3:I:246:THR:HG22	1.64	0.77
3:C:108:LYS:HE3	3:C:112:ASP:OD2	1.84	0.77
1:G:29:SER:HA	1:G:55:PRO:HB3	1.66	0.77
1:D:29:SER:HA	1:D:55:PRO:HB3	1.66	0.77
2:B:265:HIS:HB2	2:B:399:LEU:HD21	1.64	0.77
2:H:524:ASP:HA	2:H:527:LEU:CD1	2.15	0.77
3:C:74:PHE:O	3:C:78:VAL:HG23	1.85	0.77
1:A:63:HIS:HD2	1:A:65:LYS:HB2	1.50	0.77
2:B:522:THR:HA	2:B:525:HIS:HB2	1.66	0.77
1:G:131:LYS:CE	1:G:137:SER:HB2	2.15	0.77
2:B:524:ASP:HA	2:B:527:LEU:CD1	2.15	0.77
1:A:212:TRP:HA	1:A:222:LEU:HD23	1.62	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:108:LYS:HE3	3:I:112:ASP:OD2	1.83	0.76
3:F:74:PHE:O	3:F:78:VAL:HG23	1.84	0.76
2:E:524:ASP:HA	2:E:527:LEU:CD1	2.15	0.76
1:A:131:LYS:CE	1:A:137:SER:HB2	2.15	0.76
2:H:522:THR:HA	2:H:525:HIS:HB2	1.66	0.76
3:F:416:TYR:HE2	3:F:432:TYR:CE2	2.02	0.76
2:E:522:THR:HA	2:E:525:HIS:HB2	1.66	0.76
3:I:74:PHE:O	3:I:78:VAL:HG23	1.85	0.76
1:A:225:VAL:HG13	1:A:257:LEU:HB2	1.67	0.75
3:C:116:LEU:HD21	3:C:294:LEU:HD11	1.69	0.75
1:A:208:ARG:NH2	2:B:143:ARG:HB2	2.01	0.75
1:D:131:LYS:CE	1:D:137:SER:HB2	2.15	0.75
3:C:18:THR:HG23	3:C:41:GLU:OE1	1.86	0.75
3:I:269:GLY:HA3	3:I:295:GLN:HG2	1.68	0.75
1:G:259:ARG:HD2	2:H:152:LYS:HE3	1.69	0.74
3:C:269:GLY:HA3	3:C:295:GLN:HG2	1.68	0.74
1:D:275:ASP:O	1:D:276:ASN:HB2	1.86	0.74
2:B:165:VAL:O	2:B:165:VAL:HG12	1.84	0.74
3:F:269:GLY:HA3	3:F:295:GLN:HG2	1.69	0.74
2:H:523:ASN:O	2:H:527:LEU:HG	1.87	0.74
2:B:155:THR:HG22	2:B:513:ARG:HD2	1.69	0.74
3:I:116:LEU:HD21	3:I:294:LEU:HD11	1.69	0.74
2:E:340:LEU:HD22	2:E:370:PHE:CD1	2.23	0.74
1:G:10:GLU:O	1:G:11:LEU:HG	1.88	0.74
1:D:225:VAL:HG13	1:D:257:LEU:HB2	1.67	0.74
1:G:285:LEU:HD12	1:G:285:LEU:H	1.53	0.74
2:E:369:LEU:CG	2:E:369:LEU:O	2.23	0.74
2:H:207:TYR:CE1	2:H:504:GLU:HG3	2.23	0.74
3:C:11:ARG:CG	3:C:12:PHE:N	2.50	0.74
2:E:207:TYR:CE1	2:E:504:GLU:HG3	2.23	0.74
1:D:24:LEU:CD2	2:E:170:VAL:HG21	2.18	0.74
2:E:523:ASN:O	2:E:527:LEU:HG	1.88	0.74
1:D:10:GLU:O	1:D:11:LEU:HG	1.88	0.74
1:A:285:LEU:H	1:A:285:LEU:HD12	1.53	0.74
1:G:225:VAL:HG13	1:G:257:LEU:HB2	1.67	0.73
1:G:275:ASP:O	1:G:276:ASN:HB2	1.86	0.73
1:A:275:ASP:O	1:A:276:ASN:HB2	1.86	0.73
1:D:285:LEU:HD12	1:D:285:LEU:H	1.53	0.73
1:G:265:SER:HB2	2:H:509:ARG:HH22	1.52	0.73
3:I:293:ILE:HD11	3:I:327:VAL:HG21	1.70	0.73
1:D:57:TRP:NE1	2:E:142:ARG:NH2	2.35	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:MET:HA	2:B:540:ALA:HB1	1.69	0.73
3:C:384:TYR:HA	3:C:387:ARG:NH1	2.04	0.73
2:H:512:MET:HA	2:H:540:ALA:HB1	1.69	0.73
2:H:530:LEU:O	2:H:531:LYS:HG2	1.89	0.73
2:B:207:TYR:CE1	2:B:504:GLU:HG3	2.23	0.73
1:A:180:ASN:HA	1:A:207:VAL:HG23	1.71	0.73
1:G:17:LEU:HD12	2:H:154:SER:HA	1.70	0.73
3:F:116:LEU:HD21	3:F:294:LEU:HD11	1.68	0.73
2:H:340:LEU:HD23	2:H:370:PHE:CD1	2.24	0.73
2:B:523:ASN:O	2:B:527:LEU:HG	1.88	0.73
1:G:180:ASN:HA	1:G:207:VAL:HG23	1.71	0.73
2:B:442:THR:HG22	2:B:443:ASN:N	2.04	0.73
3:F:293:ILE:HD11	3:F:327:VAL:HG21	1.70	0.73
2:B:530:LEU:O	2:B:531:LYS:HG2	1.89	0.72
2:E:512:MET:HA	2:E:540:ALA:HB1	1.69	0.72
2:H:167:LYS:O	2:H:167:LYS:HD3	1.89	0.72
3:C:11:ARG:HG2	3:C:12:PHE:H	1.54	0.72
2:E:320:VAL:CA	3:F:246:THR:HG21	2.19	0.72
3:C:8:GLN:C	3:C:10:GLU:H	1.92	0.72
2:B:167:LYS:O	2:B:167:LYS:HD3	1.89	0.72
2:E:507:ILE:O	2:E:511:VAL:HG23	1.90	0.72
2:H:136:LYS:CA	2:H:139:MET:HB3	2.18	0.72
2:H:162:LYS:CE	2:H:164:ILE:HD11	2.20	0.72
3:C:139:VAL:HG13	3:C:140:PRO:HD2	1.72	0.72
2:E:530:LEU:O	2:E:531:LYS:HG2	1.90	0.72
1:A:103:ASN:OD1	2:B:142:ARG:NH2	2.22	0.72
2:E:162:LYS:CE	2:E:164:ILE:HD11	2.20	0.72
2:E:167:LYS:O	2:E:167:LYS:HD3	1.89	0.72
1:G:138:PRO:HB2	1:G:140:ILE:HD11	1.72	0.72
1:A:261:SER:HB3	2:B:152:LYS:HA	1.72	0.72
3:C:20:LYS:HG2	3:C:431:ILE:HG12	1.70	0.72
3:C:293:ILE:HD11	3:C:327:VAL:HG21	1.71	0.72
2:E:442:THR:HG22	2:E:443:ASN:N	2.04	0.72
3:F:406:GLU:HA	3:F:409:LYS:HE3	1.72	0.72
2:B:187:ASP:HB3	2:B:523:ASN:ND2	2.05	0.71
3:I:384:TYR:HA	3:I:387:ARG:NH1	2.04	0.71
3:C:8:GLN:O	3:C:10:GLU:N	2.23	0.71
1:D:180:ASN:HA	1:D:207:VAL:HG23	1.71	0.71
3:I:89:LEU:HD13	3:I:114:LYS:HE2	1.71	0.71
2:E:494:SER:O	2:E:497:LEU:HD13	1.90	0.71
3:I:406:GLU:HA	3:I:409:LYS:HE3	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:7:TYR:O	3:F:9:THR:N	2.23	0.71
2:B:204:SER:O	2:B:205:ASN:HB3	1.91	0.71
2:E:187:ASP:HB3	2:E:523:ASN:ND2	2.05	0.71
3:C:20:LYS:NZ	3:C:428:ASN:OD1	2.23	0.71
2:B:507:ILE:O	2:B:511:VAL:HG23	1.90	0.71
3:C:8:GLN:HE22	3:C:53:LEU:HG	1.54	0.71
3:I:385:LEU:O	3:I:389:VAL:HG23	1.91	0.71
3:F:384:TYR:HA	3:F:387:ARG:NH1	2.04	0.71
2:E:160:LEU:HD23	2:E:171:SER:O	1.91	0.71
2:H:507:ILE:O	2:H:511:VAL:HG23	1.90	0.71
2:H:442:THR:HG22	2:H:443:ASN:N	2.04	0.71
3:I:139:VAL:HG13	3:I:140:PRO:HD2	1.72	0.71
3:F:139:VAL:HG13	3:F:140:PRO:HD2	1.72	0.71
2:H:187:ASP:HB3	2:H:523:ASN:ND2	2.05	0.71
3:F:350:VAL:HG22	3:F:355:LEU:HD22	1.73	0.71
1:G:57:TRP:HE1	2:H:142:ARG:HH21	1.37	0.71
1:A:259:ARG:HH12	2:B:150:PHE:HB2	1.55	0.71
3:I:11:ARG:HG3	3:I:12:PHE:CD1	2.26	0.71
3:C:93:GLU:HG3	3:C:94:MET:N	2.06	0.71
2:B:158:MET:HB2	2:B:173:LYS:O	1.91	0.71
2:E:159:LEU:HD13	2:E:160:LEU:H	1.56	0.71
1:D:138:PRO:HB2	1:D:140:ILE:HD11	1.72	0.70
1:G:126:SER:CB	1:G:140:ILE:HG13	2.20	0.70
2:H:204:SER:O	2:H:205:ASN:HB3	1.91	0.70
3:C:350:VAL:HG22	3:C:355:LEU:HD22	1.73	0.70
1:D:17:LEU:HD21	2:E:160:LEU:HD11	1.72	0.70
2:H:494:SER:O	2:H:497:LEU:HD13	1.91	0.70
3:I:409:LYS:O	3:I:413:ILE:HG13	1.91	0.70
2:B:494:SER:O	2:B:497:LEU:HD13	1.90	0.70
1:A:83:LYS:HD3	1:A:92:ILE:HD12	1.73	0.70
2:B:160:LEU:HD23	2:B:171:SER:O	1.91	0.70
1:D:217:LEU:HD13	1:D:218:LEU:N	2.07	0.70
3:I:350:VAL:HG22	3:I:355:LEU:HD22	1.73	0.70
2:E:521:SER:O	2:E:524:ASP:HB2	1.92	0.70
1:A:138:PRO:HB2	1:A:140:ILE:HD11	1.72	0.70
2:H:158:MET:HB2	2:H:173:LYS:O	1.91	0.70
3:I:293:ILE:HD11	3:I:327:VAL:CG2	2.21	0.70
3:F:327:VAL:O	3:F:331:VAL:HG23	1.92	0.70
3:I:23:LYS:HZ3	3:I:431:ILE:HA	1.54	0.70
2:B:521:SER:O	2:B:524:ASP:HB2	1.92	0.70
3:I:70:LEU:HD21	3:I:344:ARG:NH1	2.05	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:ARG:HH11	2:H:267:ARG:HG3	1.56	0.70
3:C:435:PHE:O	3:C:436:LEU:HD23	1.92	0.70
3:C:406:GLU:HA	3:C:409:LYS:HE3	1.72	0.70
3:C:11:ARG:CG	3:C:12:PHE:H	2.04	0.70
2:E:204:SER:O	2:E:205:ASN:HB3	1.91	0.70
3:C:385:LEU:O	3:C:389:VAL:HG23	1.91	0.70
1:G:217:LEU:HD13	1:G:218:LEU:N	2.07	0.70
3:I:434:THR:O	3:I:434:THR:HG22	1.91	0.70
2:E:391:TYR:O	2:E:393:GLN:N	2.25	0.70
2:E:327:SER:OG	3:F:238:LYS:HG3	1.91	0.70
1:A:126:SER:CB	1:A:140:ILE:HG13	2.21	0.70
2:B:159:LEU:HD13	2:B:160:LEU:H	1.56	0.70
3:C:409:LYS:O	3:C:413:ILE:HG13	1.91	0.70
3:I:327:VAL:O	3:I:331:VAL:HG23	1.92	0.70
2:H:533:PRO:O	2:H:537:ILE:HG13	1.92	0.70
2:H:521:SER:O	2:H:524:ASP:HB2	1.92	0.69
2:E:544:LYS:O	2:E:548:GLU:HG3	1.92	0.69
3:F:293:ILE:HD11	3:F:327:VAL:CG2	2.22	0.69
2:E:299:LEU:HD23	2:E:387:LEU:HD21	1.74	0.69
2:E:267:ARG:HG3	2:E:267:ARG:HH11	1.56	0.69
1:A:20:TYR:HD2	2:B:544:LYS:HZ2	1.38	0.69
1:A:217:LEU:HD13	1:A:218:LEU:N	2.07	0.69
3:C:382:LYS:HD3	3:C:384:TYR:OH	1.92	0.69
2:E:158:MET:HB2	2:E:173:LYS:O	1.91	0.69
3:F:409:LYS:O	3:F:413:ILE:HG13	1.91	0.69
2:B:533:PRO:O	2:B:537:ILE:HG13	1.92	0.69
3:F:385:LEU:O	3:F:389:VAL:HG23	1.91	0.69
2:H:544:LYS:O	2:H:548:GLU:HG3	1.92	0.69
2:H:159:LEU:HD13	2:H:160:LEU:H	1.56	0.69
1:A:12:ILE:HD13	2:B:168:SER:O	1.92	0.69
2:H:155:THR:HG22	2:H:513:ARG:CG	2.22	0.69
1:A:262:TRP:O	2:B:153:PHE:HB2	1.92	0.69
3:C:327:VAL:O	3:C:331:VAL:HG23	1.91	0.69
1:G:83:LYS:HD3	1:G:92:ILE:HD12	1.73	0.69
3:C:70:LEU:CD2	3:C:343:ILE:HD11	2.20	0.69
1:A:24:LEU:HD21	2:B:170:VAL:HG21	1.73	0.69
2:H:160:LEU:HD23	2:H:171:SER:O	1.91	0.69
1:D:83:LYS:HD3	1:D:92:ILE:HD12	1.73	0.69
2:E:533:PRO:O	2:E:537:ILE:HG13	1.92	0.69
1:G:77:GLY:HA2	1:G:100:ALA:O	1.93	0.69
3:F:363:VAL:HG11	3:F:408:ASP:OD1	1.92	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:21:GLU:HB3	3:I:25:GLU:OE1	1.93	0.69
3:F:434:THR:HG22	3:F:434:THR:O	1.92	0.69
2:B:544:LYS:O	2:B:548:GLU:HG3	1.92	0.69
3:C:434:THR:O	3:C:434:THR:HG22	1.92	0.69
2:B:491:LEU:HD11	2:B:507:ILE:HG23	1.75	0.68
1:A:77:GLY:HA2	1:A:100:ALA:O	1.93	0.68
2:H:287:SER:OG	2:H:293:GLN:HG2	1.93	0.68
2:H:457:LEU:HD13	2:H:463:ARG:HB2	1.76	0.68
2:H:299:LEU:HD23	2:H:387:LEU:HD21	1.74	0.68
3:I:102:ARG:HD3	3:I:302:LEU:HD13	1.76	0.68
3:I:435:PHE:O	3:I:436:LEU:HG	1.92	0.68
2:E:457:LEU:HD13	2:E:463:ARG:HB2	1.75	0.68
2:H:391:TYR:O	2:H:393:GLN:N	2.26	0.68
3:C:227:ILE:C	3:C:229:ASN:H	1.96	0.68
1:G:35:ILE:HB	1:G:47:ASP:HB2	1.75	0.68
2:E:491:LEU:HD11	2:E:507:ILE:HG23	1.75	0.68
2:B:457:LEU:HD13	2:B:463:ARG:HB2	1.76	0.68
3:C:293:ILE:HD11	3:C:327:VAL:CG2	2.22	0.68
2:B:267:ARG:HH11	2:B:267:ARG:HG3	1.56	0.68
2:E:329:ASP:OD2	3:F:236:GLY:N	2.25	0.68
1:D:77:GLY:HA2	1:D:100:ALA:O	1.93	0.68
1:D:35:ILE:HB	1:D:47:ASP:HB2	1.75	0.68
3:F:319:SER:OG	2:H:337:GLU:HG2	1.94	0.68
1:G:20:TYR:CE2	2:H:544:LYS:HD3	2.29	0.68
2:B:314:LYS:HG2	3:C:162:LEU:O	1.94	0.68
2:B:287:SER:OG	2:B:293:GLN:HG2	1.93	0.68
2:H:418:ILE:H	2:H:418:ILE:HD13	1.59	0.67
2:B:391:TYR:O	2:B:393:GLN:N	2.26	0.67
3:C:8:GLN:NE2	3:C:53:LEU:HG	2.10	0.67
3:I:23:LYS:NZ	3:I:434:THR:OG1	2.25	0.67
3:F:102:ARG:HD3	3:F:302:LEU:HD13	1.76	0.67
2:E:202:ARG:HG3	2:E:500:ASP:OD1	1.95	0.67
3:F:227:ILE:C	3:F:229:ASN:H	1.96	0.67
3:F:438:GLU:HA	3:F:438:GLU:OE1	1.94	0.67
1:A:63:HIS:HD2	1:A:65:LYS:CB	2.08	0.67
2:E:287:SER:OG	2:E:293:GLN:HG2	1.93	0.67
2:B:418:ILE:H	2:B:418:ILE:HD13	1.60	0.67
2:B:299:LEU:HD23	2:B:387:LEU:HD21	1.75	0.67
2:H:340:LEU:HD22	2:H:370:PHE:CD1	2.29	0.67
3:I:227:ILE:C	3:I:229:ASN:H	1.96	0.67
1:G:200:LEU:HD13	1:G:234:TRP:CE3	2.30	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:417:ILE:HG23	3:I:429:ILE:HG23	1.76	0.67
3:C:171:VAL:O	3:C:175:GLU:HG3	1.94	0.67
3:I:89:LEU:HD22	3:I:114:LYS:HZ1	1.59	0.67
2:H:320:VAL:CA	3:I:246:THR:HG21	2.23	0.66
3:F:91:LEU:HG	3:F:92:ASP:H	1.60	0.66
2:B:153:PHE:HA	2:B:159:LEU:HD22	1.77	0.66
1:D:200:LEU:HD13	1:D:234:TRP:CE3	2.30	0.66
2:B:320:VAL:HG22	3:C:246:THR:HG22	1.76	0.66
3:C:83:VAL:O	3:C:87:ALA:CB	2.43	0.66
3:F:171:VAL:O	3:F:175:GLU:HG3	1.95	0.66
2:E:549:GLY:O	2:E:551:TYR:N	2.28	0.66
1:A:35:ILE:HB	1:A:47:ASP:HB2	1.75	0.66
2:B:202:ARG:HG3	2:B:500:ASP:OD1	1.94	0.66
1:G:78:LYS:HA	1:G:96:ALA:CB	2.25	0.66
1:A:200:LEU:HD13	1:A:234:TRP:CE3	2.30	0.66
2:H:491:LEU:HD11	2:H:507:ILE:HG23	1.75	0.66
2:B:476:ALA:O	2:B:480:GLN:HG2	1.95	0.66
1:D:38:VAL:O	1:D:39:GLU:HG3	1.95	0.66
3:C:24:ILE:HG22	3:C:24:ILE:O	1.94	0.66
2:H:442:THR:HG22	2:H:443:ASN:H	1.60	0.66
3:I:77:LEU:HD12	3:I:125:TRP:CH2	2.31	0.66
2:H:476:ALA:O	2:H:480:GLN:HG2	1.95	0.66
2:E:418:ILE:H	2:E:418:ILE:HD13	1.59	0.66
1:G:217:LEU:HD13	1:G:218:LEU:H	1.61	0.66
2:H:202:ARG:HG3	2:H:500:ASP:OD1	1.95	0.66
2:B:416:ASP:O	2:B:420:VAL:HG23	1.95	0.66
1:A:217:LEU:HD13	1:A:218:LEU:H	1.61	0.66
2:B:178:GLU:HB2	2:B:480:GLN:OE1	1.95	0.66
2:B:327:SER:O	2:B:329:ASP:N	2.29	0.66
2:H:416:ASP:O	2:H:420:VAL:HG23	1.95	0.66
2:H:347:GLY:O	2:H:349:SER:N	2.29	0.66
3:F:34:ASP:HB3	3:F:35:PRO:CD	2.26	0.66
2:E:175:LEU:HD12	2:E:176:PRO:CD	2.26	0.66
2:E:327:SER:HA	3:F:238:LYS:HE3	1.76	0.66
2:H:178:GLU:HB2	2:H:480:GLN:OE1	1.95	0.66
2:H:155:THR:CG2	2:H:513:ARG:HG3	2.25	0.66
2:H:159:LEU:CD1	2:H:160:LEU:H	2.09	0.66
2:E:442:THR:HG22	2:E:443:ASN:H	1.61	0.66
1:G:38:VAL:O	1:G:39:GLU:HG3	1.95	0.66
3:I:171:VAL:O	3:I:175:GLU:HG3	1.94	0.66
3:I:382:LYS:N	3:I:383:PRO:CD	2.58	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:136:LYS:HE3	2:H:139:MET:SD	2.36	0.65
2:H:162:LYS:HE2	2:H:164:ILE:HD11	1.78	0.65
1:A:83:LYS:HD3	1:A:92:ILE:CD1	2.26	0.65
1:G:284:ASN:OD1	1:G:286:GLU:HB2	1.96	0.65
3:C:102:ARG:HD3	3:C:302:LEU:HD13	1.77	0.65
2:B:347:GLY:O	2:B:349:SER:N	2.29	0.65
2:E:314:LYS:HG3	3:F:162:LEU:HB3	1.78	0.65
2:E:347:GLY:O	2:E:349:SER:N	2.29	0.65
1:G:229:ARG:HH12	1:G:252:LYS:CD	2.09	0.65
1:D:57:TRP:HE1	2:E:142:ARG:HH21	1.43	0.65
2:B:159:LEU:CD1	2:B:160:LEU:H	2.09	0.65
2:B:512:MET:O	2:B:514:GLU:N	2.29	0.65
3:I:34:ASP:HB3	3:I:35:PRO:CD	2.25	0.65
2:H:153:PHE:HA	2:H:159:LEU:HD22	1.77	0.65
1:D:78:LYS:HA	1:D:96:ALA:CB	2.25	0.65
2:E:178:GLU:HB2	2:E:480:GLN:OE1	1.95	0.65
1:A:284:ASN:OD1	1:A:286:GLU:HB2	1.96	0.65
1:A:78:LYS:HA	1:A:96:ALA:CB	2.25	0.65
2:B:442:THR:HG22	2:B:443:ASN:H	1.61	0.65
2:E:476:ALA:O	2:E:480:GLN:HG2	1.95	0.65
1:G:20:TYR:HE2	2:H:544:LYS:HD3	1.62	0.65
1:A:38:VAL:O	1:A:39:GLU:HG3	1.95	0.65
2:H:512:MET:O	2:H:514:GLU:N	2.29	0.65
1:G:265:SER:HB2	2:H:509:ARG:NH2	2.11	0.65
1:D:284:ASN:OD1	1:D:286:GLU:HB2	1.96	0.65
1:D:49:LEU:HD13	1:D:82:TRP:CE3	2.32	0.65
2:E:159:LEU:CD1	2:E:160:LEU:H	2.09	0.65
2:H:175:LEU:HD12	2:H:176:PRO:CD	2.26	0.65
3:C:11:ARG:HG2	3:C:12:PHE:CD1	2.32	0.65
1:G:49:LEU:HD13	1:G:82:TRP:CE3	2.32	0.65
3:F:8:GLN:C	3:F:10:GLU:H	2.00	0.65
1:D:83:LYS:HD3	1:D:92:ILE:CD1	2.26	0.65
1:D:229:ARG:HH12	1:D:252:LYS:CD	2.09	0.65
1:A:205:ASP:HB3	1:A:227:GLN:HB3	1.79	0.65
2:E:512:MET:O	2:E:514:GLU:N	2.29	0.64
1:G:83:LYS:HD3	1:G:92:ILE:CD1	2.27	0.64
2:H:392:GLY:O	2:H:393:GLN:CB	2.45	0.64
1:A:229:ARG:HH12	1:A:252:LYS:CD	2.10	0.64
3:F:416:TYR:CE2	3:F:432:TYR:HE2	2.15	0.64
1:D:24:LEU:HD21	2:E:170:VAL:HG21	1.77	0.64
2:B:392:GLY:O	2:B:393:GLN:CB	2.46	0.64

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:THR:HG21	2:B:484:ALA:HB2	1.79	0.64
3:I:58:ASP:HB3	3:I:61:ASN:OD1	1.97	0.64
3:C:429:ILE:N	3:C:430:PRO:CD	2.60	0.64
2:E:416:ASP:O	2:E:420:VAL:HG23	1.96	0.64
3:I:429:ILE:N	3:I:430:PRO:CD	2.59	0.64
2:E:327:SER:O	2:E:329:ASP:N	2.29	0.64
1:D:57:TRP:CZ2	2:E:142:ARG:HG2	2.32	0.64
2:E:320:VAL:CG2	3:F:246:THR:HG22	2.26	0.64
2:E:153:PHE:HA	2:E:159:LEU:HD22	1.77	0.64
1:D:217:LEU:HD22	1:D:218:LEU:N	2.12	0.64
3:F:429:ILE:N	3:F:430:PRO:CD	2.60	0.64
3:F:20:LYS:HE2	3:F:431:ILE:HD11	1.79	0.64
2:E:392:GLY:O	2:E:393:GLN:CB	2.46	0.64
1:A:140:ILE:HG22	1:A:141:ILE:N	2.13	0.64
2:B:175:LEU:HD12	2:B:176:PRO:CD	2.26	0.64
2:H:259:LEU:HD11	3:I:99:TYR:CD1	2.33	0.64
1:D:140:ILE:HG22	1:D:141:ILE:N	2.13	0.64
3:F:437:ASN:O	3:F:440:ASP:CB	2.45	0.64
3:C:77:LEU:O	3:C:77:LEU:HD23	1.98	0.64
3:F:431:ILE:H	3:F:431:ILE:CD1	2.11	0.64
1:D:208:ARG:NH2	2:E:143:ARG:HG3	2.12	0.64
1:A:229:ARG:CB	1:A:229:ARG:HH11	2.09	0.64
3:I:431:ILE:N	3:I:431:ILE:HD12	2.13	0.64
2:B:221:LEU:HD22	2:B:231:TYR:CE1	2.32	0.64
1:G:140:ILE:HG22	1:G:141:ILE:N	2.13	0.64
2:H:320:VAL:HA	3:I:246:THR:CG2	2.23	0.64
1:A:49:LEU:HD13	1:A:82:TRP:CE3	2.32	0.64
2:E:162:LYS:HE2	2:E:164:ILE:HD11	1.78	0.64
2:H:252:ASN:OD1	2:H:253:ASP:N	2.31	0.64
3:I:8:GLN:HE22	3:I:53:LEU:CD2	2.11	0.64
1:A:17:LEU:HD21	2:B:160:LEU:HD11	1.79	0.64
3:C:431:ILE:N	3:C:431:ILE:HD12	2.13	0.64
1:A:144:HIS:HB2	1:A:148:VAL:HG22	1.80	0.64
1:D:126:SER:CB	1:D:140:ILE:HG13	2.20	0.63
1:D:286:GLU:HG2	2:E:440:GLN:OE1	1.97	0.63
2:H:327:SER:O	2:H:329:ASP:N	2.29	0.63
2:H:202:ARG:HG2	2:H:209:GLN:HE22	1.63	0.63
2:E:210:ILE:HD11	2:E:495:CYS:HB2	1.79	0.63
2:E:221:LEU:HD22	2:E:231:TYR:CE1	2.33	0.63
1:D:205:ASP:HB3	1:D:227:GLN:HB3	1.79	0.63
1:D:227:GLN:OE1	1:D:256:VAL:HG11	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:LYS:HG2	3:C:431:ILE:HG13	1.79	0.63
3:I:62:VAL:HG12	3:I:66:LYS:HE3	1.80	0.63
1:G:65:LYS:HA	2:H:546:ARG:HH21	1.64	0.63
3:F:77:LEU:O	3:F:77:LEU:HD23	1.98	0.63
1:G:205:ASP:HB3	1:G:227:GLN:HB3	1.79	0.63
3:I:431:ILE:CD1	3:I:431:ILE:H	2.11	0.63
1:G:105:VAL:O	1:G:105:VAL:HG13	1.99	0.63
2:E:252:ASN:OD1	2:E:253:ASP:N	2.31	0.63
2:E:521:SER:HB2	2:E:523:ASN:OD1	1.99	0.63
3:I:387:ARG:HH11	3:I:387:ARG:HB3	1.63	0.63
2:H:259:LEU:HD23	3:I:223:ILE:HD13	1.80	0.63
3:C:62:VAL:HG12	3:C:66:LYS:HE3	1.80	0.63
3:F:431:ILE:N	3:F:431:ILE:HD12	2.13	0.63
3:C:416:TYR:HE2	3:C:432:TYR:CE2	2.17	0.63
3:C:431:ILE:H	3:C:431:ILE:CD1	2.11	0.63
2:H:210:ILE:HD11	2:H:495:CYS:HB2	1.80	0.63
3:I:416:TYR:CE2	3:I:432:TYR:HE2	2.16	0.63
1:D:217:LEU:HD13	1:D:218:LEU:H	1.60	0.63
1:A:217:LEU:HD22	1:A:218:LEU:N	2.12	0.63
3:C:116:LEU:HD21	3:C:294:LEU:CD1	2.29	0.63
3:I:77:LEU:O	3:I:77:LEU:HD23	1.98	0.63
2:E:202:ARG:HG2	2:E:209:GLN:HE22	1.63	0.63
2:H:521:SER:HB2	2:H:523:ASN:OD1	1.99	0.63
1:G:55:PRO:HB2	1:G:57:TRP:CZ3	2.34	0.63
3:F:387:ARG:HH11	3:F:387:ARG:HB3	1.64	0.63
2:H:221:LEU:HD22	2:H:231:TYR:CE1	2.33	0.63
3:C:20:LYS:HE2	3:C:431:ILE:CD1	2.29	0.63
1:D:105:VAL:HG13	1:D:105:VAL:O	1.99	0.63
3:C:387:ARG:HB3	3:C:387:ARG:HH11	1.63	0.62
1:G:227:GLN:OE1	1:G:256:VAL:HG11	1.99	0.62
1:A:55:PRO:HB2	1:A:57:TRP:CZ3	2.34	0.62
3:F:102:ARG:HD2	3:F:217:GLU:OE2	1.99	0.62
1:G:73:CYS:HB2	1:G:102:VAL:HG12	1.81	0.62
1:A:73:CYS:HB2	1:A:102:VAL:HG12	1.81	0.62
1:D:55:PRO:HB2	1:D:57:TRP:CZ3	2.34	0.62
1:G:282:LYS:HE2	1:G:292:ALA:HB2	1.80	0.62
1:G:144:HIS:HB2	1:G:148:VAL:HG22	1.80	0.62
2:B:252:ASN:OD1	2:B:253:ASP:N	2.31	0.62
2:B:521:SER:HB2	2:B:523:ASN:OD1	1.99	0.62
1:G:64:PRO:CB	2:H:543:LEU:HD11	2.29	0.62
1:G:217:LEU:HD22	1:G:218:LEU:N	2.12	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:VAL:HG21	2:H:151:ALA:CB	2.29	0.62
3:C:70:LEU:HB3	3:C:343:ILE:CD1	2.30	0.62
1:A:259:ARG:NH1	2:B:150:PHE:CB	2.60	0.62
1:D:217:LEU:CD2	1:D:218:LEU:H	2.13	0.62
3:F:62:VAL:HG12	3:F:66:LYS:HE3	1.80	0.62
1:G:229:ARG:HH11	1:G:229:ARG:CB	2.09	0.62
2:B:210:ILE:HD11	2:B:495:CYS:HB2	1.80	0.62
3:F:116:LEU:HD21	3:F:294:LEU:CD1	2.29	0.62
3:I:363:VAL:HG11	3:I:408:ASP:OD1	1.99	0.62
1:A:8:HIS:O	1:A:9:ASN:HB2	1.97	0.62
3:I:10:GLU:O	3:I:13:THR:HB	1.99	0.62
3:F:93:GLU:HG2	3:F:94:MET:H	1.65	0.62
3:I:426:TYR:HA	3:I:429:ILE:HG13	1.81	0.62
2:B:314:LYS:HG3	3:C:162:LEU:HB3	1.80	0.62
3:C:102:ARG:HD2	3:C:217:GLU:OE2	1.99	0.62
3:C:20:LYS:HE2	3:C:431:ILE:HG12	1.82	0.62
1:A:13:HIS:NE2	2:B:144:PHE:CE1	2.68	0.62
1:D:73:CYS:HB2	1:D:102:VAL:HG12	1.81	0.62
1:D:229:ARG:CB	1:D:229:ARG:HH11	2.09	0.62
1:A:227:GLN:OE1	1:A:256:VAL:HG11	1.99	0.62
2:E:142:ARG:C	2:E:143:ARG:HG2	2.19	0.62
3:C:426:TYR:HA	3:C:429:ILE:HG13	1.81	0.62
3:F:8:GLN:O	3:F:10:GLU:N	2.32	0.62
3:F:11:ARG:HB2	3:F:12:PHE:CD1	2.35	0.62
3:F:12:PHE:CD1	3:F:12:PHE:N	2.63	0.62
1:A:217:LEU:CD2	1:A:218:LEU:H	2.13	0.62
3:I:102:ARG:HD2	3:I:217:GLU:OE2	1.99	0.62
1:A:282:LYS:HE2	1:A:292:ALA:HB2	1.80	0.62
2:B:202:ARG:HG2	2:B:209:GLN:HE22	1.62	0.62
1:A:13:HIS:HE1	2:B:144:PHE:CE2	2.18	0.62
2:B:179:LEU:HD11	2:B:477:PHE:HE1	1.65	0.62
3:I:79:GLU:O	3:I:83:VAL:HG23	2.00	0.62
2:E:354:ILE:HD13	3:F:157:ASP:CG	2.20	0.62
3:F:426:TYR:HA	3:F:429:ILE:HG13	1.81	0.61
1:D:144:HIS:HB2	1:D:148:VAL:HG22	1.80	0.61
2:E:340:LEU:HD23	2:E:370:PHE:CD1	2.35	0.61
3:C:11:ARG:HG3	3:C:12:PHE:N	2.15	0.61
2:H:179:LEU:HD21	2:H:184:LEU:HD13	1.82	0.61
2:H:179:LEU:HD11	2:H:477:PHE:HE1	1.65	0.61
3:F:438:GLU:C	3:F:440:ASP:H	2.00	0.61
3:I:116:LEU:HD21	3:I:294:LEU:CD1	2.30	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:O	1:A:105:VAL:HG13	1.98	0.61
3:C:34:ASP:HB3	3:C:35:PRO:CD	2.25	0.61
2:B:267:ARG:NH1	2:B:267:ARG:HG3	2.15	0.61
2:H:325:LEU:CD2	2:H:361:LEU:HD23	2.30	0.61
3:C:20:LYS:HZ3	3:C:428:ASN:CG	2.02	0.61
3:I:417:ILE:HG23	3:I:429:ILE:CG2	2.30	0.61
3:F:21:GLU:O	3:F:25:GLU:HG3	2.01	0.61
2:H:547:TYR:CE2	2:H:548:GLU:HG2	2.36	0.61
2:E:325:LEU:CD2	2:E:361:LEU:HD23	2.29	0.61
3:F:16:SER:HA	3:F:19:LEU:HD12	1.83	0.61
1:G:227:GLN:HA	1:G:256:VAL:CG1	2.28	0.61
3:C:79:GLU:O	3:C:83:VAL:HG23	2.00	0.61
2:B:226:LYS:HA	2:B:231:TYR:CD2	2.36	0.61
3:C:310:THR:HG23	3:C:311:ASP:N	2.15	0.61
2:H:226:LYS:HA	2:H:231:TYR:CD2	2.36	0.60
3:I:387:ARG:NH1	3:I:387:ARG:HB3	2.17	0.60
1:G:19:TYR:O	2:H:155:THR:HG21	2.01	0.60
2:E:226:LYS:HA	2:E:231:TYR:CD2	2.36	0.60
3:C:431:ILE:H	3:C:431:ILE:HD12	1.66	0.60
1:G:264:LEU:HD22	2:H:509:ARG:HD2	1.83	0.60
2:H:210:ILE:HD12	2:H:495:CYS:HB2	1.84	0.60
1:D:282:LYS:HE2	1:D:292:ALA:HB2	1.80	0.60
3:C:387:ARG:HB3	3:C:387:ARG:NH1	2.17	0.60
3:I:431:ILE:HD12	3:I:431:ILE:H	1.66	0.60
1:G:282:LYS:CE	1:G:292:ALA:HB2	2.32	0.60
2:E:280:ILE:HG21	2:E:300:LEU:HG	1.83	0.60
3:C:341:HIS:O	3:C:345:VAL:HG23	2.02	0.60
3:F:431:ILE:H	3:F:431:ILE:HD12	1.66	0.60
3:I:341:HIS:O	3:I:345:VAL:HG23	2.02	0.60
2:E:179:LEU:HD11	2:E:477:PHE:HE1	1.65	0.60
3:F:77:LEU:HD12	3:F:125:TRP:CH2	2.37	0.60
1:A:79:VAL:HG22	1:A:102:VAL:HG11	1.82	0.60
1:D:285:LEU:HD12	1:D:285:LEU:N	2.17	0.60
2:H:267:ARG:HG3	2:H:267:ARG:NH1	2.15	0.60
2:E:142:ARG:HH11	2:E:142:ARG:HG3	1.67	0.60
3:I:89:LEU:HD22	3:I:114:LYS:NZ	2.17	0.60
3:I:34:ASP:CB	3:I:35:PRO:HD3	2.29	0.60
1:D:140:ILE:H	1:D:140:ILE:HD12	1.67	0.60
3:F:341:HIS:O	3:F:345:VAL:HG23	2.02	0.60
1:G:217:LEU:CD2	1:G:218:LEU:H	2.13	0.60
3:F:79:GLU:O	3:F:83:VAL:HG23	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ILE:O	1:A:146:ILE:HG22	2.02	0.60
2:B:314:LYS:HE3	3:C:162:LEU:HB3	1.84	0.60
1:G:79:VAL:HG22	1:G:102:VAL:HG11	1.82	0.60
1:D:282:LYS:CE	1:D:292:ALA:HB2	2.32	0.60
2:E:402:LEU:O	2:E:405:SER:HB3	2.02	0.60
1:A:140:ILE:H	1:A:140:ILE:HD12	1.67	0.59
3:C:34:ASP:CB	3:C:35:PRO:HD3	2.29	0.59
3:I:70:LEU:HB3	3:I:343:ILE:CD1	2.32	0.59
1:D:259:ARG:HD2	2:E:152:LYS:HE3	1.84	0.59
2:B:179:LEU:HD21	2:B:184:LEU:HD13	1.83	0.59
1:A:264:LEU:HD12	2:B:155:THR:O	2.01	0.59
1:A:285:LEU:N	1:A:285:LEU:HD12	2.17	0.59
2:B:280:ILE:HG21	2:B:300:LEU:HG	1.84	0.59
2:H:402:LEU:O	2:H:405:SER:HB3	2.02	0.59
2:E:466:SER:HB2	2:E:469:THR:H	1.67	0.59
3:C:364:GLU:C	3:C:366:LEU:H	2.05	0.59
1:G:146:ILE:O	1:G:146:ILE:HG22	2.02	0.59
1:A:227:GLN:HA	1:A:256:VAL:CG1	2.28	0.59
3:I:15:PHE:CD1	3:I:387:ARG:HD3	2.36	0.59
3:F:387:ARG:HB3	3:F:387:ARG:NH1	2.17	0.59
1:D:79:VAL:HG22	1:D:102:VAL:HG11	1.83	0.59
1:A:282:LYS:CE	1:A:292:ALA:HB2	2.32	0.59
1:A:259:ARG:HH11	2:B:150:PHE:HB2	1.61	0.59
3:I:11:ARG:HG3	3:I:12:PHE:CE1	2.37	0.59
2:E:179:LEU:HD21	2:E:184:LEU:HD13	1.83	0.59
3:C:349:SER:OG	3:C:358:VAL:HG21	2.02	0.59
1:D:57:TRP:HE1	2:E:142:ARG:CZ	2.14	0.59
3:F:438:GLU:C	3:F:440:ASP:N	2.54	0.59
3:C:417:ILE:HG23	3:C:429:ILE:HD13	1.84	0.59
3:I:349:SER:OG	3:I:358:VAL:HG21	2.02	0.59
1:D:227:GLN:NE2	2:E:143:ARG:HH12	2.01	0.59
3:C:319:SER:OG	2:E:337:GLU:HG2	2.03	0.59
2:B:466:SER:HB2	2:B:469:THR:H	1.67	0.59
1:D:212:TRP:CG	1:D:222:LEU:HD21	2.37	0.59
2:E:210:ILE:HD12	2:E:495:CYS:HB2	1.84	0.59
2:B:402:LEU:O	2:B:405:SER:HB3	2.02	0.59
1:D:146:ILE:O	1:D:146:ILE:HG22	2.02	0.59
2:H:138:ILE:HA	2:H:141:GLU:HG2	1.84	0.59
1:D:15:ALA:HB2	1:D:26:THR:HG22	1.84	0.59
2:H:466:SER:HB2	2:H:469:THR:H	1.67	0.59
1:A:212:TRP:CG	1:A:222:LEU:HD21	2.38	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LEU:HD11	1:A:243:TRP:CD1	2.38	0.59
3:C:11:ARG:O	3:C:13:THR:N	2.36	0.59
1:A:63:HIS:CD2	1:A:65:LYS:HB2	2.36	0.59
1:D:200:LEU:HD11	1:D:243:TRP:CD1	2.38	0.58
3:F:349:SER:OG	3:F:358:VAL:HG21	2.02	0.58
1:D:17:LEU:HD12	2:E:154:SER:CA	2.32	0.58
1:A:272:SER:OG	2:B:151:ALA:HB3	2.03	0.58
2:H:304:VAL:HG13	3:I:314:ILE:HD11	1.83	0.58
3:I:406:GLU:HG2	3:I:409:LYS:NZ	2.18	0.58
2:H:177:THR:HG21	2:H:484:ALA:HB2	1.85	0.58
3:F:366:LEU:HB2	3:F:379:ILE:HG21	1.85	0.58
2:E:515:ILE:HD13	2:E:540:ALA:C	2.23	0.58
3:C:11:ARG:C	3:C:13:THR:N	2.55	0.58
1:G:15:ALA:HB2	1:G:26:THR:HG22	1.84	0.58
2:H:280:ILE:HG21	2:H:300:LEU:HG	1.84	0.58
1:G:200:LEU:HD11	1:G:243:TRP:CD1	2.38	0.58
3:C:406:GLU:HG2	3:C:409:LYS:NZ	2.18	0.58
1:G:157:THR:HG21	2:H:501:LYS:NZ	2.19	0.58
2:E:269:THR:O	2:E:273:VAL:HG23	2.04	0.58
1:A:15:ALA:HB2	1:A:26:THR:HG22	1.84	0.58
1:A:20:TYR:HD2	2:B:544:LYS:NZ	2.01	0.58
2:B:515:ILE:HD13	2:B:540:ALA:C	2.23	0.58
3:F:359:ILE:HG21	3:F:404:VAL:HG11	1.85	0.58
2:H:285:ARG:HG3	2:H:285:ARG:HH11	1.68	0.58
1:D:9:ASN:HD22	1:D:9:ASN:H	1.52	0.58
2:B:269:THR:O	2:B:273:VAL:HG23	2.04	0.58
1:A:37:GLU:HG2	1:A:46:ILE:HD12	1.86	0.58
1:G:140:ILE:H	1:G:140:ILE:HD12	1.67	0.58
3:I:8:GLN:CD	3:I:53:LEU:HG	2.22	0.58
2:H:515:ILE:HD13	2:H:540:ALA:C	2.24	0.58
1:A:258:TRP:NE1	2:B:148:TYR:HA	2.18	0.58
1:G:212:TRP:CG	1:G:222:LEU:HD21	2.38	0.58
2:E:425:TYR:O	2:E:463:ARG:NH2	2.37	0.58
2:B:213:SER:HB3	2:B:459:PHE:CG	2.39	0.58
2:B:250:THR:HG21	2:B:255:VAL:HB	1.86	0.58
1:A:12:ILE:CD1	2:B:168:SER:O	2.52	0.57
2:H:340:LEU:CD2	2:H:370:PHE:CG	2.87	0.57
1:G:285:LEU:HD12	1:G:285:LEU:N	2.17	0.57
2:E:285:ARG:HH11	2:E:285:ARG:HG3	1.69	0.57
2:B:285:ARG:HG3	2:B:285:ARG:HH11	1.68	0.57
3:F:34:ASP:CB	3:F:35:PRO:HD3	2.30	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:425:TYR:O	2:H:463:ARG:NH2	2.38	0.57
3:F:91:LEU:CG	3:F:92:ASP:H	2.17	0.57
2:H:250:THR:HG21	2:H:255:VAL:HB	1.86	0.57
1:D:181:LEU:HD22	1:D:199:THR:HG22	1.87	0.57
1:D:43:HIS:CD2	2:E:168:SER:HB3	2.39	0.57
3:F:406:GLU:HG2	3:F:409:LYS:NZ	2.18	0.57
2:E:267:ARG:HG3	2:E:267:ARG:NH1	2.15	0.57
2:H:259:LEU:CD2	3:I:223:ILE:HD13	2.34	0.57
1:D:37:GLU:HG2	1:D:46:ILE:HD12	1.86	0.57
2:H:291:ILE:CD1	2:H:291:ILE:H	2.16	0.57
1:A:181:LEU:HD22	1:A:199:THR:CG2	2.35	0.57
1:A:13:HIS:CE1	2:B:144:PHE:CE2	2.90	0.57
2:B:198:THR:CB	2:B:212:GLU:HB2	2.29	0.57
1:A:153:TRP:HH2	1:A:194:TYR:HH	1.52	0.57
3:I:94:MET:HE3	3:I:96:LEU:HD21	1.85	0.57
2:H:213:SER:HB3	2:H:459:PHE:CG	2.39	0.57
1:D:73:CYS:HB2	1:D:102:VAL:CG1	2.35	0.57
1:A:20:TYR:CE2	2:B:544:LYS:CD	2.84	0.57
2:B:165:VAL:O	2:B:165:VAL:CG1	2.52	0.57
2:B:202:ARG:CG	2:B:209:GLN:NE2	2.60	0.57
3:I:418:SER:O	3:I:422:LEU:HG	2.03	0.57
3:C:22:PHE:C	3:C:24:ILE:H	2.08	0.57
2:B:210:ILE:HD12	2:B:495:CYS:HB2	1.84	0.57
2:B:425:TYR:O	2:B:463:ARG:NH2	2.37	0.57
2:E:133:ASP:O	2:E:137:LEU:HG	2.05	0.57
2:H:202:ARG:CG	2:H:209:GLN:NE2	2.60	0.57
1:D:181:LEU:HD22	1:D:199:THR:CG2	2.35	0.57
2:H:269:THR:O	2:H:273:VAL:HG23	2.04	0.57
1:G:227:GLN:O	1:G:256:VAL:HG22	2.05	0.57
2:B:160:LEU:HA	2:B:171:SER:O	2.05	0.57
1:A:16:VAL:HG21	1:A:59:VAL:O	2.05	0.57
2:E:205:ASN:OD1	2:E:207:TYR:HB2	2.05	0.57
1:A:73:CYS:HB2	1:A:102:VAL:CG1	2.35	0.57
3:F:50:ALA:HB1	3:F:69:GLU:HG2	1.86	0.57
2:E:213:SER:HB3	2:E:459:PHE:CG	2.40	0.57
2:E:198:THR:CB	2:E:212:GLU:HB2	2.29	0.56
3:F:116:LEU:CD2	3:F:294:LEU:HD11	2.35	0.56
1:D:112:TYR:HA	1:D:171:ARG:NH2	2.19	0.56
3:I:160:PHE:CE2	3:I:168:VAL:HG11	2.40	0.56
1:D:227:GLN:O	1:D:256:VAL:HG22	2.05	0.56
3:I:416:TYR:HE2	3:I:432:TYR:HE2	1.47	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD12	1:A:185:TRP:CE3	2.40	0.56
3:F:379:ILE:HG13	3:F:385:LEU:HG	1.87	0.56
1:D:16:VAL:HG21	1:D:59:VAL:O	2.05	0.56
2:H:369:LEU:O	2:H:370:PHE:HB2	2.05	0.56
1:A:96:ALA:C	1:A:98:HIS:H	2.09	0.56
2:H:320:VAL:CG2	3:I:246:THR:HG22	2.35	0.56
2:H:340:LEU:HD22	2:H:370:PHE:CG	2.40	0.56
3:C:116:LEU:CD2	3:C:294:LEU:HD11	2.35	0.56
1:D:10:GLU:O	1:D:11:LEU:CG	2.54	0.56
1:G:181:LEU:HD22	1:G:199:THR:HG22	1.86	0.56
3:F:326:GLU:O	3:F:330:ARG:HG3	2.06	0.56
2:E:358:TYR:HE2	3:F:210:MET:HE1	1.70	0.56
2:H:138:ILE:HA	2:H:141:GLU:CG	2.35	0.56
1:D:227:GLN:HA	1:D:256:VAL:CG1	2.28	0.56
1:A:227:GLN:O	1:A:256:VAL:HG22	2.05	0.56
1:A:261:SER:CB	2:B:152:LYS:HG2	2.32	0.56
1:G:16:VAL:HG21	1:G:59:VAL:O	2.05	0.56
1:G:96:ALA:C	1:G:98:HIS:H	2.09	0.56
2:E:325:LEU:HD23	2:E:361:LEU:HD23	1.88	0.56
1:G:37:GLU:HG2	1:G:46:ILE:HD12	1.86	0.56
3:I:70:LEU:HB3	3:I:343:ILE:HD11	1.87	0.56
1:G:20:TYR:CE2	2:H:544:LYS:HA	2.41	0.56
2:B:512:MET:C	2:B:514:GLU:H	2.09	0.56
2:E:324:TYR:CE2	3:F:237:ILE:HG21	2.39	0.56
1:G:181:LEU:HD22	1:G:199:THR:CG2	2.35	0.56
3:C:387:ARG:HG2	3:C:391:HIS:CE1	2.41	0.56
3:F:387:ARG:HG2	3:F:391:HIS:CE1	2.41	0.56
2:B:291:ILE:CD1	2:B:291:ILE:H	2.16	0.56
2:H:205:ASN:OD1	2:H:207:TYR:HB2	2.05	0.56
2:B:205:ASN:OD1	2:B:207:TYR:HB2	2.05	0.56
1:A:181:LEU:HD22	1:A:199:THR:HG22	1.87	0.56
1:G:237:ASP:OD1	1:G:244:LYS:HE3	2.06	0.56
3:F:160:PHE:CE2	3:F:168:VAL:HG11	2.40	0.56
3:F:441:CYS:O	3:F:442:LEU:HG	2.06	0.56
1:A:12:ILE:CD1	2:B:169:GLY:HA3	2.35	0.56
3:F:23:LYS:O	3:F:26:GLN:HB2	2.06	0.56
2:H:512:MET:C	2:H:514:GLU:H	2.09	0.56
1:A:13:HIS:ND1	2:B:148:TYR:CE2	2.74	0.56
1:G:233:ILE:HD11	1:G:248:LEU:HD13	1.88	0.56
3:I:116:LEU:CD2	3:I:294:LEU:HD11	2.35	0.56
2:E:162:LYS:HE3	2:E:164:ILE:HD11	1.88	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:GLU:O	3:C:330:ARG:HG3	2.06	0.56
3:C:160:PHE:CE2	3:C:168:VAL:HG11	2.40	0.56
3:C:50:ALA:HB1	3:C:69:GLU:HG2	1.87	0.56
2:E:202:ARG:NE	2:E:202:ARG:HA	2.21	0.55
2:H:325:LEU:HD23	2:H:361:LEU:HD23	1.89	0.55
2:E:250:THR:HG21	2:E:255:VAL:HB	1.86	0.55
2:E:202:ARG:CG	2:E:209:GLN:NE2	2.61	0.55
1:D:138:PRO:HB2	1:D:140:ILE:CD1	2.37	0.55
1:G:221:TYR:O	1:G:222:LEU:HD23	2.06	0.55
1:D:221:TYR:O	1:D:222:LEU:HD23	2.06	0.55
3:I:387:ARG:HG2	3:I:391:HIS:CE1	2.41	0.55
1:D:209:ASP:OD1	1:D:259:ARG:HD3	2.06	0.55
1:G:209:ASP:OD1	1:G:259:ARG:HD3	2.06	0.55
2:E:512:MET:C	2:E:514:GLU:H	2.09	0.55
3:I:326:GLU:O	3:I:330:ARG:HG3	2.07	0.55
2:H:160:LEU:HA	2:H:171:SER:O	2.05	0.55
3:C:11:ARG:C	3:C:13:THR:H	2.09	0.55
1:D:19:TYR:O	2:E:155:THR:HG21	2.06	0.55
3:F:94:MET:CE	3:F:108:LYS:HB2	2.35	0.55
1:G:105:VAL:HA	1:G:117:LEU:O	2.07	0.55
1:D:9:ASN:ND2	1:D:9:ASN:N	2.54	0.55
1:G:109:PRO:HD2	1:G:112:TYR:CD1	2.42	0.55
3:I:110:MET:SD	3:I:116:LEU:HD22	2.47	0.55
1:G:73:CYS:HB2	1:G:102:VAL:CG1	2.35	0.55
2:E:160:LEU:HA	2:E:171:SER:O	2.05	0.55
2:H:162:LYS:HE3	2:H:164:ILE:HD11	1.88	0.55
2:B:320:VAL:CA	3:C:246:THR:HG21	2.35	0.55
2:B:207:TYR:HE2	2:B:536:LEU:HD22	1.72	0.55
1:D:96:ALA:C	1:D:98:HIS:H	2.09	0.55
2:B:155:THR:HG22	2:B:513:ARG:CD	2.37	0.55
1:G:10:GLU:O	1:G:11:LEU:CG	2.54	0.55
1:A:117:LEU:HB2	1:A:153:TRP:HE1	1.72	0.55
1:A:127:VAL:HG21	1:A:194:TYR:CE1	2.41	0.55
1:A:109:PRO:HD2	1:A:112:TYR:CD1	2.42	0.55
2:E:369:LEU:O	2:E:370:PHE:HB2	2.07	0.55
1:D:139:ILE:HG22	1:D:139:ILE:O	2.07	0.55
1:D:57:TRP:NE1	2:E:142:ARG:CZ	2.70	0.55
3:F:16:SER:O	3:F:19:LEU:HB2	2.07	0.55
2:E:303:VAL:HG13	2:E:322:ILE:HG22	1.89	0.55
1:A:209:ASP:OD1	1:A:259:ARG:HD3	2.06	0.55
2:B:150:PHE:CE2	2:B:162:LYS:HB2	2.41	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:PRO:HB2	1:G:140:ILE:CD1	2.37	0.55
3:I:8:GLN:C	3:I:10:GLU:N	2.53	0.55
2:E:291:ILE:CD1	2:E:291:ILE:H	2.17	0.55
2:H:207:TYR:HE2	2:H:536:LEU:HD22	1.72	0.55
1:A:112:TYR:HA	1:A:171:ARG:NH2	2.22	0.55
1:A:237:ASP:OD1	1:A:244:LYS:HE3	2.06	0.55
3:I:143:LYS:HE3	3:I:144:TRP:NE1	2.22	0.55
3:F:143:LYS:HE3	3:F:144:TRP:NE1	2.22	0.55
1:A:139:ILE:O	1:A:139:ILE:HG22	2.07	0.55
3:I:7:TYR:HB3	3:I:10:GLU:OE1	2.06	0.55
1:D:105:VAL:HA	1:D:117:LEU:O	2.07	0.55
1:D:109:PRO:HD2	1:D:112:TYR:CD1	2.42	0.55
2:E:339:GLN:HB2	3:F:206:ILE:HG21	1.89	0.55
2:B:202:ARG:NE	2:B:202:ARG:HA	2.21	0.55
1:A:138:PRO:HB2	1:A:140:ILE:CD1	2.37	0.55
1:A:233:ILE:HD11	1:A:248:LEU:HD13	1.88	0.55
1:D:19:TYR:CD2	1:D:20:TYR:CE1	2.88	0.55
3:C:110:MET:SD	3:C:116:LEU:HD22	2.47	0.55
1:D:117:LEU:HB2	1:D:153:TRP:HE1	1.72	0.55
3:F:16:SER:HA	3:F:19:LEU:CD1	2.36	0.55
2:B:303:VAL:HG13	2:B:322:ILE:HG22	1.89	0.55
1:D:237:ASP:OD1	1:D:244:LYS:HE3	2.06	0.55
3:C:184:ILE:O	3:C:188:ILE:HG13	2.07	0.55
2:H:202:ARG:HA	2:H:202:ARG:NE	2.21	0.54
3:F:20:LYS:O	3:F:23:LYS:N	2.40	0.54
1:A:221:TYR:O	1:A:222:LEU:HD23	2.06	0.54
1:G:19:TYR:CD2	1:G:20:TYR:CE1	2.89	0.54
2:H:474:THR:HG21	2:H:497:LEU:HD12	1.89	0.54
2:E:207:TYR:HE2	2:E:536:LEU:HD22	1.72	0.54
3:I:89:LEU:CD1	3:I:114:LYS:HZ3	2.13	0.54
1:G:217:LEU:HG	2:H:475:PHE:CE1	2.42	0.54
1:G:140:ILE:HD12	1:G:140:ILE:N	2.23	0.54
3:I:206:ILE:O	3:I:209:CYS:HB3	2.08	0.54
1:G:117:LEU:HB2	1:G:153:TRP:HE1	1.72	0.54
3:I:184:ILE:O	3:I:188:ILE:HG13	2.08	0.54
3:I:421:LYS:C	3:I:423:GLN:H	2.09	0.54
1:D:233:ILE:HD11	1:D:248:LEU:HD13	1.88	0.54
3:F:110:MET:SD	3:F:116:LEU:HD22	2.47	0.54
3:C:206:ILE:O	3:C:209:CYS:HB3	2.07	0.54
3:C:143:LYS:HE3	3:C:144:TRP:NE1	2.22	0.54
1:G:279:THR:CB	1:G:281:TRP:HE1	2.21	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:416:TYR:CD2	3:F:432:TYR:CE2	2.95	0.54
2:B:221:LEU:HB3	2:B:231:TYR:HE1	1.73	0.54
2:E:342:LYS:HD2	3:F:206:ILE:HD11	1.90	0.54
2:H:303:VAL:HG13	2:H:322:ILE:HG22	1.89	0.54
1:A:140:ILE:N	1:A:140:ILE:HD12	2.23	0.54
1:G:139:ILE:O	1:G:139:ILE:HG22	2.07	0.54
2:B:484:ALA:O	2:B:485:GLN:HB2	2.08	0.54
1:G:153:TRP:HH2	1:G:194:TYR:HH	1.56	0.54
1:A:105:VAL:HA	1:A:117:LEU:O	2.07	0.54
1:G:31:LYS:HG2	1:G:54:GLY:O	2.08	0.54
3:I:70:LEU:HD11	3:I:344:ARG:NH2	2.23	0.54
2:E:509:ARG:HH11	2:E:509:ARG:HG2	1.72	0.54
1:G:109:PRO:HD2	1:G:112:TYR:CE1	2.43	0.54
1:D:279:THR:HB	1:D:281:TRP:HE1	1.73	0.54
1:D:140:ILE:N	1:D:140:ILE:HD12	2.23	0.54
3:F:23:LYS:HA	3:F:26:GLN:OE1	2.07	0.54
1:G:247:LEU:O	1:G:248:LEU:C	2.46	0.54
2:H:509:ARG:HH11	2:H:509:ARG:HG2	1.72	0.54
1:D:9:ASN:HD22	1:D:9:ASN:N	2.05	0.54
3:I:160:PHE:HE2	3:I:168:VAL:HG11	1.73	0.54
1:D:279:THR:CB	1:D:281:TRP:HE1	2.21	0.54
3:C:384:TYR:CD1	3:C:385:LEU:N	2.76	0.54
1:D:138:PRO:C	1:D:139:ILE:HD12	2.29	0.54
2:B:474:THR:HG21	2:B:497:LEU:HD12	1.90	0.54
1:A:279:THR:HB	1:A:281:TRP:HE1	1.73	0.54
1:A:31:LYS:HG2	1:A:54:GLY:O	2.08	0.53
2:E:546:ARG:HB2	2:E:551:TYR:CE1	2.42	0.53
2:H:233:LEU:HD21	2:H:421:ILE:HD11	1.90	0.53
2:B:233:LEU:HD21	2:B:421:ILE:HD11	1.90	0.53
3:C:227:ILE:C	3:C:229:ASN:N	2.61	0.53
3:F:227:ILE:C	3:F:229:ASN:N	2.61	0.53
1:D:95:HIS:CE1	1:D:97:VAL:HG22	2.43	0.53
1:G:138:PRO:C	1:G:139:ILE:HD12	2.29	0.53
2:H:207:TYR:CE2	2:H:536:LEU:HD22	2.44	0.53
2:B:442:THR:CG2	2:B:443:ASN:N	2.72	0.53
1:G:225:VAL:HG21	1:G:271:LEU:HD22	1.91	0.53
1:A:225:VAL:CG2	1:A:271:LEU:HD22	2.38	0.53
3:I:102:ARG:NH2	3:I:241:SER:H	2.06	0.53
1:D:109:PRO:HD2	1:D:112:TYR:CE1	2.43	0.53
2:B:145:THR:HG22	2:B:147:SER:H	1.72	0.53
2:B:449:PHE:CE2	2:B:453:LEU:HD12	2.43	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:HIS:CE1	1:G:97:VAL:HG22	2.43	0.53
1:D:31:LYS:HG2	1:D:54:GLY:O	2.08	0.53
1:A:247:LEU:O	1:A:248:LEU:C	2.46	0.53
2:E:207:TYR:CE2	2:E:536:LEU:HD22	2.43	0.53
2:E:150:PHE:CE2	2:E:162:LYS:HB2	2.44	0.53
3:F:160:PHE:HE2	3:F:168:VAL:HG11	1.74	0.53
3:I:148:ILE:CD1	3:I:153:LEU:HD12	2.39	0.53
3:F:184:ILE:O	3:F:188:ILE:HG13	2.08	0.53
2:E:484:ALA:O	2:E:485:GLN:HB2	2.09	0.53
1:D:262:TRP:CZ3	1:D:269:LEU:HB2	2.44	0.53
1:A:138:PRO:C	1:A:139:ILE:HD12	2.29	0.53
1:A:103:ASN:HD21	2:B:142:ARG:HH22	1.57	0.53
2:H:515:ILE:CD1	2:H:544:LYS:HB2	2.38	0.53
3:I:77:LEU:CD2	3:I:81:LEU:HD12	2.39	0.53
3:C:77:LEU:CD2	3:C:81:LEU:HD12	2.39	0.53
1:G:112:TYR:HA	1:G:171:ARG:NH2	2.23	0.53
1:A:95:HIS:CE1	1:A:97:VAL:HG22	2.43	0.53
2:H:449:PHE:CE2	2:H:453:LEU:HD12	2.43	0.53
3:F:384:TYR:CD1	3:F:385:LEU:N	2.76	0.53
2:E:474:THR:HG21	2:E:497:LEU:HD12	1.90	0.53
1:G:225:VAL:CG2	1:G:271:LEU:HD22	2.38	0.53
3:I:23:LYS:HA	3:I:27:ASN:OD1	2.09	0.53
2:E:221:LEU:HB3	2:E:231:TYR:HE1	1.73	0.53
1:A:181:LEU:HD23	1:A:201:GLU:HG2	1.91	0.53
3:F:70:LEU:HB3	3:F:343:ILE:CD1	2.38	0.53
1:D:225:VAL:CG2	1:D:271:LEU:HD22	2.38	0.53
3:I:227:ILE:C	3:I:229:ASN:N	2.61	0.53
3:F:83:VAL:O	3:F:87:ALA:HB3	2.09	0.53
3:C:160:PHE:HE2	3:C:168:VAL:HG11	1.73	0.53
3:C:148:ILE:CD1	3:C:153:LEU:HD12	2.39	0.53
2:H:538:PHE:C	2:H:538:PHE:CD1	2.82	0.53
3:F:117:TYR:O	3:F:120:TRP:HB3	2.09	0.53
3:C:35:PRO:HB2	3:C:399:ILE:HG12	1.90	0.53
2:B:509:ARG:HH11	2:B:509:ARG:HG2	1.72	0.53
1:A:225:VAL:HG21	1:A:271:LEU:HD22	1.91	0.53
2:H:221:LEU:HB3	2:H:231:TYR:HE1	1.73	0.53
1:A:279:THR:CB	1:A:281:TRP:HE1	2.21	0.53
1:G:262:TRP:CZ3	1:G:269:LEU:HB2	2.44	0.53
2:H:297:TYR:CE2	2:H:305:ARG:HD2	2.44	0.53
1:A:262:TRP:CZ3	1:A:269:LEU:HB2	2.44	0.53
2:E:515:ILE:CD1	2:E:544:LYS:HB2	2.39	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:77:LEU:CD2	3:F:81:LEU:HD12	2.38	0.53
2:H:484:ALA:O	2:H:485:GLN:HB2	2.08	0.53
1:D:181:LEU:HD23	1:D:201:GLU:HG2	1.91	0.53
1:A:265:SER:O	2:B:483:PHE:CE2	2.62	0.53
3:C:365:MET:HB3	3:C:379:ILE:CG2	2.39	0.53
1:D:27:CYS:HB2	1:D:56:VAL:HB	1.91	0.53
1:A:261:SER:HB2	2:B:152:LYS:CG	2.33	0.53
2:H:415:ASP:HA	2:H:442:THR:HG21	1.91	0.53
1:D:225:VAL:HG13	1:D:257:LEU:CB	2.39	0.53
1:D:225:VAL:HG21	1:D:271:LEU:HD22	1.91	0.53
1:A:121:SER:O	1:A:147:GLY:HA2	2.09	0.53
3:C:102:ARG:NH2	3:C:241:SER:H	2.06	0.53
2:B:138:ILE:O	2:B:141:GLU:HG2	2.09	0.53
2:B:538:PHE:CD1	2:B:538:PHE:C	2.82	0.53
3:F:86:ASN:C	3:F:88:ASP:H	2.13	0.53
2:E:538:PHE:CD1	2:E:538:PHE:C	2.82	0.53
3:I:86:ASN:O	3:I:86:ASN:ND2	2.42	0.52
1:D:217:LEU:CD1	1:D:218:LEU:H	2.22	0.52
2:E:415:ASP:HA	2:E:442:THR:HG21	1.91	0.52
2:E:442:THR:CG2	2:E:443:ASN:N	2.72	0.52
3:F:428:ASN:C	3:F:430:PRO:HD2	2.29	0.52
3:F:102:ARG:NH2	3:F:241:SER:H	2.07	0.52
2:E:297:TYR:CE2	2:E:305:ARG:HD2	2.44	0.52
1:A:191:ALA:C	1:A:193:THR:H	2.13	0.52
1:G:29:SER:C	1:G:31:LYS:H	2.13	0.52
2:B:207:TYR:CE2	2:B:536:LEU:HD22	2.43	0.52
2:E:551:TYR:CD2	2:E:552:LEU:HG	2.44	0.52
3:I:160:PHE:HB3	3:I:161:PRO:HD3	1.92	0.52
1:G:181:LEU:HD23	1:G:201:GLU:HG2	1.91	0.52
3:F:206:ILE:O	3:F:209:CYS:HB3	2.07	0.52
1:D:191:ALA:C	1:D:193:THR:H	2.13	0.52
2:E:233:LEU:HD21	2:E:421:ILE:HD11	1.90	0.52
1:A:259:ARG:HB2	1:A:272:SER:HB2	1.92	0.52
1:D:29:SER:C	1:D:31:LYS:H	2.13	0.52
3:C:416:TYR:CE2	3:C:432:TYR:CE2	2.98	0.52
2:H:442:THR:CG2	2:H:443:ASN:N	2.72	0.52
1:D:9:ASN:OD1	1:D:12:ILE:HD11	2.10	0.52
2:H:335:LEU:HD12	3:I:206:ILE:HG23	1.92	0.52
3:I:117:TYR:O	3:I:120:TRP:HB3	2.10	0.52
3:I:243:TRP:O	3:I:247:VAL:HG23	2.09	0.52
3:C:20:LYS:NZ	3:C:428:ASN:CG	2.62	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:431:ILE:N	3:C:431:ILE:CD1	2.72	0.52
2:H:150:PHE:CE2	2:H:162:LYS:HB2	2.44	0.52
3:C:117:TYR:O	3:C:120:TRP:HB3	2.10	0.52
2:E:449:PHE:CE2	2:E:453:LEU:HD12	2.44	0.52
3:C:342:PRO:HG2	3:C:382:LYS:CD	2.39	0.52
2:E:448:GLN:HG3	2:E:477:PHE:CZ	2.45	0.52
1:D:40:GLY:O	2:E:172:ILE:HD13	2.09	0.52
1:A:29:SER:C	1:A:31:LYS:H	2.13	0.52
3:C:143:LYS:HG3	3:C:144:TRP:N	2.25	0.52
1:G:191:ALA:C	1:G:193:THR:H	2.13	0.52
2:E:320:VAL:HA	3:F:246:THR:CG2	2.34	0.52
1:D:259:ARG:HB2	1:D:272:SER:HB2	1.91	0.52
3:C:20:LYS:HE2	3:C:431:ILE:CG1	2.39	0.52
3:C:428:ASN:C	3:C:430:PRO:HD2	2.30	0.52
1:D:247:LEU:O	1:D:248:LEU:C	2.46	0.52
2:B:415:ASP:HA	2:B:442:THR:HG21	1.91	0.52
1:D:121:SER:O	1:D:147:GLY:HA2	2.09	0.52
1:A:109:PRO:HD2	1:A:112:TYR:CE1	2.43	0.52
2:B:551:TYR:CD2	2:B:552:LEU:HG	2.44	0.52
2:B:369:LEU:O	2:B:370:PHE:HB2	2.10	0.52
2:H:527:LEU:HA	2:H:530:LEU:HD13	1.92	0.52
1:D:118:VAL:O	1:D:125:VAL:HA	2.10	0.52
2:E:142:ARG:HB3	2:E:144:PHE:CD1	2.44	0.52
2:B:515:ILE:CD1	2:B:544:LYS:HB2	2.39	0.52
2:E:442:THR:HG22	2:E:444:ALA:N	2.21	0.52
3:F:148:ILE:CD1	3:F:153:LEU:HD12	2.39	0.52
2:B:525:HIS:C	2:B:527:LEU:N	2.62	0.52
2:H:448:GLN:HG3	2:H:477:PHE:CZ	2.45	0.52
2:B:442:THR:HG22	2:B:444:ALA:N	2.21	0.52
3:C:77:LEU:HD12	3:C:125:TRP:CH2	2.45	0.52
1:A:118:VAL:O	1:A:125:VAL:HA	2.10	0.52
3:I:35:PRO:HB2	3:I:399:ILE:HG12	1.92	0.52
2:B:448:GLN:HG3	2:B:477:PHE:CZ	2.45	0.52
2:B:327:SER:C	2:B:329:ASP:H	2.13	0.52
1:D:283:GLU:HB2	1:D:289:TRP:CZ3	2.45	0.52
3:C:243:TRP:O	3:C:247:VAL:HG23	2.10	0.52
2:B:297:TYR:CE2	2:B:305:ARG:HD2	2.44	0.52
3:F:243:TRP:O	3:F:247:VAL:HG23	2.09	0.52
1:G:27:CYS:HB2	1:G:56:VAL:HB	1.91	0.51
1:A:19:TYR:CD2	1:A:20:TYR:CE1	2.88	0.51
2:H:442:THR:HG22	2:H:444:ALA:N	2.21	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:SER:O	1:G:147:GLY:HA2	2.10	0.51
3:I:77:LEU:HB2	3:I:125:TRP:CE2	2.45	0.51
1:G:279:THR:HB	1:G:281:TRP:HE1	1.73	0.51
3:C:70:LEU:HB3	3:C:343:ILE:HD11	1.91	0.51
1:A:24:LEU:HD21	2:B:170:VAL:CG2	2.38	0.51
2:E:320:VAL:HG22	3:F:246:THR:CG2	2.38	0.51
3:C:20:LYS:CG	3:C:431:ILE:HG12	2.39	0.51
3:I:428:ASN:C	3:I:430:PRO:HD2	2.30	0.51
2:B:289:ASN:O	2:B:293:GLN:HG3	2.11	0.51
1:A:283:GLU:HB2	1:A:289:TRP:CZ3	2.46	0.51
1:A:15:ALA:CB	2:B:170:VAL:HG11	2.41	0.51
3:I:384:TYR:CD1	3:I:385:LEU:N	2.78	0.51
1:G:217:LEU:CD1	1:G:218:LEU:H	2.22	0.51
1:G:268:VAL:HG12	1:G:269:LEU:N	2.25	0.51
1:G:62:ALA:HB2	1:G:107:TRP:CE2	2.45	0.51
3:C:363:VAL:HG11	3:C:408:ASP:OD1	2.09	0.51
3:I:166:THR:O	3:I:166:THR:HG22	2.10	0.51
1:G:57:TRP:HE1	2:H:142:ARG:NH2	2.07	0.51
2:H:141:GLU:HG3	2:H:142:ARG:N	2.26	0.51
2:E:152:LYS:O	2:E:159:LEU:HD13	2.11	0.51
2:B:511:VAL:HG21	2:B:536:LEU:HD21	1.93	0.51
1:D:217:LEU:HG	2:E:475:PHE:CE1	2.45	0.51
2:E:225:GLU:C	2:E:227:THR:H	2.14	0.51
2:E:358:TYR:HE2	3:F:210:MET:CE	2.24	0.51
3:C:160:PHE:HB3	3:C:161:PRO:HD3	1.92	0.51
1:A:151:ALA:HB2	1:A:175:THR:HG22	1.91	0.51
2:H:525:HIS:C	2:H:527:LEU:N	2.62	0.51
1:A:103:ASN:HD21	2:B:142:ARG:NH2	2.08	0.51
1:D:229:ARG:HD2	1:D:253:PHE:O	2.11	0.51
1:A:229:ARG:HD2	1:A:253:PHE:O	2.11	0.51
2:B:152:LYS:N	2:B:159:LEU:HD11	2.26	0.51
1:G:225:VAL:HG13	1:G:257:LEU:CB	2.39	0.51
1:G:118:VAL:O	1:G:125:VAL:HA	2.10	0.51
3:F:160:PHE:HB3	3:F:161:PRO:HD3	1.93	0.51
3:F:143:LYS:HG3	3:F:144:TRP:N	2.25	0.51
1:D:268:VAL:HG12	1:D:269:LEU:N	2.25	0.51
3:I:359:ILE:HG21	3:I:404:VAL:CG1	2.40	0.51
3:I:18:THR:HG23	3:I:41:GLU:OE1	2.10	0.51
1:G:54:GLY:HA3	1:G:75:TYR:HB3	1.93	0.51
2:B:202:ARG:NH2	2:B:209:GLN:O	2.44	0.51
1:G:229:ARG:HD2	1:G:253:PHE:O	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:GLY:HA3	1:D:75:TYR:HB3	1.93	0.51
2:H:512:MET:HA	2:H:540:ALA:CB	2.41	0.51
2:E:511:VAL:HG21	2:E:536:LEU:HD21	1.93	0.51
3:I:294:LEU:O	3:I:298:ILE:CD1	2.58	0.51
3:I:235:GLN:HG2	3:I:236:GLY:N	2.25	0.51
1:G:180:ASN:ND2	1:G:205:ASP:N	2.59	0.51
3:F:384:TYR:CA	3:F:387:ARG:HH12	2.15	0.51
2:H:152:LYS:N	2:H:159:LEU:HD11	2.26	0.51
2:H:255:VAL:HG22	3:I:222:VAL:O	2.11	0.51
1:D:63:HIS:C	1:D:65:LYS:H	2.14	0.51
1:G:283:GLU:HB2	1:G:289:TRP:CZ3	2.46	0.51
2:H:198:THR:CB	2:H:212:GLU:HB2	2.29	0.51
2:H:547:TYR:CD2	2:H:548:GLU:HG2	2.46	0.51
2:E:152:LYS:N	2:E:159:LEU:HD11	2.26	0.51
1:G:63:HIS:C	1:G:65:LYS:H	2.14	0.51
1:A:54:GLY:HA3	1:A:75:TYR:HB3	1.93	0.51
3:F:71:GLU:O	3:F:74:PHE:HB3	2.11	0.51
3:I:431:ILE:N	3:I:431:ILE:CD1	2.72	0.51
2:E:314:LYS:NZ	3:F:253:GLN:HB3	2.26	0.51
2:B:225:GLU:C	2:B:227:THR:H	2.14	0.51
3:I:359:ILE:HG21	3:I:404:VAL:HG11	1.92	0.51
3:I:400:ASN:HB2	3:I:403:SER:OG	2.10	0.51
1:G:8:HIS:O	1:G:9:ASN:ND2	2.43	0.51
2:E:525:HIS:C	2:E:527:LEU:N	2.62	0.51
3:F:417:ILE:HG23	3:F:429:ILE:HG23	1.93	0.51
2:E:272:ILE:HG23	2:E:382:LEU:HG	1.93	0.51
3:C:226:GLN:CD	3:C:226:GLN:H	2.14	0.51
1:D:180:ASN:ND2	1:D:205:ASP:N	2.59	0.51
1:A:63:HIS:C	1:A:65:LYS:H	2.15	0.51
2:E:289:ASN:O	2:E:293:GLN:HG3	2.11	0.51
1:A:27:CYS:HB2	1:A:56:VAL:HB	1.91	0.51
2:H:202:ARG:NH2	2:H:209:GLN:O	2.44	0.50
2:B:522:THR:HA	2:B:525:HIS:CB	2.39	0.50
2:B:527:LEU:HA	2:B:530:LEU:HD13	1.92	0.50
2:E:138:ILE:HG22	2:E:138:ILE:O	2.11	0.50
1:G:259:ARG:HB2	1:G:272:SER:HB2	1.92	0.50
3:I:71:GLU:O	3:I:74:PHE:HB3	2.11	0.50
2:H:327:SER:C	2:H:329:ASP:H	2.13	0.50
2:H:453:LEU:C	2:H:453:LEU:HD23	2.32	0.50
1:D:62:ALA:HB2	1:D:107:TRP:CE2	2.45	0.50
2:E:142:ARG:HG2	2:E:144:PHE:HE1	1.77	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASN:ND2	1:A:205:ASP:N	2.59	0.50
2:B:152:LYS:O	2:B:159:LEU:HD13	2.11	0.50
2:E:172:ILE:HD12	2:E:172:ILE:N	2.27	0.50
2:H:289:ASN:O	2:H:293:GLN:HG3	2.11	0.50
1:D:153:TRP:HH2	1:D:194:TYR:HH	1.59	0.50
2:B:272:ILE:HG23	2:B:382:LEU:HG	1.93	0.50
3:F:166:THR:HG22	3:F:166:THR:O	2.10	0.50
3:C:342:PRO:HG2	3:C:382:LYS:HD2	1.92	0.50
3:F:70:LEU:CD2	3:F:343:ILE:HD11	2.30	0.50
1:A:236:GLN:HB2	1:A:243:TRP:CE3	2.46	0.50
3:F:294:LEU:O	3:F:298:ILE:CD1	2.59	0.50
2:E:453:LEU:HD23	2:E:453:LEU:C	2.32	0.50
1:A:62:ALA:HB2	1:A:107:TRP:CE2	2.45	0.50
1:A:268:VAL:HG12	1:A:269:LEU:N	2.25	0.50
3:C:24:ILE:CG2	3:C:24:ILE:O	2.60	0.50
1:A:217:LEU:CD1	1:A:218:LEU:H	2.23	0.50
1:A:225:VAL:HG13	1:A:257:LEU:CB	2.39	0.50
2:E:427:ALA:O	2:E:429:GLU:N	2.45	0.50
2:E:202:ARG:NH2	2:E:209:GLN:O	2.44	0.50
2:E:527:LEU:HA	2:E:530:LEU:HD13	1.92	0.50
2:H:142:ARG:O	2:H:143:ARG:HB2	2.12	0.50
2:H:546:ARG:CG	2:H:546:ARG:O	2.60	0.50
2:B:354:ILE:HD13	3:C:157:ASP:CG	2.32	0.50
1:G:53:GLU:HB2	1:G:76:ASP:CB	2.42	0.50
3:C:25:GLU:O	3:C:25:GLU:HG2	2.12	0.50
2:B:142:ARG:HH11	2:B:142:ARG:HA	1.77	0.50
1:A:263:SER:HB3	2:B:153:PHE:CE1	2.47	0.50
1:D:236:GLN:HB2	1:D:243:TRP:CE3	2.46	0.50
1:G:154:ALA:HB2	1:G:212:TRP:CE3	2.46	0.50
1:A:249:LYS:HE2	1:A:253:PHE:CE2	2.47	0.50
3:I:237:ILE:HD12	3:I:237:ILE:O	2.12	0.50
2:H:442:THR:CG2	2:H:443:ASN:H	2.25	0.50
1:D:271:LEU:C	1:D:278:VAL:HG13	2.32	0.50
3:I:382:LYS:N	3:I:383:PRO:HD2	2.26	0.50
3:I:143:LYS:HG3	3:I:144:TRP:N	2.25	0.50
2:B:453:LEU:C	2:B:453:LEU:HD23	2.32	0.50
2:B:427:ALA:O	2:B:429:GLU:N	2.45	0.50
2:B:435:TYR:CE2	2:B:454:ILE:HD11	2.47	0.50
1:A:140:ILE:HG22	1:A:141:ILE:H	1.77	0.50
1:G:249:LYS:HE2	1:G:253:PHE:CE2	2.47	0.50
2:B:512:MET:HA	2:B:540:ALA:CB	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:VAL:HG13	3:C:314:ILE:HD11	1.94	0.50
1:G:236:GLN:HB2	1:G:243:TRP:CE3	2.47	0.50
2:H:152:LYS:O	2:H:159:LEU:HD13	2.11	0.50
3:F:9:THR:O	3:F:9:THR:HG22	2.11	0.50
2:H:272:ILE:HG23	2:H:382:LEU:HG	1.93	0.50
2:E:165:VAL:O	2:E:165:VAL:HG12	2.11	0.50
3:F:380:ILE:HG22	3:F:380:ILE:O	2.12	0.50
3:C:166:THR:HG22	3:C:166:THR:O	2.10	0.50
3:I:421:LYS:C	3:I:423:GLN:N	2.66	0.50
2:E:320:VAL:N	3:F:246:THR:HG21	2.26	0.50
2:B:172:ILE:HD12	2:B:172:ILE:N	2.27	0.50
3:C:20:LYS:HE2	3:C:431:ILE:HD11	1.94	0.50
2:H:511:VAL:HG21	2:H:536:LEU:HD21	1.93	0.50
2:E:512:MET:HA	2:E:540:ALA:CB	2.41	0.50
3:C:71:GLU:O	3:C:74:PHE:HB3	2.11	0.50
1:D:249:LYS:HE2	1:D:253:PHE:CE2	2.47	0.49
3:F:8:GLN:C	3:F:10:GLU:N	2.65	0.49
2:E:435:TYR:CE2	2:E:454:ILE:HD11	2.47	0.49
2:H:427:ALA:O	2:H:429:GLU:N	2.45	0.49
1:D:53:GLU:HB2	1:D:76:ASP:CB	2.42	0.49
2:H:165:VAL:O	2:H:165:VAL:HG12	2.11	0.49
3:F:431:ILE:N	3:F:431:ILE:CD1	2.72	0.49
2:E:442:THR:CG2	2:E:443:ASN:H	2.25	0.49
3:C:93:GLU:HG3	3:C:94:MET:H	1.76	0.49
2:H:225:GLU:C	2:H:227:THR:H	2.14	0.49
2:E:159:LEU:O	2:E:173:LYS:HB2	2.12	0.49
3:C:294:LEU:O	3:C:298:ILE:CD1	2.59	0.49
3:I:350:VAL:HG22	3:I:355:LEU:CD2	2.41	0.49
2:H:419:GLY:O	2:H:423:GLN:HG3	2.12	0.49
1:A:14:ASP:HB3	1:A:58:ARG:HA	1.95	0.49
1:G:129:GLU:HG2	1:G:130:PHE:N	2.27	0.49
2:B:320:VAL:HA	3:C:246:THR:CG2	2.38	0.49
3:C:237:ILE:O	3:C:237:ILE:HD12	2.12	0.49
2:E:327:SER:C	2:E:329:ASP:H	2.13	0.49
2:E:546:ARG:O	2:E:546:ARG:CG	2.59	0.49
2:B:327:SER:OG	3:C:238:LYS:HG3	2.13	0.49
2:E:530:LEU:O	2:E:531:LYS:CG	2.59	0.49
1:G:140:ILE:HG22	1:G:141:ILE:H	1.77	0.49
1:D:154:ALA:HB2	1:D:212:TRP:CE3	2.48	0.49
3:I:384:TYR:O	3:I:388:ILE:HG13	2.13	0.49
3:I:387:ARG:HG2	3:I:391:HIS:ND1	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:387:ARG:HG2	3:F:391:HIS:ND1	2.27	0.49
2:B:159:LEU:O	2:B:173:LYS:HB2	2.12	0.49
2:B:466:SER:HB3	2:B:468:GLU:HG2	1.94	0.49
2:H:466:SER:HB3	2:H:468:GLU:HG2	1.95	0.49
1:G:271:LEU:C	1:G:278:VAL:HG13	2.32	0.49
1:A:271:LEU:C	1:A:278:VAL:HG13	2.32	0.49
3:F:353:ASP:O	3:F:355:LEU:N	2.43	0.49
3:I:381:ASP:N	3:I:383:PRO:HD2	2.27	0.49
3:I:226:GLN:CD	3:I:226:GLN:H	2.14	0.49
2:B:419:GLY:O	2:B:423:GLN:HG3	2.13	0.49
2:B:546:ARG:CG	2:B:546:ARG:O	2.60	0.49
3:F:237:ILE:HD12	3:F:237:ILE:O	2.12	0.49
3:I:23:LYS:NZ	3:I:431:ILE:HA	2.26	0.49
3:C:282:TRP:HE3	3:C:283:GLU:OE2	1.96	0.49
2:H:435:TYR:CE2	2:H:454:ILE:HD11	2.47	0.49
1:A:53:GLU:HB2	1:A:76:ASP:CB	2.42	0.49
3:F:226:GLN:CD	3:F:226:GLN:H	2.13	0.49
1:A:48:THR:O	1:A:49:LEU:HD23	2.13	0.49
2:B:512:MET:C	2:B:514:GLU:N	2.66	0.49
2:H:304:VAL:CG1	3:I:314:ILE:HD11	2.43	0.49
2:H:172:ILE:HD12	2:H:172:ILE:N	2.27	0.49
2:B:442:THR:CG2	2:B:443:ASN:H	2.25	0.49
3:I:353:ASP:O	3:I:355:LEU:N	2.44	0.49
3:C:77:LEU:HD21	3:C:81:LEU:HD12	1.95	0.49
2:H:522:THR:HA	2:H:525:HIS:CB	2.39	0.49
1:G:31:LYS:HD3	1:G:52:HIS:O	2.13	0.49
3:C:387:ARG:HG2	3:C:391:HIS:ND1	2.28	0.49
3:C:410:SER:HA	3:C:436:LEU:HD11	1.94	0.49
1:D:259:ARG:HH11	1:D:259:ARG:HG3	1.78	0.49
2:B:197:VAL:HG12	2:B:210:ILE:HG23	1.94	0.49
1:D:112:TYR:CZ	1:D:171:ARG:HG2	2.48	0.49
3:I:92:ASP:O	3:I:93:GLU:C	2.51	0.49
2:H:524:ASP:CA	2:H:527:LEU:HD12	2.35	0.49
2:B:530:LEU:O	2:B:531:LYS:CG	2.59	0.49
1:A:259:ARG:HH11	1:A:259:ARG:HG3	1.78	0.49
3:I:12:PHE:HD1	3:I:12:PHE:H	1.49	0.49
1:G:259:ARG:HG3	1:G:259:ARG:HH11	1.78	0.49
2:E:197:VAL:HG12	2:E:210:ILE:HG23	1.94	0.49
1:A:57:TRP:HE3	1:A:57:TRP:HA	1.78	0.49
1:G:11:LEU:HD23	2:H:162:LYS:NZ	2.28	0.49
3:F:50:ALA:HB1	3:F:69:GLU:CG	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:THR:O	1:D:49:LEU:HD23	2.13	0.48
2:H:155:THR:HG22	2:H:513:ARG:CD	2.43	0.48
3:C:433:ALA:O	3:C:435:PHE:N	2.46	0.48
2:H:159:LEU:O	2:H:173:LYS:HB2	2.12	0.48
3:I:237:ILE:HD11	3:I:240:HIS:HA	1.95	0.48
3:C:434:THR:O	3:C:434:THR:CG2	2.61	0.48
2:E:419:GLY:O	2:E:423:GLN:HG3	2.13	0.48
3:C:384:TYR:CA	3:C:387:ARG:HH12	2.15	0.48
1:D:205:ASP:CB	1:D:227:GLN:HB3	2.44	0.48
2:E:508:LYS:HG2	2:E:509:ARG:N	2.28	0.48
2:H:530:LEU:O	2:H:531:LYS:CG	2.59	0.48
2:E:160:LEU:HD23	2:E:172:ILE:HA	1.96	0.48
3:F:148:ILE:HD13	3:F:153:LEU:HD12	1.95	0.48
2:B:145:THR:O	2:B:147:SER:N	2.46	0.48
3:C:365:MET:HB3	3:C:379:ILE:HG22	1.94	0.48
1:D:202:GLY:HA2	1:D:245:LYS:NZ	2.29	0.48
1:G:57:TRP:HA	1:G:57:TRP:HE3	1.78	0.48
1:D:140:ILE:HG22	1:D:141:ILE:H	1.77	0.48
2:H:197:VAL:HG12	2:H:210:ILE:HG23	1.94	0.48
2:E:399:LEU:HB3	2:E:425:TYR:OH	2.14	0.48
3:C:350:VAL:HG22	3:C:355:LEU:CD2	2.41	0.48
3:F:77:LEU:HD21	3:F:81:LEU:HD12	1.95	0.48
3:C:148:ILE:HD13	3:C:153:LEU:HD12	1.95	0.48
3:I:282:TRP:HE3	3:I:283:GLU:OE2	1.97	0.48
1:D:129:GLU:HG2	1:D:130:PHE:N	2.27	0.48
1:A:129:GLU:HG2	1:A:130:PHE:N	2.27	0.48
2:B:172:ILE:H	2:B:172:ILE:HD12	1.79	0.48
1:D:270:ALA:HB2	2:E:153:PHE:CE1	2.49	0.48
2:E:154:SER:HB3	2:E:158:MET:H	1.79	0.48
3:I:433:ALA:O	3:I:435:PHE:N	2.46	0.48
3:C:11:ARG:HG2	3:C:12:PHE:HD1	1.78	0.48
3:F:416:TYR:HE2	3:F:432:TYR:CZ	2.32	0.48
2:E:466:SER:HB3	2:E:468:GLU:HG2	1.94	0.48
2:H:449:PHE:HE2	2:H:453:LEU:HD12	1.78	0.48
2:E:449:PHE:HE2	2:E:453:LEU:HD12	1.79	0.48
3:F:282:TRP:HE3	3:F:283:GLU:OE2	1.96	0.48
2:E:522:THR:HA	2:E:525:HIS:CB	2.39	0.48
2:E:491:LEU:HD12	2:E:507:ILE:HD13	1.95	0.48
1:A:31:LYS:HD3	1:A:52:HIS:O	2.13	0.48
3:C:7:TYR:C	3:C:7:TYR:CD1	2.87	0.48
3:C:355:LEU:N	3:C:356:PRO:HD2	2.29	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:HIS:CE1	1:G:80:LEU:HD12	2.49	0.48
1:G:20:TYR:CE2	2:H:544:LYS:CD	2.97	0.48
2:B:508:LYS:HG2	2:B:509:ARG:N	2.29	0.48
2:B:174:ARG:O	2:B:175:LEU:C	2.52	0.48
3:F:237:ILE:HD11	3:F:240:HIS:HA	1.95	0.48
3:C:237:ILE:HD11	3:C:240:HIS:HA	1.95	0.48
3:F:355:LEU:N	3:F:356:PRO:HD2	2.29	0.48
2:E:327:SER:OG	3:F:238:LYS:CG	2.62	0.48
1:G:117:LEU:HB2	1:G:153:TRP:NE1	2.29	0.48
1:G:157:THR:HG21	2:H:501:LYS:HZ2	1.79	0.48
2:B:135:ALA:O	2:B:138:ILE:N	2.46	0.48
2:H:314:LYS:HE3	3:I:162:LEU:HB3	1.95	0.48
3:I:189:LEU:HA	3:I:189:LEU:HD23	1.71	0.48
1:D:31:LYS:HD3	1:D:52:HIS:O	2.13	0.48
1:G:48:THR:O	1:G:49:LEU:HD23	2.13	0.48
3:C:8:GLN:C	3:C:10:GLU:N	2.60	0.48
3:F:406:GLU:HG2	3:F:409:LYS:HZ1	1.78	0.48
2:E:392:GLY:O	2:E:393:GLN:HB2	2.14	0.48
1:A:280:LEU:HB2	1:A:292:ALA:O	2.14	0.48
3:F:113:ASN:OD1	3:F:113:ASN:C	2.52	0.48
3:I:86:ASN:OD1	3:I:399:ILE:HG22	2.14	0.48
3:F:433:ALA:O	3:F:435:PHE:N	2.45	0.48
3:F:355:LEU:H	3:F:356:PRO:HD2	1.79	0.48
2:H:392:GLY:O	2:H:393:GLN:HB2	2.14	0.48
1:G:171:ARG:O	1:G:172:LYS:HG3	2.14	0.48
1:A:171:ARG:O	1:A:172:LYS:HG3	2.14	0.48
1:A:205:ASP:CB	1:A:227:GLN:HB3	2.43	0.47
2:B:508:LYS:HA	2:B:536:LEU:HD11	1.96	0.47
2:H:172:ILE:H	2:H:172:ILE:HD12	1.79	0.47
2:E:515:ILE:HD12	2:E:544:LYS:HB2	1.95	0.47
1:D:273:GLY:C	1:D:275:ASP:H	2.17	0.47
1:A:273:GLY:C	1:A:275:ASP:H	2.17	0.47
3:I:104:LEU:CD1	3:I:224:ASP:HB3	2.44	0.47
1:G:253:PHE:O	1:G:255:ASP:N	2.48	0.47
1:G:127:VAL:HG21	1:G:194:TYR:CE1	2.49	0.47
3:F:437:ASN:O	3:F:437:ASN:OD1	2.33	0.47
2:H:508:LYS:HG2	2:H:509:ARG:N	2.29	0.47
3:C:355:LEU:H	3:C:356:PRO:HD2	1.79	0.47
1:G:280:LEU:HB2	1:G:292:ALA:O	2.14	0.47
3:I:148:ILE:HD13	3:I:153:LEU:HD12	1.96	0.47
1:A:290:GLU:HG3	1:A:291:PRO:HD2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:ASP:OD1	3:C:172:LYS:N	2.47	0.47
3:F:341:HIS:CE1	3:F:343:ILE:HD12	2.50	0.47
1:D:253:PHE:O	1:D:255:ASP:N	2.48	0.47
1:D:57:TRP:HA	1:D:57:TRP:HE3	1.78	0.47
2:B:154:SER:HB3	2:B:158:MET:H	1.79	0.47
2:B:515:ILE:O	2:B:519:ARG:HG3	2.15	0.47
2:H:160:LEU:HD23	2:H:172:ILE:HA	1.96	0.47
3:I:355:LEU:N	3:I:356:PRO:HD2	2.30	0.47
3:I:77:LEU:HD21	3:I:81:LEU:HD12	1.95	0.47
3:F:242:LEU:HB2	3:F:312:GLU:HG2	1.96	0.47
1:G:57:TRP:HA	1:G:57:TRP:CE3	2.49	0.47
1:A:253:PHE:O	1:A:255:ASP:N	2.48	0.47
2:H:515:ILE:HD12	2:H:544:LYS:HB2	1.94	0.47
2:B:160:LEU:HD23	2:B:172:ILE:HA	1.95	0.47
2:H:210:ILE:H	2:H:210:ILE:CD1	2.21	0.47
2:B:491:LEU:HD12	2:B:507:ILE:HD13	1.95	0.47
3:F:10:GLU:O	3:F:11:ARG:C	2.52	0.47
3:F:350:VAL:HG22	3:F:355:LEU:CD2	2.41	0.47
3:I:355:LEU:H	3:I:356:PRO:HD2	1.80	0.47
3:I:434:THR:O	3:I:434:THR:CG2	2.61	0.47
1:D:117:LEU:HB2	1:D:153:TRP:NE1	2.29	0.47
1:A:202:GLY:HA2	1:A:245:LYS:NZ	2.29	0.47
2:H:522:THR:O	2:H:526:ILE:HG13	2.15	0.47
2:B:515:ILE:HD12	2:B:544:LYS:HB2	1.95	0.47
1:D:14:ASP:HB3	1:D:58:ARG:HA	1.95	0.47
2:E:324:TYR:CD2	3:F:237:ILE:HG21	2.48	0.47
2:H:221:LEU:HD22	2:H:231:TYR:CD1	2.49	0.47
1:G:202:GLY:HA2	1:G:245:LYS:NZ	2.29	0.47
2:B:522:THR:O	2:B:526:ILE:HG13	2.15	0.47
1:D:140:ILE:CG2	1:D:141:ILE:N	2.78	0.47
1:D:57:TRP:HA	1:D:57:TRP:CE3	2.49	0.47
1:D:52:HIS:CE1	1:D:80:LEU:HD12	2.49	0.47
2:H:512:MET:C	2:H:514:GLU:N	2.66	0.47
2:H:491:LEU:HD12	2:H:507:ILE:HD13	1.96	0.47
2:H:154:SER:HB3	2:H:158:MET:H	1.79	0.47
1:G:14:ASP:HB3	1:G:58:ARG:HA	1.95	0.47
2:H:399:LEU:HB3	2:H:425:TYR:OH	2.14	0.47
1:G:273:GLY:C	1:G:275:ASP:H	2.17	0.47
3:C:104:LEU:CD1	3:C:224:ASP:HB3	2.44	0.47
3:I:24:ILE:HG22	3:I:25:GLU:N	2.28	0.47
2:B:392:GLY:O	2:B:393:GLN:HB2	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:250:THR:HG23	3:I:99:TYR:OH	2.13	0.47
1:D:280:LEU:HB2	1:D:292:ALA:O	2.14	0.47
2:B:449:PHE:HE2	2:B:453:LEU:HD12	1.78	0.47
1:D:290:GLU:HG3	1:D:291:PRO:HD2	1.97	0.47
3:F:104:LEU:CD1	3:F:224:ASP:HB3	2.44	0.47
3:I:113:ASN:C	3:I:113:ASN:OD1	2.53	0.47
3:I:317:LEU:HD23	3:I:317:LEU:HA	1.59	0.47
3:C:235:GLN:HG2	3:C:236:GLY:N	2.30	0.47
2:B:366:PHE:O	2:B:368:GLY:N	2.43	0.47
1:A:215:THR:O	1:A:215:THR:HG23	2.15	0.47
1:G:57:TRP:NE1	2:H:142:ARG:NH2	2.62	0.47
1:G:205:ASP:CB	1:G:227:GLN:HB3	2.44	0.47
1:D:208:ARG:HH21	2:E:143:ARG:HG3	1.80	0.47
3:C:16:SER:HB2	3:C:432:TYR:HE1	1.79	0.47
2:E:512:MET:C	2:E:514:GLU:N	2.66	0.47
1:D:217:LEU:CG	1:D:218:LEU:H	2.28	0.47
2:E:508:LYS:HA	2:E:536:LEU:HD11	1.97	0.47
1:D:11:LEU:HD23	2:E:162:LYS:NZ	2.29	0.47
3:C:313:LEU:HD13	2:E:341:GLN:HB3	1.97	0.47
2:E:341:GLN:O	2:E:342:LYS:C	2.53	0.47
1:G:74:SER:HB3	1:G:76:ASP:OD1	2.15	0.47
3:I:242:LEU:HB2	3:I:312:GLU:HG2	1.96	0.47
1:G:141:ILE:HD12	1:G:185:TRP:CE3	2.50	0.47
3:I:7:TYR:O	3:I:9:THR:N	2.47	0.47
3:C:11:ARG:CG	3:C:12:PHE:CD1	2.97	0.47
1:A:52:HIS:CE1	1:A:80:LEU:HD12	2.49	0.47
1:G:102:VAL:HG13	1:G:118:VAL:HG13	1.97	0.47
2:H:435:TYR:OH	2:H:450:CYS:HB3	2.15	0.47
1:D:215:THR:O	1:D:215:THR:HG23	2.15	0.47
1:G:43:HIS:N	1:G:43:HIS:ND1	2.63	0.47
2:H:515:ILE:O	2:H:519:ARG:HG3	2.14	0.47
2:E:172:ILE:H	2:E:172:ILE:HD12	1.79	0.47
1:A:217:LEU:CG	1:A:218:LEU:H	2.28	0.47
1:A:57:TRP:CE3	1:A:57:TRP:HA	2.49	0.47
2:B:399:LEU:HB3	2:B:425:TYR:OH	2.14	0.47
1:A:117:LEU:HB2	1:A:153:TRP:NE1	2.29	0.47
2:H:364:SER:HB3	2:H:367:GLU:HB2	1.97	0.47
3:C:113:ASN:C	3:C:113:ASN:OD1	2.53	0.47
3:C:341:HIS:CE1	3:C:343:ILE:HD12	2.50	0.46
2:E:142:ARG:O	2:E:143:ARG:HG2	2.14	0.46
3:C:284:SER:O	3:C:287:HIS:HB3	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:ARG:O	2:H:175:LEU:C	2.52	0.46
1:D:171:ARG:O	1:D:172:LYS:HG3	2.14	0.46
3:F:58:ASP:C	3:F:60:SER:N	2.69	0.46
3:C:274:GLN:O	3:C:278:GLN:HB3	2.15	0.46
2:E:333:ARG:HG2	2:E:362:SER:O	2.15	0.46
2:E:522:THR:O	2:E:526:ILE:HG13	2.15	0.46
2:E:174:ARG:O	2:E:175:LEU:C	2.53	0.46
2:E:515:ILE:O	2:E:519:ARG:HG3	2.15	0.46
3:C:139:VAL:CG1	3:C:140:PRO:HD2	2.43	0.46
2:E:206:PRO:O	2:E:533:PRO:HG3	2.15	0.46
3:C:310:THR:CG2	3:C:311:ASP:N	2.78	0.46
3:F:274:GLN:O	3:F:278:GLN:HB3	2.15	0.46
1:A:43:HIS:ND1	1:A:43:HIS:N	2.63	0.46
3:I:341:HIS:CE1	3:I:343:ILE:HD12	2.50	0.46
3:F:12:PHE:HD2	3:F:416:TYR:HH	1.62	0.46
2:E:221:LEU:HD22	2:E:231:TYR:CD1	2.50	0.46
3:I:170:ASP:OD1	3:I:172:LYS:N	2.48	0.46
3:C:439:SER:C	3:C:441:CYS:H	2.18	0.46
2:E:340:LEU:HD22	2:E:370:PHE:CG	2.50	0.46
2:H:508:LYS:HA	2:H:536:LEU:HD11	1.96	0.46
1:G:65:LYS:CA	2:H:546:ARG:NH2	2.73	0.46
2:B:221:LEU:HD22	2:B:231:TYR:CD1	2.49	0.46
2:B:134:ASN:O	2:B:138:ILE:HG13	2.15	0.46
1:D:63:HIS:O	1:D:65:LYS:N	2.49	0.46
3:F:170:ASP:OD1	3:F:172:LYS:N	2.48	0.46
3:I:274:GLN:O	3:I:278:GLN:HB3	2.15	0.46
1:G:215:THR:HG23	1:G:215:THR:O	2.15	0.46
2:B:206:PRO:O	2:B:533:PRO:HG3	2.15	0.46
1:G:37:GLU:CG	1:G:46:ILE:HD12	2.45	0.46
1:G:53:GLU:HB2	1:G:76:ASP:HB3	1.98	0.46
2:B:435:TYR:OH	2:B:450:CYS:HB3	2.15	0.46
2:H:333:ARG:HG2	2:H:362:SER:O	2.15	0.46
3:F:313:LEU:HB3	2:H:338:LEU:HD11	1.98	0.46
2:B:526:ILE:O	2:B:529:ARG:HB2	2.16	0.46
1:D:229:ARG:HH11	1:D:252:LYS:HB3	1.81	0.46
2:H:546:ARG:O	2:H:546:ARG:HG2	2.15	0.46
2:H:206:PRO:O	2:H:533:PRO:HG3	2.15	0.46
2:E:546:ARG:O	2:E:546:ARG:HG2	2.15	0.46
3:F:441:CYS:SG	3:F:441:CYS:O	2.74	0.46
2:E:250:THR:CG2	2:E:255:VAL:HB	2.45	0.46
1:A:151:ALA:CB	1:A:175:THR:HG22	2.46	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:TRP:O	1:A:107:TRP:CD1	2.69	0.46
1:A:53:GLU:HB2	1:A:76:ASP:HB3	1.98	0.46
1:G:290:GLU:HG3	1:G:291:PRO:HD2	1.97	0.46
2:B:460:ASN:C	2:B:462:THR:H	2.19	0.46
3:I:54:ALA:O	3:I:55:ASN:C	2.53	0.46
2:E:514:GLU:O	2:E:516:THR:N	2.49	0.46
3:F:7:TYR:CD1	3:F:7:TYR:N	2.84	0.46
2:B:327:SER:HA	3:C:238:LYS:HE3	1.98	0.46
2:H:348:CYS:O	2:H:349:SER:OG	2.30	0.46
2:H:259:LEU:HD11	3:I:99:TYR:CG	2.50	0.46
3:F:59:GLU:HA	3:F:62:VAL:HG23	1.98	0.46
1:A:37:GLU:CG	1:A:46:ILE:HD12	2.45	0.46
1:D:37:GLU:CG	1:D:46:ILE:HD12	2.45	0.46
3:I:36:PHE:HB3	3:I:40:ARG:HH21	1.81	0.46
1:G:229:ARG:HH11	1:G:252:LYS:HB3	1.80	0.46
2:E:142:ARG:NH1	2:E:142:ARG:HG3	2.31	0.46
1:A:78:LYS:CA	1:A:96:ALA:HB2	2.41	0.46
3:F:10:GLU:HG3	3:F:11:ARG:N	2.31	0.46
1:A:63:HIS:O	1:A:65:LYS:N	2.49	0.46
3:C:104:LEU:HD23	3:C:104:LEU:HA	1.72	0.46
3:F:434:THR:O	3:F:434:THR:CG2	2.61	0.46
2:B:452:TYR:O	2:B:452:TYR:HD2	1.98	0.46
3:F:36:PHE:HB3	3:F:40:ARG:HH21	1.80	0.46
2:H:526:ILE:O	2:H:529:ARG:HB2	2.16	0.46
1:D:57:TRP:CH2	2:E:144:PHE:CE1	3.04	0.46
3:F:68:TRP:CH2	3:F:387:ARG:NH2	2.84	0.46
1:A:261:SER:HB2	2:B:152:LYS:HA	1.91	0.46
2:B:417:PRO:HG2	2:B:418:ILE:HD13	1.98	0.46
2:E:435:TYR:OH	2:E:450:CYS:HB3	2.15	0.46
2:H:452:TYR:O	2:H:452:TYR:HD2	1.99	0.46
2:E:234:TRP:CH2	2:E:452:TYR:CD1	3.04	0.46
2:B:164:ILE:HG13	2:B:164:ILE:O	2.15	0.46
3:F:13:THR:O	3:F:17:ASP:CB	2.51	0.46
3:C:406:GLU:HA	3:C:409:LYS:CE	2.45	0.46
2:E:210:ILE:HD12	2:E:495:CYS:CB	2.46	0.46
2:H:417:PRO:HG2	2:H:418:ILE:HD13	1.98	0.46
2:H:250:THR:CG2	2:H:255:VAL:HB	2.45	0.46
2:H:338:LEU:O	2:H:342:LYS:HG3	2.16	0.46
2:E:318:LEU:HD23	2:E:318:LEU:O	2.16	0.46
1:A:140:ILE:CG2	1:A:141:ILE:N	2.78	0.45
1:G:140:ILE:CG2	1:G:141:ILE:N	2.78	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:284:SER:O	3:I:287:HIS:HB3	2.16	0.45
2:B:420:VAL:CG1	2:B:438:VAL:HG11	2.46	0.45
1:D:10:GLU:N	1:D:10:GLU:OE1	2.45	0.45
3:I:139:VAL:CG1	3:I:140:PRO:HD2	2.42	0.45
3:F:139:VAL:CG1	3:F:140:PRO:HD2	2.43	0.45
3:F:77:LEU:C	3:F:77:LEU:HD23	2.36	0.45
1:A:102:VAL:HG13	1:A:118:VAL:HG13	1.98	0.45
2:B:250:THR:CG2	2:B:255:VAL:HB	2.45	0.45
2:B:546:ARG:HG2	2:B:546:ARG:O	2.15	0.45
2:H:234:TRP:CH2	2:H:452:TYR:CD1	3.04	0.45
2:E:460:ASN:C	2:E:462:THR:H	2.19	0.45
2:B:333:ARG:HG2	2:B:362:SER:O	2.16	0.45
2:B:338:LEU:O	2:B:342:LYS:HG3	2.16	0.45
3:C:242:LEU:HB2	3:C:312:GLU:HG2	1.97	0.45
2:H:460:ASN:C	2:H:462:THR:H	2.19	0.45
1:A:8:HIS:O	1:A:9:ASN:CB	2.65	0.45
1:D:102:VAL:HG13	1:D:118:VAL:HG13	1.97	0.45
3:F:284:SER:O	3:F:287:HIS:HB3	2.16	0.45
1:G:217:LEU:CG	1:G:218:LEU:H	2.28	0.45
3:I:294:LEU:O	3:I:298:ILE:HD12	2.17	0.45
2:E:342:LYS:HD2	3:F:206:ILE:CD1	2.47	0.45
2:E:338:LEU:O	2:E:342:LYS:HG3	2.16	0.45
1:A:151:ALA:HA	1:A:174:VAL:O	2.16	0.45
1:D:61:TRP:O	1:D:107:TRP:CD1	2.69	0.45
2:H:318:LEU:O	2:H:318:LEU:HD23	2.16	0.45
3:C:269:GLY:HA3	3:C:295:GLN:CG	2.42	0.45
3:I:413:ILE:O	3:I:417:ILE:HG13	2.17	0.45
2:H:225:GLU:O	2:H:231:TYR:HB2	2.15	0.45
3:C:54:ALA:O	3:C:55:ASN:C	2.55	0.45
1:G:61:TRP:O	1:G:107:TRP:CD1	2.69	0.45
3:C:36:PHE:HB3	3:C:40:ARG:HH21	1.81	0.45
3:C:413:ILE:O	3:C:417:ILE:HG13	2.17	0.45
2:B:210:ILE:HD12	2:B:495:CYS:CB	2.46	0.45
3:F:406:GLU:HA	3:F:409:LYS:CE	2.45	0.45
2:E:417:PRO:HG2	2:E:418:ILE:HD13	1.98	0.45
2:E:225:GLU:O	2:E:231:TYR:HB2	2.16	0.45
3:C:144:TRP:O	3:C:148:ILE:HG12	2.17	0.45
2:E:366:PHE:O	2:E:368:GLY:N	2.44	0.45
3:F:233:THR:HG22	3:F:234:GLN:O	2.17	0.45
3:C:23:LYS:O	3:C:26:GLN:OE1	2.34	0.45
3:I:77:LEU:C	3:I:77:LEU:HD23	2.36	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:TYR:HA	2:B:247:PRO:HD2	1.76	0.45
3:C:183:TYR:CE2	3:C:199:GLU:HG3	2.52	0.45
2:E:526:ILE:O	2:E:529:ARG:HB2	2.16	0.45
2:B:529:ARG:O	2:B:530:LEU:C	2.55	0.45
2:H:210:ILE:HD12	2:H:495:CYS:CB	2.46	0.45
2:B:210:ILE:CD1	2:B:210:ILE:H	2.22	0.45
2:E:265:HIS:HB2	2:E:399:LEU:CD2	2.42	0.45
3:F:294:LEU:O	3:F:298:ILE:HD12	2.17	0.45
2:B:364:SER:HB3	2:B:367:GLU:HB2	1.98	0.45
1:A:126:SER:HB3	1:A:140:ILE:CG1	2.28	0.45
3:F:42:PHE:CZ	3:F:391:HIS:HB3	2.52	0.45
1:G:63:HIS:O	1:G:65:LYS:N	2.49	0.45
3:C:227:ILE:C	3:C:227:ILE:HD12	2.37	0.45
1:D:43:HIS:N	1:D:43:HIS:ND1	2.63	0.45
3:F:144:TRP:O	3:F:148:ILE:HG12	2.17	0.45
1:D:74:SER:HB3	1:D:76:ASP:OD1	2.16	0.45
3:F:58:ASP:C	3:F:60:SER:H	2.20	0.45
2:H:215:LEU:HB3	2:H:452:TYR:CE2	2.52	0.45
3:C:189:LEU:HD23	3:C:189:LEU:HA	1.70	0.45
2:E:340:LEU:CD2	2:E:370:PHE:CG	2.99	0.45
1:D:232:ILE:HG12	1:D:247:LEU:CD2	2.38	0.45
2:E:420:VAL:CG1	2:E:438:VAL:HG11	2.46	0.45
2:H:420:VAL:CG1	2:H:438:VAL:HG11	2.46	0.45
3:C:353:ASP:O	3:C:355:LEU:N	2.44	0.45
3:I:102:ARG:NH2	3:I:241:SER:OG	2.45	0.45
3:I:144:TRP:O	3:I:148:ILE:HG12	2.17	0.45
3:C:206:ILE:HD12	3:C:206:ILE:H	1.82	0.45
1:A:74:SER:HB3	1:A:76:ASP:OD1	2.15	0.45
2:B:215:LEU:HB3	2:B:452:TYR:CE2	2.52	0.45
2:E:526:ILE:C	2:E:529:ARG:HB2	2.37	0.45
2:H:142:ARG:O	2:H:143:ARG:CB	2.65	0.45
1:A:229:ARG:HH11	1:A:252:LYS:HB3	1.81	0.45
2:B:514:GLU:O	2:B:516:THR:N	2.50	0.45
3:C:22:PHE:C	3:C:24:ILE:N	2.69	0.45
1:D:217:LEU:HD13	1:D:218:LEU:HB2	1.99	0.45
2:E:197:VAL:HG11	2:E:210:ILE:CG1	2.47	0.45
3:F:319:SER:CB	2:H:337:GLU:HG2	2.47	0.45
3:F:54:ALA:O	3:F:55:ASN:C	2.54	0.45
3:C:313:LEU:O	2:E:342:LYS:HE2	2.17	0.45
2:B:234:TRP:CH2	2:B:452:TYR:CD1	3.04	0.45
2:E:215:LEU:HB3	2:E:452:TYR:CE2	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:452:TYR:HD2	2:E:452:TYR:O	1.98	0.45
3:C:135:ARG:HG3	3:C:183:TYR:CE2	2.52	0.45
1:G:151:ALA:HB2	1:G:175:THR:HG22	1.99	0.45
1:G:10:GLU:N	1:G:10:GLU:OE1	2.45	0.45
3:F:413:ILE:O	3:F:417:ILE:HG13	2.17	0.45
2:B:327:SER:OG	3:C:238:LYS:N	2.33	0.45
3:C:77:LEU:HD23	3:C:77:LEU:C	2.37	0.45
1:D:127:VAL:HG21	1:D:194:TYR:CE1	2.52	0.45
2:E:233:LEU:HD21	2:E:421:ILE:CD1	2.47	0.45
1:G:9:ASN:HD21	1:G:34:LYS:HE3	1.81	0.45
3:C:58:ASP:C	3:C:60:SER:H	2.20	0.45
3:F:48:GLN:HA	3:F:51:LEU:HD12	1.99	0.45
2:E:529:ARG:O	2:E:530:LEU:C	2.55	0.44
3:F:70:LEU:HB3	3:F:343:ILE:HD11	1.99	0.44
1:D:17:LEU:HD21	2:E:160:LEU:CD1	2.43	0.44
1:G:58:ARG:NH2	1:G:259:ARG:HE	2.14	0.44
3:I:227:ILE:HD12	3:I:227:ILE:C	2.37	0.44
3:F:77:LEU:HD12	3:F:125:TRP:CZ2	2.52	0.44
1:D:53:GLU:HB2	1:D:76:ASP:HB3	1.98	0.44
3:F:183:TYR:CE2	3:F:199:GLU:HG3	2.52	0.44
3:F:329:ASN:O	3:F:332:ALA:HB3	2.17	0.44
2:H:526:ILE:C	2:H:529:ARG:HB2	2.37	0.44
2:H:529:ARG:O	2:H:530:LEU:C	2.55	0.44
3:I:11:ARG:C	3:I:13:THR:N	2.71	0.44
2:H:514:GLU:O	2:H:516:THR:N	2.50	0.44
2:H:153:PHE:HA	2:H:159:LEU:CD2	2.46	0.44
3:C:12:PHE:H	3:C:12:PHE:HD1	1.61	0.44
1:A:217:LEU:HD13	1:A:218:LEU:HB2	1.99	0.44
2:B:155:THR:HG22	2:B:513:ARG:CG	2.48	0.44
2:H:538:PHE:O	2:H:541:GLN:HB3	2.17	0.44
2:H:341:GLN:O	2:H:342:LYS:C	2.52	0.44
3:F:135:ARG:HG3	3:F:183:TYR:CE2	2.52	0.44
2:B:318:LEU:O	2:B:318:LEU:HD23	2.16	0.44
3:I:183:TYR:CE2	3:I:199:GLU:HG3	2.52	0.44
3:I:329:ASN:O	3:I:332:ALA:HB3	2.17	0.44
2:H:366:PHE:O	2:H:368:GLY:N	2.47	0.44
1:D:208:ARG:HD3	1:D:208:ARG:HA	1.81	0.44
1:G:19:TYR:CD2	2:H:543:LEU:HD21	2.52	0.44
2:H:184:LEU:HA	2:H:184:LEU:HD23	1.85	0.44
2:B:197:VAL:HG11	2:B:210:ILE:CG1	2.47	0.44
2:B:225:GLU:O	2:B:231:TYR:HB2	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:233:LEU:HD21	2:H:421:ILE:CD1	2.48	0.44
2:E:538:PHE:O	2:E:541:GLN:HB3	2.18	0.44
1:D:151:ALA:HB2	1:D:175:THR:HG22	1.99	0.44
3:C:39:ILE:HD11	3:C:399:ILE:HD11	1.99	0.44
2:B:142:ARG:HG3	2:B:142:ARG:NH1	2.33	0.44
1:G:126:SER:HB3	1:G:140:ILE:CG1	2.28	0.44
1:A:232:ILE:HG12	1:A:247:LEU:CD2	2.38	0.44
2:B:175:LEU:CD1	2:B:176:PRO:HD2	2.42	0.44
1:G:281:TRP:N	1:G:281:TRP:CD1	2.86	0.44
3:C:225:THR:HG22	3:C:226:GLN:N	2.32	0.44
2:B:263:GLU:HA	2:B:263:GLU:OE1	2.17	0.44
3:C:34:ASP:CB	3:C:35:PRO:CD	2.93	0.44
3:I:384:TYR:CA	3:I:387:ARG:HH12	2.15	0.44
2:H:174:ARG:HE	2:H:174:ARG:HA	1.82	0.44
1:D:273:GLY:O	1:D:275:ASP:N	2.46	0.44
3:I:23:LYS:CE	3:I:434:THR:OG1	2.65	0.44
1:A:38:VAL:HG12	1:A:39:GLU:N	2.33	0.44
2:H:255:VAL:HG13	3:I:223:ILE:HA	1.99	0.44
3:C:358:VAL:O	3:C:361:SER:HB3	2.18	0.44
3:F:317:LEU:HD23	3:F:317:LEU:HA	1.58	0.44
2:H:263:GLU:OE1	2:H:263:GLU:HA	2.18	0.44
2:E:159:LEU:CD1	2:E:160:LEU:N	2.79	0.44
1:G:78:LYS:CA	1:G:96:ALA:HB2	2.41	0.44
2:H:265:HIS:CB	2:H:399:LEU:HD21	2.42	0.44
3:I:77:LEU:HD12	3:I:125:TRP:CZ3	2.52	0.44
3:I:135:ARG:HG3	3:I:183:TYR:CE2	2.52	0.44
3:C:233:THR:HG22	3:C:234:GLN:O	2.17	0.44
2:E:304:VAL:HG21	3:F:311:ASP:HB3	1.99	0.44
1:A:66:PHE:CZ	1:A:113:GLY:O	2.71	0.44
3:C:382:LYS:HA	3:C:383:PRO:HD3	1.47	0.44
2:B:516:THR:OG1	2:B:544:LYS:HE2	2.18	0.44
3:C:7:TYR:O	3:C:10:GLU:HB2	2.18	0.44
2:E:299:LEU:CD2	2:E:387:LEU:HD21	2.46	0.44
3:F:227:ILE:HD12	3:F:227:ILE:C	2.37	0.44
1:A:109:PRO:O	1:A:111:GLU:N	2.51	0.44
1:A:279:THR:HB	1:A:281:TRP:NE1	2.33	0.44
1:G:95:HIS:ND1	1:G:128:VAL:HG21	2.33	0.44
1:A:9:ASN:HA	1:A:9:ASN:HD22	1.49	0.44
3:C:16:SER:O	3:C:19:LEU:HB2	2.18	0.44
1:D:58:ARG:NH2	1:D:259:ARG:HE	2.16	0.44
1:G:217:LEU:HD13	1:G:218:LEU:HB2	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:399:LEU:O	2:H:403:VAL:HG23	2.18	0.44
2:B:265:HIS:CB	2:B:399:LEU:HD21	2.42	0.44
3:C:116:LEU:CD2	3:C:294:LEU:CD1	2.95	0.44
3:F:269:GLY:HA3	3:F:295:GLN:CG	2.42	0.44
3:F:298:ILE:HD12	3:F:298:ILE:N	2.33	0.44
3:I:144:TRP:CZ2	3:I:169:LEU:HD11	2.53	0.44
1:A:95:HIS:ND1	1:A:128:VAL:HG21	2.33	0.44
3:I:48:GLN:HA	3:I:51:LEU:HD12	1.99	0.44
2:H:381:TRP:CD2	2:H:412:LEU:HD22	2.53	0.44
2:B:381:TRP:CD2	2:B:412:LEU:HD22	2.52	0.44
1:D:66:PHE:CZ	1:D:113:GLY:O	2.71	0.44
1:A:10:GLU:OE1	1:A:10:GLU:HA	2.18	0.44
1:A:154:ALA:HB2	1:A:212:TRP:CE3	2.53	0.44
2:E:153:PHE:HA	2:E:159:LEU:CD2	2.46	0.44
1:D:236:GLN:HG3	1:D:241:GLY:O	2.18	0.44
2:H:197:VAL:HG11	2:H:210:ILE:CG1	2.47	0.44
3:I:416:TYR:CD2	3:I:432:TYR:CE2	3.06	0.44
3:C:294:LEU:HG	3:C:298:ILE:HD11	1.99	0.44
1:G:38:VAL:HG12	1:G:39:GLU:N	2.33	0.44
3:F:358:VAL:O	3:F:361:SER:HB3	2.18	0.44
2:E:193:GLU:HG3	2:E:215:LEU:HD11	2.00	0.44
3:C:329:ASN:O	3:C:332:ALA:HB3	2.18	0.44
3:C:164:GLU:O	3:C:165:ASN:O	2.36	0.44
1:G:57:TRP:CH2	2:H:144:PHE:CE1	3.05	0.43
1:A:12:ILE:HG21	1:A:26:THR:HB	2.00	0.43
3:I:419:LEU:O	3:I:423:GLN:HB2	2.18	0.43
3:F:436:LEU:HB3	3:F:437:ASN:H	1.46	0.43
3:C:406:GLU:HG2	3:C:409:LYS:HZ1	1.83	0.43
2:H:340:LEU:HD22	2:H:370:PHE:CB	2.48	0.43
2:H:340:LEU:HD23	2:H:370:PHE:CE1	2.53	0.43
1:A:273:GLY:O	1:A:275:ASP:N	2.47	0.43
3:F:144:TRP:CZ2	3:F:169:LEU:HD11	2.53	0.43
1:D:95:HIS:ND1	1:D:128:VAL:HG21	2.33	0.43
2:B:193:GLU:HG3	2:B:215:LEU:HD11	2.00	0.43
3:I:164:GLU:O	3:I:165:ASN:O	2.36	0.43
2:E:263:GLU:OE1	2:E:263:GLU:HA	2.17	0.43
3:F:212:LEU:HA	3:F:212:LEU:HD23	1.74	0.43
2:H:135:ALA:O	2:H:139:MET:HB2	2.18	0.43
1:G:20:TYR:N	1:G:20:TYR:CD1	2.86	0.43
1:G:233:ILE:HD11	1:G:248:LEU:CD1	2.48	0.43
2:E:174:ARG:HE	2:E:174:ARG:HA	1.82	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:294:LEU:HG	3:I:298:ILE:HD11	1.99	0.43
2:H:150:PHE:CZ	2:H:170:VAL:HG12	2.53	0.43
2:H:150:PHE:HZ	2:H:170:VAL:HG12	1.83	0.43
2:E:393:GLN:HG2	2:E:396:GLU:HB2	2.00	0.43
1:G:112:TYR:CZ	1:G:171:ARG:HG2	2.54	0.43
3:I:104:LEU:HA	3:I:104:LEU:HD23	1.72	0.43
1:G:170:SER:HA	1:G:186:LYS:HE3	2.00	0.43
3:C:9:THR:O	3:C:9:THR:HG22	2.17	0.43
2:B:527:LEU:C	2:B:529:ARG:N	2.72	0.43
3:F:384:TYR:O	3:F:388:ILE:HG13	2.18	0.43
1:A:20:TYR:N	1:A:20:TYR:CD1	2.87	0.43
1:G:219:ARG:HB2	1:G:236:GLN:O	2.19	0.43
1:A:219:ARG:HB2	1:A:236:GLN:O	2.19	0.43
2:B:174:ARG:HE	2:B:174:ARG:HA	1.82	0.43
2:E:150:PHE:HZ	2:E:170:VAL:HG12	1.83	0.43
3:F:298:ILE:H	3:F:298:ILE:HD12	1.83	0.43
2:H:393:GLN:HG2	2:H:396:GLU:HB2	2.00	0.43
1:D:38:VAL:HG12	1:D:39:GLU:N	2.33	0.43
3:C:354:SER:O	3:C:358:VAL:HG23	2.19	0.43
3:I:354:SER:O	3:I:358:VAL:HG23	2.19	0.43
3:C:316:PRO:HB3	2:E:338:LEU:HB2	1.99	0.43
3:I:206:ILE:HD12	3:I:206:ILE:H	1.84	0.43
2:B:145:THR:C	2:B:147:SER:H	2.22	0.43
2:E:381:TRP:CD2	2:E:412:LEU:HD22	2.53	0.43
3:F:305:ASN:O	3:F:306:ASN:C	2.56	0.43
3:C:317:LEU:HA	3:C:317:LEU:HD23	1.58	0.43
2:H:527:LEU:C	2:H:529:ARG:N	2.71	0.43
2:B:526:ILE:C	2:B:529:ARG:HB2	2.37	0.43
3:F:343:ILE:HD13	3:F:344:ARG:N	2.34	0.43
3:F:24:ILE:HD13	3:F:24:ILE:N	2.34	0.43
1:G:227:GLN:C	1:G:229:ARG:H	2.22	0.43
2:H:516:THR:OG1	2:H:544:LYS:HE2	2.18	0.43
1:D:233:ILE:HD11	1:D:248:LEU:CD1	2.48	0.43
2:B:265:HIS:HB2	2:B:399:LEU:CD2	2.42	0.43
3:C:294:LEU:O	3:C:298:ILE:HD13	2.18	0.43
3:C:364:GLU:C	3:C:366:LEU:N	2.69	0.43
3:C:144:TRP:CZ2	3:C:169:LEU:HD11	2.54	0.43
1:A:274:GLY:O	2:B:147:SER:HB2	2.19	0.43
2:B:538:PHE:O	2:B:541:GLN:HB3	2.18	0.43
2:H:330:PRO:HA	2:H:333:ARG:HB2	2.00	0.43
2:B:341:GLN:O	2:B:342:LYS:C	2.52	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:233:THR:HG22	3:I:234:GLN:O	2.17	0.43
2:H:467:LYS:HD2	2:H:498:ASN:HB3	2.01	0.43
1:A:185:TRP:CE2	1:A:196:LEU:HD13	2.54	0.43
3:I:421:LYS:O	3:I:423:GLN:N	2.52	0.43
3:I:343:ILE:HD13	3:I:344:ARG:N	2.34	0.43
1:D:232:ILE:HG21	1:D:234:TRP:CZ2	2.53	0.43
3:I:298:ILE:N	3:I:298:ILE:HD12	2.33	0.43
3:F:294:LEU:HD12	3:F:294:LEU:HA	1.81	0.43
3:F:102:ARG:NH2	3:F:241:SER:OG	2.45	0.43
1:A:281:TRP:CD1	1:A:281:TRP:N	2.86	0.43
3:I:225:THR:HG22	3:I:226:GLN:N	2.33	0.43
2:H:314:LYS:HG2	3:I:162:LEU:O	2.19	0.43
1:G:66:PHE:CZ	1:G:113:GLY:O	2.71	0.43
1:D:170:SER:HA	1:D:186:LYS:HE3	2.00	0.43
2:B:202:ARG:HE	2:B:209:GLN:HB2	1.84	0.43
3:C:384:TYR:O	3:C:388:ILE:HG13	2.19	0.43
1:D:185:TRP:CE2	1:D:196:LEU:HD13	2.54	0.43
1:D:208:ARG:HE	1:D:258:TRP:HZ3	1.67	0.43
1:D:264:LEU:HD12	2:E:155:THR:O	2.19	0.43
2:E:399:LEU:O	2:E:403:VAL:HG23	2.19	0.43
3:C:298:ILE:N	3:C:298:ILE:HD12	2.34	0.43
3:C:94:MET:HE3	3:C:104:LEU:HD22	2.01	0.43
1:G:279:THR:HB	1:G:281:TRP:NE1	2.33	0.43
2:E:297:TYR:HE2	2:E:305:ARG:HH11	1.67	0.43
1:G:289:TRP:CD1	1:G:289:TRP:N	2.87	0.43
3:F:104:LEU:HA	3:F:104:LEU:HD23	1.72	0.43
2:H:193:GLU:HG3	2:H:215:LEU:HD11	2.00	0.43
2:H:318:LEU:HD11	2:H:357:ILE:HD12	2.00	0.43
1:A:103:ASN:ND2	2:B:142:ARG:NH2	2.66	0.43
3:C:16:SER:HB3	3:C:432:TYR:OH	2.17	0.43
1:G:232:ILE:HG21	1:G:234:TRP:CZ2	2.54	0.43
3:I:435:PHE:O	3:I:436:LEU:CG	2.65	0.43
2:E:150:PHE:CZ	2:E:170:VAL:HG12	2.53	0.43
3:F:294:LEU:HG	3:F:298:ILE:HD11	2.00	0.43
2:E:468:GLU:N	2:E:468:GLU:OE1	2.47	0.43
3:I:143:LYS:HE3	3:I:144:TRP:CD1	2.54	0.43
3:F:206:ILE:HD12	3:F:206:ILE:H	1.83	0.43
3:I:305:ASN:O	3:I:306:ASN:C	2.56	0.43
2:E:246:TYR:HA	2:E:247:PRO:HD2	1.76	0.43
3:C:212:LEU:HD23	3:C:212:LEU:HA	1.75	0.43
1:A:208:ARG:HA	1:A:208:ARG:HD3	1.81	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ARG:O	2:B:143:ARG:CB	2.66	0.43
2:B:150:PHE:HZ	2:B:170:VAL:HG12	1.83	0.43
1:A:227:GLN:C	1:A:229:ARG:H	2.22	0.43
3:F:34:ASP:CB	3:F:35:PRO:CD	2.93	0.43
3:C:428:ASN:C	3:C:430:PRO:CD	2.87	0.43
3:I:116:LEU:CD2	3:I:294:LEU:CD1	2.96	0.43
1:A:102:VAL:CG1	1:A:118:VAL:HG13	2.49	0.43
2:H:285:ARG:HG3	2:H:285:ARG:NH1	2.33	0.43
3:C:143:LYS:HE3	3:C:144:TRP:CD1	2.54	0.43
3:F:225:THR:HG22	3:F:226:GLN:N	2.32	0.43
3:F:164:GLU:O	3:F:165:ASN:O	2.36	0.43
2:B:325:LEU:CD2	2:B:361:LEU:HD23	2.49	0.43
2:B:340:LEU:HA	2:B:340:LEU:HD12	1.80	0.43
2:B:467:LYS:HD2	2:B:498:ASN:HB3	2.01	0.43
1:G:236:GLN:HG3	1:G:241:GLY:O	2.18	0.43
3:I:294:LEU:O	3:I:298:ILE:HD13	2.19	0.43
1:G:273:GLY:O	1:G:275:ASP:N	2.46	0.43
3:F:428:ASN:C	3:F:430:PRO:CD	2.87	0.43
2:H:327:SER:OG	3:I:238:LYS:HG3	2.19	0.43
2:B:233:LEU:HD21	2:B:421:ILE:CD1	2.47	0.43
2:B:318:LEU:HD11	2:B:357:ILE:HD12	2.01	0.43
2:E:524:ASP:CA	2:E:527:LEU:HD12	2.35	0.43
2:H:138:ILE:HG23	2:H:141:GLU:OE2	2.18	0.43
1:D:102:VAL:CG1	1:D:118:VAL:HG13	2.49	0.43
2:B:159:LEU:CD1	2:B:160:LEU:N	2.79	0.43
1:D:219:ARG:HB2	1:D:236:GLN:O	2.19	0.43
1:G:264:LEU:HB3	2:H:509:ARG:NH1	2.33	0.43
1:D:121:SER:C	1:D:123:GLY:H	2.22	0.43
2:B:314:LYS:HE3	3:C:162:LEU:CB	2.47	0.43
2:B:393:GLN:HG2	2:B:396:GLU:HB2	2.00	0.43
1:G:102:VAL:CG1	1:G:118:VAL:HG13	2.49	0.43
1:G:108:ALA:HB1	1:G:112:TYR:HD1	1.84	0.43
1:D:279:THR:HB	1:D:281:TRP:NE1	2.33	0.43
1:D:281:TRP:CD1	1:D:281:TRP:N	2.86	0.43
3:C:48:GLN:HA	3:C:51:LEU:HD12	1.99	0.43
1:G:229:ARG:NH1	1:G:252:LYS:HB3	2.34	0.42
1:D:229:ARG:NH1	1:D:252:LYS:HB3	2.34	0.42
2:E:516:THR:OG1	2:E:544:LYS:HE2	2.18	0.42
2:E:197:VAL:HG11	2:E:210:ILE:HG12	2.01	0.42
3:C:294:LEU:O	3:C:298:ILE:HD12	2.18	0.42
1:D:108:ALA:HB1	1:D:112:TYR:HD1	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:297:TYR:HE2	2:H:305:ARG:HH11	1.67	0.42
2:H:359:LYS:HG3	2:H:365:PRO:HA	2.01	0.42
1:G:208:ARG:HE	1:G:258:TRP:HZ3	1.67	0.42
3:C:343:ILE:HD13	3:C:344:ARG:N	2.34	0.42
1:G:185:TRP:CE2	1:G:196:LEU:HD13	2.53	0.42
1:D:227:GLN:C	1:D:229:ARG:H	2.22	0.42
1:D:57:TRP:CH2	2:E:144:PHE:HE1	2.37	0.42
3:C:11:ARG:HD2	3:C:12:PHE:CE1	2.54	0.42
3:I:59:GLU:HA	3:I:62:VAL:CG2	2.42	0.42
3:I:269:GLY:HA3	3:I:295:GLN:CG	2.42	0.42
3:I:21:GLU:HG2	3:I:25:GLU:OE2	2.18	0.42
2:B:396:GLU:N	2:B:396:GLU:OE1	2.51	0.42
2:B:177:THR:CG2	2:B:484:ALA:HB2	2.45	0.42
3:I:358:VAL:O	3:I:361:SER:HB3	2.18	0.42
1:G:12:ILE:HG21	1:G:26:THR:HB	2.01	0.42
3:F:316:PRO:HB2	2:H:334:ASP:HB3	2.00	0.42
2:E:202:ARG:HE	2:E:209:GLN:HB2	1.84	0.42
2:H:136:LYS:HB3	2:H:136:LYS:HE2	1.82	0.42
3:C:42:PHE:CZ	3:C:391:HIS:HB3	2.55	0.42
2:B:198:THR:O	2:B:211:SER:HB3	2.19	0.42
2:H:320:VAL:HG11	3:I:211:ILE:HD13	2.02	0.42
1:A:229:ARG:NH1	1:A:252:LYS:HB3	2.34	0.42
2:B:153:PHE:HA	2:B:159:LEU:CD2	2.46	0.42
2:H:495:CYS:C	2:H:497:LEU:H	2.23	0.42
1:D:217:LEU:CD2	2:E:475:PHE:HE1	2.31	0.42
2:B:399:LEU:O	2:B:403:VAL:HG23	2.19	0.42
1:A:108:ALA:HB1	1:A:112:TYR:HD1	1.85	0.42
2:B:330:PRO:HA	2:B:333:ARG:HB2	2.02	0.42
2:H:295:PHE:CE1	2:H:356:LYS:HB3	2.55	0.42
3:I:16:SER:O	3:I:19:LEU:HB2	2.20	0.42
2:B:142:ARG:O	2:B:143:ARG:HB2	2.19	0.42
2:B:150:PHE:CZ	2:B:170:VAL:HG12	2.54	0.42
3:I:53:LEU:O	3:I:61:ASN:HB3	2.20	0.42
3:F:364:GLU:C	3:F:366:LEU:H	2.23	0.42
1:A:233:ILE:HD11	1:A:248:LEU:CD1	2.48	0.42
1:A:236:GLN:HG3	1:A:241:GLY:O	2.18	0.42
2:E:495:CYS:C	2:E:497:LEU:H	2.23	0.42
3:F:10:GLU:O	3:F:12:PHE:N	2.52	0.42
3:F:294:LEU:O	3:F:298:ILE:HD13	2.20	0.42
1:G:100:ALA:CB	1:G:121:SER:HB2	2.49	0.42
1:A:100:ALA:CB	1:A:121:SER:HB2	2.50	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:LYS:HE3	3:C:162:LEU:HD22	2.01	0.42
3:F:354:SER:O	3:F:358:VAL:HG23	2.19	0.42
1:G:109:PRO:O	1:G:111:GLU:N	2.52	0.42
3:I:28:ASN:O	3:I:29:GLU:O	2.38	0.42
3:F:150:SER:O	3:F:151:GLY:O	2.37	0.42
1:D:212:TRP:HA	1:D:222:LEU:HD22	1.92	0.42
3:F:93:GLU:CG	3:F:94:MET:H	2.31	0.42
3:I:428:ASN:C	3:I:430:PRO:CD	2.87	0.42
1:A:121:SER:C	1:A:123:GLY:H	2.22	0.42
2:H:396:GLU:OE1	2:H:396:GLU:N	2.52	0.42
2:H:250:THR:HG23	3:I:99:TYR:CZ	2.55	0.42
2:E:330:PRO:HA	2:E:333:ARG:HB2	2.01	0.42
3:C:220:ASN:HA	3:C:221:PRO:HD3	1.88	0.42
3:F:221:PRO:HG3	3:F:231:PHE:HB2	2.01	0.42
2:B:295:PHE:CE1	2:B:356:LYS:HB3	2.54	0.42
2:B:527:LEU:O	2:B:530:LEU:HB2	2.20	0.42
1:D:141:ILE:HD12	1:D:185:TRP:CE3	2.54	0.42
3:I:9:THR:HG22	3:I:423:GLN:OE1	2.20	0.42
3:I:8:GLN:O	3:I:10:GLU:N	2.52	0.42
1:A:232:ILE:HG21	1:A:234:TRP:CZ2	2.53	0.42
2:H:197:VAL:HG21	2:H:492:PHE:CZ	2.55	0.42
2:H:175:LEU:CD1	2:H:176:PRO:HD2	2.42	0.42
3:C:298:ILE:H	3:C:298:ILE:HD12	1.85	0.42
3:I:355:LEU:HA	3:I:355:LEU:HD12	1.84	0.42
3:C:227:ILE:O	3:C:229:ASN:N	2.53	0.42
1:D:15:ALA:CB	1:D:26:THR:HG22	2.49	0.42
1:G:15:ALA:CB	1:G:26:THR:HG22	2.49	0.42
1:D:109:PRO:O	1:D:111:GLU:N	2.52	0.42
1:D:61:TRP:CD1	1:D:61:TRP:N	2.87	0.42
3:I:82:LEU:HA	3:I:82:LEU:HD23	1.80	0.42
2:B:208:PRO:HB3	2:B:531:LYS:CB	2.24	0.42
1:G:229:ARG:CG	1:G:256:VAL:HA	2.50	0.42
2:B:491:LEU:O	2:B:494:SER:HB2	2.19	0.42
3:I:237:ILE:CD1	3:I:237:ILE:C	2.75	0.42
3:C:7:TYR:O	3:C:7:TYR:CD1	2.72	0.42
3:C:355:LEU:HD12	3:C:355:LEU:HA	1.83	0.42
1:G:121:SER:C	1:G:123:GLY:H	2.22	0.42
1:D:100:ALA:CB	1:D:121:SER:HB2	2.49	0.42
2:H:225:GLU:C	2:H:227:THR:N	2.73	0.42
1:D:12:ILE:HG21	1:D:26:THR:HB	2.01	0.42
1:A:289:TRP:CD1	1:A:289:TRP:N	2.87	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:TRP:N	1:G:61:TRP:CD1	2.87	0.42
2:E:234:TRP:CZ3	2:E:452:TYR:CD1	3.08	0.42
3:C:305:ASN:O	3:C:306:ASN:C	2.56	0.42
2:E:467:LYS:HD2	2:E:498:ASN:HB3	2.01	0.42
2:B:202:ARG:CG	2:B:500:ASP:OD1	2.67	0.42
3:F:35:PRO:HB2	3:F:399:ILE:HG12	2.00	0.42
2:E:175:LEU:CD1	2:E:176:PRO:HD2	2.42	0.42
1:D:20:TYR:CD1	1:D:20:TYR:N	2.87	0.42
2:E:197:VAL:HG21	2:E:492:PHE:CZ	2.55	0.42
2:E:265:HIS:CB	2:E:399:LEU:HD21	2.42	0.42
3:C:206:ILE:N	3:C:206:ILE:HD12	2.35	0.42
1:D:289:TRP:CD1	1:D:289:TRP:N	2.87	0.42
1:A:170:SER:HA	1:A:186:LYS:HE3	2.00	0.42
3:I:150:SER:O	3:I:151:GLY:O	2.37	0.42
1:A:141:ILE:HD12	1:A:185:TRP:CZ3	2.54	0.42
1:G:205:ASP:CG	1:G:227:GLN:HB3	2.40	0.42
1:A:205:ASP:CG	1:A:227:GLN:HB3	2.40	0.42
2:B:197:VAL:HG11	2:B:210:ILE:HG12	2.02	0.42
2:B:495:CYS:C	2:B:497:LEU:H	2.23	0.42
1:G:282:LYS:NZ	2:H:178:GLU:OE2	2.53	0.42
1:G:79:VAL:CG2	1:G:102:VAL:HG11	2.49	0.42
2:E:318:LEU:HD11	2:E:357:ILE:HD12	2.01	0.42
3:C:221:PRO:HG3	3:C:231:PHE:HB2	2.01	0.42
2:E:276:ILE:O	2:E:277:GLY:C	2.58	0.42
2:E:359:LYS:HG3	2:E:365:PRO:HA	2.01	0.42
2:H:202:ARG:HE	2:H:209:GLN:HB2	1.84	0.42
3:C:42:PHE:HD2	3:C:42:PHE:HA	1.76	0.42
3:F:17:ASP:O	3:F:20:LYS:HB2	2.20	0.42
3:F:20:LYS:O	3:F:24:ILE:HG12	2.20	0.42
1:D:229:ARG:CG	1:D:256:VAL:HA	2.50	0.42
1:D:55:PRO:HD3	2:E:138:ILE:HD13	2.00	0.42
1:A:277:LYS:HG3	1:A:278:VAL:N	2.35	0.42
1:G:285:LEU:CD1	1:G:285:LEU:H	2.27	0.42
1:A:285:LEU:CD1	1:A:285:LEU:H	2.27	0.42
3:F:116:LEU:CD2	3:F:294:LEU:CD1	2.95	0.42
2:B:299:LEU:HD23	2:B:299:LEU:HA	1.79	0.42
3:F:125:TRP:O	3:F:128:GLU:HB3	2.20	0.42
1:A:282:LYS:CD	1:A:292:ALA:HB2	2.50	0.42
1:A:112:TYR:CZ	1:A:171:ARG:HG2	2.54	0.42
1:A:202:GLY:HA3	1:A:245:LYS:HE3	2.02	0.42
1:G:216:VAL:HG23	2:H:505:ASP:OD2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:CYS:O	2:B:132:ILE:HG13	2.20	0.42
3:F:419:LEU:HA	3:F:422:LEU:HB2	2.00	0.42
2:H:317:HIS:ND1	3:I:159:ASP:OD1	2.53	0.42
3:F:195:GLU:OE2	3:F:195:GLU:N	2.44	0.42
2:H:527:LEU:O	2:H:530:LEU:HB2	2.20	0.41
3:I:8:GLN:O	3:I:11:ARG:HG2	2.21	0.41
2:E:198:THR:O	2:E:211:SER:HB3	2.19	0.41
2:H:291:ILE:HD12	2:H:291:ILE:N	2.20	0.41
2:H:491:LEU:O	2:H:494:SER:HB2	2.20	0.41
2:B:197:VAL:HG21	2:B:492:PHE:CZ	2.55	0.41
3:C:102:ARG:HH22	3:C:241:SER:H	1.68	0.41
2:B:297:TYR:HE2	2:B:305:ARG:HH11	1.67	0.41
3:I:235:GLN:HG2	3:I:236:GLY:H	1.85	0.41
3:C:439:SER:C	3:C:441:CYS:N	2.73	0.41
3:F:259:TYR:O	3:F:263:ILE:HG13	2.20	0.41
3:C:378:ASP:HB3	3:C:381:ASP:OD2	2.19	0.41
3:C:187:LEU:HD23	3:C:187:LEU:HA	1.93	0.41
2:E:295:PHE:CE1	2:E:356:LYS:HB3	2.55	0.41
2:E:527:LEU:O	2:E:530:LEU:HB2	2.19	0.41
2:B:187:ASP:HB3	2:B:523:ASN:HD22	1.82	0.41
3:C:341:HIS:HA	3:C:342:PRO:HD3	1.90	0.41
2:B:142:ARG:HH11	2:B:142:ARG:HG3	1.84	0.41
1:D:205:ASP:CG	1:D:227:GLN:HB3	2.40	0.41
2:H:198:THR:O	2:H:211:SER:HB3	2.19	0.41
1:A:229:ARG:CG	1:A:256:VAL:HA	2.50	0.41
1:G:200:LEU:HD11	1:G:243:TRP:CG	2.55	0.41
1:A:200:LEU:HD11	1:A:243:TRP:CG	2.55	0.41
3:C:323:THR:O	3:C:327:VAL:HG23	2.20	0.41
3:I:227:ILE:O	3:I:229:ASN:N	2.53	0.41
3:C:125:TRP:O	3:C:128:GLU:HB3	2.20	0.41
1:D:282:LYS:CD	1:D:292:ALA:HB2	2.50	0.41
3:F:288:ILE:O	3:F:291:ASN:HB3	2.21	0.41
3:C:150:SER:O	3:C:151:GLY:O	2.37	0.41
2:B:359:LYS:HG3	2:B:365:PRO:HA	2.01	0.41
3:C:359:ILE:HG21	3:C:404:VAL:HG11	2.03	0.41
2:E:527:LEU:C	2:E:529:ARG:N	2.71	0.41
2:H:139:MET:CG	2:H:144:PHE:O	2.47	0.41
1:A:140:ILE:CG2	1:A:141:ILE:H	2.33	0.41
3:C:39:ILE:HA	3:C:42:PHE:HB2	2.02	0.41
3:I:12:PHE:CD1	3:I:12:PHE:N	2.70	0.41
3:F:39:ILE:HA	3:F:42:PHE:HB2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:THR:C	2:H:513:ARG:HD2	2.38	0.41
1:D:233:ILE:HG22	1:D:235:THR:HG23	2.03	0.41
1:G:277:LYS:HG3	1:G:278:VAL:N	2.35	0.41
3:I:298:ILE:H	3:I:298:ILE:HD12	1.84	0.41
3:I:125:TRP:O	3:I:128:GLU:HB3	2.20	0.41
2:B:225:GLU:C	2:B:227:THR:N	2.73	0.41
2:B:468:GLU:OE1	2:B:468:GLU:N	2.47	0.41
1:G:151:ALA:HA	1:G:174:VAL:O	2.20	0.41
2:B:359:LYS:HA	2:B:359:LYS:HD2	1.80	0.41
2:B:276:ILE:O	2:B:277:GLY:C	2.59	0.41
3:F:322:LEU:HA	3:F:322:LEU:HD23	1.77	0.41
3:I:39:ILE:HA	3:I:42:PHE:HB2	2.02	0.41
2:H:208:PRO:HB3	2:H:531:LYS:CB	2.25	0.41
2:H:208:PRO:O	2:H:209:GLN:CB	2.68	0.41
3:C:68:TRP:CH2	3:C:387:ARG:NH2	2.89	0.41
1:D:79:VAL:CG2	1:D:102:VAL:HG11	2.49	0.41
2:B:512:MET:O	2:B:515:ILE:HG12	2.20	0.41
2:B:291:ILE:HD12	2:B:291:ILE:N	2.21	0.41
2:H:159:LEU:CD1	2:H:160:LEU:N	2.79	0.41
2:E:197:VAL:CG1	2:E:210:ILE:HG23	2.51	0.41
1:D:277:LYS:HG3	1:D:278:VAL:N	2.35	0.41
3:C:50:ALA:HB1	3:C:69:GLU:CG	2.49	0.41
3:I:281:ASP:O	3:I:282:TRP:C	2.59	0.41
1:A:208:ARG:HE	1:A:258:TRP:HZ3	1.67	0.41
1:G:212:TRP:HA	1:G:222:LEU:HD22	1.92	0.41
2:H:198:THR:HG22	2:H:198:THR:O	2.20	0.41
1:G:233:ILE:HG22	1:G:235:THR:HG23	2.03	0.41
1:D:200:LEU:HD11	1:D:243:TRP:CG	2.55	0.41
2:E:291:ILE:N	2:E:291:ILE:HD12	2.21	0.41
3:F:432:TYR:O	3:F:435:PHE:HD1	2.04	0.41
3:F:323:THR:O	3:F:327:VAL:HG23	2.20	0.41
3:I:102:ARG:HH22	3:I:241:SER:H	1.68	0.41
3:F:143:LYS:HE3	3:F:144:TRP:CD1	2.54	0.41
1:D:283:GLU:HB2	1:D:289:TRP:CH2	2.56	0.41
1:A:283:GLU:HB2	1:A:289:TRP:CH2	2.56	0.41
2:H:359:LYS:HD2	2:H:359:LYS:HA	1.80	0.41
3:C:288:ILE:O	3:C:291:ASN:HB3	2.21	0.41
3:C:421:LYS:O	3:C:424:GLY:N	2.44	0.41
2:H:276:ILE:O	2:H:277:GLY:C	2.59	0.41
3:I:259:TYR:O	3:I:263:ILE:HG13	2.20	0.41
2:E:202:ARG:CG	2:E:500:ASP:OD1	2.67	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:PHE:C	1:A:255:ASP:H	2.24	0.41
3:F:363:VAL:HG12	3:F:364:GLU:N	2.35	0.41
1:G:19:TYR:CD2	2:H:543:LEU:CD2	3.03	0.41
2:E:319:SER:OG	3:F:246:THR:HG23	2.21	0.41
2:B:320:VAL:CG2	3:C:246:THR:HG22	2.45	0.41
2:H:197:VAL:HG11	2:H:210:ILE:HG12	2.02	0.41
1:G:63:HIS:C	1:G:65:LYS:N	2.74	0.41
3:I:21:GLU:HA	3:I:25:GLU:HG3	2.02	0.41
3:F:227:ILE:O	3:F:229:ASN:N	2.53	0.41
2:B:329:ASP:OD1	2:B:331:ARG:HB2	2.20	0.41
1:D:63:HIS:C	1:D:65:LYS:N	2.74	0.41
1:D:202:GLY:HA3	1:D:245:LYS:HE3	2.02	0.41
1:G:202:GLY:HA3	1:G:245:LYS:HE3	2.02	0.41
2:H:406:HIS:CE1	2:H:410:PHE:CE1	3.09	0.41
2:B:545:ASP:O	2:B:549:GLY:N	2.49	0.41
3:C:15:PHE:H	3:C:15:PHE:HD1	1.68	0.41
2:E:248:TYR:CD2	2:E:248:TYR:N	2.88	0.41
1:G:31:LYS:HA	1:G:56:VAL:HG23	2.03	0.41
3:F:379:ILE:C	3:F:381:ASP:H	2.23	0.41
2:H:513:ARG:HG2	2:H:513:ARG:O	2.21	0.41
3:C:432:TYR:O	3:C:435:PHE:HD1	2.03	0.41
2:H:197:VAL:CG1	2:H:210:ILE:HG23	2.51	0.41
2:B:197:VAL:CG1	2:B:210:ILE:HG23	2.51	0.41
2:E:491:LEU:O	2:E:494:SER:HB2	2.19	0.41
1:A:63:HIS:C	1:A:65:LYS:N	2.74	0.41
3:I:21:GLU:HB3	3:I:25:GLU:CD	2.40	0.41
1:G:282:LYS:CD	1:G:292:ALA:HB2	2.50	0.41
2:H:468:GLU:OE1	2:H:468:GLU:N	2.46	0.41
3:F:50:ALA:O	3:F:54:ALA:HB2	2.21	0.41
3:C:50:ALA:O	3:C:54:ALA:HB2	2.21	0.41
3:I:50:ALA:O	3:I:54:ALA:HB2	2.21	0.41
2:H:234:TRP:CZ3	2:H:452:TYR:CD1	3.08	0.41
3:F:317:LEU:HA	3:F:318:PRO:HD2	1.90	0.41
2:E:364:SER:HB3	2:E:367:GLU:HB2	2.02	0.41
3:I:221:PRO:HG3	3:I:231:PHE:HB2	2.01	0.41
3:C:259:TYR:O	3:C:263:ILE:HG13	2.20	0.41
2:H:187:ASP:HB3	2:H:523:ASN:HD22	1.82	0.41
1:D:118:VAL:O	1:D:125:VAL:HG13	2.21	0.41
2:B:160:LEU:CD2	2:B:172:ILE:HA	2.50	0.41
2:H:160:LEU:CD2	2:H:172:ILE:HA	2.50	0.41
2:E:225:GLU:C	2:E:227:THR:N	2.73	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:HIS:CE1	2:B:410:PHE:CE1	3.09	0.41
2:E:199:ILE:HG22	2:E:209:GLN:H	1.86	0.41
2:E:208:PRO:O	2:E:209:GLN:CB	2.68	0.41
1:A:9:ASN:OD1	1:A:12:ILE:HD11	2.21	0.41
3:F:14:LYS:O	3:F:17:ASP:HB3	2.21	0.41
2:B:198:THR:HG22	2:B:198:THR:O	2.20	0.41
1:D:31:LYS:HA	1:D:56:VAL:HG23	2.03	0.41
2:E:198:THR:O	2:E:198:THR:HG22	2.20	0.41
2:H:512:MET:O	2:H:515:ILE:HG12	2.20	0.41
3:C:280:SER:CB	3:C:284:SER:HB3	2.41	0.41
1:A:233:ILE:HG22	1:A:235:THR:HG23	2.03	0.41
2:B:495:CYS:O	2:B:497:LEU:N	2.54	0.41
1:G:270:ALA:HB2	2:H:153:PHE:CE1	2.55	0.41
2:E:512:MET:O	2:E:515:ILE:HG12	2.21	0.41
1:A:96:ALA:O	1:A:98:HIS:N	2.52	0.41
1:D:78:LYS:CA	1:D:96:ALA:HB2	2.42	0.41
2:E:495:CYS:O	2:E:497:LEU:N	2.54	0.41
2:H:265:HIS:HB2	2:H:399:LEU:CD2	2.42	0.41
1:D:271:LEU:O	1:D:278:VAL:HG13	2.21	0.41
3:I:323:THR:O	3:I:327:VAL:HG23	2.20	0.41
2:H:299:LEU:CD2	2:H:387:LEU:HD21	2.46	0.41
1:D:77:GLY:CA	1:D:100:ALA:O	2.67	0.41
2:H:250:THR:HG21	2:H:255:VAL:CB	2.50	0.41
1:A:118:VAL:O	1:A:125:VAL:HG13	2.21	0.41
2:E:342:LYS:CD	3:F:206:ILE:HD11	2.51	0.41
1:A:265:SER:O	2:B:483:PHE:CZ	2.74	0.41
1:G:283:GLU:HB2	1:G:289:TRP:CH2	2.55	0.41
3:F:220:ASN:HA	3:F:221:PRO:HD3	1.87	0.41
3:I:145:LEU:HD12	3:I:145:LEU:HA	1.75	0.41
2:E:513:ARG:HG2	2:E:513:ARG:O	2.21	0.41
3:F:187:LEU:HA	3:F:187:LEU:HD23	1.92	0.41
3:C:145:LEU:HA	3:C:145:LEU:HD12	1.75	0.41
2:H:199:ILE:HG22	2:H:209:GLN:H	1.86	0.41
2:B:162:LYS:HE2	2:B:164:ILE:CG2	2.51	0.41
1:D:253:PHE:C	1:D:255:ASP:H	2.24	0.41
2:B:513:ARG:HG2	2:B:513:ARG:O	2.21	0.41
3:F:355:LEU:HD12	3:F:355:LEU:HA	1.84	0.41
2:B:392:GLY:O	2:B:393:GLN:HB3	2.19	0.41
2:E:314:LYS:HG2	3:F:162:LEU:O	2.21	0.41
2:B:250:THR:HG21	2:B:255:VAL:CB	2.50	0.41
1:A:61:TRP:CD1	1:A:61:TRP:N	2.87	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:281:ASP:O	3:C:282:TRP:C	2.60	0.41
3:F:58:ASP:HB2	3:F:60:SER:H	1.85	0.41
2:B:234:TRP:CZ3	2:B:452:TYR:CD1	3.08	0.41
3:F:419:LEU:O	3:F:423:GLN:HB2	2.21	0.41
2:H:343:TRP:C	2:H:345:THR:H	2.24	0.41
1:G:60:ASP:H	1:G:70:LEU:CD1	2.34	0.41
3:I:362:SER:O	3:I:365:MET:HB3	2.21	0.41
3:I:288:ILE:O	3:I:291:ASN:HB3	2.21	0.41
2:E:525:HIS:O	2:E:527:LEU:N	2.54	0.40
2:B:199:ILE:HG22	2:B:209:GLN:H	1.86	0.40
3:I:432:TYR:O	3:I:435:PHE:HD1	2.04	0.40
2:H:153:PHE:HE2	2:H:175:LEU:HD22	1.86	0.40
1:A:79:VAL:CG2	1:A:102:VAL:HG11	2.49	0.40
3:F:88:ASP:O	3:F:90:ASP:N	2.54	0.40
1:D:151:ALA:HA	1:D:174:VAL:O	2.20	0.40
3:C:48:GLN:O	3:C:51:LEU:HB2	2.21	0.40
2:B:389:LEU:HA	2:B:389:LEU:HD23	1.86	0.40
2:E:202:ARG:HD2	2:E:500:ASP:OD1	2.21	0.40
2:H:138:ILE:O	2:H:142:ARG:HB2	2.20	0.40
2:B:208:PRO:O	2:B:209:GLN:CB	2.69	0.40
2:E:142:ARG:HG2	2:E:144:PHE:CE1	2.54	0.40
2:H:495:CYS:O	2:H:497:LEU:N	2.54	0.40
1:D:285:LEU:CD1	1:D:285:LEU:H	2.27	0.40
3:I:23:LYS:O	3:I:27:ASN:HB2	2.21	0.40
1:D:95:HIS:CG	1:D:128:VAL:HG21	2.57	0.40
1:G:71:ALA:HB2	1:G:107:TRP:CZ2	2.56	0.40
1:A:71:ALA:HB2	1:A:107:TRP:CZ2	2.57	0.40
1:D:151:ALA:CB	1:D:175:THR:HG22	2.51	0.40
1:G:155:PRO:HG3	1:G:214:PRO:HA	2.02	0.40
2:E:517:LEU:HD12	2:E:517:LEU:N	2.36	0.40
2:B:202:ARG:HD2	2:B:500:ASP:OD1	2.21	0.40
3:I:10:GLU:O	3:I:10:GLU:HG3	2.22	0.40
1:G:253:PHE:C	1:G:255:ASP:H	2.24	0.40
1:D:80:LEU:O	1:D:82:TRP:CD1	2.75	0.40
2:H:515:ILE:HD11	2:H:544:LYS:HB2	2.04	0.40
2:E:160:LEU:CD2	2:E:172:ILE:HA	2.50	0.40
2:H:190:LEU:CD1	2:H:492:PHE:HD1	2.35	0.40
1:G:264:LEU:HB3	2:H:509:ARG:CZ	2.51	0.40
2:E:392:GLY:O	2:E:393:GLN:HB3	2.19	0.40
2:E:285:ARG:NH1	2:E:285:ARG:HG3	2.33	0.40
2:H:220:ALA:O	2:H:224:MET:HG3	2.22	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:ASP:O	1:G:206:TRP:C	2.60	0.40
1:D:205:ASP:O	1:D:206:TRP:C	2.60	0.40
3:C:18:THR:O	3:C:19:LEU:C	2.59	0.40
3:C:81:LEU:CD2	3:C:118:GLN:HG2	2.51	0.40
1:D:71:ALA:HB2	1:D:107:TRP:CZ2	2.56	0.40
1:D:81:ILE:HG12	1:D:130:PHE:HZ	1.86	0.40
2:B:325:LEU:HD23	2:B:361:LEU:HD23	2.03	0.40
3:F:390:THR:O	3:F:394:ILE:HG12	2.22	0.40
3:I:251:SER:O	3:I:261:ARG:HD2	2.21	0.40
2:B:517:LEU:N	2:B:517:LEU:HD12	2.37	0.40
3:I:90:ASP:OD1	3:I:90:ASP:N	2.54	0.40
2:B:525:HIS:O	2:B:527:LEU:N	2.54	0.40
1:D:57:TRP:HD1	1:D:102:VAL:O	2.05	0.40
2:E:153:PHE:HE2	2:E:175:LEU:HD22	1.86	0.40
1:A:271:LEU:O	1:A:278:VAL:HG13	2.21	0.40
3:F:102:ARG:HH22	3:F:241:SER:H	1.68	0.40
1:G:118:VAL:O	1:G:125:VAL:HG13	2.21	0.40
3:F:206:ILE:HD12	3:F:206:ILE:N	2.36	0.40
1:G:81:ILE:HG12	1:G:130:PHE:HZ	1.86	0.40
1:A:81:ILE:HG12	1:A:130:PHE:HZ	1.86	0.40
2:B:374:GLU:C	2:B:376:GLU:H	2.25	0.40
3:I:212:LEU:HA	3:I:212:LEU:HD23	1.76	0.40
2:H:517:LEU:N	2:H:517:LEU:HD12	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	270/297 (91%)	199 (74%)	51 (19%)	20 (7%)	1	9
1	D	270/297 (91%)	200 (74%)	51 (19%)	19 (7%)	1	10

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	270/297 (91%)	200 (74%)	50 (18%)	20 (7%)	1	9
2	B	432/442 (98%)	346 (80%)	55 (13%)	31 (7%)	1	10
2	E	421/442 (95%)	343 (82%)	48 (11%)	30 (7%)	1	10
2	H	418/442 (95%)	339 (81%)	49 (12%)	30 (7%)	1	10
3	C	413/460 (90%)	341 (83%)	55 (13%)	17 (4%)	3	27
3	F	413/460 (90%)	343 (83%)	53 (13%)	17 (4%)	3	27
3	I	408/460 (89%)	334 (82%)	56 (14%)	18 (4%)	3	24
All	All	3315/3597 (92%)	2645 (80%)	468 (14%)	202 (6%)	2	15

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	254	PRO
2	B	209	GLN
2	B	348	CYS
2	B	367	GLU
2	B	370	PHE
2	B	392	GLY
2	B	393	GLN
2	B	428	ASN
2	B	513	ARG
3	C	9	THR
3	C	11	ARG
3	C	55	ASN
3	C	90	ASP
3	C	165	ASN
3	C	434	THR
1	D	254	PRO
2	E	209	GLN
2	E	348	CYS
2	E	367	GLU
2	E	370	PHE
2	E	392	GLY
2	E	393	GLN
2	E	428	ASN
2	E	513	ARG
2	E	550	ASN
3	F	8	GLN
3	F	9	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	F	11	ARG
3	F	55	ASN
3	F	165	ASN
3	F	434	THR
1	G	254	PRO
2	H	209	GLN
2	H	348	CYS
2	H	367	GLU
2	H	370	PHE
2	H	392	GLY
2	H	393	GLN
2	H	428	ASN
2	H	513	ARG
3	I	8	GLN
3	I	29	GLU
3	I	165	ASN
3	I	434	THR
1	A	97	VAL
1	A	110	HIS
1	A	248	LEU
2	B	139	MET
2	B	146	ALA
2	B	157	SER
2	B	182	LYS
2	B	183	PHE
2	B	205	ASN
2	B	220	ALA
2	B	277	GLY
2	B	328	ASN
2	B	347	GLY
2	B	515	ILE
2	B	531	LYS
2	B	535	GLN
3	C	151	GLY
3	C	226	GLN
1	D	97	VAL
1	D	110	HIS
1	D	248	LEU
2	E	157	SER
2	E	182	LYS
2	E	183	PHE
2	E	205	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	220	ALA
2	E	277	GLY
2	E	328	ASN
2	E	347	GLY
2	E	515	ILE
2	E	531	LYS
2	E	535	GLN
3	F	90	ASP
3	F	151	GLY
3	F	226	GLN
1	G	97	VAL
1	G	110	HIS
1	G	248	LEU
2	H	143	ARG
2	H	157	SER
2	H	182	LYS
2	H	183	PHE
2	H	205	ASN
2	H	220	ALA
2	H	277	GLY
2	H	328	ASN
2	H	347	GLY
2	H	515	ILE
2	H	531	LYS
2	H	535	GLN
3	I	55	ASN
3	I	59	GLU
3	I	151	GLY
3	I	226	GLN
1	A	19	TYR
1	A	51	GLY
1	A	105	VAL
1	A	115	LEU
1	A	202	GLY
1	A	206	TRP
1	A	207	VAL
1	A	208	ARG
2	B	162	LYS
2	B	530	LEU
2	B	536	LEU
3	C	12	PHE
3	C	19	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	19	TYR
1	D	51	GLY
1	D	105	VAL
1	D	115	LEU
1	D	202	GLY
1	D	206	TRP
1	D	207	VAL
1	D	208	ARG
2	E	162	LYS
2	E	530	LEU
2	E	536	LEU
3	F	21	GLU
3	F	87	ALA
1	G	19	TYR
1	G	51	GLY
1	G	105	VAL
1	G	115	LEU
1	G	202	GLY
1	G	206	TRP
1	G	207	VAL
1	G	208	ARG
2	H	162	LYS
2	H	530	LEU
2	H	536	LEU
3	I	57	GLY
3	I	93	GLU
3	I	383	PRO
2	B	144	PHE
2	B	164	ILE
2	B	496	PHE
2	B	508	LYS
2	B	516	THR
2	B	527	LEU
3	C	21	GLU
3	C	59	GLU
3	C	403	SER
1	D	11	LEU
2	E	164	ILE
2	E	496	PHE
2	E	508	LYS
2	E	516	THR
2	E	527	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	F	403	SER
1	G	11	LEU
2	H	164	ILE
2	H	496	PHE
2	H	508	LYS
2	H	516	THR
2	H	527	LEU
3	I	92	ASP
3	I	403	SER
1	A	114	PRO
3	C	152	GLY
3	C	354	SER
1	D	114	PRO
3	F	20	LYS
3	F	152	GLY
3	F	354	SER
1	G	114	PRO
3	I	152	GLY
3	I	354	SER
3	I	422	LEU
1	A	64	PRO
1	A	83	LYS
1	A	192	GLN
1	A	243	TRP
1	A	276	ASN
3	C	333	SER
1	D	64	PRO
1	D	83	LYS
1	D	243	TRP
1	D	276	ASN
3	F	333	SER
1	G	64	PRO
1	G	83	LYS
1	G	192	GLN
1	G	243	TRP
1	G	276	ASN
3	I	333	SER
1	A	216	VAL
1	D	216	VAL
3	F	383	PRO
1	G	216	VAL
2	B	208	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	208	PRO
2	H	208	PRO
2	E	329	ASP
2	H	329	ASP
3	C	383	PRO
3	I	382	LYS

### 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	233/252 (92%)	221 (95%)	12 (5%)	29	69
1	D	233/252 (92%)	222 (95%)	11 (5%)	32	73
1	G	233/252 (92%)	223 (96%)	10 (4%)	35	75
2	B	397/404 (98%)	362 (91%)	35 (9%)	12	45
2	E	386/404 (96%)	352 (91%)	34 (9%)	12	45
2	H	383/404 (95%)	350 (91%)	33 (9%)	13	46
3	C	387/425 (91%)	361 (93%)	26 (7%)	20	60
3	F	387/425 (91%)	359 (93%)	28 (7%)	18	57
3	I	382/425 (90%)	358 (94%)	24 (6%)	22	63
All	All	3021/3243 (93%)	2808 (93%)	213 (7%)	18	57

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	13	HIS
1	A	20	TYR
1	A	30	ASP
1	A	43	HIS
1	A	46	ILE
1	A	57	TRP
1	A	85	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	188	ASN
1	A	217	LEU
1	A	237	ASP
1	A	275	ASP
2	B	142	ARG
2	B	144	PHE
2	B	159	LEU
2	B	177	THR
2	B	197	VAL
2	B	199	ILE
2	B	202	ARG
2	B	227	THR
2	B	233	LEU
2	B	282	GLU
2	B	307	SER
2	B	328	ASN
2	B	335	LEU
2	B	340	LEU
2	B	350	ILE
2	B	367	GLU
2	B	369	LEU
2	B	370	PHE
2	B	399	LEU
2	B	407	LEU
2	B	414	TYR
2	B	418	ILE
2	B	430	ASN
2	B	439	ARG
2	B	447	VAL
2	B	452	TYR
2	B	455	GLN
2	B	463	ARG
2	B	468	GLU
2	B	490	SER
2	B	492	PHE
2	B	515	ILE
2	B	538	PHE
2	B	547	TYR
2	B	550	ASN
3	C	18	THR
3	C	26	GLN
3	C	34	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	39	ILE
3	C	42	PHE
3	C	58	ASP
3	C	71	GLU
3	C	86	ASN
3	C	92	ASP
3	C	118	GLN
3	C	225	THR
3	C	226	GLN
3	C	232	ASN
3	C	237	ILE
3	C	274	GLN
3	C	278	GLN
3	C	284	SER
3	C	293	ILE
3	C	343	ILE
3	C	365	MET
3	C	379	ILE
3	C	387	ARG
3	C	395	CYS
3	C	404	VAL
3	C	422	LEU
3	C	429	ILE
1	D	9	ASN
1	D	20	TYR
1	D	30	ASP
1	D	43	HIS
1	D	46	ILE
1	D	57	TRP
1	D	85	GLU
1	D	188	ASN
1	D	217	LEU
1	D	237	ASP
1	D	275	ASP
2	E	142	ARG
2	E	143	ARG
2	E	145	THR
2	E	159	LEU
2	E	197	VAL
2	E	199	ILE
2	E	202	ARG
2	E	227	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	233	LEU
2	E	282	GLU
2	E	307	SER
2	E	328	ASN
2	E	335	LEU
2	E	340	LEU
2	E	350	ILE
2	E	367	GLU
2	E	369	LEU
2	E	370	PHE
2	E	399	LEU
2	E	407	LEU
2	E	414	TYR
2	E	418	ILE
2	E	430	ASN
2	E	439	ARG
2	E	447	VAL
2	E	452	TYR
2	E	455	GLN
2	E	463	ARG
2	E	468	GLU
2	E	490	SER
2	E	492	PHE
2	E	515	ILE
2	E	538	PHE
2	E	550	ASN
3	F	7	TYR
3	F	12	PHE
3	F	19	LEU
3	F	34	ASP
3	F	39	ILE
3	F	42	PHE
3	F	58	ASP
3	F	71	GLU
3	F	86	ASN
3	F	118	GLN
3	F	225	THR
3	F	226	GLN
3	F	232	ASN
3	F	237	ILE
3	F	274	GLN
3	F	278	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	F	284	SER
3	F	293	ILE
3	F	310	THR
3	F	343	ILE
3	F	363	VAL
3	F	365	MET
3	F	387	ARG
3	F	395	CYS
3	F	400	ASN
3	F	404	VAL
3	F	423	GLN
3	F	429	ILE
1	G	20	TYR
1	G	30	ASP
1	G	43	HIS
1	G	46	ILE
1	G	57	TRP
1	G	85	GLU
1	G	188	ASN
1	G	217	LEU
1	G	237	ASP
1	G	275	ASP
2	H	132	ILE
2	H	139	MET
2	H	159	LEU
2	H	197	VAL
2	H	199	ILE
2	H	202	ARG
2	H	227	THR
2	H	233	LEU
2	H	282	GLU
2	H	307	SER
2	H	328	ASN
2	H	335	LEU
2	H	340	LEU
2	H	350	ILE
2	H	367	GLU
2	H	369	LEU
2	H	370	PHE
2	H	399	LEU
2	H	407	LEU
2	H	414	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	418	ILE
2	H	430	ASN
2	H	439	ARG
2	H	447	VAL
2	H	452	TYR
2	H	455	GLN
2	H	463	ARG
2	H	468	GLU
2	H	490	SER
2	H	492	PHE
2	H	515	ILE
2	H	538	PHE
2	H	547	TYR
3	I	9	THR
3	I	12	PHE
3	I	34	ASP
3	I	39	ILE
3	I	42	PHE
3	I	71	GLU
3	I	86	ASN
3	I	90	ASP
3	I	93	GLU
3	I	118	GLN
3	I	225	THR
3	I	226	GLN
3	I	232	ASN
3	I	237	ILE
3	I	274	GLN
3	I	278	GLN
3	I	284	SER
3	I	293	ILE
3	I	310	THR
3	I	343	ILE
3	I	387	ARG
3	I	395	CYS
3	I	404	VAL
3	I	429	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	13	HIS
1	A	63	HIS
3	C	235	GLN
1	D	9	ASN
1	D	149	ASN
2	E	328	ASN
3	F	300	ASN
1	G	9	ASN
2	H	328	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	274/297 (92%)	1.71	92 (33%) 0 0	103, 167, 201, 202	0
1	D	274/297 (92%)	1.85	102 (37%) 0 0	101, 185, 202, 202	0
1	G	274/297 (92%)	1.97	116 (42%) 0 0	127, 193, 202, 202	0
2	B	434/442 (98%)	0.21	12 (2%) 56 42	44, 102, 181, 202	2 (0%)
2	E	423/442 (95%)	0.43	35 (8%) 14 7	49, 94, 192, 202	2 (0%)
2	H	420/442 (95%)	0.87	80 (19%) 2 1	46, 122, 200, 202	2 (0%)
3	C	419/460 (91%)	0.15	13 (3%) 52 38	9, 95, 175, 202	19 (4%)
3	F	419/460 (91%)	0.22	21 (5%) 32 19	11, 96, 178, 201	19 (4%)
3	I	414/460 (90%)	0.14	17 (4%) 41 27	48, 95, 181, 202	0
All	All	3351/3597 (93%)	0.71	488 (14%) 3 2	9, 124, 201, 202	44 (1%)

All (488) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	148	VAL	11.0
1	D	73	CYS	10.7
1	D	41	GLU	10.3
1	D	136	THR	10.0
2	E	138	ILE	9.5
1	A	223	ALA	9.3
2	E	134	ASN	9.2
1	A	127	VAL	9.1
1	D	272	SER	8.9
2	H	132	ILE	8.9
1	D	223	ALA	8.7
1	D	72	SER	8.6
2	H	133	ASP	8.6
1	G	272	SER	8.5
1	A	194	TYR	8.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	170	VAL	8.1
1	G	134	GLY	8.0
2	H	145	THR	8.0
2	H	523	ASN	7.9
1	D	273	GLY	7.9
1	G	133	ASN	7.8
1	A	128	VAL	7.6
1	G	72	SER	7.4
2	E	133	ASP	7.3
1	A	136	THR	7.2
1	D	224	SER	7.2
1	D	117	LEU	7.1
1	D	118	VAL	7.1
1	G	273	GLY	7.1
2	E	136	LYS	7.1
1	A	185	TRP	7.0
1	G	112	TYR	6.9
1	A	126	SER	6.9
2	H	172	ILE	6.8
1	A	70	LEU	6.7
1	A	138	PRO	6.7
1	G	201	GLU	6.6
1	G	147	GLY	6.6
2	H	135	ALA	6.6
1	G	144	HIS	6.5
2	H	150	PHE	6.5
2	H	547	TYR	6.5
2	H	134	ASN	6.5
1	G	41	GLU	6.3
1	D	135	THR	6.3
2	E	130	ASP	6.2
1	D	210	VAL	6.2
2	H	169	GLY	6.1
2	H	149	THR	6.1
1	A	200	LEU	6.1
1	G	149	ASN	6.1
1	D	40	GLY	6.0
1	D	143	ALA	6.0
1	G	177	GLY	6.0
2	H	162	LYS	5.9
1	G	82	TRP	5.9
1	G	135	THR	5.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	95	HIS	5.8
1	G	143	ALA	5.8
2	E	135	ALA	5.8
2	E	144	PHE	5.8
1	G	89	TRP	5.8
1	D	74	SER	5.7
1	D	32	THR	5.7
2	E	139	MET	5.7
2	H	532	ILE	5.5
1	D	225	VAL	5.5
3	F	432	TYR	5.4
1	G	73	CYS	5.4
1	A	50	THR	5.4
2	H	208	PRO	5.4
1	G	98	HIS	5.3
1	A	193	THR	5.2
2	H	161	THR	5.2
2	E	168	SER	5.2
2	E	145	THR	5.1
2	E	131	GLU	5.1
1	D	248	LEU	5.1
1	G	70	LEU	5.1
1	G	119	ALA	5.0
1	D	138	PRO	5.0
2	E	132	ILE	5.0
2	H	163	ASP	5.0
1	G	33	ILE	5.0
2	H	537	ILE	5.0
1	D	271	LEU	5.0
3	I	432	TYR	4.9
2	E	167	LYS	4.9
1	A	125	VAL	4.9
1	A	260	ALA	4.9
2	H	489	HIS	4.8
3	F	53	LEU	4.8
1	G	185	TRP	4.8
1	D	126	SER	4.8
1	D	201	GLU	4.8
2	H	543	LEU	4.7
1	G	29	SER	4.6
1	D	176	GLY	4.6
2	H	171	SER	4.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	178	ALA	4.6
2	H	131	GLU	4.6
2	H	146	ALA	4.6
2	H	527	LEU	4.6
1	G	271	LEU	4.6
1	A	182	VAL	4.6
1	A	143	ALA	4.6
1	G	132	GLU	4.5
1	G	12	ILE	4.5
1	A	231	CYS	4.5
2	H	148	TYR	4.5
1	G	125	VAL	4.5
1	A	71	ALA	4.5
3	C	15	PHE	4.5
1	G	16	VAL	4.4
1	D	15	ALA	4.4
1	D	187	TYR	4.4
1	A	221	TYR	4.4
1	D	270	ALA	4.4
1	D	209	ASP	4.4
1	A	135	THR	4.3
2	E	146	ALA	4.3
1	D	289	TRP	4.3
1	A	44	LYS	4.3
2	H	130	ASP	4.3
1	G	118	VAL	4.3
1	D	208	ARG	4.3
1	A	195	VAL	4.3
1	D	59	VAL	4.3
1	G	56	VAL	4.3
1	G	13	HIS	4.3
1	A	98	HIS	4.3
1	D	96	ALA	4.2
1	D	151	ALA	4.2
1	G	281	TRP	4.2
1	G	90	SER	4.2
1	G	136	THR	4.1
1	G	28	SER	4.1
1	G	59	VAL	4.1
1	A	32	THR	4.1
1	A	272	SER	4.1
1	A	144	HIS	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	103	ASN	4.0
2	H	136	LYS	4.0
1	A	270	ALA	4.0
2	H	536	LEU	4.0
1	A	206	TRP	4.0
3	F	15	PHE	4.0
1	D	13	HIS	4.0
1	D	125	VAL	4.0
1	D	98	HIS	4.0
2	H	189	TYR	4.0
1	D	279	THR	3.9
2	H	147	SER	3.9
2	H	348	CYS	3.9
1	A	149	ASN	3.9
2	E	170	VAL	3.9
1	A	147	GLY	3.9
2	E	148	TYR	3.8
2	E	149	THR	3.8
1	D	33	ILE	3.8
1	D	173	PHE	3.8
1	G	69	ILE	3.8
1	D	102	VAL	3.8
2	H	166	GLY	3.8
2	E	137	LEU	3.7
1	A	196	LEU	3.7
1	D	275	ASP	3.7
1	G	141	ILE	3.7
2	E	147	SER	3.7
2	B	145	THR	3.7
1	A	148	VAL	3.7
1	A	254	PRO	3.7
1	D	274	GLY	3.6
2	H	183	PHE	3.6
1	A	234	TRP	3.6
1	G	243	TRP	3.6
1	G	274	GLY	3.6
3	C	53	LEU	3.6
1	D	226	SER	3.6
3	C	440	ASP	3.6
1	G	8	HIS	3.6
1	A	141	ILE	3.5
2	E	163	ASP	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	533	PRO	3.5
2	B	144	PHE	3.5
2	H	477	PHE	3.5
1	D	116	LEU	3.5
1	D	119	ALA	3.5
1	A	199	THR	3.5
1	D	114	PRO	3.5
1	A	243	TRP	3.4
1	D	26	THR	3.4
1	G	11	LEU	3.4
2	H	206	PRO	3.4
1	G	52	HIS	3.4
1	G	176	GLY	3.4
1	D	80	LEU	3.4
1	D	281	TRP	3.3
2	E	523	ASN	3.3
1	D	12	ILE	3.3
1	A	69	ILE	3.3
3	I	15	PHE	3.3
1	A	208	ARG	3.3
2	H	518	LEU	3.3
1	A	103	ASN	3.3
1	A	274	GLY	3.3
1	G	71	ALA	3.3
1	G	260	ALA	3.3
1	G	92	ILE	3.3
2	H	510	LEU	3.3
1	D	259	ARG	3.3
1	A	248	LEU	3.3
1	D	149	ASN	3.2
2	H	165	VAL	3.2
2	E	172	ILE	3.2
1	A	37	GLU	3.2
1	D	127	VAL	3.2
2	H	173	LYS	3.2
1	A	201	GLU	3.2
1	G	197	GLU	3.2
1	D	177	GLY	3.2
1	A	150	SER	3.2
1	A	140	ILE	3.2
1	A	118	VAL	3.2
1	D	140	ILE	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	26	THR	3.2
3	I	433	ALA	3.2
3	C	87	ALA	3.2
3	I	430	PRO	3.2
2	B	149	THR	3.2
1	G	102	VAL	3.2
1	D	97	VAL	3.1
2	E	140	LYS	3.1
1	A	181	LEU	3.1
2	H	164	ILE	3.1
1	D	185	TRP	3.1
1	D	69	ILE	3.1
3	I	59	GLU	3.1
1	G	87	GLY	3.1
3	F	8	GLN	3.1
1	D	52	HIS	3.1
2	E	150	PHE	3.1
2	H	196	LYS	3.1
1	D	194	TYR	3.0
1	D	133	ASN	3.0
1	A	241	GLY	3.0
2	B	527	LEU	3.0
2	H	178	GLU	3.0
1	A	176	GLY	3.0
1	G	113	GLY	3.0
1	A	129	GLU	3.0
3	I	435	PHE	3.0
1	D	250	GLU	3.0
1	G	15	ALA	3.0
1	G	248	LEU	3.0
1	D	81	ILE	3.0
1	G	86	ASN	3.0
1	D	56	VAL	3.0
2	H	157	SER	3.0
1	G	276	ASN	3.0
2	H	137	LEU	3.0
1	D	78	LYS	3.0
3	F	379	ILE	2.9
2	B	546	ARG	2.9
2	E	348	CYS	2.9
2	H	207	TYR	2.9
2	H	144	PHE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	209	ASP	2.9
1	A	225	VAL	2.9
1	G	189	SER	2.9
1	D	153	TRP	2.9
3	F	423	GLN	2.9
2	H	199	ILE	2.9
3	C	420	LEU	2.9
1	G	193	THR	2.9
2	H	139	MET	2.9
1	A	224	SER	2.9
1	D	189	SER	2.9
1	A	175	THR	2.8
1	D	95	HIS	2.8
1	G	47	ASP	2.8
1	G	194	TYR	2.8
1	D	204	SER	2.8
1	G	35	ILE	2.8
1	G	50	THR	2.8
1	D	28	SER	2.8
1	G	25	ALA	2.8
1	G	257	LEU	2.8
1	D	137	SER	2.8
1	D	58	ARG	2.8
1	G	226	SER	2.8
1	G	45	LEU	2.8
1	D	180	ASN	2.8
1	A	192	GLN	2.8
1	G	51	GLY	2.7
2	H	177	THR	2.7
1	G	192	GLN	2.7
2	B	547	TYR	2.7
1	D	128	VAL	2.7
1	G	57	TRP	2.7
1	G	293	GLY	2.7
1	A	276	ASN	2.7
1	G	80	LEU	2.7
1	D	103	ASN	2.7
3	C	19	LEU	2.7
1	G	88	ARG	2.7
1	D	252	LYS	2.7
3	C	39	ILE	2.7
3	F	380	ILE	2.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	207	VAL	2.7
1	G	188	ASN	2.6
1	A	269	LEU	2.6
2	B	179	LEU	2.6
1	A	222	LEU	2.6
2	H	548	GLU	2.6
1	G	9	ASN	2.6
1	G	150	SER	2.6
1	D	144	HIS	2.6
3	F	64	SER	2.6
2	H	484	ALA	2.6
1	A	210	VAL	2.6
1	G	97	VAL	2.6
2	H	168	SER	2.6
1	A	212	TRP	2.6
3	F	59	GLU	2.6
1	G	157	THR	2.6
3	I	416	TYR	2.6
1	G	122	ASP	2.6
1	G	202	GLY	2.6
2	E	392	GLY	2.6
2	E	162	LYS	2.6
1	G	104	SER	2.6
3	I	53	LEU	2.5
3	I	425	LEU	2.5
1	A	96	ALA	2.5
1	A	49	LEU	2.5
3	F	394	ILE	2.5
1	A	99	SER	2.5
1	G	279	THR	2.5
2	E	518	LEU	2.5
2	H	517	LEU	2.5
1	G	34	LYS	2.5
1	G	110	HIS	2.5
3	C	54	ALA	2.5
1	G	91	GLN	2.5
3	C	398	ILE	2.5
1	G	275	ASP	2.5
2	H	138	ILE	2.5
3	I	381	ASP	2.5
3	F	431	ILE	2.5
2	H	215	LEU	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	F	384	TYR	2.5
2	H	201	ALA	2.5
1	A	187	TYR	2.5
1	D	243	TRP	2.5
1	D	203	HIS	2.5
2	E	164	ILE	2.5
1	A	89	TRP	2.4
1	D	179	ASP	2.4
3	I	412	LEU	2.4
1	A	114	PRO	2.4
2	H	174	ARG	2.4
1	G	49	LEU	2.4
3	F	412	LEU	2.4
3	I	428	ASN	2.4
3	F	435	PHE	2.4
1	D	57	TRP	2.4
1	A	198	SER	2.4
2	E	522	THR	2.4
1	A	48	THR	2.4
1	G	240	GLN	2.4
1	A	13	HIS	2.4
1	D	269	LEU	2.4
1	G	128	VAL	2.4
2	H	480	GLN	2.4
2	H	496	PHE	2.4
3	C	439	SER	2.4
1	A	233	ILE	2.4
1	G	146	ILE	2.4
2	H	185	PHE	2.4
2	H	522	THR	2.4
1	A	130	PHE	2.4
2	H	481	LEU	2.4
1	A	261	SER	2.3
1	G	32	THR	2.3
1	A	227	GLN	2.3
1	D	184	ILE	2.3
1	D	245	LYS	2.3
1	D	47	ASP	2.3
1	G	99	SER	2.3
1	G	280	LEU	2.3
2	H	167	LYS	2.3
3	F	68	TRP	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	142	ASP	2.3
1	G	27	CYS	2.3
1	D	71	ALA	2.3
1	A	245	LYS	2.3
2	E	169	GLY	2.3
3	C	417	ILE	2.3
1	A	204	SER	2.3
1	A	116	LEU	2.3
1	G	53	GLU	2.3
2	B	140	LYS	2.3
2	H	516	THR	2.3
1	A	82	TRP	2.3
2	H	530	LEU	2.3
1	G	140	ILE	2.3
1	D	178	ALA	2.3
1	D	42	THR	2.3
1	D	70	LEU	2.3
1	D	105	VAL	2.3
1	G	124	LYS	2.3
3	I	426	TYR	2.3
1	A	174	VAL	2.3
1	G	130	PHE	2.2
1	G	196	LEU	2.2
2	H	190	LEU	2.2
1	A	220	SER	2.2
2	H	367	GLU	2.2
3	F	19	LEU	2.2
1	D	278	VAL	2.2
1	G	171	ARG	2.2
1	A	137	SER	2.2
1	G	17	LEU	2.2
2	H	159	LEU	2.2
3	F	359	ILE	2.2
3	I	429	ILE	2.2
3	F	391	HIS	2.2
2	B	147	SER	2.2
1	D	14	ASP	2.2
2	H	540	ALA	2.2
1	A	258	TRP	2.2
2	H	153	PHE	2.2
1	G	131	LYS	2.2
1	A	251	GLU	2.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	150	SER	2.2
1	G	225	VAL	2.2
2	B	392	GLY	2.2
1	G	74	SER	2.2
3	F	362	SER	2.2
1	G	184	ILE	2.2
1	A	191	ALA	2.2
3	C	436	LEU	2.2
3	I	19	LEU	2.2
1	G	14	ASP	2.2
2	H	392	GLY	2.2
1	D	132	GLU	2.2
2	H	209	GLN	2.2
2	H	524	ASP	2.1
1	D	234	TRP	2.1
3	F	75	TRP	2.1
2	H	521	SER	2.1
1	G	63	HIS	2.1
1	A	173	PHE	2.1
1	D	251	GLU	2.1
1	G	19	TYR	2.1
2	H	184	LEU	2.1
1	A	84	GLU	2.1
1	G	81	ILE	2.1
2	H	160	LEU	2.1
2	H	187	ASP	2.1
3	C	399	ILE	2.1
1	A	184	ILE	2.1
1	A	289	TRP	2.1
1	D	258	TRP	2.1
3	I	366	LEU	2.1
2	E	142	ARG	2.1
1	D	17	LEU	2.1
2	B	367	GLU	2.1
1	A	255	ASP	2.0
1	D	229	ARG	2.0
2	H	179	LEU	2.0
1	G	114	PRO	2.0
3	I	39	ILE	2.0
3	F	392	LEU	2.0
1	G	224	SER	2.0
2	E	367	GLU	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	348	CYS	2.0
1	G	145	ALA	2.0
1	G	292	ALA	2.0
1	D	25	ALA	2.0
2	H	193	GLU	2.0
1	D	113	GLY	2.0
1	D	104	SER	2.0
1	G	107	TRP	2.0
2	E	197	VAL	2.0
2	E	521	SER	2.0
1	A	211	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.