



## wwPDB EM Map/Model Validation Report ⓘ

Sep 27, 2016 – 02:27 PM EDT

PDB ID : 5SVA  
EMDB ID: : EMD-8305  
Title : Mediator-RNA Polymerase II Pre-Initiation Complex  
Authors : Robinson, P.J.; Bushnell, D.A.; Kornberg, R.D.  
Deposited on : 2016-08-05  
Resolution : 15.30 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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/EMValidationReportHelp>

---

MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

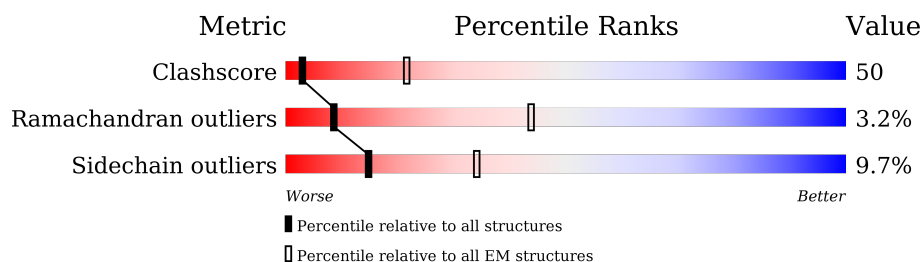
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 15.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	J	70	
11	K	120	
12	L	70	
13	M	295	
14	N	223	
15	O	115	
16	P	687	
17	Q	307	
18	R	210	
19	S	121	
20	T	284	
21	U	222	
22	V	149	
23	W	140	
24	X	127	
25	Y	778	
26	Z	843	
27	a	513	
28	b	72	
29	c	345	
30	d	286	
31	e	122	
32	f	735	
33	g	400	
34	h	482	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
35	i	328	<div><div></div><div>28%8%63%</div></div>
36	j	240	<div><div></div><div>70%25%</div></div>
37	k	25	<div><div></div><div>68%32%</div></div>
38	l	108	<div><div></div><div>57%43%</div></div>
39	m	108	<div><div></div><div>57%43%</div></div>
40	n	244	<div><div></div><div>82%18%</div></div>

## 2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 66759 atoms, of which 626 are hydrogens and 0 are deuteriums.

In the tables below, 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1422	Total	C	N	O	S	0	0
			11174	7036	1954	2122	62		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1156	Total	C	N	O	S	0	0
			9140	5781	1606	1697	56		

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	266	Total	C	N	O	S	0	0
			2095	1317	348	417	13		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	178	Total	C	N	O	S	0	0
			1434	887	257	288	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1752	1111	309	321	11		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	84	Total	C	N	O	S	0	0
			679	434	115	127	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	133	Total	C	N	O	S	0	0
			1068	673	180	211	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	119	Total	C	N	O	S	0	0
			971	596	179	186	10		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	65	Total	C	N	O	S	0	0
			532	339	93	94	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	115	Total	C	N	O	S	0	1
			920	590	157	171	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			363	224	72	63	4		

- Molecule 13 is a protein called Mediator of RNA polymerase II transcription subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	156	Total	C	N	O	S	0	0
			777	464	156	156	1		

- Molecule 14 is a protein called Mediator of RNA polymerase II transcription subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	168	Total	C	N	O	0	0
			891	542	172	177		

- Molecule 15 is a protein called Mediator of RNA polymerase II transcription subunit 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	O	103	Total	C	N	O	0	0
			511	305	103	103		

- Molecule 16 is a protein called Mediator of RNA polymerase II transcription subunit 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	487	Total	C	N	O	0	0
			2421	1447	487	487		

- Molecule 17 is a protein called Mediator of RNA polymerase II transcription subunit 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	253	Total	C	N	O	S	0	0
			1979	1255	330	384	10		

- Molecule 18 is a protein called Mediator of RNA polymerase II transcription subunit 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	209	Total	C	N	O	S	0	0
			1600	1011	269	315	5		

- Molecule 19 is a protein called Mediator of RNA polymerase II transcription subunit 22.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	109	Total	C	N	O	0	0
			544	326	109	109		

- Molecule 20 is a protein called Mediator of RNA polymerase II transcription subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	91	Total	C	N	O	S	0	0
			756	475	125	154	2		

- Molecule 21 is a protein called Mediator of RNA polymerase II transcription subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	156	Total	C	N	O	S	0	0
			1310	847	220	238	5		

- Molecule 22 is a protein called Mediator of RNA polymerase II transcription subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	85	Total	C	N	O	S	0	0
			720	451	133	135	1		

- Molecule 23 is a protein called Mediator of RNA polymerase II transcription subunit 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	119	Total	C	N	O	S	0	0
			965	608	160	193	4		

- Molecule 24 is a protein called Mediator of RNA polymerase II transcription subunit 31.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	92	Total	C	N	O	S	0	0
			767	506	116	141	4		

- Molecule 25 is a protein called DNA repair helicase RAD3.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Y	562	Total	C	H	N	O	S	0	0
			5175	2901	626	777	838	33		

- Molecule 26 is a protein called DNA repair helicase RAD25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	469	Total	C	N	O	S	0	0
			3769	2370	660	716	23		

- Molecule 27 is a protein called RNA polymerase II transcription factor B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	62	Total	C	N	O	0	0
			518	334	83	101		

- Molecule 28 is a protein called RNA polymerase II transcription factor B subunit 5.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	63	Total	C	N	O	S	0	0
			499	316	88	93	2		

- Molecule 29 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	189	Total	C	N	O	S	0	0
			1357	838	240	267	12		

- Molecule 30 is a protein called Transcription initiation factor IIA large subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	116	Total	C	N	O	S	0	0
			956	599	159	195	3		

- Molecule 31 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	101	Total	C	N	O	S	0	0
			792	500	132	156	4		

- Molecule 32 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	149	Total	C	N	O	S	0	0
			1243	788	222	229	4		

- Molecule 33 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	172	Total	C	N	O	S	0	0
			1443	922	248	267	6		

- Molecule 34 is a protein called Transcription initiation factor IIE subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	118	Total	C	N	O	S	0	0
			960	625	158	172	5		

- Molecule 35 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	120	Total	C	N	O	S	0	0
			987	636	161	187	3		

- Molecule 36 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	180	Total	C	N	O	S	0	0
			1416	921	242	247	6		

- Molecule 37 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	25	Total	C	N	O	0	0
			184	116	25	43		

- Molecule 38 is a DNA chain called 108bp HIS4 Promoter Non-template Strand (-92/+16).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	62	Total	C	N	O	P	0	0
			1271	609	222	378	62		

- Molecule 39 is a DNA chain called 108bp HIS4 Promoter Template Strand (+16/-92).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	62	Total	C	N	O	P	0	0
			1271	607	236	366	62		

- Molecule 40 is a protein called Transcription initiation factor TFIID subunit 14.

Mol	Chain	Residues	Atoms		AltConf	Trace
40	n	200	Total	C	0	200
			200	200		

- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
41	J	1	Total	Zn	0
			1	1	
41	B	1	Total	Zn	0
			1	1	
41	I	2	Total	Zn	0
			2	2	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
41	C	1	Total 1	Zn 1	0
41	A	2	Total 2	Zn 2	0
41	L	1	Total 1	Zn 1	0

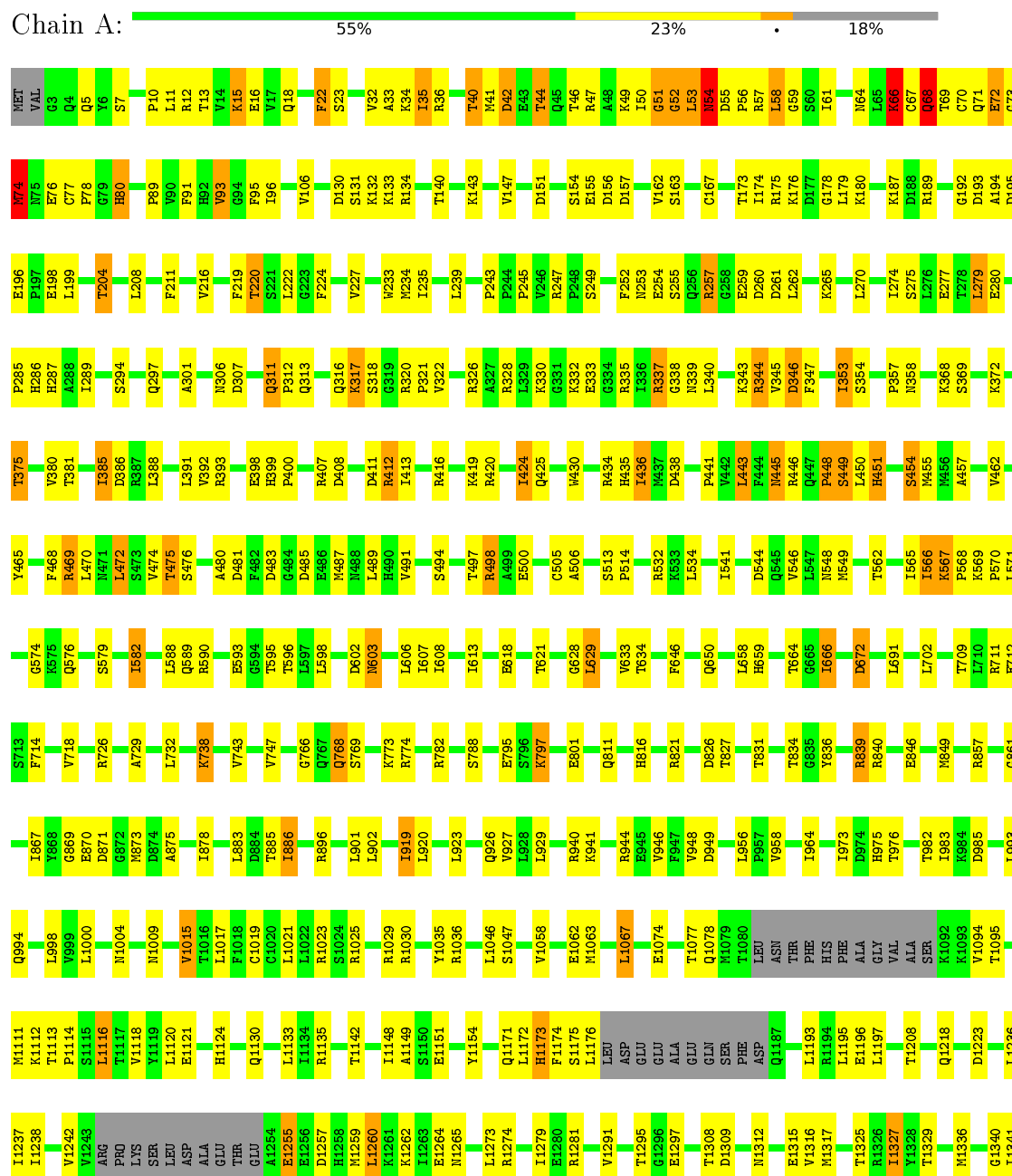
- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

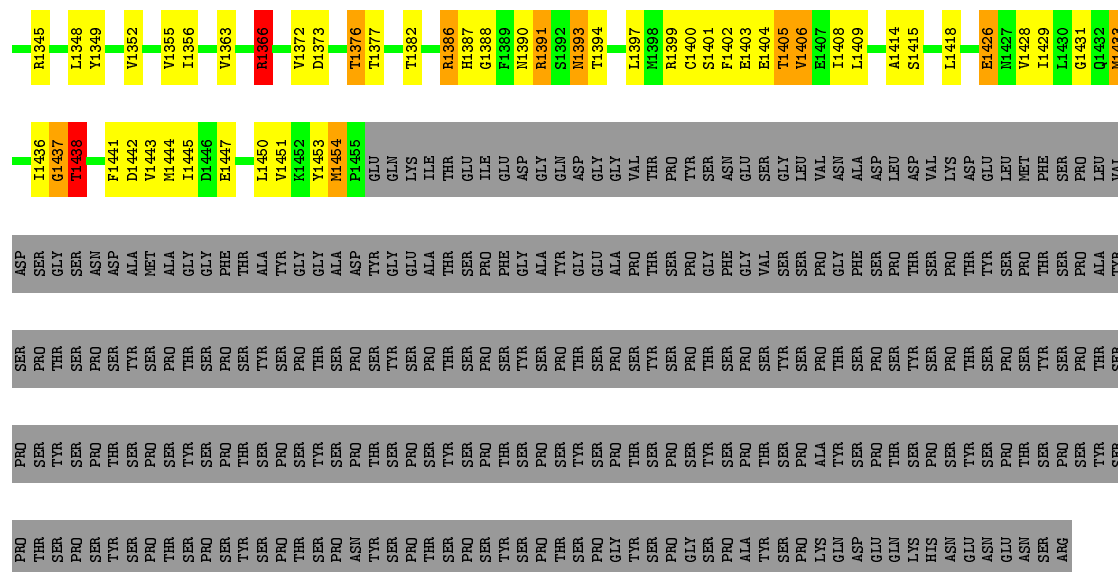
Mol	Chain	Residues	Atoms		AltConf
42	A	1	Total 1	Mg 1	0

### 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. 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. 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.

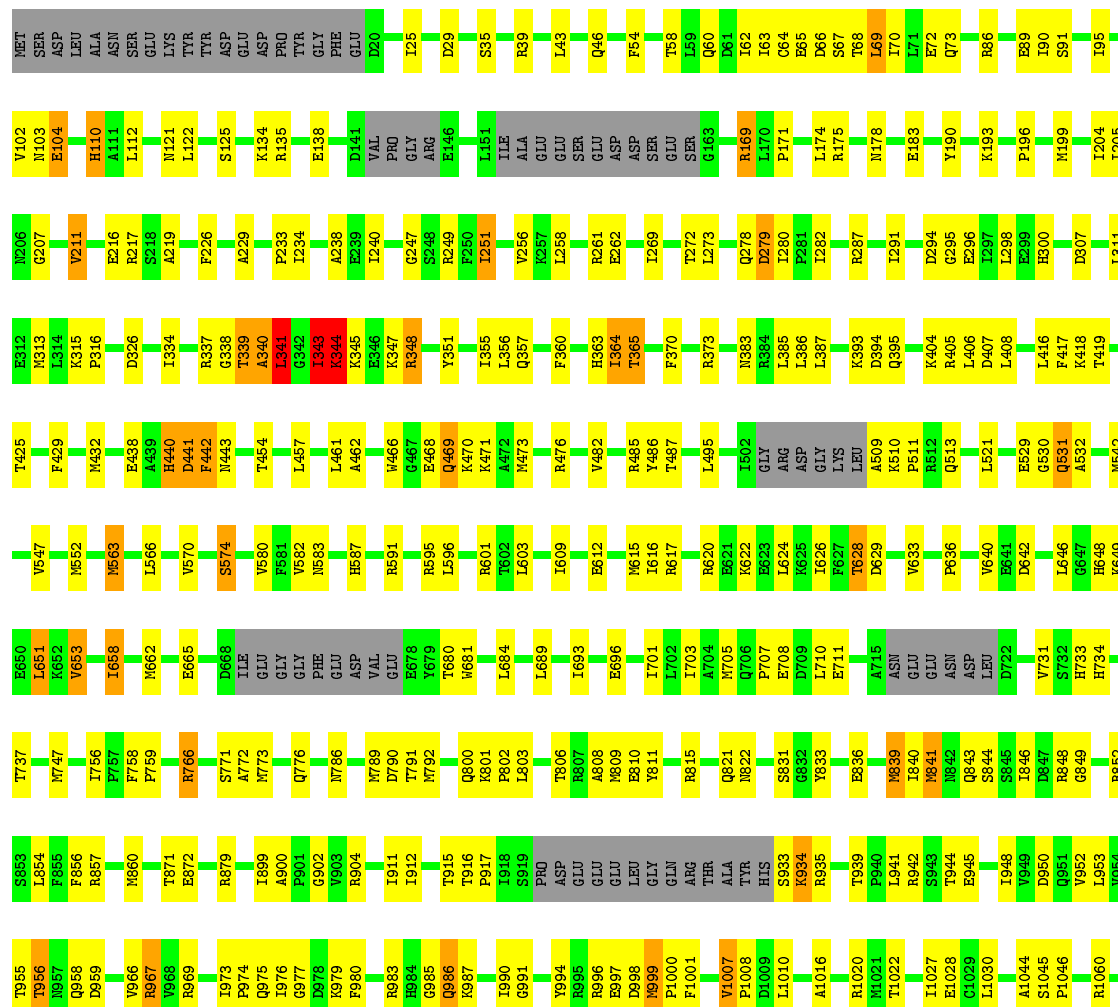
- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

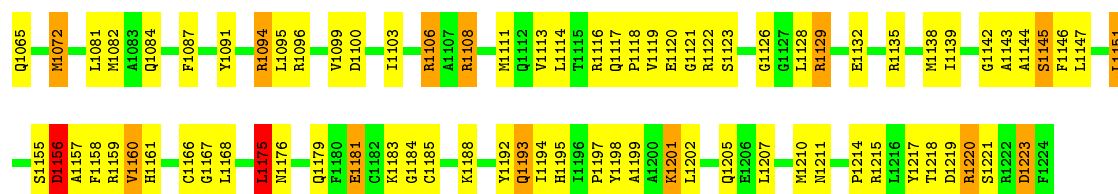




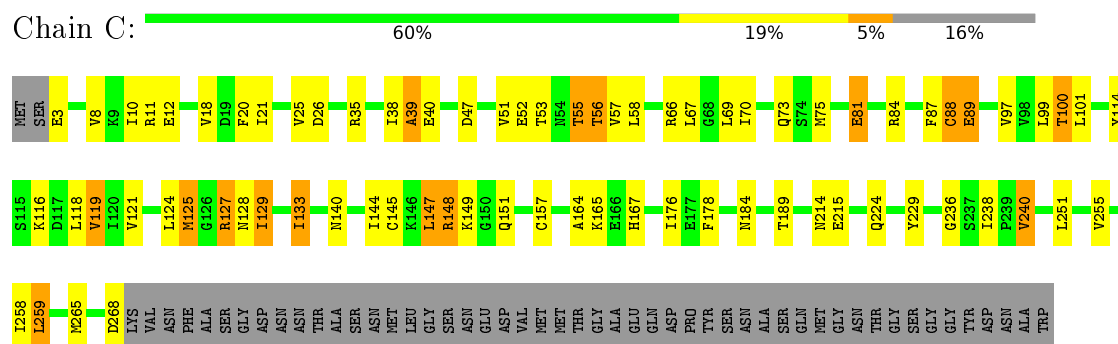
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B: 62% 28% 6%

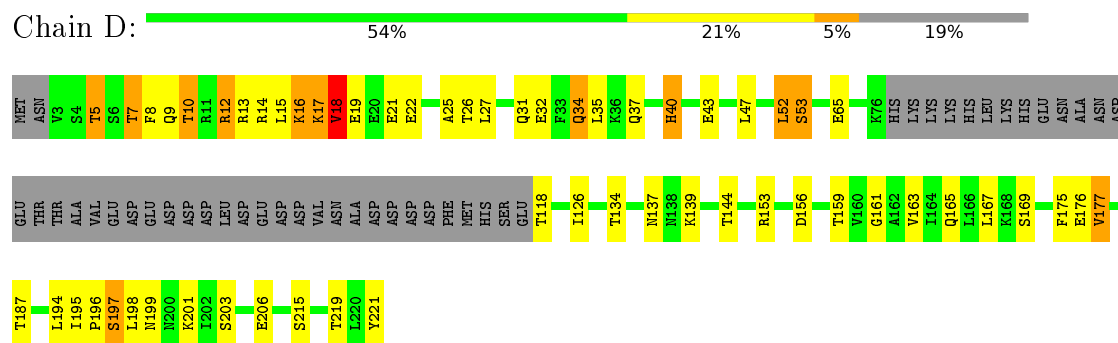




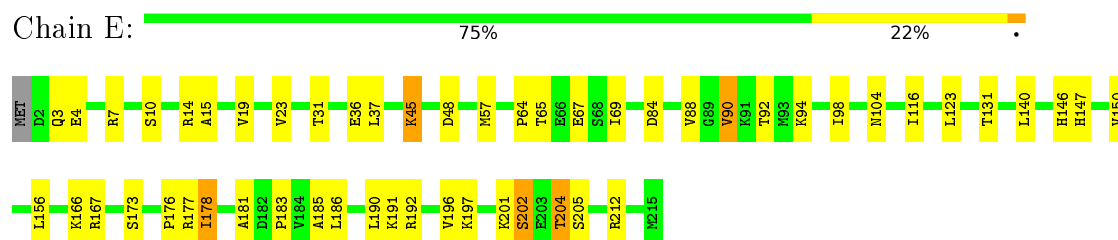
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



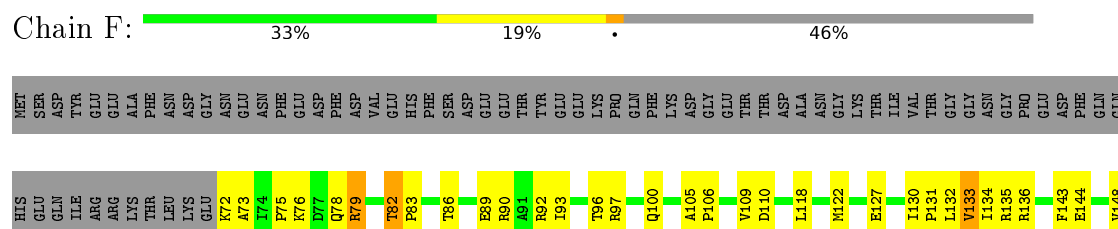
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



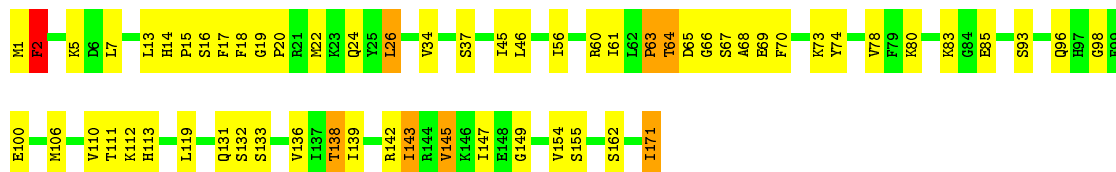
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2





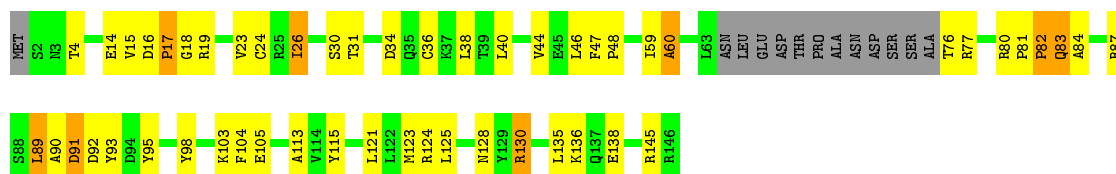
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G: 64% 31%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 55% 30% 5% 9%



- Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I: 75% 20%



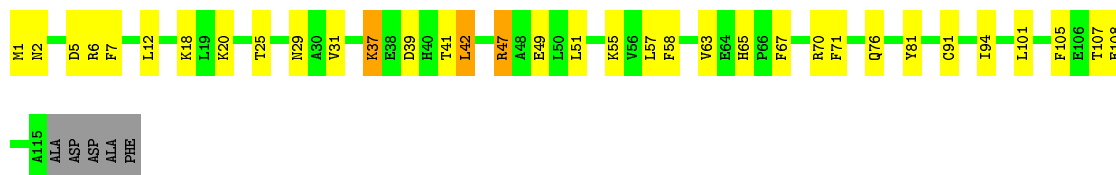
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 56% 26% 11% 7%



- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

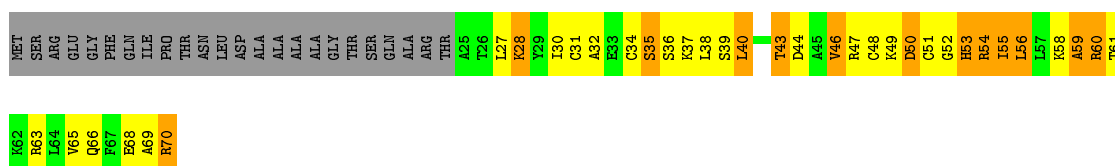
Chain K: 68% 26%



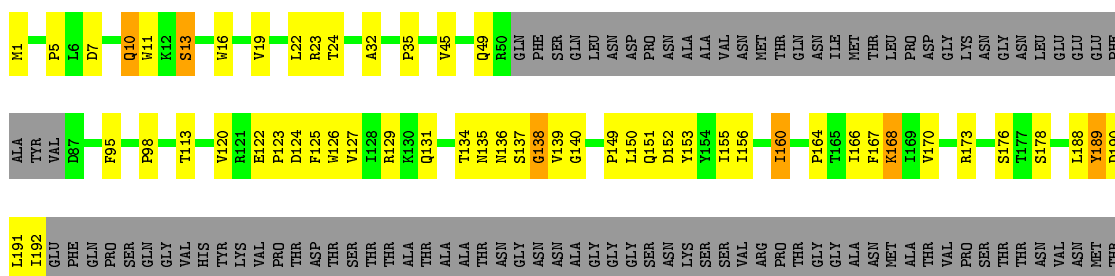
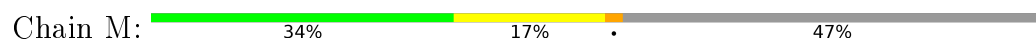
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L: 16% 31% 19% 34%

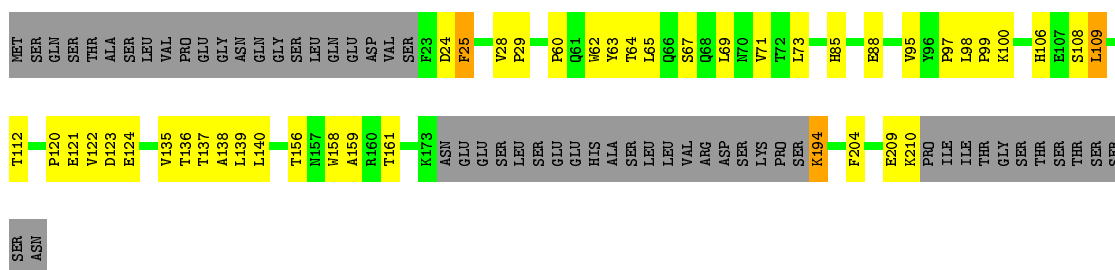




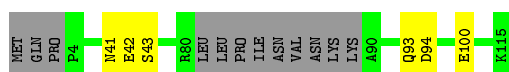
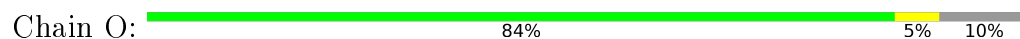
- Molecule 13: Mediator of RNA polymerase II transcription subunit 6



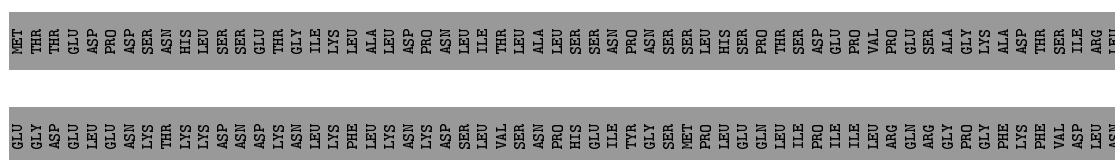
- Molecule 14: Mediator of RNA polymerase II transcription subunit 8



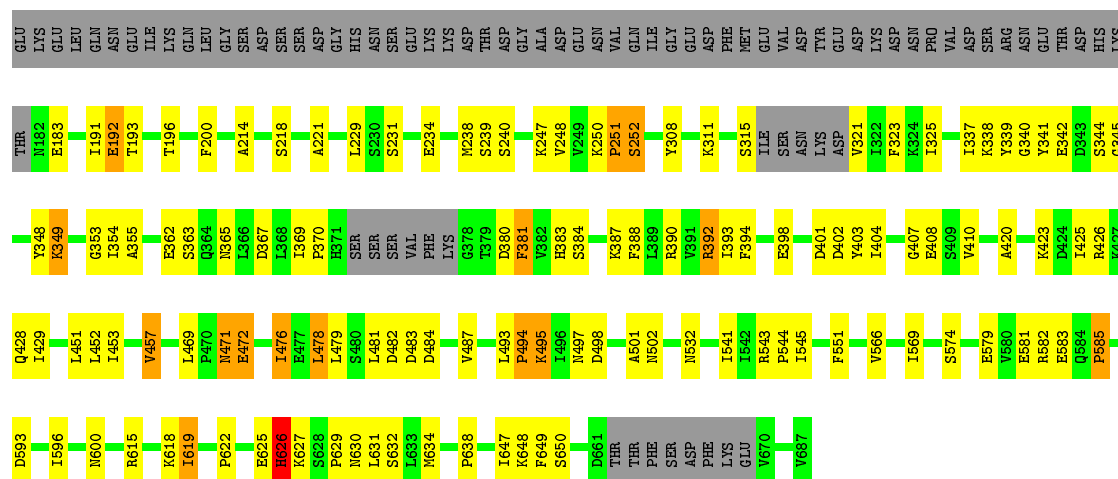
- Molecule 15: Mediator of RNA polymerase II transcription subunit 11



- Molecule 16: Mediator of RNA polymerase II transcription subunit 17

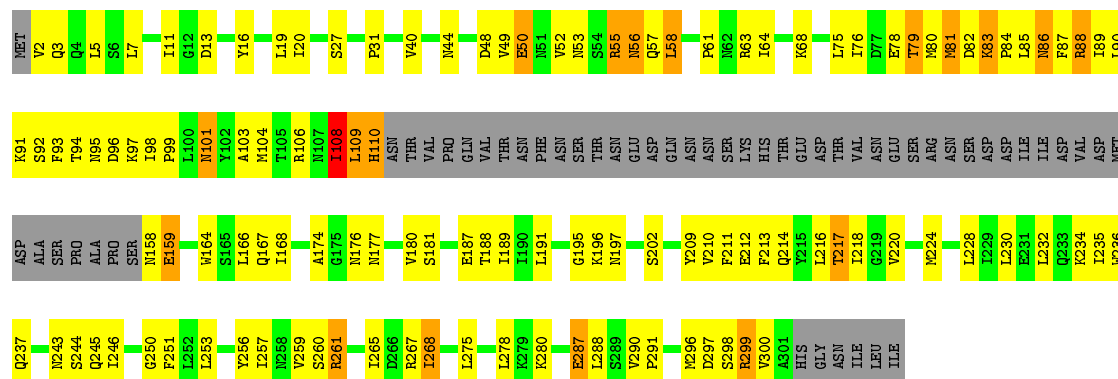






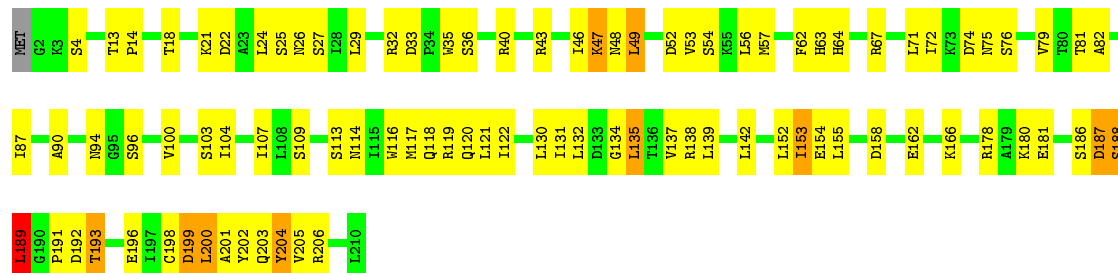
- Molecule 17: Mediator of RNA polymerase II transcription subunit 18

Chain Q: 43% 33% 6% 18%



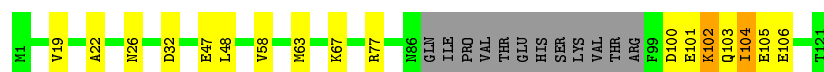
- Molecule 18: Mediator of RNA polymerase II transcription subunit 20

Chain R: 56% 39% 5%



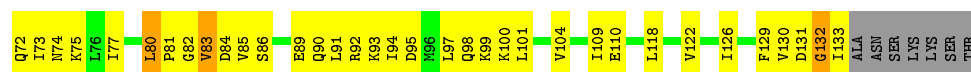
- Molecule 19: Mediator of RNA polymerase II transcription subunit 22

Chain S: 76% 12% 10%



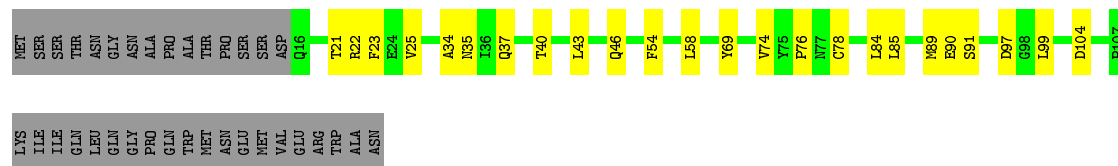
- Molecule 20: Mediator of RNA polymerase II transcription subunit 4





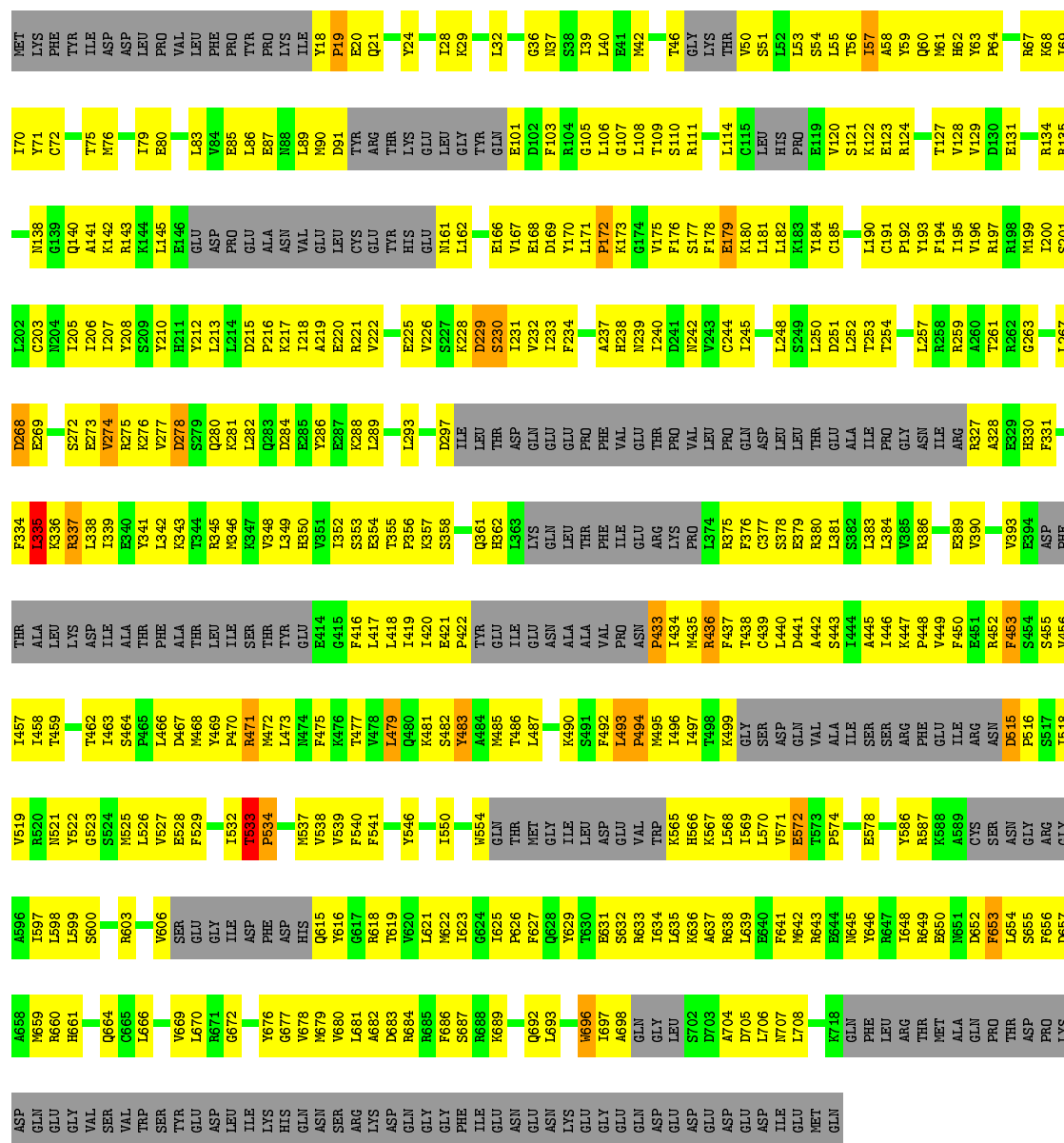
• Molecule 24: Mediator of RNA polymerase II transcription subunit 31

Chain X: 54% 19% 28%



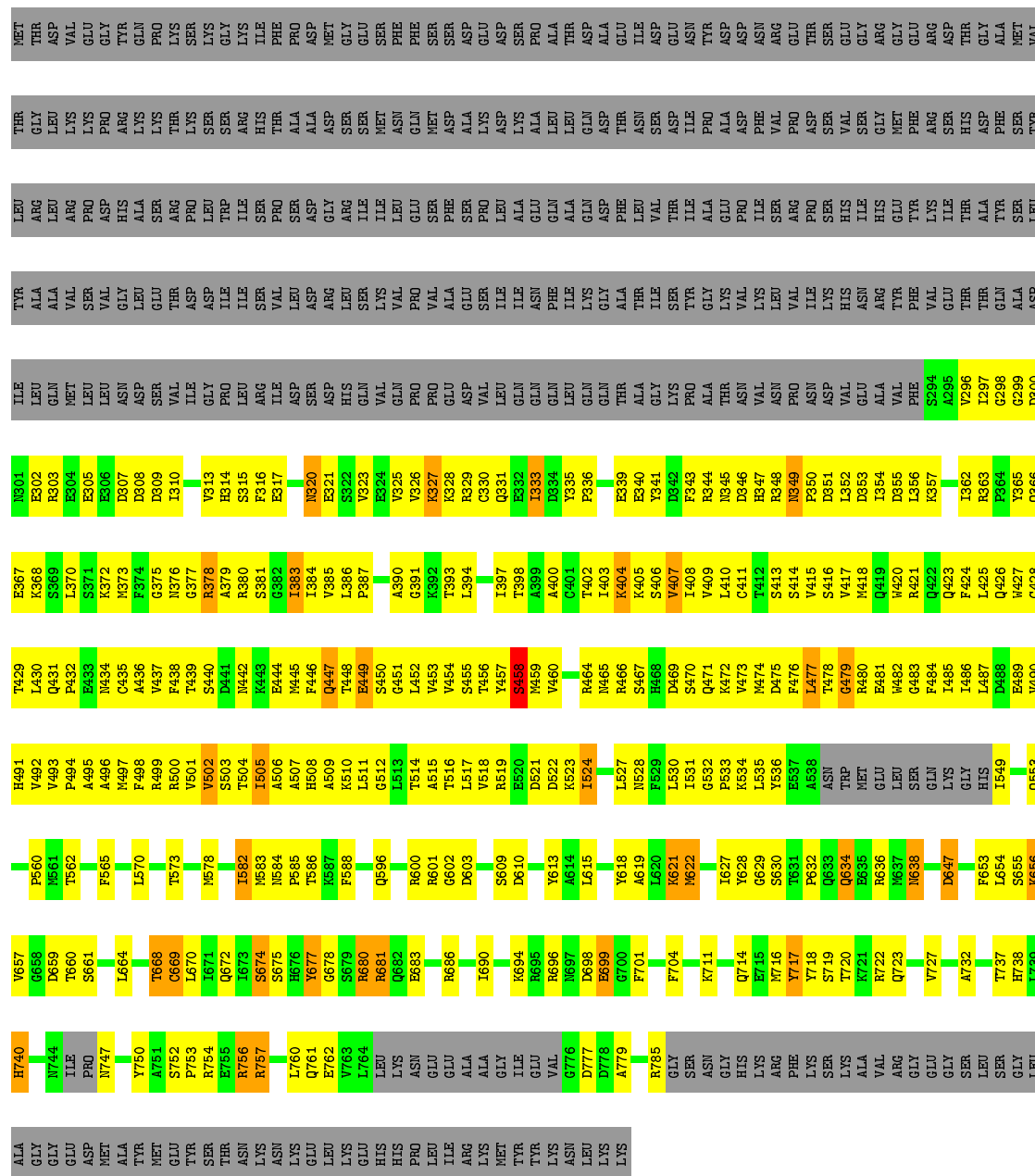
• Molecule 25: DNA repair helicase RAD3

Chain Y: 25% 44% 28%



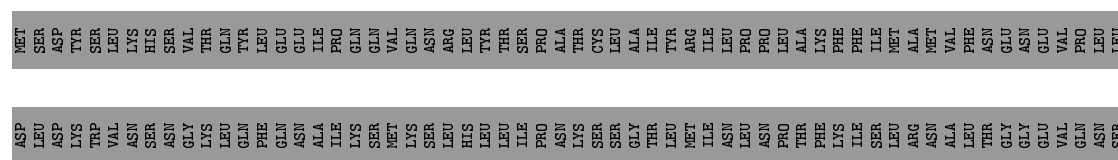
- Molecule 26: DNA repair helicase RAD25

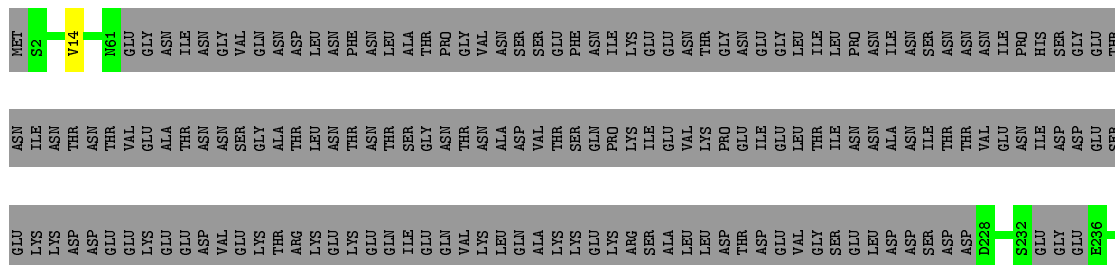
Chain Z:  22% 30% . 44%



- Molecule 27: RNA polymerase II transcription factor B subunit 2

Chain a:  12% 88%









M1	T137	GLU	GLU	THR	THR	ASN	THR	GLY	ILE	GLY	LNS	ARG	ARG	THR	THR	ASN	THR	THR	ALA	GLU	PRO	LNS	ALA	LYS	ARG	ALA	LNS	GLY	SER	ALA	SER	SER	THR	VAL	LNS	GLY	SER	VAL	D178	E240	LNS	ASN	THR	VAL
----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	170600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI 20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.51	1/11374 (0.0%)	0.79	5/15384 (0.0%)
10	J	0.54	0/541	0.88	1/727 (0.1%)
11	K	0.48	0/938	0.71	0/1267
12	L	0.54	0/365	0.79	0/485
13	M	0.61	0/775	0.83	0/1077
14	N	0.53	0/893	0.76	0/1237
15	O	0.52	0/509	0.67	0/707
16	P	0.58	0/2417	0.79	2/3369 (0.1%)
17	Q	0.56	0/2014	0.75	0/2728
18	R	0.50	2/1626 (0.1%)	0.66	0/2205
19	S	0.57	0/542	0.73	0/755
2	B	0.48	0/9317	0.74	4/12567 (0.0%)
20	T	0.69	0/763	1.10	2/1025 (0.2%)
21	U	0.43	0/1339	0.60	0/1808
22	V	0.73	0/732	1.01	4/984 (0.4%)
23	W	0.47	0/973	0.64	0/1308
24	X	0.39	0/789	0.53	0/1077
25	Y	0.55	2/4616 (0.0%)	0.79	13/6196 (0.2%)
26	Z	0.78	0/3837	0.98	8/5177 (0.2%)
27	a	0.67	0/527	0.68	0/704
28	b	0.60	0/504	0.69	1/679 (0.1%)
29	c	0.29	0/1373	0.47	0/1863
3	C	0.49	0/2133	0.78	2/2891 (0.1%)
30	d	0.40	0/970	0.57	0/1310
31	e	0.42	0/800	0.63	0/1080
32	f	0.33	0/1267	0.82	9/1700 (0.5%)
33	g	0.66	0/1469	0.73	3/1972 (0.2%)
34	h	0.96	0/978	1.11	1/1321 (0.1%)
35	i	0.37	0/1003	0.61	0/1345
36	j	0.41	0/1443	0.62	0/1942
37	k	0.77	0/194	0.69	0/270
38	l	0.43	0/1423	0.89	0/2195

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	m	0.47	0/1427	0.89	0/2199
4	D	0.51	0/1444	0.83	2/1935 (0.1%)
5	E	0.48	0/1788	0.72	0/2406
6	F	0.58	0/691	0.79	0/933
7	G	0.51	0/1368	0.81	0/1844
8	H	0.51	0/1086	0.80	0/1470
9	I	0.47	0/989	0.78	0/1331
All	All	0.54	5/67237 (0.0%)	0.78	57/91473 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	M	0	2
16	P	0	3
17	Q	0	1
2	B	0	1
25	Y	0	1
26	Z	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1394	THR	C-N	-6.29	1.21	1.33
25	Y	172	PRO	N-CD	5.61	1.55	1.47
25	Y	19	PRO	N-CD	5.51	1.55	1.47
18	R	35	TRP	CD2-CE2	5.06	1.47	1.41
18	R	116	TRP	CD2-CE2	5.04	1.47	1.41

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	493	LEU	C-N-CD	-13.71	90.45	120.60
25	Y	533	THR	C-N-CD	-13.65	90.57	120.60
32	f	135	LEU	C-N-CD	-11.09	96.21	120.60
26	Z	505	ILE	CB-CA-C	-9.99	91.62	111.60
25	Y	433	PRO	CA-N-CD	-9.03	98.86	111.50
32	f	129	PRO	CA-N-CD	-8.28	99.90	111.50
32	f	349	PRO	CA-N-CD	-7.96	100.35	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	102	PRO	CA-N-CD	-7.60	100.86	111.50
1	A	346	ASP	O-C-N	-7.53	110.65	122.70
34	h	123	MET	CG-SD-CE	-7.14	88.78	100.20
25	Y	471	ARG	NE-CZ-NH2	6.60	123.60	120.30
25	Y	436	ARG	NE-CZ-NH2	6.55	123.58	120.30
25	Y	337	ARG	NE-CZ-NH2	6.55	123.57	120.30
26	Z	477	LEU	C-N-CA	-6.26	106.04	121.70
22	V	87	LEU	CB-CA-C	-6.13	98.54	110.20
20	T	115	LEU	CB-CA-C	-6.12	98.57	110.20
4	D	25	ALA	C-N-CA	6.11	136.98	121.70
26	Z	670	LEU	CB-CG-CD1	-6.10	100.63	111.00
25	Y	453	PHE	N-CA-C	-5.91	95.05	111.00
20	T	94	TYR	CA-CB-CG	-5.81	102.36	113.40
22	V	136	LYS	N-CA-CB	-5.77	100.22	110.60
25	Y	696	TRP	CZ3-CH2-CZ2	5.71	128.46	121.60
1	A	58	LEU	CA-CB-CG	5.70	128.40	115.30
1	A	194	ALA	C-N-CA	5.66	135.86	121.70
33	g	69	TRP	CZ3-CH2-CZ2	5.65	128.38	121.60
2	B	340	ALA	C-N-CA	5.65	135.83	121.70
33	g	81	TRP	CZ3-CH2-CZ2	5.64	128.37	121.60
32	f	361	TRP	CZ3-CH2-CZ2	5.62	128.35	121.60
33	g	313	TRP	CZ3-CH2-CZ2	5.57	128.28	121.60
26	Z	632	PRO	N-CA-CB	5.55	109.96	103.30
22	V	141	ASP	CB-CG-OD1	5.50	123.25	118.30
4	D	26	THR	N-CA-C	-5.49	96.19	111.00
2	B	628	THR	C-N-CA	5.47	135.36	121.70
3	C	39	ALA	N-CA-C	5.46	125.75	111.00
3	C	89	GLU	N-CA-C	-5.29	96.70	111.00
1	A	1394	THR	C-N-CA	5.29	133.40	122.30
25	Y	229	ASP	CB-CG-OD2	5.24	123.02	118.30
32	f	354	ASP	CB-CG-OD2	5.24	123.01	118.30
32	f	336	ASP	CB-CG-OD2	5.23	123.01	118.30
25	Y	91	ASP	CB-CG-OD2	5.21	122.99	118.30
25	Y	515	ASP	CB-CG-OD2	5.21	122.99	118.30
25	Y	297	ASP	CB-CG-OD2	5.21	122.99	118.30
26	Z	777	ASP	CB-CG-OD2	5.21	122.99	118.30
32	f	110	ASP	CB-CG-OD2	5.21	122.99	118.30
32	f	132	ASP	CB-CG-OD2	5.21	122.99	118.30
2	B	1181	GLU	N-CA-C	5.14	124.88	111.00
26	Z	458	SER	N-CA-CB	5.13	118.20	110.50
26	Z	479	GLY	N-CA-C	5.13	125.91	113.10
25	Y	278	ASP	CB-CG-OD2	5.11	122.90	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	502	VAL	CB-CA-C	-5.10	101.71	111.40
16	P	457	VAL	N-CA-C	5.09	124.75	111.00
16	P	342	GLU	N-CA-C	5.08	124.71	111.00
22	V	139	VAL	CA-CB-CG1	-5.04	103.34	110.90
28	b	3	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	346	ASP	CA-C-N	5.02	128.24	117.20
2	B	1156	ASP	N-CA-C	5.01	124.52	111.00
10	J	5	VAL	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	43	LEU	Mainchain
13	M	10	GLN	Peptide
13	M	138	GLY	Peptide
16	P	471	ASN	Peptide
16	P	532	ASN	Peptide
16	P	626	HIS	Peptide
17	Q	101	ASN	Peptide
25	Y	335	LEU	Peptide
26	Z	661	SER	Peptide

## 5.2 Too-close contacts [i](#)

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	11174	0	11225	498	0
2	B	9140	0	9111	297	0
3	C	2095	0	2051	62	0
4	D	1434	0	1460	70	0
5	E	1752	0	1776	26	0
6	F	679	0	698	109	0
7	G	1340	0	1355	228	0
8	H	1068	0	1040	25	0
9	I	971	0	927	15	0
10	J	532	0	542	14	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	920	0	929	21	0
12	L	363	0	386	54	0
13	M	777	0	329	39	0
14	N	891	0	455	25	0
15	O	511	0	215	3	0
16	P	2421	0	1017	101	0
17	Q	1979	0	1977	245	0
18	R	1600	0	1614	107	0
19	S	544	0	241	10	0
20	T	756	0	761	265	0
21	U	1310	0	1339	106	0
22	V	720	0	725	280	0
23	W	965	0	987	136	0
24	X	767	0	752	22	0
25	Y	4549	626	4642	1289	0
26	Z	3769	0	3697	845	0
27	a	518	0	514	0	0
28	b	499	0	525	0	0
29	c	1357	0	1266	0	0
30	d	956	0	916	0	0
31	e	792	0	806	0	0
32	f	1243	0	1238	0	0
33	g	1443	0	1461	0	0
34	h	960	0	973	0	0
35	i	987	0	999	0	0
36	j	1416	0	1491	0	0
37	k	184	0	163	0	0
38	l	1271	0	705	0	0
39	m	1271	0	699	0	0
40	n	200	0	0	0	0
41	A	2	0	0	0	0
41	B	1	0	0	0	0
41	C	1	0	0	0	0
41	I	2	0	0	0	0
41	J	1	0	0	0	0
41	L	1	0	0	0	0
42	A	1	0	0	0	0
All	All	66133	626	62007	4244	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 50.

All (4244) 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)
25:Y:254:THR:HG23	25:Y:286:TYR:CE1	1.20	1.71
25:Y:352:ILE:HB	25:Y:380:ARG:CZ	1.23	1.66
26:Z:757:ARG:HH12	26:Z:760:LEU:CG	1.04	1.66
25:Y:550:ILE:HG22	25:Y:554:TRP:CZ2	1.17	1.63
25:Y:639:LEU:HD12	25:Y:653:PHE:CE2	1.32	1.61
22:V:119:PRO:HA	22:V:122:TRP:CD1	1.14	1.60
25:Y:518:ILE:CG2	25:Y:522:TYR:HE2	1.00	1.59
26:Z:717:TYR:CE2	26:Z:718:TYR:CE1	1.89	1.58
20:T:93:ILE:HD12	22:V:122:TRP:CE3	1.29	1.57
25:Y:416:PHE:CE2	25:Y:440:LEU:HD22	1.39	1.57
17:Q:81:MET:CE	17:Q:92:SER:HB3	1.21	1.57
25:Y:639:LEU:CD2	25:Y:649:ARG:HD2	1.30	1.57
1:A:1447:GLU:HA	7:G:22:MET:CE	1.32	1.57
25:Y:59:TYR:HA	25:Y:62:HIS:CD2	1.40	1.56
26:Z:757:ARG:NH2	26:Z:760:LEU:CD2	1.67	1.56
25:Y:254:THR:CG2	25:Y:286:TYR:HE1	1.06	1.55
20:T:122:HIS:HA	23:W:130:VAL:CG1	1.36	1.55
25:Y:68:LYS:HD2	25:Y:228:LYS:CG	1.36	1.55
22:V:119:PRO:CA	22:V:122:TRP:CD1	1.82	1.55
26:Z:585:PRO:CB	26:Z:756:ARG:NH1	1.69	1.55
20:T:93:ILE:CD1	22:V:122:TRP:HE3	1.14	1.54
1:A:1445:ILE:CG2	6:F:132:LEU:HD23	1.38	1.54
25:Y:499:LYS:NZ	25:Y:522:TYR:CA	1.68	1.54
25:Y:393:VAL:HB	25:Y:437:PHE:CZ	1.38	1.53
25:Y:518:ILE:CG2	25:Y:522:TYR:CE2	1.90	1.53
1:A:1445:ILE:HB	7:G:18:PHE:CE2	1.42	1.52
25:Y:639:LEU:CD1	25:Y:653:PHE:CE2	1.89	1.52
22:V:146:LYS:HD3	23:W:129:PHE:CZ	1.42	1.52
25:Y:499:LYS:CE	25:Y:522:TYR:HA	1.38	1.52
25:Y:550:ILE:CG2	25:Y:554:TRP:HZ2	1.12	1.51
1:A:1443:VAL:HG12	7:G:61:ILE:CG2	1.37	1.51
17:Q:97:LYS:CE	17:Q:243:ASN:HB3	1.36	1.51
25:Y:200:ILE:CB	25:Y:226:VAL:CG2	1.84	1.50
25:Y:37:ASN:CB	25:Y:456:VAL:HB	1.06	1.50
25:Y:68:LYS:CD	25:Y:228:LYS:HG3	1.37	1.50
2:B:1185:CYS:SG	4:D:17:LYS:HD3	1.52	1.50
25:Y:518:ILE:HG22	25:Y:522:TYR:CE2	1.39	1.49
25:Y:200:ILE:HB	25:Y:226:VAL:CB	1.22	1.49
25:Y:200:ILE:HB	25:Y:226:VAL:CG2	1.03	1.49
25:Y:639:LEU:CG	25:Y:653:PHE:CE2	1.96	1.48
2:B:1215:ARG:CD	4:D:15:LEU:CD1	1.91	1.47
1:A:1445:ILE:HD13	7:G:18:PHE:CZ	1.49	1.47

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:122:HIS:CB	23:W:130:VAL:HG12	1.40	1.46
6:F:92:ARG:NH2	7:G:63:PRO:CB	1.75	1.46
25:Y:440:LEU:HD21	25:Y:641:PHE:CB	1.43	1.46
1:A:1447:GLU:CB	7:G:22:MET:HE2	1.42	1.45
25:Y:393:VAL:HB	25:Y:437:PHE:CE2	1.49	1.45
25:Y:257:LEU:CD2	25:Y:383:LEU:HD11	1.44	1.45
1:A:1443:VAL:CG1	7:G:61:ILE:HG21	1.45	1.44
6:F:92:ARG:CZ	7:G:63:PRO:HB2	1.44	1.44
22:V:119:PRO:CB	22:V:122:TRP:HE1	1.31	1.44
17:Q:97:LYS:HE2	17:Q:243:ASN:CB	1.47	1.44
18:R:72:ILE:HG21	18:R:202:TYR:CE1	1.49	1.44
26:Z:717:TYR:HE2	26:Z:718:TYR:CE1	1.28	1.44
25:Y:59:TYR:CA	25:Y:62:HIS:NE2	1.80	1.43
26:Z:757:ARG:NH1	26:Z:760:LEU:HG	1.17	1.43
25:Y:420:ILE:CG1	25:Y:633:ARG:NH2	1.79	1.42
25:Y:357:LYS:HE3	25:Y:376:PHE:CD1	1.51	1.42
25:Y:200:ILE:CB	25:Y:226:VAL:HG21	1.42	1.42
1:A:1443:VAL:N	7:G:63:PRO:HG3	1.17	1.42
20:T:122:HIS:HB3	23:W:131:ASP:C	1.06	1.42
25:Y:190:LEU:HD13	25:Y:195:ILE:CD1	1.47	1.42
20:T:122:HIS:CA	23:W:130:VAL:CG1	1.96	1.42
25:Y:639:LEU:HD21	25:Y:649:ARG:CD	1.45	1.41
17:Q:81:MET:CE	17:Q:92:SER:CB	1.95	1.41
25:Y:352:ILE:HB	25:Y:380:ARG:NH1	1.20	1.41
26:Z:668:THR:HG21	26:Z:694:LYS:CB	1.50	1.41
25:Y:499:LYS:NZ	25:Y:522:TYR:HA	1.10	1.40
25:Y:550:ILE:CG2	25:Y:554:TRP:CZ2	1.85	1.40
25:Y:420:ILE:HG13	25:Y:633:ARG:NH2	1.13	1.39
25:Y:288:LYS:CG	25:Y:335:LEU:HB3	1.23	1.39
26:Z:585:PRO:HB2	26:Z:756:ARG:CZ	1.50	1.39
25:Y:37:ASN:HB3	25:Y:456:VAL:CB	1.50	1.39
25:Y:493:LEU:CD2	25:Y:696:TRP:HE1	1.35	1.39
1:A:1447:GLU:OE2	7:G:26:LEU:HD11	1.22	1.38
17:Q:97:LYS:NZ	17:Q:244:SER:N	1.70	1.38
25:Y:135:ARG:NH2	25:Y:143:ARG:HE	1.19	1.38
25:Y:631:GLU:HA	25:Y:636:LYS:CE	1.52	1.38
26:Z:757:ARG:NH2	26:Z:760:LEU:HD23	1.09	1.38
1:A:1445:ILE:CD1	7:G:18:PHE:CZ	2.07	1.38
1:A:1447:GLU:CA	7:G:22:MET:CE	2.02	1.38
25:Y:349:LEU:CA	25:Y:380:ARG:NH2	1.86	1.37
25:Y:349:LEU:HA	25:Y:380:ARG:NH2	1.04	1.37

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:119:PRO:CA	22:V:122:TRP:NE1	1.83	1.37
25:Y:639:LEU:HB2	25:Y:653:PHE:CD2	1.57	1.36
26:Z:757:ARG:CZ	26:Z:760:LEU:HD23	1.53	1.36
25:Y:37:ASN:CB	25:Y:456:VAL:CB	2.02	1.36
1:A:1445:ILE:CG1	7:G:18:PHE:CZ	2.09	1.36
25:Y:493:LEU:HD23	25:Y:696:TRP:NE1	1.34	1.36
2:B:1215:ARG:HD2	4:D:15:LEU:CD1	1.50	1.36
17:Q:97:LYS:HZ3	17:Q:244:SER:N	1.16	1.36
6:F:96:THR:HG23	7:G:65:ASP:C	1.42	1.36
20:T:122:HIS:CB	23:W:131:ASP:C	1.92	1.35
16:P:315:SER:CB	16:P:426:ARG:H	1.37	1.35
17:Q:97:LYS:CD	17:Q:243:ASN:HB2	1.54	1.35
26:Z:585:PRO:HB2	26:Z:756:ARG:NH2	1.40	1.35
13:M:10:GLN:CB	13:M:160:ILE:O	1.71	1.34
17:Q:20:ILE:CD1	17:Q:87:PHE:CE2	2.10	1.34
22:V:146:LYS:CD	23:W:129:PHE:CZ	2.09	1.34
1:A:1451:VAL:CG1	7:G:20:PRO:HA	1.54	1.34
1:A:1445:ILE:HD13	7:G:18:PHE:CE1	1.62	1.34
25:Y:124:ARG:NH2	25:Y:381:LEU:HD23	1.38	1.34
26:Z:560:PRO:O	26:Z:586:THR:HG21	1.21	1.34
1:A:1447:GLU:CG	7:G:22:MET:HE2	1.57	1.34
25:Y:683:ASP:O	25:Y:686:PHE:CD2	1.79	1.34
25:Y:288:LYS:HG3	25:Y:335:LEU:CB	1.51	1.34
25:Y:420:ILE:HG13	25:Y:633:ARG:CZ	1.55	1.34
25:Y:526:LEU:HD23	25:Y:554:TRP:CH2	1.62	1.34
1:A:1445:ILE:CG2	6:F:132:LEU:CD2	2.06	1.34
1:A:1445:ILE:CB	7:G:18:PHE:CE2	2.10	1.34
25:Y:499:LYS:HB3	25:Y:522:TYR:CE1	1.64	1.33
25:Y:229:ASP:CB	25:Y:453:PHE:HB3	1.57	1.33
25:Y:103:PHE:CE1	25:Y:205:ILE:HD12	1.64	1.32
1:A:1443:VAL:H	7:G:63:PRO:CG	1.41	1.32
2:B:1215:ARG:NE	4:D:15:LEU:HD11	1.45	1.32
17:Q:16:TYR:HE2	17:Q:87:PHE:CB	1.11	1.32
25:Y:419:ILE:N	25:Y:633:ARG:NH1	1.71	1.32
25:Y:349:LEU:HA	25:Y:380:ARG:CZ	1.60	1.32
22:V:146:LYS:CD	23:W:129:PHE:HZ	1.41	1.31
22:V:146:LYS:HD3	23:W:129:PHE:CE1	1.65	1.31
2:B:1221:SER:OG	4:D:14:ARG:NH1	1.59	1.31
2:B:1220:ARG:CA	4:D:14:ARG:HH22	1.43	1.31
17:Q:75:LEU:O	17:Q:98:ILE:CG2	1.78	1.31
1:A:1447:GLU:CA	7:G:22:MET:HE1	1.56	1.31

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:289:LEU:CD2	25:Y:435:MET:SD	2.19	1.31
7:G:60:ARG:NH2	7:G:69:GLU:OE1	1.65	1.30
18:R:62:PHE:CZ	18:R:201:ALA:HB1	1.66	1.30
20:T:122:HIS:HB2	23:W:131:ASP:N	1.45	1.30
25:Y:349:LEU:HD12	25:Y:380:ARG:NE	1.44	1.30
25:Y:67:ARG:HB3	25:Y:230:SER:CB	1.61	1.30
2:B:193:LYS:NZ	12:L:32:ALA:O	1.61	1.30
1:A:1445:ILE:CG1	7:G:18:PHE:HZ	1.40	1.30
17:Q:97:LYS:CG	17:Q:243:ASN:HB2	1.61	1.29
25:Y:257:LEU:HD23	25:Y:383:LEU:CD1	1.62	1.29
22:V:119:PRO:O	22:V:122:TRP:CD1	1.86	1.29
17:Q:16:TYR:CE2	17:Q:87:PHE:HB3	1.48	1.29
25:Y:440:LEU:CD2	25:Y:641:PHE:HB2	1.60	1.29
1:A:1444:MET:HG2	7:G:60:ARG:CB	1.34	1.29
20:T:63:PHE:O	20:T:66:ASN:ND2	1.66	1.29
25:Y:28:ILE:CG2	25:Y:57:ILE:HG13	1.62	1.29
25:Y:352:ILE:O	25:Y:356:PRO:CD	1.79	1.29
26:Z:696:ARG:NH1	26:Z:704:PHE:CE1	1.98	1.29
25:Y:352:ILE:CB	25:Y:380:ARG:CZ	2.10	1.28
25:Y:420:ILE:CD1	25:Y:633:ARG:HH21	1.44	1.28
17:Q:97:LYS:CE	17:Q:243:ASN:CB	2.07	1.28
2:B:1220:ARG:C	4:D:14:ARG:NH2	1.86	1.27
17:Q:106:ARG:HH21	17:Q:214:GLN:CD	1.34	1.27
1:A:1450:LEU:C	7:G:18:PHE:O	1.71	1.27
20:T:122:HIS:HB3	23:W:131:ASP:O	1.27	1.27
25:Y:193:TYR:CZ	25:Y:197:ARG:HD2	1.69	1.27
25:Y:419:ILE:C	25:Y:633:ARG:HH12	1.36	1.27
1:A:344:ARG:NH2	2:B:1120:GLU:HG3	1.48	1.26
6:F:105:ALA:CB	7:G:14:HIS:CE1	2.18	1.26
22:V:119:PRO:C	22:V:122:TRP:CD1	2.08	1.26
26:Z:757:ARG:NH1	26:Z:760:LEU:CG	1.76	1.26
1:A:1442:ASP:HA	7:G:63:PRO:CG	1.64	1.26
16:P:619:ILE:CB	16:P:634:MET:HA	1.64	1.26
17:Q:97:LYS:CD	17:Q:243:ASN:CB	2.13	1.26
25:Y:232:VAL:CG2	25:Y:453:PHE:HE2	1.48	1.25
1:A:1451:VAL:CG1	7:G:20:PRO:CA	2.13	1.25
25:Y:229:ASP:CA	25:Y:453:PHE:HB3	1.64	1.25
25:Y:631:GLU:CA	25:Y:636:LYS:HE3	1.67	1.25
25:Y:200:ILE:CB	25:Y:226:VAL:CB	1.79	1.25
2:B:110:HIS:CE1	12:L:54:ARG:HH22	1.55	1.25
20:T:122:HIS:CA	23:W:130:VAL:HG12	1.59	1.24

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:585:PRO:HB3	26:Z:756:ARG:NH1	1.33	1.24
6:F:92:ARG:CZ	7:G:63:PRO:CB	2.12	1.24
25:Y:639:LEU:CB	25:Y:653:PHE:CD2	2.19	1.24
25:Y:272:SER:OG	25:Y:281:LYS:HE3	1.28	1.24
25:Y:352:ILE:CB	25:Y:380:ARG:NH1	2.00	1.24
25:Y:518:ILE:O	25:Y:522:TYR:CD2	1.90	1.24
1:A:1447:GLU:OE2	7:G:26:LEU:CD1	1.86	1.24
25:Y:639:LEU:CD1	25:Y:653:PHE:HE2	1.34	1.24
25:Y:357:LYS:CE	25:Y:376:PHE:CD1	2.21	1.23
25:Y:419:ILE:C	25:Y:633:ARG:NH1	1.90	1.23
2:B:1215:ARG:NE	4:D:15:LEU:CD1	1.99	1.23
25:Y:135:ARG:NH2	25:Y:143:ARG:NE	1.85	1.23
25:Y:28:ILE:HG22	25:Y:57:ILE:CG1	1.67	1.23
7:G:19:GLY:O	7:G:22:MET:HG3	1.38	1.23
17:Q:75:LEU:O	17:Q:98:ILE:HG23	1.08	1.22
25:Y:353:SER:O	25:Y:356:PRO:HG2	1.34	1.22
25:Y:499:LYS:NZ	25:Y:522:TYR:C	1.92	1.22
25:Y:419:ILE:CA	25:Y:633:ARG:HH12	1.50	1.22
26:Z:668:THR:CG2	26:Z:694:LYS:CB	2.18	1.22
25:Y:420:ILE:CD1	25:Y:633:ARG:NH2	2.02	1.21
25:Y:418:LEU:CD1	25:Y:634:ILE:HG12	1.68	1.21
25:Y:244:CYS:CB	25:Y:442:ALA:HB1	1.68	1.21
25:Y:59:TYR:HA	25:Y:62:HIS:NE2	0.90	1.21
1:A:317:LYS:O	2:B:471:LYS:NZ	1.73	1.21
25:Y:254:THR:CG2	25:Y:286:TYR:CE1	1.94	1.21
25:Y:639:LEU:CB	25:Y:653:PHE:CE2	2.23	1.21
26:Z:717:TYR:CE2	26:Z:718:TYR:CD1	2.28	1.20
25:Y:393:VAL:CB	25:Y:437:PHE:CZ	2.22	1.20
6:F:96:THR:CG2	7:G:65:ASP:O	1.90	1.20
26:Z:477:LEU:HA	26:Z:501:VAL:HB	1.20	1.19
25:Y:327:ARG:HB2	25:Y:330:HIS:CE1	1.78	1.19
25:Y:357:LYS:HE3	25:Y:376:PHE:CE1	1.76	1.19
25:Y:59:TYR:CA	25:Y:62:HIS:CD2	2.21	1.19
25:Y:639:LEU:HB2	25:Y:653:PHE:CE2	1.77	1.19
17:Q:97:LYS:HG2	17:Q:243:ASN:CB	1.71	1.19
17:Q:20:ILE:HD11	17:Q:87:PHE:CE2	1.69	1.19
1:A:1445:ILE:HG23	6:F:132:LEU:CD2	1.71	1.19
17:Q:85:LEU:O	17:Q:89:ILE:HG23	1.43	1.19
26:Z:621:LYS:HB3	26:Z:621:LYS:NZ	1.40	1.19
25:Y:639:LEU:HD12	25:Y:653:PHE:CZ	1.77	1.18
17:Q:81:MET:HE1	17:Q:92:SER:CB	1.66	1.18

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:68:LYS:CG	25:Y:228:LYS:HG3	1.72	1.18
1:A:1450:LEU:O	7:G:18:PHE:O	1.59	1.18
2:B:1220:ARG:C	4:D:14:ARG:HH22	1.41	1.18
20:T:97:LEU:HD12	20:T:100:ILE:HD11	1.18	1.18
1:A:1447:GLU:CB	7:G:22:MET:CE	2.20	1.18
6:F:92:ARG:HE	7:G:64:THR:N	1.40	1.18
25:Y:586:TYR:CD2	25:Y:598:LEU:CD1	2.27	1.18
26:Z:527:LEU:HD22	26:Z:531:ILE:HD12	1.21	1.17
1:A:227:VAL:CG2	4:D:16:LYS:HE3	1.72	1.17
25:Y:28:ILE:HG22	25:Y:57:ILE:CD1	1.72	1.17
25:Y:350:HIS:CE1	25:Y:381:LEU:HD11	1.79	1.17
25:Y:353:SER:HA	25:Y:356:PRO:HG3	1.19	1.17
25:Y:416:PHE:HE2	25:Y:440:LEU:CD2	1.56	1.16
25:Y:352:ILE:O	25:Y:356:PRO:HD3	0.98	1.16
25:Y:418:LEU:HD11	25:Y:634:ILE:HG12	1.26	1.16
25:Y:639:LEU:CD1	25:Y:653:PHE:CZ	2.28	1.16
1:A:1451:VAL:HG13	7:G:20:PRO:CA	1.75	1.16
25:Y:526:LEU:CD2	25:Y:554:TRP:CH2	2.29	1.16
25:Y:231:ILE:HA	25:Y:455:SER:CB	1.76	1.16
1:A:1445:ILE:CG1	7:G:68:ALA:N	2.04	1.16
25:Y:67:ARG:HB3	25:Y:230:SER:HB3	1.17	1.16
25:Y:272:SER:OG	25:Y:281:LYS:CE	1.93	1.15
1:A:1447:GLU:HG3	7:G:70:PHE:CZ	1.80	1.15
6:F:92:ARG:NH2	7:G:63:PRO:HB2	0.84	1.15
26:Z:757:ARG:CZ	26:Z:760:LEU:HB3	1.76	1.15
18:R:62:PHE:CE2	18:R:201:ALA:HB1	1.80	1.15
25:Y:393:VAL:CB	25:Y:437:PHE:CE2	2.29	1.15
17:Q:81:MET:HE2	17:Q:92:SER:CB	1.59	1.14
25:Y:193:TYR:CE2	25:Y:197:ARG:HD2	1.80	1.14
20:T:122:HIS:HA	23:W:130:VAL:HG11	1.27	1.14
20:T:122:HIS:HB2	23:W:130:VAL:HG12	1.23	1.14
1:A:49:LYS:HE2	1:A:61:ILE:HD11	1.26	1.14
26:Z:474:MET:HB3	26:Z:482:TRP:H	1.13	1.14
26:Z:668:THR:CG2	26:Z:694:LYS:HB3	1.76	1.14
22:V:146:LYS:CG	23:W:129:PHE:CZ	2.29	1.14
25:Y:68:LYS:O	25:Y:230:SER:OG	1.63	1.14
1:A:1444:MET:CG	7:G:60:ARG:HB2	1.77	1.13
2:B:1215:ARG:CZ	4:D:15:LEU:HD11	1.77	1.13
1:A:1447:GLU:CG	7:G:70:PHE:HZ	1.60	1.13
25:Y:567:LYS:HE2	25:Y:597:ILE:HG21	1.21	1.13
17:Q:75:LEU:HA	17:Q:98:ILE:HG21	1.19	1.13

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:421:ARG:HG2	26:Z:430:LEU:HG	1.30	1.13
1:A:36:ARG:NH2	1:A:57:ARG:HH12	1.45	1.13
22:V:117:LYS:NZ	22:V:121:GLU:HG2	1.41	1.13
25:Y:269:GLU:HG2	25:Y:277:VAL:HG11	1.28	1.13
25:Y:327:ARG:CZ	25:Y:330:HIS:CE1	2.31	1.13
25:Y:231:ILE:HA	25:Y:455:SER:HB2	1.16	1.13
25:Y:494:PRO:HD2	25:Y:679:MET:O	1.46	1.13
25:Y:71:TYR:CE2	25:Y:233:ILE:HG21	1.83	1.13
20:T:38:SER:HB2	22:V:113:ASP:OD2	1.47	1.13
25:Y:200:ILE:O	25:Y:226:VAL:HG23	1.49	1.13
6:F:96:THR:OG1	7:G:64:THR:O	1.65	1.12
25:Y:586:TYR:CD2	25:Y:598:LEU:HD11	1.84	1.12
17:Q:97:LYS:CG	17:Q:243:ASN:CB	2.24	1.12
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.28	1.12
25:Y:353:SER:HB2	25:Y:381:LEU:HB2	1.14	1.12
16:P:315:SER:CB	16:P:426:ARG:N	2.12	1.12
25:Y:232:VAL:HG21	25:Y:453:PHE:HE2	1.14	1.12
25:Y:289:LEU:HD22	25:Y:435:MET:SD	1.84	1.12
1:A:1444:MET:CG	7:G:60:ARG:CB	2.28	1.12
25:Y:518:ILE:HG23	25:Y:522:TYR:CE2	1.77	1.12
6:F:96:THR:HG21	7:G:65:ASP:O	1.48	1.11
20:T:118:LEU:HD21	23:W:129:PHE:CB	1.80	1.11
1:A:227:VAL:HG21	4:D:16:LYS:HE3	1.18	1.11
1:A:1445:ILE:CG2	7:G:18:PHE:HE2	1.62	1.11
25:Y:327:ARG:NH1	25:Y:330:HIS:CE1	2.18	1.11
25:Y:353:SER:O	25:Y:356:PRO:CG	1.99	1.11
17:Q:90:LEU:CD2	17:Q:251:PHE:HE2	1.62	1.11
13:M:1:MET:N	24:X:90:GLU:O	1.80	1.11
26:Z:455:SER:HB3	26:Z:466:ARG:HH11	1.15	1.11
26:Z:408:ILE:HG12	26:Z:475:ASP:HB3	1.28	1.11
20:T:122:HIS:HB2	23:W:130:VAL:C	1.70	1.11
20:T:114:ILE:HG13	22:V:143:LEU:HD13	1.33	1.11
25:Y:230:SER:N	25:Y:453:PHE:HB2	1.65	1.11
22:V:112:LYS:HG3	22:V:119:PRO:HD3	1.27	1.11
25:Y:499:LYS:HD3	25:Y:521:ASN:C	1.71	1.11
16:P:410:VAL:CB	16:P:502:ASN:HA	1.81	1.10
21:U:70:MET:SD	24:X:69:TYR:CE1	2.44	1.10
25:Y:60:GLN:O	25:Y:64:PRO:CD	2.00	1.10
2:B:1215:ARG:CD	4:D:15:LEU:HD13	1.62	1.10
1:A:1451:VAL:HG13	7:G:20:PRO:CB	1.80	1.10
26:Z:757:ARG:NH1	26:Z:760:LEU:CB	2.13	1.10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:200:ILE:CA	25:Y:226:VAL:CG2	2.28	1.10
25:Y:495:MET:HG2	25:Y:686:PHE:CB	1.81	1.10
17:Q:48:ASP:O	18:R:47:LYS:HE3	1.52	1.10
25:Y:254:THR:HG23	25:Y:286:TYR:CD1	1.86	1.10
1:A:1447:GLU:CD	7:G:70:PHE:CZ	2.25	1.10
25:Y:353:SER:CB	25:Y:381:LEU:HB2	1.82	1.10
25:Y:499:LYS:CD	25:Y:522:TYR:HA	1.81	1.09
1:A:1451:VAL:HG23	7:G:22:MET:SD	1.93	1.09
6:F:105:ALA:HB2	7:G:14:HIS:NE2	1.67	1.09
26:Z:428:CYS:HB2	26:Z:434:ASN:HB2	1.26	1.09
25:Y:244:CYS:HB3	25:Y:442:ALA:HB1	1.34	1.09
20:T:122:HIS:CB	23:W:131:ASP:N	2.14	1.09
25:Y:495:MET:HB3	25:Y:686:PHE:CD2	1.86	1.09
6:F:96:THR:CG2	7:G:65:ASP:C	2.18	1.09
22:V:83:LEU:HA	22:V:87:LEU:HB2	1.19	1.09
20:T:93:ILE:CD1	22:V:122:TRP:CE3	2.04	1.09
26:Z:487:LEU:HD23	26:Z:493:VAL:HG21	1.19	1.09
26:Z:410:LEU:HD11	26:Z:457:TYR:HA	1.17	1.09
25:Y:386:ARG:O	25:Y:390:VAL:HG23	1.51	1.09
17:Q:106:ARG:NH2	17:Q:214:GLN:OE1	1.84	1.09
22:V:111:THR:O	22:V:117:LYS:O	1.70	1.09
1:A:1447:GLU:HG2	7:G:22:MET:HE2	1.26	1.08
16:P:410:VAL:CB	16:P:502:ASN:CA	2.30	1.08
25:Y:232:VAL:CG2	25:Y:453:PHE:CE2	2.34	1.08
26:Z:647:ASP:N	26:Z:647:ASP:OD1	1.84	1.08
1:A:89:PRO:HG2	1:A:204:THR:HB	1.35	1.08
25:Y:586:TYR:CG	25:Y:598:LEU:HD11	1.87	1.08
6:F:105:ALA:CA	7:G:14:HIS:HE1	1.64	1.08
20:T:94:TYR:HB2	22:V:111:THR:HG22	1.35	1.08
25:Y:550:ILE:HG22	25:Y:554:TRP:CH2	1.87	1.08
25:Y:643:ARG:HB2	25:Y:649:ARG:HB3	1.26	1.08
26:Z:621:LYS:NZ	26:Z:621:LYS:CB	2.10	1.08
2:B:1220:ARG:CA	4:D:14:ARG:NH2	2.14	1.08
22:V:89:THR:HG23	22:V:90:LEU:HD12	1.32	1.08
25:Y:28:ILE:HG22	25:Y:57:ILE:HG13	1.19	1.08
26:Z:668:THR:CG2	26:Z:694:LYS:HB2	1.81	1.08
25:Y:353:SER:HB2	25:Y:381:LEU:CB	1.84	1.08
25:Y:418:LEU:HD12	25:Y:438:THR:OG1	1.52	1.08
25:Y:532:ILE:HD12	25:Y:705:ASP:HB2	1.31	1.08
26:Z:757:ARG:CZ	26:Z:760:LEU:CG	2.32	1.08
1:A:16:GLU:OE1	4:D:14:ARG:NH1	1.86	1.08

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:229:ASP:HB3	25:Y:453:PHE:HB3	1.19	1.08
26:Z:410:LEU:HD22	26:Z:477:LEU:HD11	1.35	1.08
1:A:836:TYR:OH	1:A:1403:GLU:OE2	1.69	1.07
20:T:87:LEU:HD12	20:T:90:TYR:HD2	1.18	1.07
25:Y:200:ILE:CA	25:Y:226:VAL:HG21	1.83	1.07
1:A:1445:ILE:HG12	7:G:18:PHE:HZ	1.03	1.07
25:Y:124:ARG:HA	25:Y:376:PHE:CE1	1.89	1.07
20:T:122:HIS:HB3	23:W:131:ASP:CA	1.85	1.07
25:Y:272:SER:CB	25:Y:281:LYS:NZ	2.17	1.07
26:Z:424:PHE:HB3	26:Z:449:GLU:HG2	1.28	1.07
17:Q:75:LEU:C	17:Q:98:ILE:HG23	1.74	1.07
17:Q:86:ASN:ND2	17:Q:87:PHE:CD1	2.23	1.07
18:R:43:ARG:HB2	18:R:119:ARG:HG3	1.33	1.07
25:Y:497:ILE:HG23	25:Y:684:ARG:HG2	1.29	1.07
17:Q:75:LEU:CA	17:Q:98:ILE:HG21	1.84	1.07
20:T:118:LEU:HD21	23:W:129:PHE:HB3	1.37	1.07
25:Y:328:ALA:CA	25:Y:417:LEU:HD22	1.85	1.07
20:T:93:ILE:HD13	22:V:122:TRP:HB2	1.36	1.07
25:Y:495:MET:HG2	25:Y:686:PHE:HB2	1.29	1.07
17:Q:97:LYS:HD3	17:Q:243:ASN:HB2	1.37	1.06
25:Y:639:LEU:HG	25:Y:653:PHE:CE2	1.84	1.06
16:P:341:TYR:HA	16:P:354:ILE:CB	1.84	1.06
20:T:118:LEU:CD2	23:W:129:PHE:HB3	1.85	1.06
25:Y:550:ILE:HG23	25:Y:554:TRP:HZ2	1.20	1.06
25:Y:350:HIS:CE1	25:Y:381:LEU:CD1	2.37	1.06
26:Z:405:LYS:HD3	26:Z:483:GLY:HA3	1.35	1.06
20:T:50:GLU:HG2	22:V:98:LEU:HD13	1.10	1.06
25:Y:229:ASP:HB3	25:Y:453:PHE:CB	1.85	1.06
1:A:78:PRO:O	2:B:1201:LYS:NZ	1.89	1.06
1:A:1442:ASP:C	7:G:63:PRO:HG3	1.76	1.06
22:V:119:PRO:CA	22:V:122:TRP:HE1	1.55	1.06
26:Z:476:PHE:HD1	26:Z:485:ILE:HD12	1.17	1.06
26:Z:696:ARG:NH1	26:Z:704:PHE:CZ	2.24	1.06
25:Y:293:LEU:CD1	25:Y:433:PRO:CB	2.32	1.06
25:Y:495:MET:SD	25:Y:696:TRP:CE3	2.49	1.06
20:T:42:LEU:HD23	22:V:105:ILE:HD12	1.36	1.05
25:Y:196:VAL:O	25:Y:200:ILE:HG23	1.56	1.05
20:T:55:LYS:HD2	20:T:60:VAL:HG11	1.33	1.05
21:U:70:MET:SD	24:X:69:TYR:CD1	2.49	1.05
26:Z:408:ILE:HB	26:Z:482:TRP:HD1	1.16	1.05
26:Z:515:ALA:C	26:Z:681:ARG:HD3	1.75	1.05

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:756:ARG:CG	26:Z:756:ARG:HH11	1.69	1.05
1:A:1443:VAL:N	7:G:63:PRO:CG	2.08	1.05
1:A:1442:ASP:CA	7:G:63:PRO:HG2	1.87	1.05
25:Y:440:LEU:HD11	25:Y:638:ARG:HA	1.08	1.05
1:A:1451:VAL:HG11	7:G:20:PRO:HA	1.13	1.05
2:B:1220:ARG:HA	4:D:14:ARG:HH22	1.11	1.05
22:V:119:PRO:HB2	22:V:122:TRP:HE1	1.21	1.05
26:Z:505:ILE:HG22	26:Z:507:ALA:H	1.21	1.05
25:Y:200:ILE:C	25:Y:226:VAL:HG23	1.75	1.05
25:Y:419:ILE:O	25:Y:633:ARG:NH1	1.87	1.05
25:Y:479:LEU:O	25:Y:479:LEU:HD22	1.54	1.05
25:Y:42:MET:CG	25:Y:50:VAL:HG22	1.87	1.04
1:A:1447:GLU:HG2	7:G:22:MET:CE	1.86	1.04
1:A:1447:GLU:O	7:G:22:MET:SD	2.15	1.04
17:Q:86:ASN:HA	17:Q:89:ILE:HG12	1.36	1.04
20:T:91:ASP:HA	22:V:111:THR:HG21	1.31	1.04
26:Z:472:LYS:HG2	26:Z:473:VAL:HG13	1.37	1.04
6:F:105:ALA:HA	7:G:14:HIS:HE1	1.19	1.04
25:Y:650:GLU:HA	25:Y:653:PHE:CE1	1.91	1.04
26:Z:757:ARG:HH12	26:Z:760:LEU:CB	1.70	1.04
25:Y:253:THR:HG22	25:Y:434:ILE:CG2	1.88	1.04
26:Z:578:MET:SD	26:Z:779:ALA:O	2.15	1.04
1:A:89:PRO:CG	1:A:204:THR:HB	1.88	1.04
16:P:321:VAL:CB	16:P:340:GLY:CA	2.35	1.04
17:Q:97:LYS:HZ3	17:Q:244:SER:CA	1.71	1.04
2:B:1215:ARG:CD	4:D:15:LEU:HD11	1.74	1.04
2:B:902:GLY:O	12:L:65:VAL:HG11	1.58	1.04
25:Y:200:ILE:HG21	25:Y:226:VAL:HG11	1.35	1.04
25:Y:230:SER:O	25:Y:455:SER:CB	2.06	1.04
25:Y:537:MET:SD	25:Y:621:LEU:HD13	1.98	1.04
26:Z:502:VAL:HG11	26:Z:530:LEU:HB3	1.35	1.04
25:Y:349:LEU:HD11	25:Y:380:ARG:HG3	1.40	1.04
25:Y:257:LEU:HD23	25:Y:383:LEU:HD11	1.07	1.03
25:Y:230:SER:O	25:Y:455:SER:HB2	1.55	1.03
25:Y:42:MET:SD	25:Y:50:VAL:HG22	1.97	1.03
1:A:317:LYS:O	2:B:471:LYS:CE	2.06	1.03
1:A:1444:MET:HG2	7:G:60:ARG:HB2	1.03	1.03
17:Q:98:ILE:CG2	17:Q:99:PRO:HD2	1.89	1.03
13:M:129:ARG:CB	13:M:134:THR:CB	2.35	1.03
17:Q:106:ARG:NH2	17:Q:214:GLN:CD	2.11	1.03
18:R:72:ILE:CG2	18:R:202:TYR:CE1	2.40	1.03

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:678:VAL:HG11	25:Y:708:LEU:HG	1.41	1.03
25:Y:250:LEU:O	25:Y:436:ARG:HG3	1.59	1.03
25:Y:37:ASN:HB2	25:Y:456:VAL:CB	1.79	1.03
25:Y:499:LYS:NZ	25:Y:522:TYR:O	1.90	1.03
25:Y:353:SER:C	25:Y:356:PRO:HD2	1.78	1.03
25:Y:28:ILE:CG2	25:Y:57:ILE:CG1	2.32	1.03
26:Z:756:ARG:HG2	26:Z:756:ARG:NH1	1.53	1.03
25:Y:495:MET:HG2	25:Y:686:PHE:CG	1.93	1.03
25:Y:70:ILE:HB	25:Y:208:TYR:HE2	1.23	1.02
26:Z:384:ILE:HD13	26:Z:511:LEU:HD11	1.41	1.02
26:Z:474:MET:H	26:Z:481:GLU:H	1.07	1.02
1:A:1445:ILE:HG13	7:G:68:ALA:N	1.69	1.02
26:Z:303:ARG:HG2	26:Z:504:THR:HB	1.40	1.02
20:T:122:HIS:CA	23:W:130:VAL:HG13	1.86	1.02
25:Y:103:PHE:CD1	25:Y:205:ILE:HD12	1.95	1.02
25:Y:128:VAL:CG2	25:Y:375:ARG:HA	1.88	1.02
25:Y:499:LYS:CD	25:Y:522:TYR:N	2.22	1.02
26:Z:757:ARG:NH2	26:Z:760:LEU:CB	2.22	1.02
6:F:105:ALA:CB	7:G:14:HIS:HE1	1.64	1.02
25:Y:499:LYS:CD	25:Y:522:TYR:CA	2.38	1.02
25:Y:59:TYR:HA	25:Y:62:HIS:CE1	1.95	1.02
26:Z:757:ARG:CZ	26:Z:760:LEU:CD2	2.21	1.02
26:Z:376:ASN:H	26:Z:380:ARG:HB2	1.22	1.02
1:A:1442:ASP:CA	7:G:63:PRO:CG	2.37	1.01
25:Y:68:LYS:HB2	25:Y:228:LYS:HB2	1.42	1.01
26:Z:588:PHE:CE2	26:Z:621:LYS:NZ	2.26	1.01
22:V:83:LEU:HG	22:V:87:LEU:HD13	1.41	1.01
20:T:119:ASN:N	23:W:131:ASP:CG	2.03	1.01
25:Y:603:ARG:NH1	25:Y:629:TYR:OH	1.93	1.01
25:Y:357:LYS:CE	25:Y:376:PHE:CE1	2.37	1.01
26:Z:588:PHE:CZ	26:Z:621:LYS:HE2	1.95	1.01
1:A:1447:GLU:HG3	7:G:70:PHE:HZ	0.89	1.01
25:Y:416:PHE:CE2	25:Y:440:LEU:CD2	2.35	1.01
26:Z:585:PRO:CB	26:Z:756:ARG:CZ	2.22	1.01
21:U:139:ILE:HD13	21:U:147:LYS:HE3	1.39	1.01
25:Y:681:LEU:HD22	25:Y:696:TRP:CZ3	1.95	1.01
20:T:93:ILE:HD11	22:V:126:ILE:HD13	1.42	1.01
25:Y:135:ARG:CZ	25:Y:143:ARG:HE	1.72	1.01
26:Z:621:LYS:HZ2	26:Z:621:LYS:CB	1.70	1.01
25:Y:495:MET:HG3	25:Y:681:LEU:HB2	1.38	1.01
26:Z:757:ARG:CZ	26:Z:760:LEU:CB	2.39	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:321:VAL:CB	16:P:340:GLY:HA2	1.91	1.01
25:Y:215:ASP:O	25:Y:218:ILE:HG22	1.59	1.01
25:Y:231:ILE:CG2	25:Y:457:ILE:HD11	1.91	1.01
2:B:1185:CYS:SG	4:D:17:LYS:CD	2.48	1.01
25:Y:248:LEU:HD21	25:Y:445:ALA:HB2	1.37	1.01
1:A:344:ARG:CZ	2:B:1120:GLU:HG3	1.88	1.01
17:Q:90:LEU:CD2	17:Q:251:PHE:CE2	2.44	1.01
17:Q:90:LEU:HD22	17:Q:251:PHE:HE2	1.20	1.01
18:R:62:PHE:CZ	18:R:201:ALA:CB	2.43	1.01
16:P:323:PHE:CB	16:P:339:TYR:O	2.09	1.00
1:A:1445:ILE:CB	7:G:18:PHE:CZ	2.40	1.00
25:Y:272:SER:HB2	25:Y:281:LYS:NZ	1.76	1.00
25:Y:288:LYS:NZ	25:Y:334:PHE:O	1.94	1.00
25:Y:124:ARG:HG2	25:Y:377:CYS:SG	2.01	1.00
25:Y:68:LYS:HD2	25:Y:228:LYS:HG2	1.40	1.00
20:T:63:PHE:O	20:T:66:ASN:CG	1.97	1.00
17:Q:98:ILE:HG23	17:Q:99:PRO:HD2	1.40	1.00
6:F:105:ALA:HA	7:G:14:HIS:CE1	1.96	1.00
22:V:119:PRO:HA	22:V:122:TRP:NE1	1.53	1.00
20:T:122:HIS:CB	23:W:130:VAL:CG1	2.29	1.00
25:Y:254:THR:HG21	25:Y:286:TYR:HE1	1.22	1.00
2:B:1215:ARG:HD2	4:D:15:LEU:HD13	1.03	1.00
25:Y:37:ASN:HB2	25:Y:456:VAL:HB	1.04	1.00
26:Z:560:PRO:O	26:Z:586:THR:CG2	2.09	1.00
22:V:119:PRO:CB	22:V:122:TRP:NE1	2.10	1.00
2:B:110:HIS:CE1	12:L:54:ARG:NH2	2.29	1.00
17:Q:75:LEU:HA	17:Q:98:ILE:CG2	1.92	0.99
25:Y:244:CYS:HB2	25:Y:442:ALA:HB1	1.44	0.99
26:Z:477:LEU:CA	26:Z:501:VAL:HB	1.92	0.99
25:Y:353:SER:HA	25:Y:356:PRO:CG	1.92	0.99
25:Y:481:LYS:HD3	25:Y:483:TYR:CE2	1.97	0.99
17:Q:20:ILE:HD12	17:Q:87:PHE:CZ	1.97	0.99
25:Y:328:ALA:HA	25:Y:417:LEU:CD2	1.91	0.99
26:Z:459:MET:HB2	26:Z:464:ARG:HD2	1.40	0.99
25:Y:197:ARG:O	25:Y:200:ILE:HG12	1.62	0.99
17:Q:81:MET:HE1	17:Q:92:SER:HB2	1.42	0.99
25:Y:190:LEU:HD13	25:Y:195:ILE:HD11	1.42	0.99
20:T:119:ASN:N	23:W:131:ASP:OD2	1.96	0.99
25:Y:518:ILE:O	25:Y:522:TYR:HD2	1.36	0.99
1:A:1386:ARG:NH1	1:A:1403:GLU:OE1	1.95	0.99
1:A:227:VAL:HG11	4:D:16:LYS:CG	1.91	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:588:PHE:HE2	26:Z:621:LYS:HZ1	1.01	0.99
17:Q:20:ILE:HD11	17:Q:87:PHE:HE2	1.16	0.99
25:Y:259:ARG:HB3	25:Y:379:GLU:OE1	1.62	0.99
25:Y:440:LEU:HD23	25:Y:641:PHE:CD2	1.97	0.99
1:A:1445:ILE:HG22	6:F:132:LEU:CD2	1.82	0.98
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.27	0.98
18:R:43:ARG:NH2	18:R:117:MET:CE	2.26	0.98
1:A:1451:VAL:HG13	7:G:20:PRO:CG	1.92	0.98
20:T:111:THR:HA	22:V:143:LEU:HD22	1.42	0.98
17:Q:106:ARG:NH2	17:Q:211:PHE:CZ	2.31	0.98
22:V:112:LYS:HD2	22:V:119:PRO:HB3	1.45	0.98
22:V:119:PRO:C	22:V:122:TRP:NE1	2.14	0.98
25:Y:68:LYS:HB2	25:Y:228:LYS:CB	1.92	0.98
26:Z:376:ASN:HB2	26:Z:380:ARG:HD3	1.45	0.98
26:Z:476:PHE:CD1	26:Z:485:ILE:HD12	1.98	0.98
17:Q:20:ILE:HD12	17:Q:87:PHE:CE2	1.95	0.98
1:A:1447:GLU:HB3	7:G:22:MET:HE2	1.43	0.98
21:U:130:TYR:CE2	21:U:134:ILE:HD11	1.99	0.98
25:Y:103:PHE:HE1	25:Y:205:ILE:HD12	1.20	0.98
25:Y:567:LYS:CE	25:Y:597:ILE:HG21	1.92	0.98
26:Z:553:GLN:HB2	26:Z:701:PHE:CD2	1.98	0.98
20:T:38:SER:HB2	22:V:113:ASP:CG	1.84	0.98
25:Y:350:HIS:HB2	25:Y:384:LEU:HD12	1.43	0.98
26:Z:421:ARG:HA	26:Z:424:PHE:HD2	1.29	0.98
17:Q:97:LYS:HZ1	17:Q:244:SER:H	1.08	0.98
25:Y:603:ARG:CZ	25:Y:629:TYR:OH	2.11	0.98
20:T:87:LEU:HD12	20:T:90:TYR:CD2	1.99	0.97
25:Y:231:ILE:CA	25:Y:455:SER:HB2	1.92	0.97
25:Y:499:LYS:HB3	25:Y:522:TYR:CD1	1.97	0.97
25:Y:639:LEU:CD2	25:Y:649:ARG:CD	2.19	0.97
26:Z:425:LEU:HG	26:Z:429:THR:HA	1.40	0.97
20:T:55:LYS:HB3	20:T:62:ARG:HG3	1.46	0.97
25:Y:440:LEU:CD1	25:Y:638:ARG:HA	1.94	0.97
25:Y:495:MET:HB3	25:Y:686:PHE:CE2	1.98	0.97
26:Z:408:ILE:HB	26:Z:482:TRP:CD1	1.98	0.97
17:Q:86:ASN:ND2	17:Q:87:PHE:CE1	2.33	0.97
25:Y:124:ARG:CB	25:Y:377:CYS:SG	2.53	0.97
25:Y:190:LEU:HD13	25:Y:195:ILE:HD12	1.46	0.97
26:Z:495:ALA:HB3	26:Z:498:PHE:HD2	1.29	0.97
1:A:1451:VAL:CG2	7:G:22:MET:HG3	1.95	0.97
17:Q:16:TYR:CE2	17:Q:87:PHE:CB	2.01	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:142:LYS:HA	25:Y:145:LEU:CD2	1.94	0.97
2:B:1217:TYR:OH	4:D:15:LEU:HA	1.64	0.96
25:Y:185:CYS:HB2	25:Y:192:PRO:HG3	1.47	0.96
25:Y:190:LEU:CD1	25:Y:195:ILE:CD1	2.42	0.96
26:Z:458:SER:HA	26:Z:465:ASN:HB2	1.47	0.96
25:Y:538:VAL:HG22	25:Y:598:LEU:HB2	1.47	0.96
20:T:90:TYR:HB3	22:V:112:LYS:H	1.28	0.96
25:Y:245:ILE:HG23	25:Y:439:CYS:O	1.63	0.96
25:Y:128:VAL:HG21	25:Y:375:ARG:HA	1.46	0.96
26:Z:757:ARG:NH2	26:Z:760:LEU:CG	2.27	0.96
17:Q:79:THR:O	17:Q:82:ASP:HB2	1.63	0.96
18:R:4:SER:HB2	18:R:200:LEU:HD23	1.48	0.96
25:Y:349:LEU:HD12	25:Y:380:ARG:HE	1.22	0.96
20:T:122:HIS:N	23:W:130:VAL:HG13	1.80	0.96
25:Y:603:ARG:NH2	25:Y:629:TYR:OH	1.99	0.96
26:Z:407:VAL:HG13	26:Z:452:LEU:H	1.29	0.96
20:T:87:LEU:HA	20:T:90:TYR:CE2	2.00	0.96
25:Y:586:TYR:CD2	25:Y:598:LEU:HG	2.01	0.96
26:Z:297:ILE:HG22	26:Z:308:ASP:HB2	1.47	0.96
26:Z:656:LYS:O	26:Z:656:LYS:HD2	1.65	0.96
25:Y:193:TYR:CE2	25:Y:197:ARG:CD	2.48	0.96
20:T:114:ILE:HD12	22:V:147:LEU:HD12	1.48	0.96
6:F:105:ALA:HB2	7:G:14:HIS:CE1	1.91	0.95
22:V:81:ASN:HB2	22:V:90:LEU:CD2	1.96	0.95
25:Y:162:LEU:HD23	25:Y:195:ILE:HG13	1.48	0.95
6:F:92:ARG:HE	7:G:64:THR:CA	1.77	0.95
25:Y:237:ALA:CB	25:Y:458:ILE:HG23	1.95	0.95
1:A:344:ARG:HD2	2:B:1118:PRO:O	1.64	0.95
25:Y:499:LYS:CB	25:Y:522:TYR:CE1	2.48	0.95
26:Z:410:LEU:HB2	26:Z:466:ARG:HH22	1.27	0.95
26:Z:668:THR:HG21	26:Z:694:LYS:HB3	0.97	0.95
25:Y:193:TYR:OH	25:Y:221:ARG:NH2	1.97	0.95
25:Y:467:ASP:O	25:Y:470:PRO:HG2	1.67	0.95
26:Z:584:ASN:HD21	26:Z:586:THR:CG2	1.78	0.95
17:Q:75:LEU:HB3	17:Q:98:ILE:HD13	1.48	0.95
25:Y:289:LEU:HD23	25:Y:435:MET:SD	2.04	0.95
26:Z:588:PHE:CZ	26:Z:621:LYS:CE	2.49	0.95
25:Y:259:ARG:CB	25:Y:379:GLU:OE1	2.15	0.95
22:V:83:LEU:CA	22:V:87:LEU:HB2	1.95	0.95
17:Q:85:LEU:HD12	17:Q:88:ARG:HB3	1.47	0.94
25:Y:28:ILE:CB	25:Y:57:ILE:HG13	1.96	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:37:ASN:HB3	25:Y:456:VAL:CG2	1.95	0.94
25:Y:495:MET:HB3	25:Y:686:PHE:CG	2.01	0.94
26:Z:588:PHE:CE2	26:Z:621:LYS:HE2	2.02	0.94
1:A:1450:LEU:HD11	7:G:15:PRO:O	1.65	0.94
26:Z:474:MET:HB2	26:Z:480:ARG:CA	1.97	0.94
2:B:326:ASP:HB3	14:N:60:PRO:CA	146.59	0.94
25:Y:440:LEU:CD2	25:Y:641:PHE:CB	2.31	0.94
25:Y:666:LEU:HD23	25:Y:679:MET:SD	2.07	0.94
25:Y:450:PHE:HZ	25:Y:475:PHE:HA	1.33	0.94
25:Y:649:ARG:O	25:Y:653:PHE:CD1	2.21	0.94
25:Y:420:ILE:HD11	25:Y:633:ARG:HH21	1.29	0.94
26:Z:397:ILE:HG23	26:Z:427:TRP:CZ2	2.01	0.94
25:Y:71:TYR:CD2	25:Y:233:ILE:HG21	2.01	0.94
25:Y:28:ILE:HG21	25:Y:57:ILE:HG21	1.47	0.94
25:Y:328:ALA:HA	25:Y:417:LEU:HD22	0.96	0.94
25:Y:683:ASP:O	25:Y:686:PHE:HD2	1.26	0.94
1:A:1451:VAL:HG23	7:G:22:MET:CG	1.97	0.94
25:Y:58:ALA:O	25:Y:62:HIS:CD2	2.20	0.94
17:Q:97:LYS:NZ	17:Q:244:SER:H	1.56	0.93
26:Z:410:LEU:HD11	26:Z:457:TYR:CA	1.99	0.93
26:Z:585:PRO:CB	26:Z:756:ARG:NH2	2.31	0.93
6:F:92:ARG:NE	7:G:64:THR:N	2.15	0.93
25:Y:253:THR:HG22	25:Y:434:ILE:HD13	1.48	0.93
1:A:1445:ILE:O	7:G:68:ALA:CB	2.16	0.93
1:A:1447:GLU:CG	7:G:70:PHE:CZ	2.41	0.93
6:F:105:ALA:HB1	7:G:14:HIS:CE1	2.04	0.93
25:Y:327:ARG:NH1	25:Y:330:HIS:NE2	2.16	0.93
1:A:227:VAL:HG11	4:D:16:LYS:HG3	1.50	0.93
20:T:56:LEU:HB2	20:T:69:ILE:HG21	1.50	0.93
25:Y:124:ARG:NH2	25:Y:381:LEU:CD2	2.30	0.93
25:Y:526:LEU:HD23	25:Y:554:TRP:CZ3	2.04	0.93
25:Y:639:LEU:HD23	25:Y:649:ARG:HB2	1.50	0.93
26:Z:368:LYS:HD2	26:Z:372:LYS:HE2	1.50	0.93
25:Y:349:LEU:HA	25:Y:380:ARG:HH21	1.27	0.93
25:Y:571:VAL:HG12	25:Y:572:GLU:N	1.80	0.93
25:Y:646:TYR:HB2	25:Y:648:ILE:HG12	1.51	0.93
20:T:42:LEU:HD23	22:V:105:ILE:CD1	1.99	0.93
25:Y:393:VAL:HG11	25:Y:437:PHE:CD2	2.04	0.93
6:F:96:THR:OG1	7:G:64:THR:C	2.08	0.92
17:Q:75:LEU:C	17:Q:98:ILE:CG2	2.33	0.92
25:Y:353:SER:H	25:Y:380:ARG:HH11	1.15	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:259:ARG:HB3	25:Y:379:GLU:CD	1.89	0.92
25:Y:251:ASP:HB3	25:Y:436:ARG:CZ	1.99	0.92
25:Y:492:PHE:CE2	25:Y:707:ASN:OD1	2.21	0.92
26:Z:584:ASN:OD1	26:Z:586:THR:HG22	1.67	0.92
20:T:122:HIS:CE1	23:W:133:ILE:C	2.42	0.92
20:T:100:ILE:HD12	22:V:129:ARG:CB	1.98	0.92
17:Q:16:TYR:CD2	17:Q:87:PHE:HB3	2.03	0.92
25:Y:393:VAL:HG21	25:Y:437:PHE:CE1	2.04	0.92
25:Y:586:TYR:CD2	25:Y:598:LEU:CG	2.51	0.92
25:Y:657:ASP:OD1	25:Y:660:ARG:NH2	2.02	0.92
26:Z:424:PHE:CE1	26:Z:450:SER:HB3	2.04	0.92
17:Q:108:ILE:HD13	17:Q:159:GLU:HB2	1.51	0.92
17:Q:97:LYS:HG2	17:Q:243:ASN:CG	1.89	0.92
25:Y:254:THR:OG1	25:Y:433:PRO:HG2	1.69	0.92
2:B:902:GLY:O	12:L:65:VAL:CG1	2.17	0.92
25:Y:288:LYS:CG	25:Y:335:LEU:CB	2.18	0.92
26:Z:439:THR:HG22	26:Z:440:SER:H	1.34	0.92
25:Y:253:THR:CG2	25:Y:434:ILE:HD13	1.99	0.92
25:Y:293:LEU:CD1	25:Y:433:PRO:HB3	2.00	0.92
26:Z:429:THR:HB	26:Z:432:PRO:HD2	1.50	0.92
26:Z:466:ARG:HB2	26:Z:477:LEU:HD22	1.48	0.92
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.52	0.92
22:V:117:LYS:HZ2	22:V:121:GLU:HG2	1.11	0.92
25:Y:353:SER:C	25:Y:356:PRO:CD	2.38	0.92
26:Z:376:ASN:HB3	26:Z:380:ARG:H	1.32	0.92
26:Z:668:THR:HG23	26:Z:694:LYS:HB2	1.50	0.92
25:Y:420:ILE:HG13	25:Y:633:ARG:HH22	1.33	0.92
25:Y:418:LEU:CD1	25:Y:634:ILE:CG1	2.47	0.92
25:Y:70:ILE:HD12	25:Y:208:TYR:OH	1.70	0.92
26:Z:297:ILE:CG2	26:Z:308:ASP:HB2	1.99	0.92
25:Y:499:LYS:HD2	25:Y:522:TYR:CA	2.00	0.91
26:Z:585:PRO:HB2	26:Z:756:ARG:HH22	1.28	0.91
18:R:4:SER:HB2	18:R:200:LEU:CD2	1.99	0.91
25:Y:342:LEU:HD23	25:Y:345:ARG:NH2	1.83	0.91
25:Y:42:MET:SD	25:Y:53:LEU:HD12	2.10	0.91
25:Y:567:LYS:HG2	25:Y:597:ILE:HB	1.52	0.91
25:Y:142:LYS:HA	25:Y:145:LEU:HD21	1.50	0.91
25:Y:416:PHE:CD2	25:Y:637:ALA:HB1	2.06	0.91
25:Y:639:LEU:HB2	25:Y:653:PHE:HD2	1.19	0.91
26:Z:585:PRO:CG	26:Z:756:ARG:NH1	2.33	0.91
25:Y:185:CYS:CB	25:Y:192:PRO:HG3	1.99	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:327:ARG:O	25:Y:417:LEU:HD23	1.70	0.91
25:Y:493:LEU:CD2	25:Y:696:TRP:NE1	2.11	0.91
25:Y:419:ILE:CA	25:Y:633:ARG:NH1	2.21	0.91
26:Z:588:PHE:CE2	26:Z:621:LYS:CE	2.53	0.91
17:Q:16:TYR:HE2	17:Q:87:PHE:HB3	0.81	0.91
25:Y:67:ARG:HB3	25:Y:230:SER:HB2	1.50	0.91
1:A:368:LYS:HG3	1:A:399:HIS:HD2	1.34	0.91
2:B:1220:ARG:HA	4:D:14:ARG:NH2	1.82	0.91
26:Z:424:PHE:HB3	26:Z:449:GLU:CG	2.00	0.91
25:Y:348:VAL:C	25:Y:380:ARG:HH22	1.73	0.91
26:Z:403:ILE:CG2	26:Z:405:LYS:HG2	2.00	0.91
26:Z:403:ILE:HG22	26:Z:405:LYS:HG2	1.53	0.91
21:U:132:GLU:HB3	21:U:139:ILE:HD12	1.49	0.91
26:Z:467:SER:N	26:Z:477:LEU:HD23	1.86	0.91
1:A:1445:ILE:HG22	6:F:132:LEU:HD23	0.93	0.91
25:Y:103:PHE:CE1	25:Y:205:ILE:CD1	2.53	0.91
26:Z:527:LEU:HD22	26:Z:531:ILE:CD1	2.00	0.91
20:T:122:HIS:NE2	23:W:133:ILE:C	2.24	0.90
26:Z:397:ILE:HG23	26:Z:427:TRP:CH2	2.06	0.90
26:Z:408:ILE:HD11	26:Z:466:ARG:HD3	1.53	0.90
16:P:321:VAL:CB	16:P:340:GLY:HA3	2.01	0.90
18:R:43:ARG:NH2	18:R:117:MET:HE1	1.84	0.90
25:Y:190:LEU:HD13	25:Y:195:ILE:HD13	1.52	0.90
26:Z:477:LEU:HA	26:Z:501:VAL:CB	2.00	0.90
26:Z:474:MET:HB3	26:Z:482:TRP:N	1.85	0.90
6:F:105:ALA:HB2	7:G:14:HIS:HE2	1.32	0.90
25:Y:357:LYS:HE3	25:Y:376:PHE:HD1	1.08	0.90
26:Z:417:VAL:HG13	26:Z:454:VAL:CG1	2.01	0.90
26:Z:516:THR:N	26:Z:681:ARG:HD3	1.83	0.90
25:Y:272:SER:HB2	25:Y:348:VAL:HG11	1.53	0.90
25:Y:124:ARG:HH21	25:Y:381:LEU:HD23	1.27	0.90
26:Z:516:THR:HA	26:Z:681:ARG:CZ	2.01	0.90
26:Z:717:TYR:CE2	26:Z:718:TYR:HE1	1.56	0.90
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.52	0.90
25:Y:349:LEU:CD1	25:Y:380:ARG:HG3	2.00	0.90
25:Y:60:GLN:O	25:Y:64:PRO:HD3	1.71	0.90
1:A:227:VAL:CG2	4:D:16:LYS:CE	2.50	0.90
17:Q:20:ILE:HG13	17:Q:87:PHE:CD2	2.06	0.90
25:Y:135:ARG:HH21	25:Y:143:ARG:HE	1.17	0.90
25:Y:327:ARG:HB2	25:Y:330:HIS:ND1	1.86	0.90
25:Y:378:SER:OG	25:Y:381:LEU:HB3	1.70	0.90

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:519:VAL:HG13	25:Y:550:ILE:HD13	1.53	0.90
26:Z:588:PHE:CZ	26:Z:621:LYS:NZ	2.39	0.90
1:A:1445:ILE:HB	7:G:18:PHE:CZ	2.01	0.90
25:Y:293:LEU:HD23	25:Y:419:ILE:HG22	1.53	0.90
25:Y:497:ILE:CG2	25:Y:684:ARG:HG2	2.01	0.90
25:Y:171:LEU:HB2	25:Y:172:PRO:HD3	1.52	0.90
25:Y:495:MET:CB	25:Y:686:PHE:CD1	2.55	0.90
18:R:142:LEU:HD11	18:R:152:LEU:HD12	1.53	0.90
25:Y:229:ASP:CA	25:Y:453:PHE:CB	2.49	0.90
16:P:394:PHE:HA	16:P:407:GLY:HA2	1.54	0.90
17:Q:97:LYS:HG2	17:Q:243:ASN:ND2	1.87	0.90
26:Z:698:ASP:O	26:Z:699:GLU:HG3	1.72	0.90
1:A:368:LYS:HG3	1:A:399:HIS:CD2	2.06	0.89
25:Y:60:GLN:O	25:Y:64:PRO:HD2	1.71	0.89
25:Y:416:PHE:CZ	25:Y:440:LEU:HD22	2.06	0.89
1:A:49:LYS:HE2	1:A:61:ILE:CD1	2.02	0.89
1:A:1445:ILE:CB	7:G:18:PHE:HE2	1.64	0.89
20:T:122:HIS:HB2	23:W:130:VAL:CG1	1.99	0.89
25:Y:288:LYS:HG3	25:Y:335:LEU:CG	2.02	0.89
25:Y:419:ILE:N	25:Y:633:ARG:HH11	1.71	0.89
25:Y:499:LYS:NZ	25:Y:525:MET:HB2	1.88	0.89
26:Z:459:MET:HB2	26:Z:464:ARG:CD	2.01	0.89
25:Y:418:LEU:HB3	25:Y:633:ARG:CZ	2.02	0.89
25:Y:650:GLU:HA	25:Y:653:PHE:HE1	1.34	0.89
20:T:122:HIS:CG	23:W:130:VAL:HG12	2.07	0.89
25:Y:237:ALA:HB1	25:Y:458:ILE:HG23	1.51	0.89
25:Y:293:LEU:HD23	25:Y:419:ILE:CG2	2.01	0.89
25:Y:419:ILE:CD1	25:Y:435:MET:HG2	2.01	0.89
26:Z:757:ARG:NH1	26:Z:760:LEU:HB3	1.84	0.89
1:A:1451:VAL:CG1	7:G:20:PRO:CB	2.46	0.89
1:A:1442:ASP:HA	7:G:63:PRO:HG2	0.92	0.89
25:Y:603:ARG:NH1	25:Y:629:TYR:CZ	2.40	0.89
1:A:36:ARG:NH2	1:A:57:ARG:NH1	2.21	0.89
25:Y:131:GLU:OE1	25:Y:134:ARG:NH1	2.06	0.89
25:Y:495:MET:CB	25:Y:686:PHE:CG	2.56	0.89
1:A:1451:VAL:HG23	7:G:22:MET:HG3	1.52	0.89
25:Y:272:SER:HB2	25:Y:281:LYS:HZ1	1.32	0.89
26:Z:362:ILE:HG23	26:Z:366:GLN:HB2	1.54	0.89
1:A:1445:ILE:CG2	7:G:18:PHE:CE2	2.49	0.88
18:R:62:PHE:HZ	18:R:201:ALA:HB1	1.39	0.88
25:Y:124:ARG:HG3	25:Y:376:PHE:O	1.72	0.88

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:487:LEU:CD2	26:Z:490:VAL:HG23	2.02	0.88
25:Y:248:LEU:CD2	25:Y:445:ALA:HB2	2.03	0.88
25:Y:276:LYS:HA	25:Y:280:GLN:OE1	1.73	0.88
25:Y:346:MET:HB3	25:Y:384:LEU:HD21	1.53	0.88
25:Y:124:ARG:CG	25:Y:377:CYS:SG	2.61	0.88
25:Y:68:LYS:HE3	25:Y:228:LYS:HE3	1.55	0.88
26:Z:307:ASP:HB2	26:Z:323:VAL:HB	1.53	0.88
26:Z:621:LYS:HB3	26:Z:621:LYS:HZ3	1.13	0.88
6:F:132:LEU:CD2	7:G:66:GLY:O	2.21	0.88
17:Q:90:LEU:HD22	17:Q:251:PHE:CE2	2.05	0.88
20:T:122:HIS:CB	23:W:131:ASP:CA	2.45	0.88
22:V:85:ASN:HA	22:V:88:GLU:OE2	1.73	0.88
25:Y:103:PHE:HE1	25:Y:205:ILE:CD1	1.85	0.88
26:Z:457:TYR:HB3	26:Z:498:PHE:CD1	2.08	0.88
16:P:410:VAL:CB	16:P:502:ASN:N	2.37	0.88
25:Y:419:ILE:N	25:Y:633:ARG:HH12	1.46	0.88
26:Z:347:HIS:CD2	26:Z:348:ARG:HG3	2.08	0.88
26:Z:447:GLN:N	26:Z:452:LEU:HD13	1.89	0.88
17:Q:61:PRO:HG2	17:Q:300:VAL:CG2	2.04	0.88
21:U:132:GLU:CD	21:U:139:ILE:HD11	1.92	0.88
22:V:83:LEU:HA	22:V:87:LEU:CB	2.04	0.88
20:T:50:GLU:CG	22:V:98:LEU:HD13	1.99	0.88
25:Y:200:ILE:C	25:Y:226:VAL:CG2	2.41	0.88
17:Q:85:LEU:CD1	17:Q:88:ARG:H	1.87	0.88
25:Y:259:ARG:C	25:Y:379:GLU:OE1	2.12	0.88
25:Y:393:VAL:CG1	25:Y:437:PHE:CE2	2.56	0.88
21:U:134:ILE:HD13	23:W:63:SER:HB2	1.54	0.88
26:Z:477:LEU:HG	26:Z:501:VAL:HG11	1.56	0.88
1:A:1443:VAL:HB	7:G:63:PRO:HA	1.54	0.88
17:Q:108:ILE:HG21	17:Q:159:GLU:CB	2.04	0.88
25:Y:124:ARG:HG2	25:Y:377:CYS:CA	2.04	0.88
1:A:1445:ILE:HG23	7:G:66:GLY:O	1.73	0.87
20:T:122:HIS:CG	23:W:131:ASP:C	2.46	0.87
25:Y:70:ILE:HB	25:Y:208:TYR:CE2	2.09	0.87
26:Z:421:ARG:HA	26:Z:424:PHE:CD2	2.09	0.87
26:Z:405:LYS:HD3	26:Z:483:GLY:CA	2.03	0.87
17:Q:90:LEU:HD23	17:Q:251:PHE:CE2	2.08	0.87
22:V:146:LYS:CD	23:W:129:PHE:CE1	2.46	0.87
25:Y:272:SER:CB	25:Y:281:LYS:HZ1	1.85	0.87
25:Y:567:LYS:HE2	25:Y:597:ILE:HD13	1.56	0.87
1:A:1451:VAL:HG11	7:G:20:PRO:CA	1.90	0.87

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:105:ALA:CA	7:G:14:HIS:CE1	2.48	0.87
20:T:55:LYS:HD2	20:T:60:VAL:CG1	2.04	0.87
22:V:125:ILE:HG23	22:V:126:ILE:HD12	1.56	0.87
25:Y:528:GLU:O	25:Y:532:ILE:HG13	1.72	0.87
26:Z:410:LEU:CD2	26:Z:477:LEU:HD11	2.04	0.87
26:Z:424:PHE:CD1	26:Z:450:SER:HB3	2.10	0.87
25:Y:338:LEU:HD12	25:Y:341:TYR:CD1	2.08	0.87
1:A:419:LYS:HA	17:Q:58:LEU:HD22	1.57	0.87
25:Y:352:ILE:HB	25:Y:380:ARG:NE	1.87	0.87
25:Y:67:ARG:NH1	25:Y:455:SER:OG	2.07	0.87
26:Z:408:ILE:HG21	26:Z:475:ASP:CA	2.04	0.87
26:Z:757:ARG:NH2	26:Z:760:LEU:HD22	1.88	0.87
17:Q:16:TYR:HE2	17:Q:87:PHE:CA	1.86	0.87
25:Y:231:ILE:HG21	25:Y:457:ILE:HD11	1.54	0.87
25:Y:269:GLU:CG	25:Y:277:VAL:HG11	2.04	0.87
25:Y:353:SER:O	25:Y:356:PRO:CD	2.22	0.87
25:Y:440:LEU:HD11	25:Y:638:ARG:CA	2.00	0.87
25:Y:393:VAL:CG2	25:Y:437:PHE:CE1	2.56	0.87
25:Y:656:PHE:HD1	25:Y:659:MET:SD	1.98	0.87
20:T:91:ASP:HB3	22:V:66:ILE:HG13	1.57	0.87
22:V:76:ILE:HD13	22:V:97:ARG:HB2	1.56	0.87
25:Y:200:ILE:CG2	25:Y:226:VAL:HG11	1.89	0.87
25:Y:499:LYS:HD2	25:Y:522:TYR:CG	2.08	0.87
26:Z:446:PHE:HB2	26:Z:452:LEU:HD21	1.54	0.87
26:Z:584:ASN:HD21	26:Z:586:THR:HG23	1.39	0.87
26:Z:621:LYS:HB3	26:Z:621:LYS:HZ2	1.17	0.87
17:Q:81:MET:HE2	17:Q:92:SER:HB3	0.87	0.86
20:T:90:TYR:CD1	22:V:112:LYS:HB3	2.10	0.86
25:Y:355:THR:N	25:Y:356:PRO:HD2	1.90	0.86
25:Y:532:ILE:CD1	25:Y:705:ASP:HB2	2.05	0.86
1:A:1436:ILE:CD1	2:B:1144:ALA:HB2	2.05	0.86
25:Y:639:LEU:HD11	25:Y:649:ARG:NH1	1.89	0.86
25:Y:440:LEU:HD12	25:Y:638:ARG:HG2	1.57	0.86
26:Z:757:ARG:NH2	26:Z:760:LEU:HB3	1.85	0.86
25:Y:357:LYS:CE	25:Y:376:PHE:HD1	1.75	0.86
25:Y:692:GLN:O	25:Y:693:LEU:HD22	1.75	0.86
26:Z:383:ILE:HG22	26:Z:512:GLY:HA3	1.57	0.86
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.57	0.86
16:P:541:ILE:O	16:P:545:ILE:CB	2.23	0.86
17:Q:265:ILE:H	17:Q:265:ILE:HD12	1.40	0.86
25:Y:418:LEU:HD13	25:Y:634:ILE:CG1	2.06	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:229:ASP:HB3	25:Y:453:PHE:CA	2.06	0.86
25:Y:495:MET:CG	25:Y:686:PHE:CG	2.58	0.86
26:Z:477:LEU:HG	26:Z:501:VAL:CG1	2.04	0.86
25:Y:50:VAL:HG11	25:Y:459:THR:HB	1.56	0.86
26:Z:421:ARG:HE	26:Z:430:LEU:HD11	1.40	0.86
26:Z:470:SER:CA	26:Z:478:THR:HG23	2.05	0.86
17:Q:86:ASN:O	17:Q:89:ILE:HG13	1.74	0.86
26:Z:425:LEU:HG	26:Z:429:THR:HG23	1.57	0.86
17:Q:81:MET:HE3	17:Q:92:SER:HB3	1.56	0.86
25:Y:248:LEU:HD11	25:Y:445:ALA:HB2	1.58	0.86
25:Y:352:ILE:CA	25:Y:380:ARG:NH1	2.38	0.86
7:G:19:GLY:O	7:G:22:MET:CG	2.24	0.86
20:T:90:TYR:CE1	22:V:112:LYS:HD3	2.11	0.86
25:Y:418:LEU:HD22	25:Y:633:ARG:HD2	1.58	0.86
26:Z:427:TRP:CH2	26:Z:450:SER:HB2	2.10	0.86
1:A:36:ARG:HH21	1:A:57:ARG:HH12	1.20	0.85
21:U:126:LEU:HB2	21:U:154:ILE:HG21	1.56	0.85
17:Q:61:PRO:HG2	17:Q:300:VAL:HG21	1.58	0.85
20:T:122:HIS:HE2	23:W:133:ILE:C	1.79	0.85
1:A:11:LEU:HD11	2:B:1195:HIS:CD2	2.11	0.85
26:Z:376:ASN:HB2	26:Z:380:ARG:CD	2.05	0.85
26:Z:487:LEU:CD2	26:Z:493:VAL:HG21	2.05	0.85
22:V:69:ILE:HD11	22:V:108:ASN:HD21	1.41	0.85
25:Y:232:VAL:HG21	25:Y:453:PHE:CE2	2.05	0.85
25:Y:631:GLU:HA	25:Y:636:LYS:HE3	0.85	0.85
26:Z:425:LEU:HG	26:Z:429:THR:CA	2.07	0.85
26:Z:717:TYR:CD2	26:Z:718:TYR:CE1	2.64	0.85
26:Z:328:LYS:HD3	26:Z:530:LEU:CD2	2.07	0.85
25:Y:393:VAL:CG2	25:Y:437:PHE:CZ	2.60	0.85
26:Z:417:VAL:HG13	26:Z:454:VAL:HG11	1.57	0.85
26:Z:474:MET:SD	26:Z:506:ALA:HB3	2.16	0.85
22:V:122:TRP:O	22:V:126:ILE:HD13	1.76	0.85
25:Y:499:LYS:HB3	25:Y:522:TYR:CZ	2.12	0.85
25:Y:493:LEU:HD21	25:Y:666:LEU:HG	1.57	0.85
20:T:122:HIS:CB	23:W:131:ASP:O	2.12	0.85
25:Y:353:SER:C	25:Y:356:PRO:CG	2.45	0.85
20:T:71:LYS:O	20:T:74:ILE:HG22	1.76	0.85
26:Z:457:TYR:HB3	26:Z:498:PHE:CE1	2.12	0.85
20:T:93:ILE:HD13	22:V:122:TRP:CE3	2.11	0.84
25:Y:499:LYS:HD3	25:Y:522:TYR:N	1.85	0.84
25:Y:124:ARG:HG2	25:Y:377:CYS:HA	1.56	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:353:SER:CB	25:Y:381:LEU:CA	2.55	0.84
26:Z:476:PHE:CE1	26:Z:502:VAL:HG22	2.13	0.84
18:R:193:THR:HG22	18:R:196:GLU:HA	1.58	0.84
25:Y:254:THR:HG21	25:Y:286:TYR:CE1	2.01	0.84
20:T:97:LEU:CD1	20:T:100:ILE:HD11	2.05	0.84
20:T:126:LYS:HG3	23:W:132:GLY:O	1.77	0.84
25:Y:67:ARG:CB	25:Y:230:SER:CB	2.53	0.84
1:A:1445:ILE:HG12	7:G:68:ALA:N	1.90	0.84
1:A:399:HIS:NE2	1:A:462:VAL:HG11	1.91	0.84
25:Y:71:TYR:HA	25:Y:233:ILE:HB	1.60	0.84
25:Y:499:LYS:HD2	25:Y:522:TYR:N	1.90	0.84
25:Y:681:LEU:CD2	25:Y:696:TRP:CZ3	2.60	0.84
26:Z:470:SER:C	26:Z:478:THR:HG23	1.97	0.84
21:U:175:ILE:O	21:U:179:GLU:HG3	1.77	0.84
21:U:73:ASN:HB2	21:U:75:GLN:HG2	1.60	0.84
25:Y:346:MET:CA	25:Y:384:LEU:HD21	2.08	0.84
25:Y:539:VAL:CG1	25:Y:623:ILE:HG12	2.07	0.84
22:V:76:ILE:HD13	22:V:97:ARG:CB	2.07	0.83
26:Z:634:GLN:HA	26:Z:634:GLN:OE1	1.75	0.83
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.61	0.83
6:F:92:ARG:HH22	7:G:63:PRO:HB2	1.02	0.83
21:U:150:ASN:O	21:U:154:ILE:HG12	1.76	0.83
20:T:50:GLU:HG2	22:V:98:LEU:CD1	2.02	0.83
25:Y:267:LEU:O	25:Y:268:ASP:HB2	1.76	0.83
26:Z:428:CYS:HB2	26:Z:434:ASN:CB	2.08	0.83
26:Z:473:VAL:H	26:Z:478:THR:HG22	1.42	0.83
26:Z:602:GLY:O	26:Z:694:LYS:NZ	2.10	0.83
25:Y:253:THR:HG22	25:Y:434:ILE:CD1	2.09	0.83
25:Y:418:LEU:HD22	25:Y:633:ARG:CD	2.07	0.83
26:Z:466:ARG:NH2	26:Z:477:LEU:HD13	1.92	0.83
22:V:89:THR:HG23	22:V:90:LEU:CD1	2.08	0.83
25:Y:353:SER:N	25:Y:380:ARG:HH11	1.75	0.83
26:Z:456:THR:HB	26:Z:465:ASN:CG	1.98	0.83
25:Y:68:LYS:CE	25:Y:228:LYS:HE3	2.08	0.83
6:F:132:LEU:HD21	7:G:66:GLY:O	1.79	0.83
25:Y:229:ASP:C	25:Y:453:PHE:CB	2.47	0.83
25:Y:272:SER:CB	25:Y:281:LYS:HZ2	1.91	0.83
26:Z:376:ASN:N	26:Z:380:ARG:HB2	1.92	0.83
26:Z:487:LEU:HD22	26:Z:490:VAL:HG23	1.59	0.83
25:Y:257:LEU:HD23	25:Y:383:LEU:HD12	1.58	0.83
25:Y:352:ILE:N	25:Y:380:ARG:HH12	1.77	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD23	1:A:54:ASN:H	1.44	0.83
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.59	0.83
20:T:42:LEU:HD12	20:T:80:LEU:HD12	1.61	0.83
25:Y:50:VAL:CG1	25:Y:459:THR:HB	2.09	0.83
25:Y:493:LEU:HD23	25:Y:696:TRP:HE1	0.69	0.83
2:B:1184:GLY:O	4:D:17:LYS:NZ	2.12	0.82
25:Y:346:MET:CB	25:Y:384:LEU:HD21	2.09	0.82
25:Y:353:SER:CA	25:Y:356:PRO:HG3	2.06	0.82
26:Z:372:LYS:O	26:Z:380:ARG:HB3	1.78	0.82
26:Z:407:VAL:CG1	26:Z:451:GLY:HA2	2.08	0.82
13:M:45:VAL:O	13:M:49:GLN:N	2.11	0.82
20:T:38:SER:CB	22:V:113:ASP:OD2	2.28	0.82
25:Y:200:ILE:HB	25:Y:226:VAL:HG21	0.95	0.82
25:Y:571:VAL:CG1	25:Y:572:GLU:N	2.42	0.82
25:Y:244:CYS:HB2	25:Y:442:ALA:CB	2.09	0.82
25:Y:349:LEU:CA	25:Y:380:ARG:CZ	2.33	0.82
26:Z:696:ARG:HH11	26:Z:704:PHE:HE1	0.83	0.82
16:P:362:GLU:O	16:P:423:LYS:HA	1.80	0.82
3:C:148:ARG:H	3:C:151:GLN:HG3	1.44	0.82
20:T:51:ASP:OD1	20:T:55:LYS:HD3	1.79	0.82
25:Y:353:SER:O	25:Y:356:PRO:HD2	1.79	0.82
25:Y:631:GLU:HA	25:Y:636:LYS:NZ	1.93	0.82
25:Y:72:CYS:SG	25:Y:234:PHE:CD1	2.72	0.82
26:Z:474:MET:HA	26:Z:478:THR:O	1.79	0.82
26:Z:478:THR:HG22	26:Z:479:GLY:H	1.43	0.82
26:Z:505:ILE:HG22	26:Z:507:ALA:N	1.94	0.82
25:Y:68:LYS:HD2	25:Y:228:LYS:HG3	0.83	0.82
17:Q:75:LEU:CA	17:Q:98:ILE:CG2	2.52	0.82
22:V:119:PRO:HA	22:V:122:TRP:HD1	0.99	0.82
25:Y:419:ILE:HD12	25:Y:435:MET:HG2	1.60	0.82
26:Z:373:MET:HG3	26:Z:381:SER:HA	1.61	0.82
25:Y:440:LEU:CD2	25:Y:641:PHE:CG	2.63	0.82
25:Y:481:LYS:HD3	25:Y:483:TYR:CD2	2.15	0.82
6:F:96:THR:CB	7:G:64:THR:O	2.27	0.82
25:Y:200:ILE:HD12	25:Y:225:GLU:C	2.00	0.82
25:Y:393:VAL:CG1	25:Y:437:PHE:CD2	2.63	0.82
26:Z:300:ASP:OD2	26:Z:480:ARG:HD3	1.80	0.82
25:Y:225:GLU:O	25:Y:226:VAL:HG12	1.80	0.81
25:Y:293:LEU:CD1	25:Y:433:PRO:HB2	2.09	0.81
25:Y:248:LEU:HD11	25:Y:445:ALA:CB	2.10	0.81
1:A:68:GLN:O	1:A:68:GLN:NE2	2.11	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1221:SER:OG	4:D:14:ARG:CZ	2.28	0.81
10:J:48:ARG:HE	10:J:49:MET:HE2	1.44	0.81
25:Y:353:SER:HB3	25:Y:381:LEU:N	1.94	0.81
25:Y:259:ARG:HB3	25:Y:379:GLU:OE2	1.80	0.81
25:Y:515:ASP:HB2	25:Y:518:ILE:HD12	1.61	0.81
26:Z:407:VAL:HG13	26:Z:452:LEU:N	1.93	0.81
2:B:849:GLY:HA2	2:B:852:ARG:HD2	1.63	0.81
21:U:155:LEU:HD13	23:W:16:THR:HG23	1.63	0.81
26:Z:408:ILE:HG21	26:Z:475:ASP:HA	1.59	0.81
26:Z:466:ARG:HB2	26:Z:477:LEU:CD2	2.10	0.81
26:Z:335:TYR:HD1	26:Z:336:PRO:HD3	1.44	0.81
1:A:344:ARG:NH2	2:B:1120:GLU:CG	2.39	0.81
17:Q:108:ILE:HG21	17:Q:159:GLU:HB3	1.62	0.81
18:R:72:ILE:CG2	18:R:202:TYR:HE1	1.81	0.81
20:T:98:GLN:O	20:T:102:LYS:HD2	1.80	0.81
25:Y:86:LEU:HD22	25:Y:103:PHE:CE1	2.15	0.81
26:Z:502:VAL:HA	26:Z:505:ILE:CD1	2.10	0.81
26:Z:384:ILE:HD13	26:Z:511:LEU:CD1	2.10	0.81
25:Y:208:TYR:CE1	25:Y:213:LEU:HB2	2.15	0.81
26:Z:331:GLN:HE22	26:Z:378:ARG:HD2	1.45	0.81
16:P:388:PHE:O	16:P:484:ASP:CB	2.29	0.81
25:Y:135:ARG:HH21	25:Y:143:ARG:NE	1.73	0.81
22:V:117:LYS:CE	22:V:121:GLU:HB3	2.09	0.81
25:Y:272:SER:OG	25:Y:281:LYS:NZ	2.10	0.81
25:Y:353:SER:CA	25:Y:356:PRO:CG	2.58	0.81
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.63	0.81
25:Y:135:ARG:NH2	25:Y:143:ARG:CZ	2.43	0.81
25:Y:67:ARG:CB	25:Y:230:SER:HB3	2.06	0.81
25:Y:639:LEU:HD11	25:Y:649:ARG:HH11	1.43	0.81
25:Y:639:LEU:HG	25:Y:653:PHE:CZ	2.15	0.81
26:Z:410:LEU:HD21	26:Z:457:TYR:CD2	2.15	0.81
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.61	0.80
18:R:130:LEU:HB2	18:R:137:VAL:HG13	1.64	0.80
25:Y:357:LYS:HG3	25:Y:376:PHE:O	1.82	0.80
25:Y:659:MET:SD	25:Y:692:GLN:HG2	2.21	0.80
1:A:1445:ILE:HG21	7:G:18:PHE:HE2	1.46	0.80
25:Y:58:ALA:HA	25:Y:231:ILE:HD13	1.63	0.80
25:Y:274:VAL:HG12	25:Y:275:ARG:H	1.46	0.80
25:Y:337:ARG:CZ	25:Y:345:ARG:HD3	2.11	0.80
25:Y:497:ILE:O	25:Y:497:ILE:HG22	1.81	0.80
26:Z:584:ASN:ND2	26:Z:586:THR:HG23	1.96	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:479:LEU:O	16:P:482:ASP:N	2.15	0.80
22:V:146:LYS:CB	23:W:129:PHE:CZ	2.64	0.80
25:Y:257:LEU:HD22	25:Y:383:LEU:HD11	1.62	0.80
16:P:380:ASP:O	16:P:383:HIS:O	2.00	0.80
21:U:139:ILE:CD1	21:U:147:LYS:HE3	2.10	0.80
25:Y:229:ASP:HA	25:Y:453:PHE:HB3	1.62	0.80
25:Y:570:LEU:HD12	25:Y:600:SER:CB	2.11	0.80
20:T:91:ASP:CB	22:V:66:ILE:HG13	2.12	0.80
25:Y:526:LEU:HD13	25:Y:623:ILE:HD11	1.64	0.80
26:Z:458:SER:CA	26:Z:465:ASN:HB2	2.12	0.80
26:Z:578:MET:O	26:Z:582:ILE:HG13	1.81	0.80
1:A:1445:ILE:HG12	7:G:18:PHE:CZ	1.90	0.80
19:S:103:GLN:O	19:S:106:GLU:N	2.14	0.80
25:Y:350:HIS:ND1	25:Y:381:LEU:HD12	1.97	0.80
25:Y:420:ILE:CG1	25:Y:633:ARG:CZ	2.40	0.80
26:Z:627:ILE:HB	26:Z:654:LEU:HD23	1.62	0.80
25:Y:193:TYR:HE2	25:Y:197:ARG:HH11	1.29	0.80
25:Y:293:LEU:HD13	25:Y:433:PRO:HB3	1.63	0.80
26:Z:458:SER:CB	26:Z:467:SER:HB3	2.11	0.80
1:A:1445:ILE:O	7:G:68:ALA:HB2	1.82	0.80
13:M:139:VAL:CB	13:M:152:ASP:CB	2.60	0.80
16:P:341:TYR:CB	16:P:354:ILE:N	2.43	0.80
17:Q:76:ILE:HG23	17:Q:93:PHE:CZ	2.17	0.80
22:V:118:SER:HB2	22:V:119:PRO:HD2	1.63	0.80
1:A:1443:VAL:H	7:G:63:PRO:CD	1.94	0.80
22:V:112:LYS:HD2	22:V:119:PRO:CB	2.12	0.80
25:Y:526:LEU:CD2	25:Y:554:TRP:CZ3	2.62	0.80
26:Z:353:ASP:OD2	26:Z:405:LYS:HA	1.80	0.80
26:Z:439:THR:HG23	26:Z:465:ASN:ND2	1.97	0.80
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.64	0.80
6:F:96:THR:HA	7:G:64:THR:O	1.82	0.80
17:Q:195:GLY:HA3	18:R:76:SER:HA	1.61	0.80
25:Y:639:LEU:CA	25:Y:653:PHE:CD2	2.65	0.80
20:T:90:TYR:CG	22:V:112:LYS:HB3	2.17	0.79
25:Y:357:LYS:HE2	25:Y:376:PHE:CD1	2.17	0.79
25:Y:586:TYR:HD2	25:Y:598:LEU:HG	1.45	0.79
1:A:227:VAL:CG1	4:D:16:LYS:HG2	2.11	0.79
18:R:4:SER:CB	18:R:200:LEU:HD23	2.11	0.79
25:Y:253:THR:CG2	25:Y:434:ILE:CG2	2.59	0.79
25:Y:124:ARG:HB3	25:Y:377:CYS:SG	2.20	0.79
26:Z:398:THR:O	26:Z:402:THR:HG23	1.82	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:400:ALA:HB1	26:Z:449:GLU:O	1.83	0.79
26:Z:584:ASN:ND2	26:Z:586:THR:CG2	2.45	0.79
1:A:1443:VAL:CG1	7:G:61:ILE:CG2	2.25	0.79
16:P:311:LYS:CB	16:P:423:LYS:O	2.30	0.79
17:Q:98:ILE:CG2	17:Q:99:PRO:CD	2.60	0.79
20:T:39:LYS:N	22:V:113:ASP:OD2	2.15	0.79
25:Y:162:LEU:HD21	25:Y:191:CYS:HB3	1.64	0.79
25:Y:244:CYS:CB	25:Y:442:ALA:CB	2.57	0.79
25:Y:353:SER:CB	25:Y:381:LEU:N	2.45	0.79
25:Y:586:TYR:HD1	25:Y:616:TYR:CE2	1.99	0.79
25:Y:565:LYS:HD3	25:Y:597:ILE:HD12	1.62	0.79
26:Z:362:ILE:HG22	26:Z:363:ARG:O	1.81	0.79
26:Z:459:MET:O	26:Z:464:ARG:HG3	1.81	0.79
26:Z:458:SER:HA	26:Z:465:ASN:CB	2.12	0.79
26:Z:502:VAL:HA	26:Z:505:ILE:HD11	1.64	0.79
1:A:89:PRO:HB2	1:A:204:THR:CG2	2.13	0.79
17:Q:97:LYS:CB	17:Q:243:ASN:HD22	1.96	0.79
20:T:93:ILE:HD13	22:V:122:TRP:CB	2.11	0.79
25:Y:111:ARG:NE	25:Y:129:VAL:HG21	1.97	0.79
26:Z:425:LEU:CG	26:Z:429:THR:HA	2.12	0.79
2:B:1215:ARG:HD2	4:D:15:LEU:HD12	1.59	0.79
1:A:1447:GLU:CD	7:G:26:LEU:HD13	2.03	0.79
1:A:1447:GLU:OE1	7:G:56:ILE:HD11	1.82	0.79
17:Q:78:GLU:OE1	17:Q:80:MET:HB3	1.82	0.79
25:Y:212:TYR:OH	25:Y:222:VAL:HG22	1.81	0.79
25:Y:479:LEU:O	25:Y:479:LEU:CD2	2.30	0.79
17:Q:97:LYS:HE3	17:Q:236:TRP:HB3	1.65	0.79
20:T:81:PHE:O	20:T:84:VAL:HG12	1.82	0.79
21:U:160:HIS:O	21:U:164:GLU:HG3	1.83	0.79
25:Y:59:TYR:CB	25:Y:62:HIS:NE2	2.46	0.79
25:Y:419:ILE:H	25:Y:633:ARG:NH1	1.76	0.79
6:F:92:ARG:CZ	7:G:63:PRO:HB3	2.12	0.79
18:R:43:ARG:NH2	18:R:117:MET:HE3	1.97	0.79
20:T:118:LEU:HD21	23:W:129:PHE:HB2	1.64	0.79
22:V:146:LYS:HB3	23:W:129:PHE:CE1	2.17	0.79
25:Y:352:ILE:CG1	25:Y:380:ARG:CZ	2.60	0.79
25:Y:499:LYS:CE	25:Y:522:TYR:CA	2.34	0.79
26:Z:378:ARG:HH21	26:Z:508:HIS:HA	1.45	0.79
26:Z:502:VAL:CG1	26:Z:530:LEU:HB3	2.12	0.79
13:M:166:ILE:HA	14:N:95:VAL:HA	1.62	0.79
22:V:140:LEU:O	22:V:143:LEU:HG	1.83	0.79

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:135:ARG:HH21	25:Y:143:ARG:HH21	1.30	0.79
25:Y:288:LYS:HZ1	25:Y:336:LYS:N	1.81	0.79
25:Y:353:SER:CB	25:Y:381:LEU:CB	2.53	0.79
26:Z:425:LEU:HG	26:Z:429:THR:CB	2.12	0.79
22:V:81:ASN:HB2	22:V:90:LEU:HD23	1.64	0.79
23:W:94:ILE:HG13	23:W:95:ASP:N	1.96	0.79
25:Y:215:ASP:HB3	25:Y:218:ILE:CG2	2.14	0.79
25:Y:253:THR:HG22	25:Y:434:ILE:HG23	1.63	0.79
25:Y:37:ASN:HB3	25:Y:456:VAL:HB	0.79	0.79
25:Y:681:LEU:HD22	25:Y:696:TRP:HZ3	1.44	0.79
13:M:139:VAL:HA	13:M:152:ASP:CB	2.14	0.78
16:P:471:ASN:O	16:P:472:GLU:O	2.00	0.78
17:Q:98:ILE:HG22	17:Q:99:PRO:CD	2.12	0.78
20:T:97:LEU:HD12	20:T:100:ILE:CD1	2.09	0.78
25:Y:39:ILE:HG12	25:Y:458:ILE:HB	1.63	0.78
26:Z:410:LEU:HA	26:Z:466:ARG:HH12	1.46	0.78
1:A:1445:ILE:O	1:A:1445:ILE:HD12	1.82	0.78
16:P:543:ARG:O	16:P:545:ILE:N	2.15	0.78
1:A:420:ARG:HH12	17:Q:174:ALA:HB2	1.47	0.78
25:Y:253:THR:HG22	25:Y:434:ILE:CG1	2.12	0.78
25:Y:639:LEU:CD2	25:Y:649:ARG:HB2	2.13	0.78
26:Z:473:VAL:H	26:Z:478:THR:CG2	1.96	0.78
26:Z:380:ARG:HA	26:Z:535:LEU:HD22	1.65	0.78
22:V:69:ILE:HG12	22:V:104:LEU:HB3	1.66	0.78
26:Z:756:ARG:HH11	26:Z:756:ARG:HG2	0.75	0.78
17:Q:106:ARG:HH21	17:Q:214:GLN:CG	1.95	0.78
26:Z:327:LYS:HE3	26:Z:327:LYS:HA	1.65	0.78
1:A:1443:VAL:HA	6:F:133:VAL:O	1.84	0.78
20:T:93:ILE:HD11	22:V:126:ILE:CD1	2.13	0.78
25:Y:135:ARG:HH21	25:Y:143:ARG:NH2	1.81	0.78
25:Y:348:VAL:O	25:Y:380:ARG:NH2	2.13	0.78
25:Y:37:ASN:O	25:Y:477:THR:OG1	2.02	0.78
20:T:55:LYS:HA	20:T:60:VAL:HG12	1.63	0.78
22:V:146:LYS:CB	23:W:129:PHE:CE1	2.67	0.78
25:Y:257:LEU:HD21	25:Y:383:LEU:HD11	1.64	0.78
26:Z:494:PRO:HB2	26:Z:519:ARG:NH1	1.98	0.78
1:A:1442:ASP:CA	7:G:63:PRO:HG3	2.09	0.78
6:F:133:VAL:O	7:G:61:ILE:HD12	1.70	0.78
25:Y:550:ILE:HG21	25:Y:554:TRP:CZ2	2.13	0.78
25:Y:58:ALA:C	25:Y:62:HIS:CD2	2.57	0.78
1:A:1447:GLU:OE2	7:G:70:PHE:CZ	2.37	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.66	0.78
25:Y:230:SER:N	25:Y:453:PHE:CB	2.47	0.78
25:Y:418:LEU:HD13	25:Y:634:ILE:HG12	1.61	0.78
7:G:17:PHE:O	7:G:22:MET:HG2	1.83	0.78
17:Q:76:ILE:HG23	17:Q:93:PHE:HZ	1.48	0.78
18:R:4:SER:OG	18:R:200:LEU:HB2	1.84	0.78
20:T:66:ASN:HB3	20:T:69:ILE:HD12	1.66	0.78
22:V:76:ILE:HD12	22:V:97:ARG:HD2	1.66	0.78
25:Y:18:TYR:HB2	25:Y:19:PRO:CD	2.14	0.78
23:W:83:VAL:HG23	23:W:84:ASP:H	1.48	0.78
25:Y:467:ASP:C	25:Y:470:PRO:HD2	2.05	0.78
20:T:55:LYS:HA	20:T:60:VAL:CG1	2.14	0.77
22:V:129:ARG:O	22:V:133:LEU:HG	1.83	0.77
26:Z:326:VAL:HG11	26:Z:503:SER:OG	1.83	0.77
6:F:92:ARG:NH2	7:G:63:PRO:CA	2.46	0.77
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.66	0.77
20:T:93:ILE:HD12	22:V:122:TRP:CZ3	2.12	0.77
22:V:146:LYS:HG2	23:W:129:PHE:CZ	2.16	0.77
25:Y:135:ARG:HB3	25:Y:143:ARG:HG3	1.66	0.77
25:Y:440:LEU:HD21	25:Y:641:PHE:HB2	0.80	0.77
17:Q:106:ARG:CZ	17:Q:211:PHE:CZ	2.67	0.77
25:Y:518:ILE:HG22	25:Y:522:TYR:HE2	0.61	0.77
25:Y:603:ARG:NH1	25:Y:629:TYR:CE2	2.53	0.77
25:Y:58:ALA:C	25:Y:62:HIS:HD2	1.86	0.77
26:Z:376:ASN:CB	26:Z:380:ARG:H	1.97	0.77
17:Q:97:LYS:HZ3	17:Q:243:ASN:C	1.88	0.77
20:T:55:LYS:HB3	20:T:62:ARG:CG	2.14	0.77
22:V:137:ARG:HD3	22:V:138:ASP:N	1.98	0.77
25:Y:288:LYS:HG2	25:Y:335:LEU:HB3	1.59	0.77
26:Z:408:ILE:HG12	26:Z:475:ASP:CB	2.13	0.77
25:Y:231:ILE:CG2	25:Y:457:ILE:CD1	2.62	0.77
25:Y:566:HIS:O	25:Y:567:LYS:HG3	1.84	0.77
26:Z:485:ILE:CD1	26:Z:510:LYS:HG2	2.14	0.77
17:Q:261:ARG:HD3	17:Q:267:ARG:HH21	1.48	0.77
17:Q:97:LYS:NZ	17:Q:243:ASN:C	2.38	0.77
25:Y:493:LEU:HD23	25:Y:696:TRP:CE2	2.20	0.77
26:Z:310:ILE:HD13	26:Z:313:VAL:HG23	1.67	0.77
1:A:1444:MET:HG2	7:G:60:ARG:CG	2.13	0.77
1:A:1447:GLU:OE1	7:G:26:LEU:HD13	1.85	0.77
25:Y:346:MET:O	25:Y:384:LEU:HG	1.84	0.77
25:Y:59:TYR:CD2	25:Y:62:HIS:CE1	2.73	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:420:ILE:HD12	25:Y:633:ARG:HH21	1.47	0.77
26:Z:406:SER:HB3	26:Z:482:TRP:CE3	2.20	0.77
26:Z:410:LEU:HD13	26:Z:477:LEU:CD1	2.15	0.77
26:Z:413:SER:O	26:Z:417:VAL:HG23	1.85	0.77
26:Z:476:PHE:HA	26:Z:485:ILE:HB	1.66	0.77
26:Z:717:TYR:CD2	26:Z:718:TYR:CD1	2.73	0.77
17:Q:86:ASN:OD1	17:Q:220:VAL:CG1	2.33	0.77
25:Y:499:LYS:HE2	25:Y:525:MET:HG3	1.66	0.77
26:Z:310:ILE:HD13	26:Z:313:VAL:CG2	2.15	0.77
26:Z:474:MET:HE2	26:Z:482:TRP:N	1.99	0.77
1:A:836:TYR:HH	1:A:1403:GLU:CD	1.86	0.76
22:V:119:PRO:CA	22:V:122:TRP:HD1	1.53	0.76
25:Y:418:LEU:HD22	25:Y:633:ARG:CG	2.15	0.76
1:A:1451:VAL:HG13	7:G:20:PRO:HG3	1.67	0.76
1:A:32:VAL:HG23	1:A:57:ARG:O	1.86	0.76
22:V:117:LYS:HE3	22:V:121:GLU:HB3	1.65	0.76
25:Y:327:ARG:CB	25:Y:330:HIS:CE1	2.65	0.76
26:Z:431:GLN:HB2	26:Z:432:PRO:HD3	1.67	0.76
26:Z:516:THR:HA	26:Z:681:ARG:NE	1.99	0.76
1:A:1116:LEU:HD12	1:A:1329:THR:HB	1.67	0.76
18:R:193:THR:CG2	18:R:196:GLU:HA	2.15	0.76
25:Y:284:ASP:O	25:Y:288:LYS:HG2	1.85	0.76
25:Y:352:ILE:H	25:Y:380:ARG:HH12	1.30	0.76
25:Y:253:THR:HG22	25:Y:434:ILE:HG21	1.68	0.76
25:Y:418:LEU:C	25:Y:633:ARG:NH1	2.38	0.76
1:A:1451:VAL:HG13	7:G:20:PRO:N	2.01	0.76
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.66	0.76
6:F:92:ARG:HH21	7:G:64:THR:H	1.31	0.76
26:Z:378:ARG:NH2	26:Z:508:HIS:HA	2.01	0.76
26:Z:407:VAL:CG2	26:Z:451:GLY:HA2	2.15	0.76
26:Z:446:PHE:C	26:Z:452:LEU:HD22	2.06	0.76
25:Y:28:ILE:CG2	25:Y:57:ILE:CD1	2.58	0.76
26:Z:363:ARG:HH21	26:Z:366:GLN:HE22	1.32	0.76
26:Z:425:LEU:CD1	26:Z:429:THR:HG23	2.15	0.76
21:U:168:HIS:HE1	23:W:82:GLY:O	1.68	0.76
25:Y:569:ILE:CG2	25:Y:571:VAL:HG22	2.15	0.76
26:Z:656:LYS:O	26:Z:656:LYS:CD	2.33	0.76
26:Z:757:ARG:NH1	26:Z:760:LEU:CD2	2.41	0.76
17:Q:7:LEU:HB3	17:Q:288:LEU:HB3	1.67	0.76
22:V:146:LYS:HB3	23:W:129:PHE:CZ	2.21	0.76
25:Y:128:VAL:HG22	25:Y:375:ARG:HA	1.68	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:ILE:HD12	2:B:1144:ALA:HB2	1.66	0.76
6:F:132:LEU:HB3	7:G:61:ILE:HD13	1.68	0.76
23:W:97:LEU:O	23:W:101:LEU:HB2	1.85	0.76
25:Y:212:TYR:OH	25:Y:222:VAL:CG2	2.33	0.76
25:Y:353:SER:H	25:Y:380:ARG:NH1	1.83	0.76
25:Y:421:GLU:N	25:Y:422:PRO:CD	2.48	0.76
25:Y:639:LEU:HD23	25:Y:649:ARG:CB	2.15	0.76
25:Y:627:PHE:CD1	25:Y:654:LEU:HD11	2.21	0.76
25:Y:693:LEU:HG	25:Y:696:TRP:CZ2	2.21	0.76
22:V:73:LEU:O	22:V:76:ILE:HG22	1.86	0.76
25:Y:352:ILE:CG1	25:Y:380:ARG:NH2	2.49	0.76
25:Y:54:SER:O	25:Y:57:ILE:HG22	1.85	0.76
1:A:1433:MET:CE	2:B:1145:SER:OG	2.33	0.76
1:A:22:PHE:HB2	2:B:1211:ASN:CG	2.06	0.76
26:Z:453:VAL:HG21	26:Z:482:TRP:CZ2	2.22	0.76
1:A:1447:GLU:CD	7:G:26:LEU:CD1	2.54	0.75
17:Q:81:MET:CE	17:Q:92:SER:HB2	1.98	0.75
25:Y:257:LEU:CD2	25:Y:383:LEU:CD1	2.32	0.75
25:Y:28:ILE:HG22	25:Y:57:ILE:HD12	1.68	0.75
25:Y:288:LYS:HG3	25:Y:335:LEU:CD1	2.16	0.75
25:Y:253:THR:CG2	25:Y:434:ILE:HG23	2.15	0.75
26:Z:485:ILE:HD11	26:Z:510:LYS:HG2	1.67	0.75
1:A:227:VAL:HG21	4:D:16:LYS:CE	2.07	0.75
25:Y:288:LYS:HD2	25:Y:334:PHE:C	2.05	0.75
26:Z:447:GLN:H	26:Z:452:LEU:HD13	1.49	0.75
25:Y:288:LYS:HG3	25:Y:335:LEU:HB3	0.76	0.75
25:Y:338:LEU:HD12	25:Y:341:TYR:CE1	2.20	0.75
25:Y:378:SER:OG	25:Y:381:LEU:CB	2.33	0.75
25:Y:550:ILE:CG2	25:Y:554:TRP:CH2	2.57	0.75
26:Z:425:LEU:HD23	26:Z:425:LEU:O	1.87	0.75
17:Q:20:ILE:CG1	17:Q:87:PHE:CE2	2.69	0.75
17:Q:49:VAL:HG21	18:R:114:ASN:O	1.86	0.75
18:R:62:PHE:CE2	18:R:201:ALA:CB	2.64	0.75
25:Y:71:TYR:CD2	25:Y:233:ILE:CD1	2.70	0.75
26:Z:297:ILE:HD11	26:Z:346:ASP:OD2	1.86	0.75
1:A:1442:ASP:O	6:F:135:ARG:N	2.13	0.75
1:A:1445:ILE:CG2	6:F:132:LEU:HD21	2.14	0.75
25:Y:276:LYS:HG3	25:Y:337:ARG:HH21	1.50	0.75
25:Y:229:ASP:C	25:Y:453:PHE:HB3	2.07	0.75
26:Z:368:LYS:HD2	26:Z:372:LYS:CE	2.16	0.75
1:A:1390:ASN:O	1:A:1399:ARG:CD	2.34	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:THR:HG22	2:B:1146:PHE:HD1	1.52	0.75
17:Q:16:TYR:CE2	17:Q:87:PHE:CA	2.67	0.75
20:T:100:ILE:HD12	22:V:129:ARG:HB2	1.67	0.75
26:Z:458:SER:HB3	26:Z:467:SER:HB3	1.68	0.75
17:Q:97:LYS:HD3	17:Q:243:ASN:C	2.07	0.75
25:Y:229:ASP:C	25:Y:453:PHE:HB2	2.05	0.75
26:Z:425:LEU:CG	26:Z:429:THR:HG23	2.16	0.75
26:Z:354:ILE:H	26:Z:447:GLN:HE22	1.34	0.75
25:Y:440:LEU:CD1	25:Y:638:ARG:HG2	2.17	0.75
26:Z:425:LEU:HG	26:Z:429:THR:CG2	2.15	0.75
25:Y:346:MET:O	25:Y:384:LEU:CG	2.35	0.75
25:Y:162:LEU:HA	25:Y:195:ILE:HG12	1.69	0.74
26:Z:315:SER:O	26:Z:323:VAL:HG13	1.87	0.74
26:Z:335:TYR:CD1	26:Z:336:PRO:HD3	2.21	0.74
26:Z:429:THR:HB	26:Z:432:PRO:CD	2.17	0.74
26:Z:476:PHE:HZ	26:Z:493:VAL:HG11	1.51	0.74
26:Z:519:ARG:HG3	26:Z:524:ILE:CG2	2.17	0.74
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.67	0.74
25:Y:162:LEU:CD2	25:Y:195:ILE:HG13	2.17	0.74
25:Y:526:LEU:HD23	25:Y:554:TRP:CZ2	2.19	0.74
17:Q:86:ASN:CA	17:Q:89:ILE:HG12	2.16	0.74
20:T:103:ASP:OD1	20:T:107:LEU:HD21	1.87	0.74
25:Y:131:GLU:CD	25:Y:134:ARG:HH12	1.91	0.74
25:Y:495:MET:HB3	25:Y:686:PHE:CZ	2.23	0.74
26:Z:351:ASP:HB2	26:Z:482:TRP:HZ3	1.53	0.74
17:Q:85:LEU:O	17:Q:89:ILE:CG2	2.30	0.74
1:A:1436:ILE:HD12	1:A:1436:ILE:O	1.87	0.74
6:F:92:ARG:HH21	7:G:64:THR:N	1.85	0.74
22:V:82:ASN:HB2	22:V:86:GLN:NE2	2.03	0.74
25:Y:185:CYS:HB3	25:Y:190:LEU:O	1.86	0.74
26:Z:470:SER:HA	26:Z:478:THR:HG23	1.67	0.74
13:M:22:LEU:O	13:M:24:THR:N	2.21	0.74
25:Y:248:LEU:CG	25:Y:445:ALA:HB2	2.18	0.74
25:Y:440:LEU:CD2	25:Y:641:PHE:CD2	2.71	0.74
25:Y:643:ARG:CB	25:Y:649:ARG:HB3	2.14	0.74
25:Y:327:ARG:O	25:Y:417:LEU:CD2	2.35	0.74
25:Y:440:LEU:HD21	25:Y:641:PHE:CG	2.19	0.74
1:A:1445:ILE:CG2	7:G:66:GLY:O	2.36	0.74
18:R:72:ILE:HG21	18:R:202:TYR:HE1	0.93	0.74
20:T:37:LEU:O	20:T:41:GLN:HB3	1.88	0.74
1:A:836:TYR:CZ	1:A:1403:GLU:OE2	2.41	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:48:ASP:O	18:R:47:LYS:CE	2.35	0.74
20:T:87:LEU:HA	20:T:90:TYR:CD2	2.23	0.74
25:Y:67:ARG:CB	25:Y:230:SER:HB2	2.18	0.74
25:Y:419:ILE:HD11	25:Y:435:MET:HE2	1.70	0.74
26:Z:476:PHE:CE1	26:Z:487:LEU:HD21	2.23	0.74
20:T:100:ILE:HD12	22:V:129:ARG:HG3	1.68	0.74
26:Z:362:ILE:CG2	26:Z:366:GLN:HB2	2.18	0.74
20:T:49:TYR:CE1	20:T:73:LEU:HG	2.22	0.73
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.23	0.73
20:T:122:HIS:CE1	20:T:126:LYS:HG3	2.23	0.73
20:T:100:ILE:HD12	22:V:129:ARG:CG	2.18	0.73
23:W:80:LEU:HD23	23:W:81:PRO:HD2	1.69	0.73
18:R:57:MET:SD	18:R:71:LEU:HD23	2.27	0.73
20:T:111:THR:O	20:T:115:LEU:HD12	1.88	0.73
25:Y:586:TYR:CD1	25:Y:616:TYR:CE2	2.75	0.73
26:Z:356:LEU:HG	26:Z:427:TRP:HD1	1.53	0.73
1:A:1447:GLU:OE2	7:G:26:LEU:HD13	1.86	0.73
25:Y:190:LEU:HD12	25:Y:190:LEU:O	1.89	0.73
25:Y:193:TYR:OH	25:Y:221:ARG:CZ	2.36	0.73
25:Y:327:ARG:HB2	25:Y:330:HIS:HE1	1.49	0.73
25:Y:352:ILE:N	25:Y:380:ARG:NH1	2.35	0.73
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.70	0.73
12:L:30:ILE:O	12:L:56:LEU:HA	1.88	0.73
12:L:48:CYS:HB3	12:L:51:CYS:O	1.88	0.73
25:Y:274:VAL:HG12	25:Y:275:ARG:N	2.02	0.73
1:A:89:PRO:HG2	1:A:204:THR:CB	2.16	0.73
2:B:1221:SER:N	4:D:14:ARG:NH2	2.36	0.73
6:F:96:THR:CA	7:G:64:THR:O	2.36	0.73
21:U:186:ARG:HH22	23:W:100:LYS:HE3	1.53	0.73
22:V:143:LEU:HD12	22:V:144:TYR:N	2.04	0.73
22:V:94:ILE:O	22:V:98:LEU:HG	1.87	0.73
26:Z:333:ILE:O	26:Z:333:ILE:HD13	1.87	0.73
1:A:346:ASP:OD1	2:B:1106:ARG:NE	2.21	0.73
18:R:4:SER:CB	18:R:200:LEU:HG	2.18	0.73
20:T:73:LEU:O	20:T:73:LEU:HD23	1.88	0.73
24:X:43:LEU:HD21	24:X:85:LEU:HD11	1.70	0.73
25:Y:293:LEU:HD13	25:Y:433:PRO:CB	2.18	0.73
25:Y:416:PHE:CE2	25:Y:637:ALA:HB1	2.23	0.73
26:Z:297:ILE:HG13	26:Z:344:ARG:HB2	1.69	0.73
17:Q:106:ARG:NH2	17:Q:211:PHE:HZ	1.85	0.73
18:R:109:SER:O	18:R:113:SER:HB3	1.88	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:585:PRO:CB	26:Z:756:ARG:HH22	1.96	0.73
25:Y:497:ILE:HG13	25:Y:686:PHE:CZ	2.24	0.73
25:Y:497:ILE:HG23	25:Y:684:ARG:CG	2.16	0.73
20:T:94:TYR:CE2	22:V:109:GLU:HB3	2.24	0.73
1:A:50:ILE:O	1:A:52:GLY:N	2.22	0.72
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.72
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.71	0.72
16:P:619:ILE:CB	16:P:634:MET:CA	2.58	0.72
13:M:139:VAL:CA	13:M:152:ASP:CB	2.66	0.72
25:Y:273:GLU:HG2	25:Y:274:VAL:HG23	1.69	0.72
25:Y:469:TYR:N	25:Y:470:PRO:HD2	2.03	0.72
26:Z:383:ILE:HG13	26:Z:517:LEU:HD13	1.71	0.72
22:V:133:LEU:HA	22:V:136:LYS:HE2	1.70	0.72
22:V:140:LEU:HD23	22:V:140:LEU:O	1.90	0.72
22:V:79:ASP:OD2	22:V:94:ILE:HG12	1.88	0.72
26:Z:446:PHE:HB2	26:Z:452:LEU:CD2	2.18	0.72
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.71	0.72
25:Y:248:LEU:CD1	25:Y:445:ALA:HB2	2.18	0.72
25:Y:59:TYR:N	25:Y:62:HIS:CD2	2.56	0.72
26:Z:455:SER:OG	26:Z:466:ARG:HG3	1.89	0.72
26:Z:717:TYR:HE2	26:Z:718:TYR:HE1	0.77	0.72
1:A:1445:ILE:O	7:G:68:ALA:HB1	1.88	0.72
26:Z:368:LYS:CD	26:Z:372:LYS:HE2	2.19	0.72
26:Z:485:ILE:HG21	26:Z:505:ILE:HD13	1.72	0.72
25:Y:200:ILE:HD12	25:Y:225:GLU:O	1.88	0.72
25:Y:231:ILE:HA	25:Y:455:SER:HB3	1.68	0.72
25:Y:467:ASP:HA	25:Y:470:PRO:HG3	1.70	0.72
25:Y:692:GLN:C	25:Y:693:LEU:HD22	2.10	0.72
26:Z:368:LYS:HZ2	26:Z:372:LYS:HD2	1.53	0.72
26:Z:618:TYR:HB3	26:Z:622:MET:HE1	1.69	0.72
3:C:66:ARG:NH2	10:J:3:VAL:O	2.23	0.72
22:V:86:GLN:HA	22:V:89:THR:HG22	1.71	0.72
25:Y:495:MET:HB2	25:Y:686:PHE:CD1	2.24	0.72
25:Y:565:LYS:HD3	25:Y:597:ILE:CD1	2.19	0.72
2:B:1215:ARG:CD	4:D:15:LEU:HD12	2.15	0.72
21:U:134:ILE:CD1	23:W:63:SER:HB2	2.20	0.72
25:Y:212:TYR:CE2	25:Y:222:VAL:HG21	2.24	0.72
25:Y:72:CYS:SG	25:Y:234:PHE:HA	2.30	0.72
25:Y:495:MET:HB3	25:Y:686:PHE:CD1	2.24	0.72
26:Z:410:LEU:HD22	26:Z:477:LEU:CD1	2.15	0.72
26:Z:475:ASP:HB2	26:Z:478:THR:H	1.54	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG22	4:D:16:LYS:CE	2.20	0.72
1:A:1450:LEU:CA	7:G:18:PHE:O	2.38	0.72
6:F:92:ARG:HD2	7:G:64:THR:OG1	1.89	0.72
25:Y:327:ARG:C	25:Y:417:LEU:HD23	2.09	0.72
26:Z:410:LEU:HB2	26:Z:466:ARG:NH2	2.01	0.72
26:Z:516:THR:N	26:Z:681:ARG:CD	2.52	0.72
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.72	0.71
20:T:90:TYR:O	20:T:93:ILE:HG22	1.90	0.71
25:Y:171:LEU:HD21	25:Y:181:LEU:HD22	1.72	0.71
25:Y:208:TYR:CE1	25:Y:213:LEU:CB	2.72	0.71
25:Y:349:LEU:HD12	25:Y:380:ARG:CD	2.20	0.71
25:Y:71:TYR:CD2	25:Y:233:ILE:HD13	2.24	0.71
26:Z:474:MET:HA	26:Z:478:THR:C	2.10	0.71
26:Z:476:PHE:CA	26:Z:485:ILE:HB	2.20	0.71
17:Q:97:LYS:NZ	17:Q:244:SER:C	2.44	0.71
20:T:42:LEU:CD1	20:T:80:LEU:HD12	2.20	0.71
25:Y:193:TYR:HH	25:Y:221:ARG:CZ	2.03	0.71
26:Z:668:THR:HG23	26:Z:694:LYS:CB	2.14	0.71
26:Z:696:ARG:HD2	26:Z:699:GLU:O	1.89	0.71
15:O:93:GLN:HA	16:P:345:GLY:H	1.54	0.71
25:Y:481:LYS:CD	25:Y:483:TYR:CE2	2.74	0.71
25:Y:419:ILE:H	25:Y:633:ARG:HH11	1.32	0.71
26:Z:447:GLN:O	26:Z:452:LEU:HB3	1.88	0.71
26:Z:473:VAL:N	26:Z:478:THR:HG22	2.05	0.71
17:Q:86:ASN:CG	17:Q:220:VAL:HG11	2.10	0.71
18:R:46:ILE:HA	18:R:47:LYS:NZ	2.04	0.71
20:T:91:ASP:HA	22:V:111:THR:CG2	2.17	0.71
25:Y:327:ARG:CZ	25:Y:330:HIS:NE2	2.52	0.71
25:Y:355:THR:N	25:Y:356:PRO:CD	2.54	0.71
26:Z:373:MET:HA	26:Z:381:SER:HA	1.72	0.71
26:Z:487:LEU:HD23	26:Z:493:VAL:CG2	2.10	0.71
17:Q:97:LYS:HE2	17:Q:243:ASN:CA	2.21	0.71
25:Y:167:VAL:CG1	25:Y:195:ILE:CG2	2.68	0.71
25:Y:167:VAL:HG22	25:Y:190:LEU:HD22	1.73	0.71
25:Y:327:ARG:NH1	25:Y:330:HIS:HE1	1.83	0.71
26:Z:429:THR:CB	26:Z:432:PRO:HD2	2.20	0.71
2:B:1215:ARG:NE	4:D:15:LEU:HD13	1.83	0.71
2:B:429:PHE:HA	2:B:432:MET:HE2	1.73	0.71
1:A:1445:ILE:CD1	7:G:18:PHE:CE1	2.52	0.71
25:Y:346:MET:C	25:Y:384:LEU:HD21	2.11	0.71
25:Y:643:ARG:HB2	25:Y:649:ARG:CB	2.14	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:462:THR:HG22	25:Y:660:ARG:HG3	1.71	0.71
2:B:1198:TYR:CE2	2:B:1201:LYS:HE3	2.25	0.71
20:T:100:ILE:CD1	22:V:129:ARG:HG3	2.21	0.71
25:Y:237:ALA:CB	25:Y:458:ILE:CG2	2.69	0.71
25:Y:230:SER:C	25:Y:455:SER:HB2	2.11	0.71
25:Y:42:MET:HG3	25:Y:50:VAL:HG22	1.71	0.71
25:Y:570:LEU:HD12	25:Y:600:SER:HB3	1.71	0.71
25:Y:28:ILE:HB	25:Y:57:ILE:HG13	1.71	0.71
26:Z:477:LEU:HG	26:Z:501:VAL:CB	2.20	0.71
16:P:311:LYS:CB	16:P:423:LYS:CB	2.68	0.71
22:V:119:PRO:O	22:V:122:TRP:CG	2.43	0.71
25:Y:293:LEU:HD11	25:Y:433:PRO:CB	2.20	0.71
25:Y:550:ILE:O	25:Y:554:TRP:CE2	2.43	0.71
26:Z:380:ARG:CA	26:Z:535:LEU:HD22	2.20	0.71
1:A:1445:ILE:HG21	7:G:18:PHE:CE2	2.21	0.71
21:U:132:GLU:OE2	21:U:139:ILE:HD11	1.91	0.71
24:X:85:LEU:O	24:X:89:MET:HG2	1.91	0.71
25:Y:135:ARG:HH21	25:Y:143:ARG:CZ	2.00	0.71
25:Y:161:ASN:O	25:Y:167:VAL:HG21	1.90	0.71
1:A:1436:ILE:HD11	2:B:1144:ALA:HB2	1.73	0.71
16:P:315:SER:CB	16:P:425:ILE:N	2.54	0.71
25:Y:215:ASP:O	25:Y:218:ILE:CG2	2.39	0.71
25:Y:272:SER:HB2	25:Y:348:VAL:CG1	2.21	0.71
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.71	0.70
25:Y:272:SER:HG	25:Y:281:LYS:HE3	1.56	0.70
25:Y:349:LEU:CD1	25:Y:380:ARG:CG	2.68	0.70
25:Y:350:HIS:CE1	25:Y:381:LEU:HD12	2.26	0.70
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.71	0.70
21:U:182:LEU:HB2	23:W:101:LEU:HD13	1.73	0.70
22:V:119:PRO:O	22:V:122:TRP:NE1	2.17	0.70
25:Y:440:LEU:HD21	25:Y:641:PHE:HB3	1.64	0.70
26:Z:495:ALA:HB3	26:Z:498:PHE:CD2	2.21	0.70
1:A:1444:MET:SD	7:G:60:ARG:HB2	2.31	0.70
1:A:52:GLY:C	1:A:56:PRO:HG3	2.12	0.70
18:R:72:ILE:HG21	18:R:202:TYR:CZ	2.21	0.70
22:V:83:LEU:O	22:V:84:SER:CB	2.39	0.70
25:Y:128:VAL:N	25:Y:376:PHE:HE2	1.82	0.70
25:Y:656:PHE:CD1	25:Y:659:MET:SD	2.84	0.70
26:Z:474:MET:HB2	26:Z:480:ARG:HA	1.73	0.70
14:N:62:TRP:O	14:N:65:LEU:N	2.24	0.70
20:T:55:LYS:CB	20:T:62:ARG:HG3	2.21	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:132:GLU:O	22:V:136:LYS:HE2	1.91	0.70
20:T:112:ARG:HA	20:T:115:LEU:HD13	1.73	0.70
25:Y:193:TYR:OH	25:Y:221:ARG:NH1	2.24	0.70
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.74	0.70
17:Q:86:ASN:HD22	17:Q:87:PHE:N	1.88	0.70
25:Y:485:MET:HG3	25:Y:486:THR:HG23	1.72	0.70
25:Y:418:LEU:HB3	25:Y:633:ARG:NE	2.06	0.70
25:Y:639:LEU:HD21	25:Y:649:ARG:CG	2.21	0.70
26:Z:500:ARG:HA	26:Z:500:ARG:HE	1.56	0.70
17:Q:97:LYS:HB3	17:Q:243:ASN:HD22	1.55	0.70
25:Y:72:CYS:SG	25:Y:234:PHE:HD1	2.14	0.70
26:Z:356:LEU:HG	26:Z:427:TRP:CD1	2.26	0.70
26:Z:475:ASP:HB2	26:Z:478:THR:N	2.06	0.70
26:Z:466:ARG:CB	26:Z:477:LEU:HB2	2.22	0.70
20:T:80:LEU:HD21	22:V:73:LEU:CD1	2.21	0.70
5:E:185:ALA:HA	5:E:190:LEU:HD12	1.74	0.70
25:Y:450:PHE:CZ	25:Y:475:PHE:CD2	2.80	0.70
25:Y:639:LEU:CG	25:Y:653:PHE:CD2	2.61	0.70
25:Y:339:ILE:HG22	25:Y:343:LYS:HE3	1.73	0.69
25:Y:495:MET:HB2	25:Y:686:PHE:CE1	2.27	0.69
26:Z:455:SER:CB	26:Z:466:ARG:HH11	2.01	0.69
25:Y:244:CYS:SG	25:Y:446:ILE:HD13	2.32	0.69
26:Z:316:PHE:CZ	26:Z:321:GLU:HA	2.27	0.69
26:Z:400:ALA:CB	26:Z:450:SER:HA	2.22	0.69
26:Z:455:SER:CB	26:Z:466:ARG:HG3	2.21	0.69
26:Z:473:VAL:O	26:Z:478:THR:HB	1.92	0.69
25:Y:200:ILE:CG2	25:Y:226:VAL:HG21	2.19	0.69
25:Y:350:HIS:HB2	25:Y:384:LEU:CD1	2.22	0.69
25:Y:463:ILE:HD11	25:Y:469:TYR:CD1	2.27	0.69
25:Y:567:LYS:HG2	25:Y:597:ILE:CB	2.23	0.69
26:Z:351:ASP:HB2	26:Z:482:TRP:CZ3	2.28	0.69
26:Z:467:SER:HA	26:Z:501:VAL:HG12	1.74	0.69
20:T:62:ARG:C	20:T:66:ASN:HD21	1.96	0.69
25:Y:122:LYS:HD3	25:Y:218:ILE:HD13	1.72	0.69
25:Y:495:MET:CB	25:Y:686:PHE:CE1	2.75	0.69
26:Z:362:ILE:HG23	26:Z:366:GLN:CB	2.23	0.69
25:Y:518:ILE:CG2	25:Y:522:TYR:CZ	2.71	0.69
25:Y:499:LYS:CD	25:Y:521:ASN:C	2.52	0.69
26:Z:448:THR:O	26:Z:452:LEU:HB2	1.92	0.69
6:F:96:THR:HG23	7:G:65:ASP:CA	2.23	0.69
6:F:96:THR:HG23	7:G:66:GLY:N	2.06	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1451:VAL:HA	7:G:19:GLY:HA2	1.75	0.69
22:V:117:LYS:HG2	22:V:121:GLU:HB3	1.72	0.69
25:Y:111:ARG:CD	25:Y:129:VAL:HG21	2.22	0.69
1:A:140:THR:HA	1:A:143:LYS:HE2	1.75	0.69
1:A:320:ARG:NH2	3:C:81:GLU:HG3	69.03	0.69
25:Y:196:VAL:O	25:Y:200:ILE:CG2	2.39	0.69
25:Y:248:LEU:HD21	25:Y:445:ALA:CB	2.20	0.69
26:Z:613:TYR:OH	26:Z:762:GLU:HG2	1.91	0.69
25:Y:124:ARG:HA	25:Y:376:PHE:CZ	2.27	0.69
25:Y:349:LEU:N	25:Y:380:ARG:NH2	2.40	0.69
26:Z:408:ILE:HG21	26:Z:476:PHE:N	2.07	0.69
26:Z:410:LEU:HD22	26:Z:476:PHE:CD2	2.27	0.69
1:A:317:LYS:O	2:B:471:LYS:HE3	1.89	0.69
17:Q:191:LEU:HD11	18:R:81:THR:HB	1.75	0.69
26:Z:476:PHE:CD1	26:Z:487:LEU:HD11	2.28	0.69
21:U:130:TYR:CE2	21:U:134:ILE:CD1	2.74	0.69
26:Z:474:MET:HB2	26:Z:480:ARG:N	2.07	0.69
20:T:114:ILE:HG13	22:V:143:LEU:CD1	2.17	0.69
20:T:42:LEU:O	20:T:46:LEU:HD13	1.93	0.69
20:T:90:TYR:CD1	22:V:112:LYS:HD3	2.28	0.69
25:Y:515:ASP:HB2	25:Y:518:ILE:CD1	2.23	0.69
26:Z:354:ILE:H	26:Z:447:GLN:NE2	1.89	0.69
23:W:68:LEU:O	23:W:72:GLN:HG3	1.92	0.68
25:Y:58:ALA:O	25:Y:62:HIS:HD2	1.68	0.68
26:Z:496:ALA:HA	26:Z:499:ARG:HH12	1.57	0.68
26:Z:495:ALA:CB	26:Z:498:PHE:HD2	2.03	0.68
1:A:344:ARG:HA	2:B:1128:LEU:O	1.93	0.68
22:V:86:GLN:HG2	22:V:90:LEU:CD1	2.23	0.68
20:T:123:ASP:N	23:W:131:ASP:O	2.26	0.68
25:Y:127:THR:CG2	25:Y:361:GLN:CD	2.61	0.68
26:Z:373:MET:CG	26:Z:381:SER:HA	2.22	0.68
1:A:412:ARG:HB3	3:C:51:VAL:CG1	45.23	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.76	0.68
2:B:1221:SER:N	4:D:14:ARG:HH22	1.91	0.68
25:Y:59:TYR:CD2	25:Y:62:HIS:HE1	2.10	0.68
26:Z:475:ASP:OD2	26:Z:478:THR:HB	1.93	0.68
21:U:130:TYR:CZ	21:U:134:ILE:HD11	2.28	0.68
25:Y:185:CYS:SG	25:Y:192:PRO:HA	2.33	0.68
25:Y:639:LEU:HD23	25:Y:649:ARG:HD2	1.62	0.68
26:Z:477:LEU:HG	26:Z:501:VAL:HB	1.74	0.68
26:Z:740:HIS:O	26:Z:740:HIS:CD2	2.47	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:85:HIS:O	14:N:88:GLU:CB	2.41	0.68
20:T:82:GLU:O	20:T:86:LEU:HD23	1.94	0.68
20:T:57:VAL:HG13	22:V:87:LEU:HD11	1.75	0.68
25:Y:167:VAL:CG1	25:Y:195:ILE:HG21	2.23	0.68
25:Y:226:VAL:HG22	25:Y:226:VAL:O	1.91	0.68
25:Y:293:LEU:HD12	25:Y:433:PRO:CB	2.22	0.68
17:Q:298:SER:O	17:Q:299:ARG:O	2.12	0.68
17:Q:97:LYS:CE	17:Q:243:ASN:CA	2.71	0.68
26:Z:298:GLY:O	26:Z:346:ASP:HB2	1.93	0.68
26:Z:407:VAL:HG12	26:Z:448:THR:HA	1.74	0.68
26:Z:477:LEU:CB	26:Z:501:VAL:HB	2.24	0.68
26:Z:527:LEU:CD2	26:Z:531:ILE:HD12	2.14	0.68
1:A:1451:VAL:CG1	7:G:20:PRO:HB3	2.24	0.68
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.76	0.68
20:T:115:LEU:O	23:W:131:ASP:OD2	2.12	0.68
22:V:117:LYS:CG	22:V:121:GLU:HB3	2.14	0.68
22:V:85:ASN:HA	22:V:88:GLU:CD	2.15	0.68
25:Y:349:LEU:CD1	25:Y:380:ARG:NE	2.40	0.68
25:Y:244:CYS:SG	25:Y:446:ILE:HB	2.34	0.68
25:Y:499:LYS:CB	25:Y:522:TYR:CD1	2.74	0.68
25:Y:567:LYS:HE2	25:Y:597:ILE:CG2	2.13	0.68
25:Y:416:PHE:CG	25:Y:637:ALA:HB1	2.28	0.68
26:Z:476:PHE:CD2	26:Z:477:LEU:HD12	2.29	0.68
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.75	0.68
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.74	0.68
25:Y:225:GLU:O	25:Y:226:VAL:CG1	2.42	0.68
25:Y:571:VAL:CG1	25:Y:572:GLU:H	2.07	0.68
1:A:1445:ILE:HG23	6:F:132:LEU:HD23	1.36	0.68
12:L:38:LEU:O	12:L:39:SER:HB3	1.93	0.68
26:Z:310:ILE:CD1	26:Z:313:VAL:HG23	2.24	0.68
26:Z:397:ILE:CD1	26:Z:423:GLN:HE21	2.05	0.68
26:Z:476:PHE:HA	26:Z:485:ILE:CB	2.24	0.68
3:C:259:LEU:HD22	11:K:91:CYS:HB3	1.75	0.67
25:Y:215:ASP:HB3	25:Y:218:ILE:HG21	1.75	0.67
25:Y:200:ILE:HA	25:Y:226:VAL:HG21	1.73	0.67
25:Y:420:ILE:HD12	25:Y:633:ARG:NH2	2.01	0.67
25:Y:656:PHE:O	25:Y:659:MET:HG2	1.93	0.67
1:A:132:LYS:HZ2	1:A:1415:SER:CB	2.07	0.67
1:A:1447:GLU:CA	7:G:22:MET:SD	2.82	0.67
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.60	0.67
17:Q:108:ILE:HG22	17:Q:109:LEU:H	1.58	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:86:ASN:OD1	17:Q:220:VAL:HG12	1.94	0.67
22:V:128:GLN:O	22:V:131:GLN:HG2	1.93	0.67
25:Y:123:GLU:OE1	25:Y:217:LYS:NZ	2.27	0.67
25:Y:170:TYR:HD2	25:Y:176:PHE:HZ	1.41	0.67
25:Y:267:LEU:O	25:Y:268:ASP:CB	2.40	0.67
25:Y:656:PHE:HA	25:Y:659:MET:CE	2.24	0.67
26:Z:373:MET:HG3	26:Z:381:SER:CA	2.23	0.67
20:T:126:LYS:CG	23:W:132:GLY:O	2.43	0.67
26:Z:421:ARG:NE	26:Z:430:LEU:HD11	2.07	0.67
26:Z:474:MET:N	26:Z:481:GLU:H	1.87	0.67
26:Z:487:LEU:HD23	26:Z:490:VAL:HG23	1.77	0.67
7:G:138:THR:HG22	7:G:139:ILE:H	1.59	0.67
22:V:117:LYS:CE	22:V:121:GLU:CB	2.58	0.67
23:W:86:SER:O	23:W:90:GLN:HG3	1.95	0.67
26:Z:485:ILE:HD11	26:Z:510:LYS:CG	2.24	0.67
26:Z:522:ASP:HA	26:Z:524:ILE:CD1	2.24	0.67
16:P:308:TYR:CB	16:P:362:GLU:CB	2.73	0.67
17:Q:20:ILE:CG1	17:Q:87:PHE:CD2	2.77	0.67
25:Y:185:CYS:SG	25:Y:192:PRO:CA	2.83	0.67
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.59	0.67
16:P:410:VAL:CB	16:P:502:ASN:CB	2.72	0.67
17:Q:86:ASN:HD22	17:Q:87:PHE:H	1.43	0.67
20:T:84:VAL:HG13	22:V:70:PHE:CE2	2.29	0.67
25:Y:212:TYR:CZ	25:Y:222:VAL:HG21	2.29	0.67
25:Y:389:GLU:O	25:Y:393:VAL:HG13	1.95	0.67
25:Y:418:LEU:CD1	25:Y:438:THR:OG1	2.39	0.67
22:V:102:LYS:O	22:V:105:ILE:HG22	1.95	0.67
25:Y:346:MET:O	25:Y:384:LEU:HD21	1.95	0.67
26:Z:303:ARG:HG2	26:Z:504:THR:CB	2.22	0.67
26:Z:403:ILE:HD13	26:Z:484:PHE:CD2	2.30	0.67
26:Z:356:LEU:CG	26:Z:427:TRP:HD1	2.07	0.67
26:Z:757:ARG:HH12	26:Z:760:LEU:HG	0.50	0.67
22:V:146:LYS:CE	23:W:129:PHE:HZ	2.07	0.67
26:Z:672:GLN:OE1	26:Z:686:ARG:NH2	2.27	0.67
7:G:1:MET:SD	7:G:2:PHE:N	2.63	0.67
25:Y:492:PHE:CE2	25:Y:494:PRO:HG3	2.30	0.67
1:A:53:LEU:CD2	1:A:54:ASN:H	2.06	0.67
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.76	0.67
17:Q:97:LYS:HD3	17:Q:243:ASN:CB	2.07	0.67
18:R:47:LYS:HZ3	18:R:47:LYS:H	1.41	0.67
21:U:165:TYR:HE2	23:W:80:LEU:HD21	1.60	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:73:ASN:HD22	21:U:75:GLN:HE21	1.40	0.67
26:Z:352:LEU:O	26:Z:447:GLN:HB3	1.95	0.67
26:Z:383:ILE:HG22	26:Z:512:GLY:CA	2.24	0.67
26:Z:407:VAL:HG13	26:Z:451:GLY:HA2	1.76	0.67
26:Z:456:THR:O	26:Z:465:ASN:HB3	1.94	0.67
26:Z:408:ILE:HD11	26:Z:466:ARG:CD	2.25	0.67
7:G:1:MET:HE3	7:G:80:LYS:O	1.94	0.66
17:Q:86:ASN:OD1	17:Q:220:VAL:HG11	1.95	0.66
22:V:132:GLU:HB3	22:V:136:LYS:HZ3	1.59	0.66
22:V:81:ASN:HB2	22:V:90:LEU:HD22	1.77	0.66
22:V:146:LYS:CG	23:W:129:PHE:HZ	1.83	0.66
23:W:60:ASP:O	23:W:64:THR:HG22	1.94	0.66
25:Y:182:LEU:HD12	25:Y:192:PRO:HG2	1.75	0.66
25:Y:346:MET:O	25:Y:384:LEU:CD2	2.42	0.66
13:M:136:ASN:N	13:M:155:ILE:O	2.20	0.66
25:Y:272:SER:CB	25:Y:348:VAL:HG11	2.24	0.66
17:Q:79:THR:O	17:Q:82:ASP:CB	2.42	0.66
25:Y:162:LEU:HD23	25:Y:195:ILE:CG1	2.24	0.66
25:Y:335:LEU:HD13	25:Y:335:LEU:H	1.60	0.66
25:Y:278:ASP:OD2	25:Y:352:ILE:HG21	1.94	0.66
25:Y:492:PHE:CZ	25:Y:707:ASN:OD1	2.48	0.66
26:Z:619:ALA:HA	26:Z:622:MET:HE2	1.77	0.66
18:R:43:ARG:HB2	18:R:119:ARG:CG	2.19	0.66
25:Y:288:LYS:HG3	25:Y:335:LEU:HD12	1.77	0.66
26:Z:386:LEU:HB3	26:Z:387:PRO:HD2	1.75	0.66
26:Z:428:CYS:CB	26:Z:434:ASN:HB2	2.15	0.66
26:Z:427:TRP:HB2	26:Z:449:GLU:CD	2.15	0.66
26:Z:452:LEU:O	26:Z:452:LEU:HD23	1.96	0.66
26:Z:466:ARG:HB2	26:Z:477:LEU:HB2	1.76	0.66
1:A:15:LYS:NZ	2:B:1220:ARG:HE	1.93	0.66
14:N:120:PRO:C	14:N:122:VAL:H	1.97	0.66
20:T:55:LYS:CE	20:T:62:ARG:HE	2.09	0.66
22:V:69:ILE:HD11	22:V:108:ASN:ND2	2.11	0.66
25:Y:171:LEU:CB	25:Y:172:PRO:HD3	2.22	0.66
25:Y:213:LEU:O	25:Y:213:LEU:HD13	1.96	0.66
26:Z:476:PHE:HB2	26:Z:485:ILE:HB	1.76	0.66
1:A:1450:LEU:HB3	7:G:22:MET:SD	2.35	0.66
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.77	0.66
25:Y:350:HIS:HE1	25:Y:381:LEU:HD11	1.57	0.66
26:Z:356:LEU:HD23	26:Z:448:THR:HG21	1.76	0.66
26:Z:370:LEU:HD11	26:Z:398:THR:CG2	2.25	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:HG3	1:A:312:PRO:HD2	1.77	0.66
25:Y:272:SER:HB2	25:Y:281:LYS:HZ2	1.57	0.66
26:Z:410:LEU:HD22	26:Z:476:PHE:HD2	1.60	0.66
1:A:1451:VAL:CG2	7:G:22:MET:CG	2.65	0.66
25:Y:357:LYS:HG3	25:Y:376:PHE:HB2	1.76	0.66
26:Z:474:MET:H	26:Z:481:GLU:N	1.89	0.66
26:Z:485:ILE:HG23	26:Z:507:ALA:CB	2.26	0.66
16:P:323:PHE:O	16:P:339:TYR:N	2.28	0.66
17:Q:97:LYS:HZ1	17:Q:244:SER:N	1.63	0.66
17:Q:3:GLN:HB2	17:Q:259:VAL:CG2	2.26	0.66
25:Y:68:LYS:HG3	25:Y:228:LYS:HG3	1.74	0.66
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.78	0.66
1:A:227:VAL:CG1	4:D:16:LYS:CG	2.65	0.66
12:L:58:LYS:HG2	12:L:58:LYS:O	1.96	0.66
14:N:85:HIS:HA	14:N:88:GLU:CB	2.25	0.66
18:R:53:VAL:HG12	18:R:54:SER:H	1.61	0.66
20:T:46:LEU:O	20:T:50:GLU:HG3	1.95	0.66
21:U:156:VAL:HG12	21:U:157:ASN:N	2.11	0.66
22:V:82:ASN:H	22:V:86:GLN:HE22	1.43	0.66
25:Y:171:LEU:HD21	25:Y:181:LEU:CD2	2.26	0.66
25:Y:337:ARG:CZ	25:Y:345:ARG:CD	2.74	0.66
25:Y:646:TYR:CB	25:Y:648:ILE:HG12	2.24	0.66
26:Z:453:VAL:HG21	26:Z:482:TRP:HZ2	1.61	0.66
26:Z:439:THR:HG23	26:Z:465:ASN:HD22	1.58	0.66
13:M:140:GLY:O	13:M:150:LEU:HA	1.95	0.65
25:Y:215:ASP:HB3	25:Y:218:ILE:HG22	1.78	0.65
25:Y:56:THR:HG22	25:Y:60:GLN:NE2	2.11	0.65
26:Z:477:LEU:CG	26:Z:501:VAL:HB	2.24	0.65
26:Z:519:ARG:HG3	26:Z:524:ILE:HG22	1.76	0.65
2:B:296:GLU:O	2:B:300:HIS:HD2	1.80	0.65
22:V:66:ILE:HB	22:V:67:PRO:HD3	1.78	0.65
25:Y:418:LEU:CD2	25:Y:633:ARG:HD2	2.26	0.65
25:Y:681:LEU:HD21	25:Y:696:TRP:CH2	2.31	0.65
26:Z:455:SER:HB3	26:Z:466:ARG:HD3	1.77	0.65
26:Z:466:ARG:HD2	26:Z:475:ASP:OD2	1.96	0.65
1:A:388:LEU:O	1:A:392:VAL:HG23	1.96	0.65
17:Q:85:LEU:HD13	17:Q:88:ARG:H	1.60	0.65
20:T:93:ILE:HD12	22:V:122:TRP:HE3	0.49	0.65
20:T:91:ASP:CG	22:V:66:ILE:HG13	2.16	0.65
22:V:149:ARG:O	23:W:126:ILE:HD11	1.96	0.65
25:Y:664:GLN:HA	25:Y:664:GLN:HE21	1.61	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:493:LEU:HB3	25:Y:696:TRP:CD1	2.31	0.65
26:Z:356:LEU:HD12	26:Z:427:TRP:HB3	1.78	0.65
26:Z:430:LEU:HD23	26:Z:430:LEU:O	1.96	0.65
26:Z:434:ASN:HB3	26:Z:449:GLU:OE1	1.95	0.65
21:U:74:GLN:HE21	21:U:77:ARG:HD3	1.60	0.65
25:Y:251:ASP:HB3	25:Y:436:ARG:NE	2.11	0.65
25:Y:357:LYS:HE2	25:Y:376:PHE:CE1	2.28	0.65
25:Y:569:ILE:HG22	25:Y:571:VAL:HG22	1.76	0.65
26:Z:505:ILE:HG21	26:Z:507:ALA:HB3	1.78	0.65
26:Z:621:LYS:HZ2	26:Z:621:LYS:HB2	1.60	0.65
26:Z:677:TYR:O	26:Z:677:TYR:CD1	2.50	0.65
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.29	0.65
25:Y:269:GLU:HG2	25:Y:277:VAL:CG1	2.18	0.65
25:Y:327:ARG:CZ	25:Y:330:HIS:HE1	2.02	0.65
25:Y:445:ALA:O	25:Y:448:PRO:HD2	1.96	0.65
26:Z:456:THR:HB	26:Z:465:ASN:ND2	2.11	0.65
1:A:316:GLN:O	1:A:318:SER:N	2.29	0.65
20:T:90:TYR:HB3	22:V:112:LYS:N	2.07	0.65
25:Y:76:MET:HA	25:Y:79:ILE:HD12	1.79	0.65
26:Z:500:ARG:O	26:Z:504:THR:HG23	1.97	0.65
2:B:1215:ARG:HD3	4:D:15:LEU:CD1	2.16	0.65
12:L:39:SER:O	12:L:40:LEU:HG	1.97	0.65
17:Q:86:ASN:O	17:Q:89:ILE:CG1	2.44	0.65
26:Z:385:VAL:O	26:Z:386:LEU:HD23	1.97	0.65
1:A:1447:GLU:HA	7:G:22:MET:SD	2.36	0.65
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.79	0.65
25:Y:467:ASP:HA	25:Y:470:PRO:CG	2.26	0.65
25:Y:497:ILE:O	25:Y:497:ILE:CG2	2.45	0.65
14:N:120:PRO:C	14:N:122:VAL:N	2.49	0.65
17:Q:104:MET:O	17:Q:108:ILE:O	2.15	0.65
25:Y:495:MET:SD	25:Y:696:TRP:HE3	2.14	0.65
25:Y:499:LYS:HE2	25:Y:525:MET:CG	2.26	0.65
25:Y:655:SER:HA	25:Y:689:LYS:HZ1	1.62	0.65
25:Y:71:TYR:HD2	25:Y:233:ILE:CD1	2.10	0.65
26:Z:373:MET:HG3	26:Z:381:SER:CB	2.27	0.65
26:Z:353:ASP:HB2	26:Z:448:THR:OG1	1.96	0.65
26:Z:473:VAL:CG1	26:Z:481:GLU:HG3	2.27	0.65
26:Z:476:PHE:CB	26:Z:485:ILE:HB	2.27	0.65
7:G:1:MET:CE	7:G:80:LYS:O	2.45	0.65
17:Q:98:ILE:HG22	17:Q:99:PRO:N	2.12	0.65
18:R:189:LEU:HD13	18:R:189:LEU:H	1.60	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:230:SER:O	25:Y:455:SER:OG	2.15	0.65
25:Y:273:GLU:HG2	25:Y:274:VAL:N	2.12	0.65
25:Y:438:THR:HG21	25:Y:634:ILE:HG23	1.79	0.65
25:Y:569:ILE:HG22	25:Y:571:VAL:CG2	2.27	0.65
26:Z:459:MET:C	26:Z:464:ARG:HG3	2.17	0.65
26:Z:502:VAL:HB	26:Z:530:LEU:HD13	1.79	0.65
3:C:56:THR:HG21	3:C:145:CYS:SG	2.36	0.64
20:T:39:LYS:CD	22:V:115:LEU:HA	2.26	0.64
25:Y:167:VAL:CG2	25:Y:190:LEU:HD22	2.27	0.64
26:Z:476:PHE:O	26:Z:505:ILE:HD11	1.97	0.64
1:A:46:THR:HG22	1:A:47:ARG:H	1.61	0.64
25:Y:135:ARG:NH2	25:Y:143:ARG:NH2	2.44	0.64
25:Y:193:TYR:HE2	25:Y:197:ARG:NH1	1.96	0.64
26:Z:351:ASP:CB	26:Z:482:TRP:HZ3	2.09	0.64
1:A:1436:ILE:HD11	2:B:1144:ALA:CA	2.28	0.64
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.27	0.64
14:N:67:SER:O	14:N:71:VAL:CB	2.46	0.64
14:N:69:LEU:O	14:N:73:LEU:CB	2.44	0.64
25:Y:493:LEU:HD22	25:Y:696:TRP:HE1	1.53	0.64
26:Z:696:ARG:CZ	26:Z:704:PHE:CZ	2.80	0.64
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.78	0.64
2:B:110:HIS:HE1	12:L:54:ARG:HH12	1.45	0.64
22:V:69:ILE:HG12	22:V:104:LEU:CB	2.26	0.64
25:Y:208:TYR:CD1	25:Y:213:LEU:HB2	2.33	0.64
25:Y:232:VAL:HG23	25:Y:453:PHE:CE2	2.29	0.64
1:A:1447:GLU:OE2	7:G:70:PHE:CE1	2.50	0.64
12:L:31:CYS:SG	12:L:34:CYS:N	2.69	0.64
17:Q:85:LEU:CD1	17:Q:88:ARG:HB3	2.25	0.64
25:Y:648:ILE:CD1	25:Y:652:ASP:OD2	2.46	0.64
25:Y:83:LEU:CD1	25:Y:177:SER:HA	2.27	0.64
26:Z:403:ILE:HG21	26:Z:405:LYS:HG2	1.78	0.64
1:A:1445:ILE:HG23	6:F:132:LEU:HD22	1.72	0.64
2:B:68:THR:HG22	2:B:91:SER:HA	1.80	0.64
20:T:91:ASP:O	20:T:95:ARG:HG3	1.96	0.64
25:Y:170:TYR:HD2	25:Y:176:PHE:CZ	2.15	0.64
25:Y:289:LEU:HD22	25:Y:435:MET:CG	2.27	0.64
25:Y:443:SER:HA	25:Y:473:LEU:HA	1.80	0.64
25:Y:518:ILE:O	25:Y:522:TYR:CE2	2.50	0.64
25:Y:567:LYS:CD	25:Y:597:ILE:HG21	2.27	0.64
25:Y:571:VAL:HG12	25:Y:572:GLU:CB	2.28	0.64
25:Y:664:GLN:HA	25:Y:664:GLN:NE2	2.13	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:3:GLN:HB2	17:Q:259:VAL:HG22	1.78	0.64
18:R:187:ASP:OD1	18:R:203:GLN:HG2	1.97	0.64
23:W:73:ILE:O	23:W:77:ILE:HG13	1.98	0.64
25:Y:200:ILE:CD1	25:Y:225:GLU:C	2.66	0.64
25:Y:339:ILE:CG2	25:Y:343:LYS:HE3	2.27	0.64
26:Z:343:PHE:HE2	26:Z:345:ASN:HB2	1.63	0.64
1:A:1451:VAL:HA	7:G:19:GLY:CA	2.28	0.64
1:A:368:LYS:CG	1:A:399:HIS:HD2	2.06	0.64
13:M:166:ILE:HA	14:N:95:VAL:CA	2.26	0.64
13:M:1:MET:N	24:X:91:SER:HA	2.13	0.64
18:R:4:SER:CB	18:R:200:LEU:CG	2.75	0.64
25:Y:28:ILE:HD11	25:Y:40:LEU:HD22	1.80	0.64
25:Y:586:TYR:HD2	25:Y:598:LEU:CG	2.02	0.64
26:Z:405:LYS:CD	26:Z:483:GLY:HA3	2.19	0.64
25:Y:185:CYS:SG	25:Y:192:PRO:HG3	2.37	0.64
25:Y:222:VAL:O	25:Y:225:GLU:O	2.16	0.64
25:Y:29:LYS:HG3	25:Y:61:MET:SD	2.38	0.64
25:Y:639:LEU:CD2	25:Y:649:ARG:CG	2.76	0.64
25:Y:656:PHE:HA	25:Y:659:MET:HE3	1.78	0.64
26:Z:415:VAL:HA	26:Z:418:MET:CE	2.27	0.64
1:A:1445:ILE:CG1	7:G:68:ALA:H	2.09	0.64
25:Y:393:VAL:HG21	25:Y:437:PHE:CD1	2.33	0.64
25:Y:469:TYR:O	25:Y:472:MET:O	2.15	0.64
26:Z:439:THR:HG22	26:Z:440:SER:N	2.10	0.63
26:Z:474:MET:HB2	26:Z:480:ARG:C	2.18	0.63
18:R:134:GLY:O	18:R:166:LYS:NZ	2.24	0.63
18:R:186:SER:O	18:R:187:ASP:HB2	1.96	0.63
20:T:55:LYS:CD	20:T:60:VAL:HG11	2.20	0.63
20:T:67:LEU:O	20:T:68:ASP:C	2.36	0.63
22:V:140:LEU:HD23	22:V:140:LEU:C	2.18	0.63
26:Z:456:THR:HG22	26:Z:457:TYR:N	2.13	0.63
1:A:867:ILE:CD1	1:A:1000:LEU:HD11	2.28	0.63
2:B:872:GLU:HG2	2:B:916:THR:HG22	1.78	0.63
12:L:31:CYS:HB3	12:L:35:SER:N	2.13	0.63
17:Q:64:ILE:HD13	17:Q:209:TYR:CE2	2.33	0.63
16:P:183:GLU:H	19:S:77:ARG:CB	2.11	0.63
20:T:108:ASP:O	20:T:112:ARG:HG3	1.97	0.63
20:T:114:ILE:HD12	22:V:147:LEU:CD1	2.27	0.63
25:Y:140:GLN:HG3	25:Y:143:ARG:NH2	2.13	0.63
26:Z:456:THR:HG22	26:Z:457:TYR:H	1.63	0.63
1:A:344:ARG:CZ	2:B:1120:GLU:CG	2.74	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:917:PRO:HA	2:B:934:LYS:HB3	1.80	0.63
16:P:341:TYR:CB	16:P:354:ILE:H	2.12	0.63
18:R:13:THR:HB	18:R:14:PRO:HD2	1.79	0.63
18:R:46:ILE:HA	18:R:47:LYS:HZ1	1.62	0.63
20:T:45:ASP:OD2	20:T:76:THR:HG23	1.99	0.63
20:T:94:TYR:HB2	22:V:111:THR:CG2	2.22	0.63
25:Y:259:ARG:CB	25:Y:379:GLU:CD	2.60	0.63
25:Y:586:TYR:CD2	25:Y:598:LEU:HD12	2.33	0.63
26:Z:455:SER:HB3	26:Z:466:ARG:NH1	2.00	0.63
26:Z:473:VAL:HB	26:Z:481:GLU:HG3	1.81	0.63
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.79	0.63
17:Q:52:VAL:HA	17:Q:57:GLN:O	1.98	0.63
25:Y:277:VAL:HG12	25:Y:278:ASP:N	2.13	0.63
25:Y:234:PHE:HZ	25:Y:449:VAL:HG21	1.62	0.63
25:Y:539:VAL:CG1	25:Y:623:ILE:CG1	2.77	0.63
26:Z:411:CYS:O	26:Z:456:THR:HA	1.97	0.63
26:Z:400:ALA:HB2	26:Z:450:SER:O	1.99	0.63
1:A:22:PHE:N	2:B:1211:ASN:O	2.32	0.63
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.81	0.63
21:U:74:GLN:NE2	21:U:77:ARG:HH11	1.97	0.63
21:U:175:ILE:HG13	23:W:94:ILE:HG22	1.80	0.63
25:Y:110:SER:HB3	25:Y:212:TYR:CD1	2.34	0.63
25:Y:683:ASP:O	25:Y:686:PHE:CE2	2.47	0.63
25:Y:68:LYS:CG	25:Y:228:LYS:CG	2.65	0.63
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.63
20:T:108:ASP:O	20:T:111:THR:HG22	1.99	0.63
20:T:64:LYS:HB2	20:T:65:PRO:HD3	1.81	0.63
20:T:91:ASP:CA	22:V:111:THR:HG21	2.18	0.63
22:V:140:LEU:HA	22:V:143:LEU:HD23	1.79	0.63
25:Y:495:MET:HB3	25:Y:686:PHE:CE1	2.34	0.63
18:R:90:ALA:O	18:R:94:ASN:OD1	2.16	0.63
21:U:70:MET:SD	24:X:23:PHE:HE2	2.22	0.63
26:Z:372:LYS:HB3	26:Z:535:LEU:HD23	1.80	0.63
26:Z:476:PHE:HD2	26:Z:477:LEU:CD1	2.11	0.63
2:B:806:THR:HG22	2:B:808:ALA:H	1.63	0.63
23:W:83:VAL:HG23	23:W:84:ASP:N	2.13	0.63
26:Z:410:LEU:HD13	26:Z:477:LEU:HD13	1.79	0.63
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.81	0.62
25:Y:653:PHE:CD1	25:Y:654:LEU:N	2.67	0.62
26:Z:409:VAL:HG22	26:Z:486:ILE:HD12	1.80	0.62
26:Z:448:THR:HG22	26:Z:449:GLU:N	2.14	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:484:PHE:HZ	26:Z:511:LEU:HB2	1.64	0.62
1:A:5:GLN:HG3	2:B:1175:LEU:HD11	1.81	0.62
6:F:92:ARG:NH2	7:G:64:THR:N	2.46	0.62
17:Q:86:ASN:CG	17:Q:220:VAL:CG1	2.66	0.62
17:Q:97:LYS:NZ	17:Q:244:SER:CA	2.44	0.62
25:Y:467:ASP:O	25:Y:470:PRO:CG	2.45	0.62
25:Y:494:PRO:CD	25:Y:679:MET:O	2.36	0.62
1:A:89:PRO:CB	1:A:204:THR:HB	2.29	0.62
1:A:1433:MET:HE2	2:B:1145:SER:OG	1.99	0.62
1:A:1445:ILE:CG1	7:G:67:SER:C	2.67	0.62
16:P:392:ARG:O	16:P:476:ILE:N	2.32	0.62
25:Y:229:ASP:CB	25:Y:452:ARG:O	2.47	0.62
26:Z:476:PHE:HZ	26:Z:493:VAL:CG1	2.12	0.62
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.81	0.62
1:A:1443:VAL:CB	7:G:61:ILE:CG2	2.77	0.62
16:P:229:LEU:O	16:P:234:GLU:CB	2.46	0.62
22:V:132:GLU:O	22:V:135:ILE:HG22	1.99	0.62
22:V:145:ARG:NH1	22:V:146:LYS:HE3	2.14	0.62
25:Y:518:ILE:HG23	25:Y:522:TYR:CZ	2.32	0.62
26:Z:408:ILE:HG21	26:Z:475:ASP:C	2.19	0.62
1:A:867:ILE:HD11	1:A:1000:LEU:HD11	1.80	0.62
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.82	0.62
6:F:132:LEU:HD22	7:G:66:GLY:O	2.00	0.62
20:T:61:ASP:O	20:T:62:ARG:HG2	1.99	0.62
20:T:104:SER:HB3	22:V:136:LYS:HZ1	1.65	0.62
25:Y:32:LEU:HD12	25:Y:57:ILE:HD11	1.80	0.62
26:Z:449:GLU:HB2	26:Z:452:LEU:HA	1.81	0.62
26:Z:499:ARG:HG3	26:Z:530:LEU:HD12	1.80	0.62
1:A:416:ARG:NH2	3:C:40:GLU:HG2	39.86	0.62
16:P:218:SER:O	16:P:221:ALA:HB3	1.98	0.62
18:R:32:ARG:HG2	18:R:33:ASP:H	1.65	0.62
21:U:132:GLU:HB3	21:U:139:ILE:CD1	2.25	0.62
25:Y:357:LYS:CG	25:Y:376:PHE:HB2	2.29	0.62
25:Y:497:ILE:HG13	25:Y:686:PHE:HZ	1.62	0.62
26:Z:397:ILE:HD11	26:Z:423:GLN:HE21	1.64	0.62
26:Z:491:HIS:O	26:Z:494:PRO:HD2	1.99	0.62
26:Z:680:ARG:NH1	26:Z:683:GLU:OE2	2.32	0.62
21:U:172:GLU:O	21:U:176:MET:HG3	1.98	0.62
22:V:112:LYS:HD2	22:V:119:PRO:CG	2.29	0.62
22:V:135:ILE:HD13	22:V:139:VAL:HG23	1.82	0.62
22:V:99:LYS:HD2	22:V:99:LYS:C	2.19	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:28:ILE:HG21	25:Y:57:ILE:CG2	2.24	0.62
25:Y:128:VAL:N	25:Y:376:PHE:CE2	2.67	0.62
25:Y:467:ASP:C	25:Y:470:PRO:CG	2.68	0.62
26:Z:326:VAL:HG12	26:Z:503:SER:O	1.99	0.62
26:Z:407:VAL:HG22	26:Z:451:GLY:HA2	1.82	0.62
26:Z:436:ALA:CB	26:Z:452:LEU:HD21	2.29	0.62
2:B:1220:ARG:O	4:D:14:ARG:NH2	2.32	0.62
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.99	0.62
17:Q:83:LYS:HG3	17:Q:84:PRO:HD2	1.80	0.62
18:R:200:LEU:O	18:R:200:LEU:HD22	2.00	0.62
25:Y:346:MET:HB3	25:Y:384:LEU:CD2	2.28	0.62
26:Z:296:VAL:HA	26:Z:309:ASP:HB2	1.81	0.62
26:Z:459:MET:HB2	26:Z:464:ARG:NE	2.14	0.62
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.82	0.62
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.81	0.62
20:T:43:TYR:OH	22:V:105:ILE:HG23	2.00	0.62
20:T:55:LYS:HE3	20:T:62:ARG:HH21	1.64	0.62
25:Y:71:TYR:CZ	25:Y:233:ILE:HG21	2.32	0.62
25:Y:352:ILE:HB	25:Y:380:ARG:HH11	1.51	0.62
26:Z:377:GLY:HA2	26:Z:381:SER:HB2	1.82	0.62
26:Z:428:CYS:HB3	26:Z:432:PRO:HB2	1.82	0.62
26:Z:603:ASP:HB3	26:Z:669:CYS:SG	2.40	0.62
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.82	0.62
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.81	0.62
13:M:126:TRP:O	13:M:137:SER:N	2.32	0.62
16:P:229:LEU:CB	16:P:250:LYS:CB	2.78	0.62
25:Y:42:MET:HG3	25:Y:50:VAL:CG2	2.30	0.62
26:Z:345:ASN:ND2	26:Z:348:ARG:HE	1.97	0.62
26:Z:348:ARG:C	26:Z:350:PRO:HD3	2.21	0.62
1:A:11:LEU:CD1	2:B:1195:HIS:CD2	2.82	0.61
1:A:317:LYS:C	2:B:471:LYS:HZ2	1.97	0.61
2:B:563:MET:HE2	2:B:580:VAL:HB	1.80	0.61
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.82	0.61
13:M:127:VAL:HA	13:M:136:ASN:HA	1.81	0.61
16:P:631:LEU:HA	16:P:648:LYS:HA	1.82	0.61
16:P:629:PRO:HA	16:P:650:SER:HA	1.82	0.61
20:T:60:VAL:HG22	20:T:61:ASP:N	2.15	0.61
22:V:82:ASN:C	22:V:83:LEU:HD12	2.21	0.61
25:Y:533:THR:HG22	25:Y:533:THR:O	2.00	0.61
25:Y:678:VAL:HG11	25:Y:708:LEU:CG	2.26	0.61
25:Y:58:ALA:HB1	25:Y:69:ILE:HD12	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:447:GLN:C	26:Z:452:LEU:HB3	2.21	0.61
26:Z:458:SER:N	26:Z:465:ASN:HB2	2.15	0.61
26:Z:501:VAL:O	26:Z:505:ILE:HG13	2.00	0.61
1:A:53:LEU:HD23	1:A:54:ASN:N	2.15	0.61
17:Q:5:LEU:HA	17:Q:181:SER:O	1.99	0.61
22:V:117:LYS:HE3	22:V:121:GLU:CB	2.29	0.61
25:Y:523:GLY:O	25:Y:527:VAL:HG23	2.00	0.61
25:Y:641:PHE:O	25:Y:645:ASN:ND2	2.32	0.61
26:Z:476:PHE:HA	26:Z:485:ILE:CG2	2.30	0.61
1:A:66:LYS:HE2	1:A:68:GLN:H	1.65	0.61
14:N:158:TRP:O	14:N:161:THR:N	2.33	0.61
16:P:380:ASP:O	16:P:381:PHE:C	2.37	0.61
23:W:70:THR:O	23:W:73:ILE:HG22	2.01	0.61
25:Y:167:VAL:CG1	25:Y:195:ILE:HG23	2.30	0.61
25:Y:190:LEU:CD1	25:Y:195:ILE:HD11	2.22	0.61
25:Y:586:TYR:CB	25:Y:598:LEU:HD11	2.30	0.61
25:Y:63:TYR:HB3	25:Y:64:PRO:HD3	1.82	0.61
26:Z:378:ARG:H	26:Z:381:SER:H	1.45	0.61
26:Z:470:SER:O	26:Z:478:THR:HG23	2.00	0.61
1:A:1445:ILE:CA	7:G:68:ALA:HB2	2.23	0.61
25:Y:193:TYR:HH	25:Y:221:ARG:NH2	1.94	0.61
25:Y:124:ARG:HH22	25:Y:381:LEU:HD23	1.54	0.61
26:Z:752:SER:HB2	26:Z:753:PRO:HD2	1.82	0.61
25:Y:124:ARG:CG	25:Y:376:PHE:O	2.47	0.61
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.83	0.61
16:P:425:ILE:O	16:P:429:ILE:N	2.33	0.61
17:Q:97:LYS:NZ	17:Q:244:SER:O	2.33	0.61
21:U:175:ILE:CG1	23:W:94:ILE:HG22	2.29	0.61
22:V:83:LEU:O	22:V:84:SER:HB2	2.01	0.61
21:U:158:ILE:HG21	23:W:12:LEU:HD11	1.81	0.61
25:Y:71:TYR:CD2	25:Y:233:ILE:HD12	2.35	0.61
1:A:95:PHE:HE1	1:A:1414:ALA:HB2	1.66	0.61
2:B:249:ARG:HH12	2:B:418:LYS:HD2	1.66	0.61
5:E:202:SER:HB3	5:E:205:SER:H	1.66	0.61
20:T:94:TYR:HE2	20:T:98:GLN:NE2	1.99	0.61
23:W:25:TYR:CZ	23:W:58:THR:HG21	2.36	0.61
25:Y:103:PHE:CZ	25:Y:105:GLY:HA3	2.36	0.61
25:Y:349:LEU:HD12	25:Y:380:ARG:CZ	2.28	0.61
25:Y:586:TYR:CE2	25:Y:598:LEU:CD1	2.83	0.61
25:Y:639:LEU:HD23	25:Y:649:ARG:CD	2.25	0.61
26:Z:484:PHE:CE1	26:Z:486:ILE:HG12	2.36	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:PRO:O	1:A:449:SER:HB2	2.01	0.61
2:B:486:TYR:HB3	2:B:1096:ARG:CZ	2.31	0.61
25:Y:288:LYS:NZ	25:Y:336:LYS:N	2.49	0.61
22:V:145:ARG:CG	22:V:149:ARG:NE	2.64	0.61
20:T:121:CYS:SG	23:W:130:VAL:HG22	2.40	0.61
25:Y:109:THR:HB	25:Y:114:LEU:CD1	2.31	0.61
25:Y:357:LYS:CE	25:Y:376:PHE:HE1	2.08	0.61
25:Y:479:LEU:C	25:Y:479:LEU:HD22	2.21	0.61
26:Z:368:LYS:CE	26:Z:372:LYS:HE2	2.31	0.61
26:Z:452:LEU:HD23	26:Z:452:LEU:C	2.21	0.61
2:B:841:MET:HB3	2:B:846:ILE:HD11	1.81	0.61
13:M:176:SER:CB	19:S:48:LEU:CB	2.79	0.61
22:V:133:LEU:HD23	22:V:136:LYS:CE	2.31	0.61
22:V:66:ILE:N	22:V:67:PRO:CD	2.63	0.61
25:Y:570:LEU:HD12	25:Y:600:SER:HB2	1.81	0.61
26:Z:424:PHE:HE1	26:Z:450:SER:HB3	1.63	0.61
26:Z:446:PHE:O	26:Z:453:VAL:HG23	2.00	0.61
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.83	0.60
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.60
18:R:43:ARG:CZ	18:R:117:MET:CE	2.79	0.60
24:X:21:THR:HG22	24:X:23:PHE:H	1.66	0.60
25:Y:251:ASP:CB	25:Y:436:ARG:CZ	2.75	0.60
25:Y:232:VAL:HG22	25:Y:453:PHE:CE2	2.33	0.60
25:Y:532:ILE:HD12	25:Y:705:ASP:CB	2.20	0.60
26:Z:619:ALA:CA	26:Z:622:MET:HE2	2.31	0.60
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.83	0.60
20:T:106:GLU:O	20:T:109:SER:HB3	2.00	0.60
20:T:117:ILE:HD11	22:V:147:LEU:CD1	2.31	0.60
20:T:39:LYS:CG	20:T:43:TYR:HE1	2.14	0.60
25:Y:190:LEU:HB2	25:Y:195:ILE:HD11	1.83	0.60
25:Y:171:LEU:HD11	25:Y:195:ILE:HG22	1.83	0.60
25:Y:493:LEU:CB	25:Y:696:TRP:CD1	2.84	0.60
26:Z:356:LEU:HD21	26:Z:448:THR:HB	1.83	0.60
26:Z:375:GLY:HA3	26:Z:380:ARG:HG2	1.82	0.60
26:Z:487:LEU:HD13	26:Z:511:LEU:O	2.01	0.60
26:Z:485:ILE:HD13	26:Z:505:ILE:CD1	2.30	0.60
1:A:1436:ILE:C	1:A:1436:ILE:HD12	2.20	0.60
16:P:408:GLU:CB	16:P:498:ASP:N	2.63	0.60
17:Q:98:ILE:HD11	17:Q:218:ILE:HD11	1.83	0.60
20:T:80:LEU:HD21	22:V:73:LEU:HD11	1.83	0.60
22:V:122:TRP:O	22:V:125:ILE:HG22	2.01	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:71:TYR:HD2	25:Y:233:ILE:HD12	1.66	0.60
26:Z:478:THR:HG22	26:Z:479:GLY:N	2.16	0.60
2:B:1221:SER:CB	4:D:14:ARG:CZ	2.80	0.60
16:P:469:LEU:O	16:P:472:GLU:HA	2.02	0.60
25:Y:111:ARG:HD3	25:Y:129:VAL:HG21	1.83	0.60
25:Y:176:PHE:N	25:Y:176:PHE:CD1	2.68	0.60
25:Y:253:THR:CA	25:Y:434:ILE:HG23	2.31	0.60
26:Z:522:ASP:C	26:Z:524:ILE:HD13	2.22	0.60
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.82	0.60
17:Q:106:ARG:NH2	17:Q:214:GLN:CG	2.61	0.60
22:V:112:LYS:CG	22:V:119:PRO:HD3	2.17	0.60
22:V:134:GLN:O	22:V:137:ARG:HG3	2.01	0.60
26:Z:370:LEU:HD11	26:Z:398:THR:HG21	1.83	0.60
1:A:839:ARG:NH2	1:A:1401:SER:O	2.35	0.60
16:P:408:GLU:CB	16:P:497:ASN:CB	2.79	0.60
25:Y:354:GLU:C	25:Y:356:PRO:HD2	2.21	0.60
25:Y:566:HIS:O	25:Y:567:LYS:CG	2.49	0.60
25:Y:90:MET:HE1	25:Y:175:VAL:HG23	1.82	0.60
26:Z:753:PRO:HD2	26:Z:754:ARG:H	1.67	0.60
2:B:110:HIS:CE1	12:L:54:ARG:HH12	2.20	0.60
2:B:205:ILE:HD11	2:B:461:LEU:HD13	1.82	0.60
18:R:40:ARG:HD3	18:R:118:GLN:NE2	2.17	0.60
20:T:126:LYS:HZ2	23:W:133:ILE:HG22	1.66	0.60
20:T:45:ASP:CG	20:T:76:THR:HG23	2.22	0.60
21:U:169:GLN:HG2	23:W:5:LEU:HB3	1.84	0.60
22:V:140:LEU:HA	22:V:143:LEU:CD2	2.30	0.60
22:V:86:GLN:HG2	22:V:90:LEU:HD13	1.84	0.60
25:Y:358:SER:O	25:Y:362:HIS:CD2	2.54	0.60
25:Y:386:ARG:O	25:Y:390:VAL:CG2	2.40	0.60
26:Z:356:LEU:CD2	26:Z:448:THR:HG21	2.32	0.60
26:Z:484:PHE:CD2	26:Z:509:ALA:HB3	2.36	0.60
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.83	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.83	0.60
17:Q:16:TYR:CE2	17:Q:87:PHE:HA	2.37	0.60
18:R:4:SER:HB2	18:R:200:LEU:CG	2.31	0.60
22:V:76:ILE:CD1	22:V:97:ARG:HD2	2.32	0.60
22:V:99:LYS:HZ2	22:V:100:LEU:N	1.99	0.60
25:Y:467:ASP:C	25:Y:470:PRO:CD	2.70	0.60
1:A:1454:MET:HG2	7:G:20:PRO:HD3	1.82	0.60
1:A:72:GLU:HB3	1:A:76:GLU:HB3	1.83	0.60
2:B:976:ILE:O	2:B:990:ILE:HB	2.02	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:100:ILE:HG13	20:T:101:ASP:N	2.17	0.60
25:Y:200:ILE:CA	25:Y:226:VAL:HG23	2.16	0.60
25:Y:467:ASP:CA	25:Y:470:PRO:CG	2.79	0.60
1:A:1387:HIS:O	1:A:1391:ARG:HG2	2.02	0.60
1:A:68:GLN:O	1:A:70:CYS:N	2.31	0.60
2:B:902:GLY:O	12:L:65:VAL:HG12	2.01	0.60
16:P:478:LEU:CB	16:P:483:ASP:HA	2.31	0.60
22:V:114:LEU:HD12	22:V:114:LEU:N	2.17	0.60
22:V:122:TRP:CH2	22:V:123:GLN:HG3	2.37	0.60
21:U:158:ILE:HG21	23:W:12:LEU:CD1	2.32	0.60
25:Y:237:ALA:HA	25:Y:240:ILE:HG12	1.83	0.60
25:Y:242:ASN:HD21	25:Y:660:ARG:HH22	1.49	0.60
25:Y:263:GLY:O	25:Y:267:LEU:HG	2.02	0.60
25:Y:586:TYR:CE2	25:Y:598:LEU:HG	2.37	0.60
26:Z:356:LEU:HD22	26:Z:356:LEU:N	2.16	0.60
1:A:132:LYS:NZ	1:A:1415:SER:CB	2.64	0.59
1:A:1390:ASN:O	1:A:1399:ARG:HG2	2.01	0.59
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.36	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.02	0.59
6:F:96:THR:OG1	7:G:64:THR:HA	2.02	0.59
8:H:82:PRO:C	8:H:84:ALA:H	2.05	0.59
17:Q:55:ARG:O	17:Q:57:GLN:HG3	2.02	0.59
21:U:73:ASN:HD22	21:U:75:GLN:NE2	2.00	0.59
22:V:107:GLU:O	22:V:107:GLU:HG3	2.01	0.59
25:Y:185:CYS:SG	25:Y:190:LEU:CD1	2.90	0.59
25:Y:28:ILE:CG2	25:Y:57:ILE:HD12	2.27	0.59
25:Y:330:HIS:O	25:Y:334:PHE:HD1	1.84	0.59
25:Y:466:LEU:HG	25:Y:479:LEU:CB	2.32	0.59
26:Z:698:ASP:O	26:Z:699:GLU:CG	2.47	0.59
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.59
22:V:112:LYS:HZ3	22:V:119:PRO:HG3	1.66	0.59
25:Y:639:LEU:CD1	25:Y:653:PHE:HZ	2.12	0.59
26:Z:424:PHE:O	26:Z:427:TRP:HE3	1.84	0.59
1:A:89:PRO:HB2	1:A:204:THR:HG21	1.83	0.59
2:B:104:GLU:OE2	12:L:54:ARG:CD	2.50	0.59
3:C:184:ASN:HD21	3:C:189:THR:H	1.50	0.59
6:F:96:THR:CG2	7:G:66:GLY:HA2	2.33	0.59
6:F:92:ARG:CZ	7:G:64:THR:N	2.65	0.59
12:L:43:THR:O	12:L:43:THR:HG22	2.03	0.59
17:Q:97:LYS:HG2	17:Q:243:ASN:HD22	1.67	0.59
25:Y:518:ILE:HG22	25:Y:522:TYR:CD2	2.22	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:373:MET:CA	26:Z:381:SER:HA	2.32	0.59
1:A:368:LYS:HE2	1:A:399:HIS:CB	2.18	0.59
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.34	0.59
6:F:92:ARG:NE	7:G:63:PRO:C	2.56	0.59
13:M:135:ASN:HA	13:M:156:ILE:HA	1.85	0.59
17:Q:167:GLN:NE2	18:R:96:SER:O	2.36	0.59
17:Q:50:GLU:CD	17:Q:50:GLU:H	2.06	0.59
25:Y:218:ILE:HD11	25:Y:221:ARG:HH21	1.68	0.59
25:Y:327:ARG:HB2	25:Y:330:HIS:HD1	1.65	0.59
25:Y:293:LEU:HD12	25:Y:433:PRO:HB2	1.83	0.59
1:A:1436:ILE:HD11	2:B:1144:ALA:CB	2.32	0.59
17:Q:108:ILE:O	17:Q:109:LEU:HB3	2.02	0.59
20:T:111:THR:HG23	20:T:112:ARG:N	2.17	0.59
20:T:39:LYS:NZ	22:V:115:LEU:HA	2.16	0.59
21:U:171:ARG:HD2	23:W:90:GLN:OE1	2.03	0.59
25:Y:253:THR:HG21	25:Y:434:ILE:HD13	1.82	0.59
25:Y:331:PHE:HB2	25:Y:435:MET:HE1	1.85	0.59
25:Y:42:MET:CG	25:Y:50:VAL:CG2	2.72	0.59
26:Z:352:LEU:H	26:Z:352:LEU:HD22	1.67	0.59
26:Z:475:ASP:CB	26:Z:478:THR:H	2.15	0.59
26:Z:385:VAL:HA	26:Z:514:THR:O	2.03	0.59
12:L:60:ARG:HG2	12:L:61:THR:H	1.67	0.59
18:R:43:ARG:HH21	18:R:117:MET:HE3	1.67	0.59
25:Y:124:ARG:CG	25:Y:377:CYS:HA	2.31	0.59
26:Z:370:LEU:CD1	26:Z:398:THR:HG21	2.32	0.59
26:Z:425:LEU:HA	26:Z:429:THR:HA	1.83	0.59
3:C:47:ASP:HA	12:L:69:ALA:CB	2.33	0.59
17:Q:97:LYS:CB	17:Q:243:ASN:HB2	2.32	0.59
18:R:47:LYS:HD2	18:R:48:ASN:N	2.18	0.59
23:W:100:LYS:O	23:W:104:VAL:HG23	2.03	0.59
25:Y:293:LEU:CD1	25:Y:433:PRO:CA	2.81	0.59
26:Z:347:HIS:HD2	26:Z:348:ARG:HG3	1.67	0.59
26:Z:394:LEU:HD12	26:Z:394:LEU:N	2.17	0.59
26:Z:410:LEU:CB	26:Z:466:ARG:HH22	2.07	0.59
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.84	0.59
6:F:133:VAL:O	7:G:61:ILE:HB	2.03	0.59
17:Q:228:LEU:HD21	17:Q:278:LEU:HD22	1.83	0.59
22:V:83:LEU:HD12	22:V:83:LEU:N	2.18	0.59
25:Y:193:TYR:CE2	25:Y:197:ARG:HD3	2.35	0.59
25:Y:353:SER:HB2	25:Y:381:LEU:CA	2.24	0.59
25:Y:468:MET:C	25:Y:470:PRO:HD2	2.23	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:376:ASN:HB3	26:Z:380:ARG:N	2.12	0.59
26:Z:386:LEU:HB3	26:Z:390:ALA:CB	2.32	0.59
26:Z:427:TRP:HB2	26:Z:449:GLU:OE2	2.01	0.59
13:M:126:TRP:N	13:M:137:SER:O	2.33	0.59
13:M:11:TRP:CB	13:M:32:ALA:HA	2.32	0.59
18:R:49:LEU:HD11	18:R:53:VAL:HB	1.84	0.59
22:V:122:TRP:CZ3	22:V:123:GLN:HG3	2.37	0.59
25:Y:135:ARG:NH2	25:Y:143:ARG:HH21	2.00	0.59
25:Y:269:GLU:O	25:Y:269:GLU:HG2	2.02	0.59
25:Y:352:ILE:HG12	25:Y:380:ARG:NH2	2.18	0.59
25:Y:493:LEU:HD21	25:Y:666:LEU:CG	2.29	0.59
26:Z:326:VAL:HG12	26:Z:327:LYS:N	2.18	0.59
26:Z:354:ILE:O	26:Z:356:LEU:HD22	2.03	0.59
26:Z:397:ILE:HG12	26:Z:427:TRP:HH2	1.67	0.59
1:A:412:ARG:HB3	3:C:51:VAL:HG11	45.10	0.59
1:A:344:ARG:CD	2:B:1118:PRO:O	2.47	0.59
1:A:22:PHE:CB	2:B:1211:ASN:OD1	2.50	0.59
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.38	0.59
25:Y:124:ARG:HG2	25:Y:377:CYS:CB	2.33	0.59
25:Y:232:VAL:O	25:Y:457:ILE:HB	2.02	0.59
25:Y:348:VAL:C	25:Y:380:ARG:NH2	2.49	0.59
25:Y:353:SER:HB2	25:Y:381:LEU:N	2.17	0.59
25:Y:567:LYS:HG2	25:Y:597:ILE:CG2	2.33	0.59
25:Y:571:VAL:CG1	25:Y:572:GLU:HG3	2.33	0.59
25:Y:586:TYR:CE1	25:Y:616:TYR:CZ	2.91	0.59
25:Y:639:LEU:CD2	25:Y:649:ARG:CB	2.78	0.59
26:Z:327:LYS:HG3	26:Z:506:ALA:CA	2.33	0.59
26:Z:373:MET:HE2	26:Z:384:ILE:CD1	2.33	0.59
26:Z:408:ILE:CG2	26:Z:475:ASP:HA	2.33	0.59
26:Z:585:PRO:C	26:Z:756:ARG:HH22	2.05	0.59
1:A:483:ASP:HB2	2:B:987:LYS:HE3	1.84	0.58
22:V:125:ILE:O	22:V:129:ARG:HG2	2.02	0.58
25:Y:289:LEU:HD21	25:Y:435:MET:SD	2.38	0.58
25:Y:479:LEU:CD2	25:Y:479:LEU:C	2.72	0.58
25:Y:586:TYR:CG	25:Y:598:LEU:CD1	2.69	0.58
25:Y:639:LEU:HD21	25:Y:649:ARG:HD2	0.61	0.58
26:Z:505:ILE:HD12	26:Z:510:LYS:NZ	2.18	0.58
6:F:97:ARG:HH12	7:G:15:PRO:HB2	1.68	0.58
18:R:47:LYS:NZ	18:R:47:LYS:H	2.00	0.58
1:A:857:ARG:HD3	1:A:861:GLY:O	2.03	0.58
2:B:846:ILE:CG2	2:B:974:PRO:HD2	2.32	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:950:ASP:HB3	2:B:967:ARG:HG2	1.84	0.58
5:E:4:GLU:HB3	5:E:7:ARG:NE	2.16	0.58
18:R:135:LEU:HD22	18:R:166:LYS:HB3	1.85	0.58
25:Y:124:ARG:HB2	25:Y:377:CYS:SG	2.43	0.58
25:Y:495:MET:CB	25:Y:686:PHE:CD2	2.75	0.58
26:Z:408:ILE:HG23	26:Z:408:ILE:O	2.03	0.58
26:Z:476:PHE:HD2	26:Z:477:LEU:HD12	1.67	0.58
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.36	0.58
18:R:4:SER:OG	18:R:200:LEU:CB	2.51	0.58
22:V:112:LYS:HA	22:V:117:LYS:O	2.02	0.58
22:V:113:ASP:O	22:V:114:LEU:HB2	2.03	0.58
25:Y:110:SER:HB3	25:Y:212:TYR:CE1	2.38	0.58
25:Y:244:CYS:HB3	25:Y:442:ALA:CB	2.22	0.58
25:Y:337:ARG:CZ	25:Y:345:ARG:NE	2.57	0.58
25:Y:353:SER:N	25:Y:380:ARG:NH1	2.45	0.58
2:B:65:GLU:OE1	2:B:247:GLY:HA2	2.04	0.58
20:T:114:ILE:O	20:T:117:ILE:HG12	2.02	0.58
22:V:146:LYS:HD3	23:W:129:PHE:HE1	1.52	0.58
25:Y:458:ILE:HD13	25:Y:469:TYR:CE2	2.38	0.58
25:Y:570:LEU:HD11	25:Y:606:VAL:HG21	1.85	0.58
26:Z:400:ALA:HB3	26:Z:450:SER:HA	1.86	0.58
1:A:1444:MET:HG3	7:G:61:ILE:O	1.99	0.58
2:B:110:HIS:NE2	12:L:54:ARG:NH2	2.52	0.58
2:B:363:HIS:O	2:B:364:ILE:HB	2.02	0.58
17:Q:27:SER:HB3	17:Q:224:MET:HE2	1.85	0.58
18:R:54:SER:HG	18:R:74:ASP:CG	2.05	0.58
20:T:55:LYS:HE3	20:T:62:ARG:HE	1.68	0.58
22:V:117:LYS:HZ3	22:V:121:GLU:HG2	1.60	0.58
25:Y:353:SER:OG	25:Y:381:LEU:HB2	2.03	0.58
25:Y:469:TYR:N	25:Y:470:PRO:CD	2.66	0.58
25:Y:87:GLU:O	25:Y:90:MET:HB3	2.04	0.58
26:Z:477:LEU:O	26:Z:501:VAL:HA	2.04	0.58
16:P:191:ILE:C	16:P:193:THR:H	2.06	0.58
23:W:74:ASN:O	23:W:77:ILE:N	2.36	0.58
21:U:168:HIS:CE1	23:W:82:GLY:O	2.55	0.58
25:Y:203:CYS:SG	25:Y:226:VAL:CG2	2.91	0.58
25:Y:499:LYS:HZ1	25:Y:525:MET:HB2	1.65	0.58
25:Y:541:PHE:HE1	25:Y:599:LEU:HD22	1.68	0.58
1:A:836:TYR:CE1	1:A:1403:GLU:OE2	2.57	0.58
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.58
16:P:363:SER:HA	16:P:423:LYS:H	1.69	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:85:LEU:HD12	17:Q:88:ARG:CB	2.29	0.58
25:Y:190:LEU:CD1	25:Y:195:ILE:HD12	2.20	0.58
25:Y:336:LYS:O	25:Y:336:LYS:HG3	2.03	0.58
25:Y:447:LYS:N	25:Y:448:PRO:CD	2.67	0.58
25:Y:450:PHE:CZ	25:Y:475:PHE:HA	2.25	0.58
25:Y:42:MET:SD	25:Y:50:VAL:HA	2.44	0.58
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.85	0.58
20:T:39:LYS:O	20:T:43:TYR:HD1	1.87	0.58
25:Y:492:PHE:CD2	25:Y:494:PRO:HG3	2.39	0.58
25:Y:639:LEU:HD11	25:Y:653:PHE:CZ	2.35	0.58
25:Y:62:HIS:CD2	25:Y:69:ILE:HD11	2.39	0.58
26:Z:378:ARG:N	26:Z:381:SER:HB3	2.18	0.58
26:Z:373:MET:HG3	26:Z:381:SER:OG	2.04	0.58
26:Z:436:ALA:HB3	26:Z:452:LEU:CD2	2.34	0.58
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.85	0.58
6:F:106:PRO:HG2	7:G:16:SER:O	1.87	0.58
1:A:1443:VAL:H	7:G:63:PRO:HG3	0.76	0.58
12:L:27:LEU:O	12:L:28:LYS:HG2	2.03	0.58
16:P:315:SER:HA	16:P:426:ARG:CB	2.34	0.58
17:Q:97:LYS:HZ3	17:Q:244:SER:C	2.06	0.58
20:T:79:ALA:O	20:T:82:GLU:HG2	2.03	0.58
21:U:73:ASN:HB2	21:U:75:GLN:CG	2.33	0.58
22:V:112:LYS:O	22:V:113:ASP:HB3	2.03	0.58
26:Z:336:PRO:HB3	26:Z:341:TYR:HB3	1.85	0.58
26:Z:333:ILE:HD11	26:Z:343:PHE:CZ	2.39	0.58
26:Z:352:LEU:HD22	26:Z:352:LEU:N	2.18	0.58
26:Z:757:ARG:O	26:Z:761:GLN:HG2	2.03	0.58
20:T:121:CYS:SG	23:W:130:VAL:HG13	2.43	0.57
21:U:159:HIS:O	21:U:163:ASN:HB2	2.04	0.57
22:V:112:LYS:NZ	22:V:119:PRO:HG3	2.19	0.57
25:Y:586:TYR:CE2	25:Y:598:LEU:HD12	2.39	0.57
26:Z:303:ARG:HD3	26:Z:504:THR:HG22	1.86	0.57
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.52	0.57
12:L:53:HIS:O	12:L:55:ILE:HG12	2.04	0.57
16:P:593:ASP:CB	16:P:600:ASN:CB	2.82	0.57
17:Q:106:ARG:CZ	17:Q:214:GLN:OE1	2.49	0.57
20:T:63:PHE:N	20:T:66:ASN:HD21	2.02	0.57
20:T:90:TYR:C	22:V:111:THR:HB	2.24	0.57
22:V:135:ILE:O	22:V:135:ILE:HD13	2.04	0.57
25:Y:167:VAL:HG11	25:Y:195:ILE:HG23	1.86	0.57
25:Y:21:GLN:HA	25:Y:53:LEU:HD21	1.85	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:499:LYS:HZ3	25:Y:525:MET:HB2	1.68	0.57
25:Y:632:SER:OG	25:Y:635:LEU:HB3	2.03	0.57
25:Y:418:LEU:HD22	25:Y:633:ARG:HG3	1.84	0.57
26:Z:328:LYS:HD3	26:Z:530:LEU:HD23	1.84	0.57
26:Z:405:LYS:HD3	26:Z:483:GLY:C	2.24	0.57
26:Z:476:PHE:CZ	26:Z:502:VAL:HG22	2.40	0.57
8:H:46:LEU:O	8:H:46:LEU:HD13	3.80	0.57
17:Q:97:LYS:CG	17:Q:243:ASN:HD22	2.16	0.57
18:R:199:ASP:O	18:R:202:TYR:HB3	2.03	0.57
20:T:107:LEU:HD23	20:T:107:LEU:N	2.19	0.57
25:Y:167:VAL:HG11	25:Y:195:ILE:CG2	2.33	0.57
25:Y:18:TYR:CB	25:Y:19:PRO:CD	2.82	0.57
25:Y:37:ASN:HB2	25:Y:456:VAL:CG1	2.32	0.57
1:A:1390:ASN:O	1:A:1399:ARG:HD3	2.04	0.57
1:A:1444:MET:HE3	6:F:135:ARG:NE	2.20	0.57
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.87	0.57
20:T:43:TYR:CE1	22:V:105:ILE:HD13	2.39	0.57
22:V:82:ASN:O	22:V:87:LEU:HA	2.03	0.57
26:Z:373:MET:HE2	26:Z:384:ILE:HD11	1.85	0.57
26:Z:411:CYS:O	26:Z:456:THR:HG23	2.04	0.57
26:Z:485:ILE:O	26:Z:485:ILE:HG13	2.03	0.57
1:A:1447:GLU:C	7:G:22:MET:SD	2.83	0.57
22:V:69:ILE:CG1	22:V:104:LEU:HB3	2.32	0.57
22:V:86:GLN:O	22:V:90:LEU:HD13	2.05	0.57
25:Y:207:ILE:HD12	25:Y:207:ILE:N	2.20	0.57
25:Y:376:PHE:CD1	25:Y:376:PHE:O	2.57	0.57
25:Y:419:ILE:HD13	25:Y:435:MET:HG2	1.87	0.57
25:Y:467:ASP:C	25:Y:470:PRO:HG2	2.23	0.57
26:Z:429:THR:N	26:Z:432:PRO:HG2	2.20	0.57
26:Z:421:ARG:CG	26:Z:430:LEU:HG	2.21	0.57
26:Z:484:PHE:HE1	26:Z:486:ILE:HG12	1.69	0.57
1:A:1063:MET:SD	1:A:1436:ILE:HG22	2.43	0.57
2:B:1215:ARG:NH1	4:D:15:LEU:HD11	2.19	0.57
17:Q:27:SER:HB2	17:Q:224:MET:HG2	1.86	0.57
18:R:4:SER:HB2	18:R:200:LEU:HG	1.84	0.57
21:U:165:TYR:CE2	23:W:80:LEU:HD21	2.39	0.57
25:Y:253:THR:CG2	25:Y:434:ILE:HG21	2.28	0.57
25:Y:515:ASP:CB	25:Y:518:ILE:HD12	2.31	0.57
25:Y:550:ILE:HG23	25:Y:554:TRP:CZ2	2.08	0.57
25:Y:56:THR:CG2	25:Y:60:GLN:NE2	2.67	0.57
25:Y:648:ILE:HD12	25:Y:652:ASP:OD2	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:83:LEU:O	25:Y:87:GLU:HG3	2.05	0.57
26:Z:349:ASN:N	26:Z:350:PRO:HD3	2.19	0.57
26:Z:487:LEU:HD12	26:Z:487:LEU:N	2.20	0.57
1:A:1436:ILE:O	1:A:1437:GLY:C	2.43	0.57
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.85	0.57
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.70	0.57
2:B:810:GLU:HA	2:B:815:ARG:HH12	1.69	0.57
13:M:125:PHE:HA	13:M:138:GLY:HA2	1.87	0.57
13:M:192:ILE:C	16:P:192:GLU:HA	2.24	0.57
25:Y:350:HIS:ND1	25:Y:381:LEU:CD1	2.58	0.57
25:Y:418:LEU:HD13	25:Y:634:ILE:HG13	1.85	0.57
25:Y:293:LEU:CD2	25:Y:419:ILE:HG22	2.31	0.57
25:Y:541:PHE:CE1	25:Y:599:LEU:HD22	2.40	0.57
25:Y:462:THR:CG2	25:Y:660:ARG:HG3	2.35	0.57
25:Y:681:LEU:CD2	25:Y:696:TRP:CH2	2.87	0.57
26:Z:335:TYR:HB3	26:Z:336:PRO:HD3	1.86	0.57
26:Z:588:PHE:HZ	26:Z:621:LYS:HZ3	1.53	0.57
6:F:96:THR:CG2	7:G:66:GLY:N	2.66	0.57
17:Q:20:ILE:HG13	17:Q:87:PHE:CE2	2.34	0.57
17:Q:63:ARG:NH1	17:Q:299:ARG:O	2.38	0.57
20:T:64:LYS:HD2	20:T:64:LYS:H	1.70	0.57
25:Y:462:THR:HB	25:Y:664:GLN:OE1	2.04	0.57
25:Y:639:LEU:HD21	25:Y:649:ARG:HH11	1.70	0.57
26:Z:473:VAL:O	26:Z:473:VAL:HG23	2.05	0.57
26:Z:485:ILE:HD13	26:Z:505:ILE:HD13	1.87	0.57
1:A:5:GLN:HG3	2:B:1175:LEU:CD1	2.35	0.57
1:A:1445:ILE:C	7:G:68:ALA:HB2	2.24	0.57
16:P:630:ASN:N	16:P:649:PHE:O	2.38	0.57
17:Q:91:LYS:O	17:Q:94:THR:HG22	2.04	0.57
20:T:43:TYR:CD2	22:V:102:LYS:HD2	2.40	0.57
25:Y:466:LEU:HG	25:Y:479:LEU:HB2	1.85	0.57
26:Z:328:LYS:HD3	26:Z:530:LEU:HD22	1.84	0.57
26:Z:303:ARG:HD3	26:Z:504:THR:CG2	2.35	0.57
26:Z:516:THR:CA	26:Z:681:ARG:NE	2.44	0.57
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.85	0.57
4:D:7:THR:HG21	7:G:5:LYS:HZ1	1.69	0.57
20:T:46:LEU:HD11	20:T:80:LEU:HD11	1.86	0.57
21:U:195:VAL:O	21:U:199:VAL:HG23	2.04	0.57
21:U:74:GLN:HE21	21:U:77:ARG:CD	2.18	0.57
25:Y:208:TYR:CZ	25:Y:213:LEU:HG	2.40	0.57
26:Z:584:ASN:CG	26:Z:586:THR:HG22	2.24	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.87	0.56
4:D:167:LEU:HB3	4:D:177:VAL:HG22	1.87	0.56
2:B:104:GLU:OE2	12:L:54:ARG:HD3	2.05	0.56
25:Y:352:ILE:HG22	25:Y:380:ARG:HD3	1.87	0.56
25:Y:443:SER:CA	25:Y:473:LEU:HA	2.35	0.56
25:Y:639:LEU:HG	25:Y:653:PHE:CD2	2.34	0.56
26:Z:368:LYS:HD2	26:Z:372:LYS:CD	2.35	0.56
26:Z:476:PHE:CZ	26:Z:487:LEU:HD21	2.38	0.56
25:Y:131:GLU:CD	25:Y:134:ARG:NH1	2.52	0.56
25:Y:185:CYS:SG	25:Y:192:PRO:CG	2.93	0.56
25:Y:495:MET:CE	25:Y:696:TRP:HB3	2.35	0.56
26:Z:425:LEU:CA	26:Z:429:THR:HA	2.35	0.56
4:D:159:THR:O	4:D:163:VAL:HG23	2.05	0.56
1:A:1445:ILE:HG12	7:G:67:SER:C	2.26	0.56
17:Q:108:ILE:HG21	17:Q:159:GLU:CG	2.35	0.56
17:Q:97:LYS:CD	17:Q:243:ASN:HB3	1.99	0.56
20:T:63:PHE:HE1	20:T:66:ASN:H	1.53	0.56
22:V:86:GLN:OE1	22:V:90:LEU:HD13	2.05	0.56
20:T:118:LEU:HD12	23:W:130:VAL:C	2.25	0.56
25:Y:229:ASP:HB3	25:Y:452:ARG:O	2.05	0.56
26:Z:475:ASP:C	26:Z:485:ILE:HG22	2.25	0.56
2:B:1215:ARG:HD3	4:D:15:LEU:HD11	1.80	0.56
17:Q:106:ARG:CZ	17:Q:211:PHE:CE2	2.88	0.56
17:Q:97:LYS:HD3	17:Q:243:ASN:O	2.05	0.56
25:Y:142:LYS:HA	25:Y:145:LEU:HD23	1.83	0.56
25:Y:129:VAL:HG11	25:Y:194:PHE:HE1	1.71	0.56
25:Y:420:ILE:C	25:Y:422:PRO:HD2	2.22	0.56
25:Y:567:LYS:HE2	25:Y:597:ILE:CD1	2.32	0.56
25:Y:569:ILE:O	25:Y:571:VAL:HG23	2.05	0.56
26:Z:378:ARG:HH21	26:Z:508:HIS:CA	2.16	0.56
26:Z:466:ARG:C	26:Z:477:LEU:HD23	2.26	0.56
26:Z:493:VAL:HB	26:Z:494:PRO:HD3	1.87	0.56
13:M:140:GLY:N	13:M:151:GLN:O	2.39	0.56
20:T:60:VAL:HG22	20:T:61:ASP:H	1.69	0.56
25:Y:127:THR:HG21	25:Y:361:GLN:OE1	2.05	0.56
25:Y:354:GLU:N	25:Y:356:PRO:HD2	2.21	0.56
25:Y:433:PRO:HD2	25:Y:433:PRO:O	2.05	0.56
26:Z:473:VAL:HB	26:Z:481:GLU:CG	2.35	0.56
26:Z:553:GLN:HB2	26:Z:701:PHE:CG	2.39	0.56
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.56
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.87	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:96:THR:HG23	7:G:65:ASP:O	1.63	0.56
16:P:196:THR:CB	16:P:200:PHE:CB	2.84	0.56
20:T:94:TYR:CZ	22:V:109:GLU:HB3	2.39	0.56
25:Y:68:LYS:CD	25:Y:228:LYS:CG	2.22	0.56
25:Y:349:LEU:N	25:Y:380:ARG:HH22	2.00	0.56
25:Y:293:LEU:HD12	25:Y:433:PRO:HB3	1.84	0.56
25:Y:479:LEU:H	25:Y:479:LEU:HD13	1.70	0.56
25:Y:646:TYR:HB2	25:Y:648:ILE:CG1	2.29	0.56
26:Z:415:VAL:HG13	26:Z:416:SER:N	2.20	0.56
26:Z:372:LYS:HB3	26:Z:535:LEU:CD2	2.35	0.56
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.88	0.56
18:R:203:GLN:O	18:R:206:ARG:N	2.39	0.56
19:S:101:GLU:O	19:S:102:LYS:CB	2.54	0.56
22:V:100:LEU:HD11	22:V:104:LEU:HD11	1.88	0.56
25:Y:237:ALA:HB1	25:Y:458:ILE:CG2	2.31	0.56
25:Y:441:ASP:HB2	25:Y:641:PHE:CZ	2.41	0.56
26:Z:376:ASN:CB	26:Z:380:ARG:HD3	2.27	0.56
26:Z:446:PHE:HB3	26:Z:452:LEU:HD11	1.88	0.56
26:Z:750:TYR:HB3	26:Z:756:ARG:NH1	2.21	0.56
17:Q:85:LEU:HD11	17:Q:88:ARG:H	1.69	0.56
17:Q:75:LEU:O	17:Q:98:ILE:HG12	2.06	0.56
22:V:86:GLN:HG2	22:V:90:LEU:HD11	1.88	0.56
25:Y:440:LEU:CD1	25:Y:638:ARG:CG	2.83	0.56
25:Y:653:PHE:HD1	25:Y:654:LEU:N	2.02	0.56
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.88	0.56
6:F:92:ARG:HE	7:G:63:PRO:C	2.06	0.56
20:T:53:LEU:HD22	22:V:94:ILE:HG21	1.88	0.56
21:U:132:GLU:CB	21:U:139:ILE:HD12	2.30	0.56
22:V:135:ILE:HG23	22:V:136:LYS:N	2.21	0.56
25:Y:276:LYS:HG3	25:Y:337:ARG:NH2	2.20	0.56
25:Y:39:ILE:CG1	25:Y:458:ILE:HD12	2.35	0.56
26:Z:394:LEU:HD12	26:Z:394:LEU:H	1.69	0.56
1:A:1445:ILE:HG13	7:G:67:SER:C	2.23	0.56
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.88	0.56
22:V:132:GLU:C	22:V:136:LYS:HE2	2.25	0.56
25:Y:550:ILE:O	25:Y:554:TRP:NE1	2.39	0.56
26:Z:436:ALA:HB1	26:Z:444:GLU:HB2	1.88	0.56
1:A:257:ARG:HB2	1:A:257:ARG:HH11	1.71	0.56
1:A:49:LYS:CE	1:A:61:ILE:CD1	2.81	0.56
1:A:74:MET:O	2:B:1116:ARG:NH2	2.39	0.56
17:Q:75:LEU:O	17:Q:98:ILE:CG1	2.54	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:97:LEU:HA	20:T:100:ILE:CD1	2.36	0.56
25:Y:420:ILE:CG1	25:Y:633:ARG:HH22	1.96	0.56
26:Z:475:ASP:O	26:Z:505:ILE:HG12	2.06	0.56
1:A:1447:GLU:HA	7:G:22:MET:HE1	0.61	0.55
25:Y:232:VAL:O	25:Y:457:ILE:N	2.39	0.55
25:Y:499:LYS:CE	25:Y:525:MET:HB2	2.35	0.55
26:Z:415:VAL:HA	26:Z:418:MET:HE3	1.88	0.55
26:Z:466:ARG:HB3	26:Z:477:LEU:HB2	1.87	0.55
26:Z:524:ILE:HD13	26:Z:524:ILE:N	2.21	0.55
26:Z:717:TYR:CZ	26:Z:718:TYR:CD1	2.91	0.55
1:A:388:LEU:HA	1:A:391:LEU:HD12	1.88	0.55
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.89	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.55
6:F:118:LEU:O	6:F:122:MET:HG3	2.06	0.55
6:F:89:GLU:O	6:F:93:ILE:HD12	2.07	0.55
6:F:96:THR:HG22	7:G:66:GLY:HA2	1.89	0.55
2:B:326:ASP:CB	14:N:60:PRO:CA	145.87	0.55
20:T:90:TYR:O	22:V:111:THR:HB	2.06	0.55
22:V:132:GLU:O	22:V:136:LYS:HG3	2.05	0.55
25:Y:124:ARG:O	25:Y:376:PHE:CE2	2.59	0.55
26:Z:310:ILE:CG1	26:Z:313:VAL:HG23	2.36	0.55
26:Z:498:PHE:O	26:Z:501:VAL:HG22	2.05	0.55
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.87	0.55
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.88	0.55
25:Y:185:CYS:SG	25:Y:190:LEU:HD12	2.46	0.55
25:Y:293:LEU:CD2	25:Y:419:ILE:CG2	2.81	0.55
25:Y:330:HIS:O	25:Y:334:PHE:CD1	2.59	0.55
25:Y:293:LEU:HD11	25:Y:433:PRO:HB2	1.81	0.55
25:Y:253:THR:HA	25:Y:434:ILE:HG23	1.88	0.55
25:Y:39:ILE:HG12	25:Y:458:ILE:HD12	1.87	0.55
25:Y:57:ILE:HG23	25:Y:58:ALA:N	2.21	0.55
25:Y:67:ARG:HD2	25:Y:230:SER:CB	2.36	0.55
26:Z:344:ARG:HE	26:Z:344:ARG:HA	1.70	0.55
26:Z:455:SER:HB3	26:Z:466:ARG:CD	2.36	0.55
1:A:368:LYS:CE	1:A:399:HIS:HB2	2.19	0.55
1:A:67:CYS:SG	1:A:77:CYS:SG	3.04	0.55
1:A:345:VAL:N	2:B:1128:LEU:O	2.39	0.55
18:R:43:ARG:CB	18:R:119:ARG:HG3	2.23	0.55
20:T:126:LYS:NZ	23:W:133:ILE:HG22	2.20	0.55
21:U:182:LEU:HD11	23:W:104:VAL:HG21	1.87	0.55
25:Y:109:THR:O	25:Y:114:LEU:HD22	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:440:LEU:HD23	25:Y:641:PHE:HD2	1.61	0.55
25:Y:479:LEU:HD13	25:Y:479:LEU:N	2.21	0.55
25:Y:70:ILE:HD11	25:Y:232:VAL:HG22	1.87	0.55
1:A:1015:VAL:HG13	1:A:1019:CYS:SG	2.47	0.55
1:A:10:PRO:HG2	2:B:1192:TYR:HA	1.89	0.55
2:B:351:TYR:CE1	2:B:355:ILE:HD12	2.42	0.55
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.88	0.55
2:B:217:ARG:NH1	2:B:407:ASP:OD1	2.40	0.55
25:Y:109:THR:HB	25:Y:114:LEU:HD13	1.89	0.55
25:Y:129:VAL:CG1	25:Y:194:PHE:HE1	2.19	0.55
25:Y:586:TYR:CD1	25:Y:616:TYR:CZ	2.94	0.55
26:Z:314:HIS:HB3	26:Z:325:VAL:HG11	1.89	0.55
26:Z:333:ILE:HD11	26:Z:343:PHE:CE1	2.41	0.55
1:A:416:ARG:HH22	3:C:40:GLU:HG2	40.58	0.55
10:J:1:MET:HB2	10:J:56:LEU:HB2	1.89	0.55
17:Q:53:ASN:ND2	17:Q:57:GLN:HB2	2.22	0.55
20:T:97:LEU:CD2	22:V:125:ILE:HD13	2.37	0.55
22:V:143:LEU:C	22:V:143:LEU:HD12	2.27	0.55
25:Y:229:ASP:OD2	25:Y:452:ARG:O	2.23	0.55
25:Y:526:LEU:HD21	25:Y:554:TRP:CZ3	2.39	0.55
25:Y:497:ILE:CG1	25:Y:686:PHE:CZ	2.89	0.55
26:Z:370:LEU:O	26:Z:370:LEU:HD23	2.06	0.55
26:Z:499:ARG:CG	26:Z:530:LEU:HD12	2.37	0.55
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.87	0.55
6:F:132:LEU:CB	7:G:61:ILE:HD13	2.28	0.55
7:G:34:VAL:O	7:G:37:SER:HB3	2.06	0.55
7:G:61:ILE:O	7:G:63:PRO:HD3	2.06	0.55
16:P:393:ILE:O	16:P:408:GLU:N	2.37	0.55
25:Y:639:LEU:CB	25:Y:653:PHE:HD2	1.92	0.55
26:Z:365:TYR:CE2	26:Z:366:GLN:HG3	2.42	0.55
16:P:566:VAL:O	16:P:569:ILE:CB	2.54	0.55
17:Q:259:VAL:HG21	17:Q:268:ILE:CD1	2.37	0.55
22:V:86:GLN:CG	22:V:90:LEU:HD13	2.37	0.55
25:Y:67:ARG:HD2	25:Y:230:SER:HB2	1.89	0.55
26:Z:408:ILE:HG12	26:Z:466:ARG:NE	2.22	0.55
26:Z:428:CYS:HB3	26:Z:432:PRO:CB	2.36	0.55
2:B:815:ARG:HH11	2:B:815:ARG:HG3	1.72	0.55
8:H:46:LEU:HD13	8:H:46:LEU:C	3.74	0.55
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.70	0.55
13:M:188:LEU:C	13:M:190:ASP:H	2.10	0.55
17:Q:97:LYS:HE2	17:Q:243:ASN:HB3	0.59	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:111:THR:CA	22:V:143:LEU:HD22	2.27	0.55
23:W:91:LEU:O	23:W:94:ILE:HG12	2.07	0.55
25:Y:490:LYS:HD2	25:Y:676:TYR:CE1	2.42	0.55
26:Z:372:LYS:C	26:Z:535:LEU:HD23	2.26	0.55
1:A:1447:GLU:CD	7:G:70:PHE:CE2	2.79	0.55
1:A:204:THR:HG22	1:A:235:ILE:HG21	1.89	0.55
2:B:486:TYR:HB3	2:B:1096:ARG:NH2	2.22	0.55
1:A:1445:ILE:CD1	7:G:18:PHE:HZ	1.72	0.55
22:V:76:ILE:HD12	22:V:79:ASP:OD2	2.07	0.55
25:Y:293:LEU:HD11	25:Y:433:PRO:CA	2.37	0.55
25:Y:570:LEU:HD11	25:Y:606:VAL:CG2	2.36	0.55
25:Y:621:LEU:HG	25:Y:680:VAL:CG1	2.36	0.55
2:B:110:HIS:CE1	12:L:54:ARG:CZ	2.90	0.54
2:B:343:ILE:O	2:B:344:LYS:HB2	2.07	0.54
16:P:387:LYS:HA	16:P:484:ASP:O	2.08	0.54
17:Q:97:LYS:CE	17:Q:243:ASN:C	2.76	0.54
17:Q:81:MET:HG3	17:Q:88:ARG:NH2	2.22	0.54
18:R:62:PHE:HZ	18:R:201:ALA:CB	2.06	0.54
20:T:104:SER:CB	22:V:136:LYS:HZ1	2.20	0.54
21:U:128:LEU:O	21:U:131:LEU:N	2.39	0.54
22:V:100:LEU:HD13	22:V:100:LEU:C	2.26	0.54
22:V:69:ILE:CD1	22:V:108:ASN:HD21	2.15	0.54
25:Y:631:GLU:CA	25:Y:636:LYS:CE	2.48	0.54
26:Z:429:THR:HG22	26:Z:430:LEU:N	2.21	0.54
26:Z:753:PRO:CD	26:Z:754:ARG:H	2.20	0.54
7:G:111:THR:HG22	7:G:113:HIS:H	1.71	0.54
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.07	0.54
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.43	0.54
16:P:471:ASN:O	16:P:472:GLU:C	2.46	0.54
17:Q:86:ASN:HA	17:Q:89:ILE:CG1	2.23	0.54
17:Q:86:ASN:O	17:Q:90:LEU:HD13	2.08	0.54
21:U:199:VAL:O	21:U:203:LEU:HB2	2.08	0.54
25:Y:176:PHE:N	25:Y:176:PHE:HD1	2.05	0.54
25:Y:185:CYS:CB	25:Y:192:PRO:CG	2.81	0.54
25:Y:242:ASN:ND2	25:Y:660:ARG:HH22	2.05	0.54
25:Y:463:ILE:HD11	25:Y:469:TYR:CG	2.43	0.54
25:Y:515:ASP:HB2	25:Y:518:ILE:CG1	2.37	0.54
25:Y:70:ILE:O	25:Y:70:ILE:HG13	2.07	0.54
6:F:92:ARG:NH1	7:G:63:PRO:CB	2.65	0.54
18:R:4:SER:HA	18:R:155:LEU:O	2.07	0.54
20:T:39:LYS:HG3	20:T:43:TYR:HE1	1.71	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:128:VAL:HG21	25:Y:375:ARG:CA	2.31	0.54
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.08	0.54
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.88	0.54
6:F:109:VAL:HG23	6:F:127:GLU:OE1	2.07	0.54
6:F:92:ARG:NH2	7:G:64:THR:H	2.01	0.54
10:J:24:LEU:O	10:J:30:LEU:HB2	2.08	0.54
17:Q:64:ILE:HD13	17:Q:209:TYR:CZ	2.42	0.54
18:R:43:ARG:CZ	18:R:117:MET:HE1	2.38	0.54
21:U:17:PRO:O	21:U:20:VAL:HG23	2.07	0.54
26:Z:345:ASN:HD21	26:Z:348:ARG:HE	1.55	0.54
26:Z:522:ASP:OD1	26:Z:524:ILE:HD11	2.06	0.54
1:A:1443:VAL:CB	7:G:61:ILE:HG22	2.37	0.54
19:S:103:GLN:O	19:S:105:GLU:N	2.41	0.54
25:Y:76:MET:HG2	25:Y:178:PHE:HE1	1.72	0.54
25:Y:86:LEU:HD13	25:Y:103:PHE:CZ	2.42	0.54
26:Z:470:SER:HA	26:Z:478:THR:CG2	2.36	0.54
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.89	0.54
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.88	0.54
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.90	0.54
12:L:36:SER:O	12:L:37:LYS:C	2.44	0.54
16:P:380:ASP:CB	16:P:384:SER:CB	2.86	0.54
20:T:90:TYR:CB	22:V:112:LYS:HB3	2.38	0.54
13:M:1:MET:H2	24:X:91:SER:HA	1.71	0.54
25:Y:288:LYS:HZ1	25:Y:336:LYS:HB2	1.72	0.54
25:Y:383:LEU:HD23	25:Y:383:LEU:C	2.28	0.54
25:Y:631:GLU:HA	25:Y:636:LYS:HZ1	1.70	0.54
25:Y:639:LEU:CG	25:Y:653:PHE:CZ	2.60	0.54
25:Y:669:VAL:CG1	25:Y:677:GLY:HA3	2.37	0.54
26:Z:320:ASN:HD22	26:Z:321:GLU:N	2.06	0.54
26:Z:410:LEU:HD13	26:Z:477:LEU:CD2	2.38	0.54
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.89	0.54
1:A:344:ARG:CA	2:B:1128:LEU:O	2.55	0.54
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.89	0.54
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.90	0.54
20:T:57:VAL:O	20:T:57:VAL:HG12	2.08	0.54
22:V:99:LYS:O	22:V:99:LYS:HD2	2.08	0.54
26:Z:505:ILE:HG21	26:Z:507:ALA:CB	2.37	0.54
2:B:338:GLY:CA	2:B:339:THR:HB	2.38	0.54
16:P:632:SER:O	16:P:647:ILE:N	2.39	0.54
26:Z:383:ILE:H	26:Z:383:ILE:HD13	1.72	0.54
26:Z:515:ALA:C	26:Z:681:ARG:CD	2.65	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1397:LEU:HB3	1:A:1429:ILE:HD12	1.90	0.54
1:A:320:ARG:HG2	1:A:321:PRO:HD2	1.90	0.54
1:A:497:THR:HG23	2:B:1146:PHE:HA	1.89	0.54
17:Q:87:PHE:CE2	17:Q:220:VAL:HG21	2.42	0.54
18:R:203:GLN:O	18:R:205:VAL:N	2.40	0.54
20:T:87:LEU:HA	20:T:90:TYR:HE2	1.63	0.54
22:V:86:GLN:HA	22:V:89:THR:CG2	2.36	0.54
25:Y:166:GLU:O	25:Y:170:TYR:HD1	1.91	0.54
25:Y:330:HIS:HB3	25:Y:334:PHE:HE1	1.73	0.54
25:Y:499:LYS:C	25:Y:522:TYR:CE1	2.81	0.54
26:Z:431:GLN:HB2	26:Z:432:PRO:CD	2.37	0.54
26:Z:521:ASP:CG	26:Z:523:LYS:HG2	2.28	0.54
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.89	0.54
5:E:156:LEU:HD11	5:E:197:LYS:HB2	1.90	0.54
17:Q:108:ILE:HG21	17:Q:159:GLU:HG2	1.90	0.54
25:Y:68:LYS:CB	25:Y:228:LYS:HG3	2.36	0.54
25:Y:230:SER:H	25:Y:453:PHE:HB2	1.64	0.54
14:N:156:THR:O	14:N:159:ALA:HB3	2.07	0.53
20:T:38:SER:O	20:T:42:LEU:HB2	2.07	0.53
25:Y:167:VAL:HG22	25:Y:190:LEU:CD2	2.37	0.53
25:Y:259:ARG:CA	25:Y:379:GLU:OE1	2.56	0.53
26:Z:354:ILE:HG22	26:Z:355:ASP:N	2.23	0.53
26:Z:458:SER:HB3	26:Z:467:SER:CB	2.37	0.53
1:A:42:ASP:OD1	1:A:46:THR:N	2.41	0.53
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.34	0.53
16:P:325:ILE:N	16:P:337:ILE:O	2.35	0.53
17:Q:75:LEU:O	17:Q:98:ILE:CB	2.52	0.53
20:T:64:LYS:N	20:T:64:LYS:HD2	2.23	0.53
21:U:162:LEU:HD23	23:W:9:GLN:HG2	1.90	0.53
21:U:73:ASN:ND2	21:U:75:GLN:HE21	2.06	0.53
25:Y:635:LEU:HD13	25:Y:635:LEU:O	2.07	0.53
25:Y:63:TYR:N	25:Y:64:PRO:CD	2.71	0.53
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.90	0.53
1:A:1390:ASN:O	1:A:1399:ARG:CG	2.57	0.53
1:A:412:ARG:CB	3:C:51:VAL:HG11	45.91	0.53
1:A:1451:VAL:CG2	7:G:22:MET:SD	2.83	0.53
17:Q:68:LYS:HG2	17:Q:164:TRP:CZ3	2.44	0.53
20:T:54:SER:OG	20:T:59:SER:HB3	2.08	0.53
22:V:118:SER:HB2	22:V:119:PRO:CD	2.38	0.53
20:T:80:LEU:CD2	22:V:73:LEU:HD12	2.39	0.53
25:Y:467:ASP:HB3	25:Y:471:ARG:HH12	1.74	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:466:ARG:HB2	26:Z:477:LEU:CB	2.38	0.53
6:F:133:VAL:O	7:G:61:ILE:CD1	2.52	0.53
25:Y:90:MET:HE1	25:Y:175:VAL:CG2	2.38	0.53
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	1.89	0.53
17:Q:97:LYS:NZ	17:Q:237:GLN:O	2.42	0.53
19:S:63:MET:O	19:S:67:LYS:CB	2.57	0.53
21:U:127:LEU:HG	21:U:131:LEU:HD23	1.91	0.53
23:W:33:GLU:HG3	23:W:33:GLU:O	2.08	0.53
25:Y:57:ILE:C	25:Y:57:ILE:HD13	2.28	0.53
25:Y:653:PHE:C	25:Y:653:PHE:CD1	2.78	0.53
26:Z:446:PHE:HB3	26:Z:452:LEU:CD1	2.38	0.53
26:Z:455:SER:HB3	26:Z:466:ARG:HG3	1.88	0.53
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.72	0.53
1:A:338:GLY:HA2	2:B:1129:ARG:HH22	1.73	0.53
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.89	0.53
3:C:164:ALA:HA	3:C:167:HIS:O	2.09	0.53
5:E:19:VAL:O	5:E:23:VAL:HG23	2.08	0.53
17:Q:108:ILE:HD13	17:Q:159:GLU:CD	2.28	0.53
25:Y:111:ARG:HE	25:Y:129:VAL:HG21	1.71	0.53
25:Y:526:LEU:HD12	25:Y:621:LEU:HD22	1.91	0.53
26:Z:305:GLU:CB	26:Z:327:LYS:HZ1	2.22	0.53
26:Z:357:LYS:HG3	26:Z:357:LYS:O	2.09	0.53
26:Z:485:ILE:CG1	26:Z:510:LYS:HG2	2.39	0.53
25:Y:253:THR:CG2	25:Y:434:ILE:CD1	2.77	0.53
25:Y:277:VAL:CG1	25:Y:278:ASP:N	2.71	0.53
25:Y:337:ARG:NH2	25:Y:345:ARG:HD3	2.24	0.53
25:Y:42:MET:SD	25:Y:53:LEU:CD1	2.93	0.53
25:Y:639:LEU:HA	25:Y:653:PHE:CD2	2.41	0.53
26:Z:356:LEU:CB	26:Z:427:TRP:HD1	2.22	0.53
26:Z:752:SER:HB2	26:Z:753:PRO:CD	2.39	0.53
2:B:510:LYS:HB2	2:B:513:GLN:OE1	2.08	0.53
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.91	0.53
17:Q:31:PRO:HG3	17:Q:87:PHE:CE1	2.43	0.53
25:Y:142:LYS:CA	25:Y:145:LEU:HD21	2.32	0.53
26:Z:473:VAL:CB	26:Z:481:GLU:HG3	2.39	0.53
1:A:340:LEU:HD21	2:B:1199:ALA:HB3	1.91	0.53
7:G:18:PHE:HA	7:G:22:MET:SD	2.49	0.53
20:T:85:LYS:O	20:T:85:LYS:HD3	2.08	0.53
20:T:90:TYR:HB3	22:V:112:LYS:HB3	1.91	0.53
25:Y:352:ILE:CG2	25:Y:380:ARG:HD3	2.39	0.53
25:Y:231:ILE:N	25:Y:455:SER:HB2	2.24	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:519:VAL:HG13	25:Y:550:ILE:CD1	2.34	0.53
25:Y:681:LEU:CD2	25:Y:696:TRP:HZ3	2.10	0.53
26:Z:421:ARG:HD3	26:Z:437:VAL:CG2	2.39	0.53
26:Z:473:VAL:HG12	26:Z:481:GLU:CG	2.39	0.53
26:Z:494:PRO:HB2	26:Z:519:ARG:HH11	1.72	0.53
26:Z:373:MET:CE	26:Z:511:LEU:HD13	2.38	0.53
1:A:1447:GLU:CG	7:G:22:MET:CE	2.42	0.53
21:U:127:LEU:HG	21:U:131:LEU:CD2	2.39	0.53
25:Y:353:SER:OG	25:Y:381:LEU:HA	2.08	0.53
25:Y:393:VAL:HG11	25:Y:437:PHE:CG	2.42	0.53
26:Z:505:ILE:HG22	26:Z:506:ALA:N	2.22	0.53
26:Z:737:THR:O	26:Z:738:HIS:HD2	1.92	0.53
1:A:36:ARG:HH21	1:A:57:ARG:NH1	1.92	0.52
1:A:22:PHE:HB3	2:B:1211:ASN:OD1	2.09	0.52
2:B:174:LEU:HD11	2:B:204:ILE:HG13	1.91	0.52
22:V:86:GLN:O	22:V:89:THR:HG22	2.10	0.52
25:Y:111:ARG:NH2	25:Y:197:ARG:NH1	2.57	0.52
25:Y:200:ILE:HD12	25:Y:226:VAL:N	2.17	0.52
25:Y:269:GLU:O	25:Y:277:VAL:HG13	2.08	0.52
26:Z:363:ARG:NH2	26:Z:366:GLN:HE22	2.02	0.52
26:Z:459:MET:H	26:Z:464:ARG:HB3	1.74	0.52
26:Z:474:MET:HE1	26:Z:480:ARG:O	2.08	0.52
26:Z:627:ILE:HB	26:Z:654:LEU:CD2	2.37	0.52
1:A:1116:LEU:H	1:A:1308:THR:HB	1.73	0.52
1:A:253:ASN:O	1:A:255:SER:N	2.38	0.52
25:Y:327:ARG:CB	25:Y:330:HIS:HE1	2.14	0.52
25:Y:357:LYS:HG3	25:Y:376:PHE:HD1	1.74	0.52
26:Z:466:ARG:HE	26:Z:475:ASP:CB	2.22	0.52
26:Z:458:SER:OG	26:Z:467:SER:HB3	2.08	0.52
1:A:91:PHE:HD2	1:A:179:LEU:O	1.93	0.52
1:A:179:LEU:HD13	1:A:297:GLN:HG3	1.91	0.52
1:A:982:THR:HB	1:A:985:ASP:H	1.73	0.52
1:A:338:GLY:HA2	2:B:1129:ARG:NH2	2.23	0.52
15:O:41:ASN:C	15:O:43:SER:H	2.12	0.52
17:Q:20:ILE:HG13	17:Q:87:PHE:CG	2.44	0.52
18:R:43:ARG:CZ	18:R:117:MET:HE3	2.38	0.52
20:T:81:PHE:CE2	22:V:77:ARG:HD2	2.44	0.52
25:Y:357:LYS:CG	25:Y:376:PHE:HD1	2.21	0.52
25:Y:458:ILE:HD13	25:Y:469:TYR:HE2	1.72	0.52
25:Y:518:ILE:C	25:Y:522:TYR:CD2	2.79	0.52
26:Z:302:GLU:O	26:Z:303:ARG:HB2	2.10	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.74	0.52
2:B:295:GLY:HA2	2:B:298:LEU:HB2	1.91	0.52
3:C:73:GLN:O	3:C:129:ILE:HA	2.08	0.52
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.89	0.52
6:F:96:THR:OG1	7:G:64:THR:CA	2.57	0.52
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.91	0.52
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.45	0.52
22:V:69:ILE:HG22	22:V:73:LEU:HD23	1.92	0.52
24:X:21:THR:HG22	24:X:23:PHE:N	2.24	0.52
25:Y:185:CYS:HB3	25:Y:192:PRO:HD3	1.90	0.52
25:Y:467:ASP:CA	25:Y:470:PRO:HG3	2.38	0.52
25:Y:655:SER:O	25:Y:689:LYS:NZ	2.43	0.52
26:Z:518:VAL:HA	26:Z:524:ILE:HG21	1.92	0.52
1:A:22:PHE:CB	2:B:1211:ASN:CG	2.78	0.52
16:P:566:VAL:HA	16:P:569:ILE:CB	2.39	0.52
17:Q:109:LEU:HG	17:Q:110:HIS:N	2.25	0.52
25:Y:288:LYS:CB	25:Y:335:LEU:HD12	2.40	0.52
26:Z:327:LYS:HG3	26:Z:506:ALA:N	2.25	0.52
26:Z:446:PHE:O	26:Z:452:LEU:HD22	2.09	0.52
26:Z:489:GLU:HB3	26:Z:491:HIS:CE1	2.45	0.52
26:Z:619:ALA:HA	26:Z:622:MET:CE	2.39	0.52
1:A:399:HIS:NE2	1:A:462:VAL:CG1	2.69	0.52
1:A:412:ARG:CB	3:C:51:VAL:CG1	46.05	0.52
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.91	0.52
2:B:90:ILE:HD11	2:B:134:LYS:HE2	1.90	0.52
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.45	0.52
2:B:110:HIS:CE1	12:L:54:ARG:NH1	2.77	0.52
16:P:380:ASP:O	16:P:381:PHE:O	2.27	0.52
16:P:402:ASP:O	16:P:404:ILE:N	2.41	0.52
17:Q:89:ILE:HG13	17:Q:90:LEU:N	2.25	0.52
18:R:4:SER:CB	18:R:200:LEU:CD2	2.74	0.52
22:V:86:GLN:CD	22:V:90:LEU:HD22	2.29	0.52
23:W:19:PHE:CE1	23:W:66:ILE:HD13	2.44	0.52
23:W:94:ILE:CG1	23:W:95:ASP:N	2.69	0.52
24:X:54:PHE:CE2	24:X:58:LEU:HD11	2.45	0.52
25:Y:190:LEU:HD12	25:Y:190:LEU:C	2.29	0.52
25:Y:129:VAL:HG11	25:Y:194:PHE:CE1	2.44	0.52
25:Y:384:LEU:O	25:Y:384:LEU:HD13	2.10	0.52
25:Y:468:MET:N	25:Y:470:PRO:HD2	2.25	0.52
25:Y:486:THR:HG21	25:Y:670:LEU:CD2	2.40	0.52
26:Z:310:ILE:O	26:Z:310:ILE:HG23	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:ARG:NH1	2:B:1218:THR:OG1	2.43	0.52
1:A:227:VAL:HG13	4:D:16:LYS:HG2	1.91	0.52
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.40	0.52
6:F:133:VAL:HG12	7:G:61:ILE:HG13	1.91	0.52
17:Q:299:ARG:HG2	17:Q:300:VAL:H	1.75	0.52
21:U:143:MET:O	21:U:146:ARG:N	2.42	0.52
25:Y:111:ARG:HH22	25:Y:197:ARG:HH12	1.57	0.52
25:Y:567:LYS:CE	25:Y:597:ILE:HD13	2.33	0.52
25:Y:705:ASP:OD1	25:Y:706:LEU:N	2.41	0.52
26:Z:476:PHE:O	26:Z:501:VAL:HG23	2.08	0.52
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.92	0.52
1:A:472:LEU:O	1:A:475:THR:HB	2.10	0.52
1:A:658:LEU:HD23	1:A:659:HIS:NE2	2.24	0.52
1:A:320:ARG:HH22	3:C:81:GLU:HG3	68.95	0.52
6:F:100:GLN:OE1	7:G:15:PRO:HG2	2.10	0.52
13:M:124:ASP:O	13:M:138:GLY:HA2	2.10	0.52
17:Q:20:ILE:CD1	17:Q:87:PHE:CD2	2.87	0.52
18:R:162:GLU:OE1	18:R:162:GLU:HA	2.10	0.52
25:Y:213:LEU:HD13	25:Y:213:LEU:C	2.30	0.52
26:Z:420:TRP:HB3	26:Z:424:PHE:CE2	2.45	0.52
26:Z:519:ARG:HH11	26:Z:523:LYS:HB2	1.73	0.52
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.42	0.52
2:B:291:ILE:HD12	2:B:291:ILE:H	1.74	0.52
12:L:34:CYS:SG	12:L:51:CYS:SG	3.08	0.52
20:T:49:TYR:CZ	20:T:73:LEU:HG	2.45	0.52
21:U:57:GLU:O	21:U:57:GLU:HG2	2.10	0.52
25:Y:193:TYR:HH	25:Y:221:ARG:NH1	2.04	0.52
25:Y:499:LYS:HZ3	25:Y:522:TYR:C	2.00	0.52
1:A:23:SER:HB2	1:A:233:TRP:CE2	2.44	0.52
2:B:405:ARG:NH2	2:B:629:ASP:OD2	2.40	0.52
12:L:40:LEU:HD22	12:L:44:ASP:CG	2.31	0.52
20:T:55:LYS:NZ	20:T:62:ARG:HE	2.08	0.52
25:Y:20:GLU:O	25:Y:24:TYR:CD2	2.63	0.52
25:Y:635:LEU:HD13	25:Y:635:LEU:C	2.31	0.52
26:Z:376:ASN:HB2	26:Z:380:ARG:HD2	1.90	0.52
26:Z:408:ILE:HG21	26:Z:476:PHE:H	1.75	0.52
26:Z:596:GLN:O	26:Z:600:ARG:HG3	2.09	0.52
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.91	0.51
1:A:494:SER:HB3	1:A:497:THR:OG1	2.10	0.51
2:B:351:TYR:CE1	2:B:355:ILE:CD1	2.93	0.51
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.45	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:398:GLU:O	16:P:401:ASP:CB	2.58	0.51
17:Q:27:SER:CB	17:Q:224:MET:HG2	2.40	0.51
17:Q:97:LYS:HZ2	17:Q:244:SER:C	2.09	0.51
18:R:36:SER:HB3	18:R:63:HIS:CD2	2.44	0.51
22:V:145:ARG:HG3	22:V:149:ARG:NE	2.25	0.51
25:Y:37:ASN:OD1	25:Y:477:THR:HB	2.10	0.51
25:Y:619:THR:HG22	25:Y:621:LEU:HD12	1.93	0.51
25:Y:627:PHE:HD1	25:Y:654:LEU:HD11	1.72	0.51
10:J:48:ARG:HE	10:J:49:MET:CE	2.19	0.51
22:V:119:PRO:HB2	22:V:122:TRP:NE1	2.04	0.51
25:Y:179:GLU:HG2	25:Y:180:LYS:N	2.24	0.51
25:Y:269:GLU:O	25:Y:277:VAL:CG1	2.59	0.51
25:Y:272:SER:CB	25:Y:281:LYS:CE	2.78	0.51
25:Y:32:LEU:HD12	25:Y:57:ILE:CD1	2.40	0.51
25:Y:348:VAL:O	25:Y:352:ILE:HG12	2.10	0.51
26:Z:370:LEU:O	26:Z:373:MET:HB3	2.11	0.51
26:Z:498:PHE:O	26:Z:501:VAL:HG13	2.10	0.51
26:Z:484:PHE:CD2	26:Z:509:ALA:CB	2.93	0.51
16:P:341:TYR:CA	16:P:354:ILE:CB	2.74	0.51
22:V:86:GLN:OE1	22:V:90:LEU:HD22	2.11	0.51
23:W:118:LEU:O	23:W:122:VAL:HG23	2.10	0.51
25:Y:200:ILE:O	25:Y:203:CYS:SG	2.68	0.51
26:Z:429:THR:H	26:Z:432:PRO:HG2	1.74	0.51
26:Z:424:PHE:CE2	26:Z:454:VAL:CG2	2.94	0.51
26:Z:476:PHE:CZ	26:Z:502:VAL:CG2	2.94	0.51
1:A:67:CYS:O	1:A:70:CYS:HB3	2.11	0.51
5:E:64:PRO:HB2	5:E:69:ILE:HD11	1.93	0.51
1:A:1443:VAL:CA	6:F:133:VAL:O	2.58	0.51
6:F:92:ARG:NE	7:G:64:THR:CA	2.60	0.51
20:T:55:LYS:HE3	20:T:62:ARG:NH2	2.24	0.51
20:T:93:ILE:HG23	20:T:94:TYR:N	2.26	0.51
25:Y:215:ASP:CB	25:Y:218:ILE:HG22	2.40	0.51
26:Z:490:VAL:HG22	26:Z:490:VAL:O	2.11	0.51
1:A:412:ARG:HB3	3:C:51:VAL:HG12	45.18	0.51
1:A:940:ARG:HB3	1:A:941:LYS:HE2	1.93	0.51
14:N:124:GLU:CB	24:X:104:ASP:OD2	2.59	0.51
16:P:365:ASN:HA	16:P:381:PHE:HA	1.92	0.51
22:V:135:ILE:C	22:V:135:ILE:HD13	2.30	0.51
24:X:74:VAL:O	24:X:76:PRO:HD3	2.10	0.51
25:Y:106:LEU:HD13	25:Y:196:VAL:HG13	1.92	0.51
25:Y:185:CYS:SG	25:Y:192:PRO:CB	2.99	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:231:ILE:CA	25:Y:455:SER:CB	2.63	0.51
25:Y:567:LYS:CD	25:Y:597:ILE:CG2	2.89	0.51
25:Y:681:LEU:HD21	25:Y:696:TRP:HH2	1.75	0.51
26:Z:446:PHE:CB	26:Z:452:LEU:HD11	2.41	0.51
1:A:1095:THR:HG23	1:A:1113:THR:HG23	1.93	0.51
1:A:646:PHE:O	1:A:650:GLN:HG2	2.10	0.51
25:Y:212:TYR:CZ	25:Y:222:VAL:CG2	2.93	0.51
25:Y:529:PHE:CD1	25:Y:529:PHE:N	2.79	0.51
26:Z:484:PHE:CE1	26:Z:486:ILE:CG1	2.94	0.51
2:B:249:ARG:HH12	2:B:418:LYS:CD	2.22	0.51
3:C:167:HIS:NE2	12:L:70:ARG:HB3	2.26	0.51
1:A:1447:GLU:HB3	7:G:22:MET:CE	2.15	0.51
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.40	0.51
16:P:362:GLU:O	16:P:423:LYS:CA	2.55	0.51
17:Q:31:PRO:HB2	17:Q:220:VAL:HB	1.92	0.51
20:T:97:LEU:HA	20:T:100:ILE:HG12	1.92	0.51
21:U:146:ARG:NH1	21:U:149:GLU:OE1	2.42	0.51
22:V:86:GLN:CD	22:V:90:LEU:HD13	2.31	0.51
25:Y:327:ARG:C	25:Y:417:LEU:CD2	2.77	0.51
26:Z:487:LEU:HD22	26:Z:490:VAL:CG2	2.33	0.51
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.93	0.51
2:B:373:ARG:HG2	2:B:566:LEU:HD23	1.93	0.51
3:C:87:PHE:CE1	18:R:120:GLN:NE2	2.79	0.51
8:H:89:LEU:C	8:H:91:ASP:H	2.14	0.51
16:P:380:ASP:O	16:P:383:HIS:N	2.43	0.51
17:Q:256:TYR:O	17:Q:257:ILE:HG13	2.11	0.51
20:T:80:LEU:HD21	22:V:73:LEU:HD12	1.93	0.51
20:T:123:ASP:OD1	23:W:132:GLY:CA	2.58	0.51
25:Y:111:ARG:HH21	25:Y:129:VAL:HG11	1.76	0.51
25:Y:193:TYR:OH	25:Y:197:ARG:HD2	2.08	0.51
26:Z:414:SER:O	26:Z:417:VAL:HB	2.10	0.51
26:Z:410:LEU:CD2	26:Z:457:TYR:CE2	2.94	0.51
26:Z:785:ARG:HG3	26:Z:785:ARG:O	2.11	0.51
17:Q:97:LYS:CD	17:Q:243:ASN:C	2.77	0.51
22:V:133:LEU:HD23	22:V:136:LYS:HE3	1.93	0.51
25:Y:622:MET:HG2	25:Y:679:MET:HE2	1.92	0.51
26:Z:534:LYS:O	26:Z:534:LYS:HG3	2.11	0.51
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.11	0.51
2:B:1008:PRO:HB3	2:B:1087:PHE:HE1	1.76	0.51
2:B:438:GLU:HG3	2:B:440:HIS:HB2	1.91	0.51
2:B:530:GLY:O	2:B:532:ALA:N	2.44	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.46	0.51
25:Y:421:GLU:N	25:Y:422:PRO:HD2	2.24	0.51
26:Z:476:PHE:CZ	26:Z:487:LEU:CD2	2.93	0.51
1:A:343:LYS:HB2	2:B:1117:GLN:OE1	2.11	0.50
20:T:118:LEU:CG	23:W:129:PHE:HB3	2.40	0.50
25:Y:18:TYR:HB2	25:Y:19:PRO:HD2	1.90	0.50
25:Y:670:LEU:HD23	25:Y:672:GLY:H	1.76	0.50
26:Z:429:THR:C	26:Z:432:PRO:HD2	2.31	0.50
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.93	0.50
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.92	0.50
2:B:1201:LYS:HD3	2:B:1205:GLN:OE1	2.11	0.50
2:B:773:MET:CE	2:B:985:GLY:HA2	2.40	0.50
5:E:15:ALA:O	5:E:19:VAL:HG23	2.10	0.50
13:M:129:ARG:CA	13:M:134:THR:CB	2.89	0.50
17:Q:181:SER:HB2	17:Q:290:VAL:HG13	1.94	0.50
18:R:199:ASP:O	18:R:203:GLN:HG3	2.11	0.50
22:V:132:GLU:HB3	22:V:136:LYS:NZ	2.24	0.50
25:Y:232:VAL:HG11	25:Y:234:PHE:CE1	2.46	0.50
25:Y:61:MET:C	25:Y:64:PRO:HD2	2.31	0.50
26:Z:436:ALA:HB3	26:Z:452:LEU:HD21	1.93	0.50
26:Z:447:GLN:CG	26:Z:448:THR:H	2.20	0.50
26:Z:476:PHE:CD1	26:Z:487:LEU:CD1	2.94	0.50
1:A:419:LYS:HA	17:Q:58:LEU:CD2	2.37	0.50
16:P:579:GLU:O	16:P:583:GLU:N	2.39	0.50
22:V:109:GLU:O	22:V:111:THR:HG23	2.11	0.50
22:V:86:GLN:CA	22:V:89:THR:HG22	2.41	0.50
25:Y:252:LEU:HD11	25:Y:383:LEU:HG	1.92	0.50
25:Y:288:LYS:CG	25:Y:335:LEU:HD12	2.41	0.50
25:Y:37:ASN:ND2	25:Y:477:THR:HG21	2.26	0.50
26:Z:466:ARG:CB	26:Z:477:LEU:CB	2.89	0.50
26:Z:467:SER:H	26:Z:477:LEU:HD23	1.70	0.50
16:P:390:ARG:CB	16:P:484:ASP:CB	2.89	0.50
18:R:18:THR:HA	18:R:21:LYS:HB3	1.93	0.50
22:V:112:LYS:CG	22:V:113:ASP:N	2.75	0.50
25:Y:18:TYR:HB2	25:Y:19:PRO:HD3	1.90	0.50
26:Z:305:GLU:OE1	26:Z:330:CYS:HA	2.11	0.50
26:Z:405:LYS:NZ	26:Z:483:GLY:HA3	2.27	0.50
1:A:1442:ASP:HB2	6:F:135:ARG:HB3	1.92	0.50
1:A:497:THR:CG2	2:B:1146:PHE:HD1	2.23	0.50
2:B:211:VAL:HG13	2:B:495:LEU:HD23	1.94	0.50
13:M:167:PHE:O	13:M:168:LYS:CB	2.60	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:582:ARG:O	16:P:585:PRO:O	2.30	0.50
20:T:85:LYS:HD3	20:T:85:LYS:C	2.32	0.50
21:U:172:GLU:OE2	23:W:90:GLN:NE2	2.33	0.50
25:Y:468:MET:HG2	25:Y:471:ARG:NH2	2.27	0.50
26:Z:303:ARG:CZ	26:Z:471:GLN:HG3	2.41	0.50
2:B:1135:ARG:HG2	2:B:1139:ILE:HD11	1.94	0.50
1:A:227:VAL:CG1	4:D:16:LYS:HE3	2.40	0.50
1:A:1444:MET:CE	6:F:135:ARG:NE	2.74	0.50
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.52	0.50
20:T:62:ARG:HB3	20:T:66:ASN:ND2	2.26	0.50
25:Y:352:ILE:H	25:Y:380:ARG:NH1	2.01	0.50
25:Y:353:SER:CB	25:Y:381:LEU:HA	2.40	0.50
25:Y:42:MET:SD	25:Y:50:VAL:CG2	2.87	0.50
25:Y:32:LEU:HD12	25:Y:61:MET:HG3	1.93	0.50
26:Z:473:VAL:HG12	26:Z:481:GLU:HG3	1.94	0.50
26:Z:484:PHE:HD2	26:Z:509:ALA:HB3	1.73	0.50
26:Z:585:PRO:HG2	26:Z:756:ARG:NH1	2.22	0.50
1:A:211:PHE:CE2	1:A:234:MET:CE	2.95	0.50
22:V:90:LEU:HD12	22:V:90:LEU:N	2.27	0.50
25:Y:140:GLN:HB3	25:Y:143:ARG:HG2	1.93	0.50
25:Y:327:ARG:CG	25:Y:330:HIS:HE1	2.25	0.50
25:Y:639:LEU:HD12	25:Y:653:PHE:HE2	0.82	0.50
26:Z:350:PRO:HA	26:Z:481:GLU:O	2.12	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.94	0.50
2:B:60:GLN:OE1	2:B:95:ILE:HG22	2.12	0.50
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.94	0.50
16:P:543:ARG:C	16:P:545:ILE:H	2.10	0.50
18:R:22:ASP:HA	18:R:25:SER:HB2	1.94	0.50
20:T:84:VAL:HG22	22:V:70:PHE:CZ	2.47	0.50
22:V:118:SER:O	22:V:122:TRP:HD1	1.95	0.50
22:V:84:SER:H	22:V:87:LEU:CB	2.25	0.50
25:Y:218:ILE:HG23	25:Y:219:ALA:N	2.27	0.50
26:Z:425:LEU:HD23	26:Z:425:LEU:C	2.31	0.50
1:A:714:PHE:O	1:A:718:VAL:HG23	2.12	0.50
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.93	0.50
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.94	0.50
13:M:13:SER:HA	13:M:16:TRP:CB	2.41	0.50
17:Q:101:ASN:O	17:Q:103:ALA:N	2.44	0.50
17:Q:108:ILE:HD13	17:Q:159:GLU:CB	2.32	0.50
22:V:76:ILE:HG23	22:V:77:ARG:N	2.27	0.50
23:W:85:VAL:HG12	23:W:86:SER:O	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:274:VAL:CG1	25:Y:275:ARG:H	2.20	0.50
25:Y:353:SER:CA	25:Y:356:PRO:CD	2.90	0.50
25:Y:59:TYR:CG	25:Y:62:HIS:CE1	2.99	0.50
25:Y:51:SER:OG	25:Y:85:GLU:HG3	2.11	0.50
26:Z:391:GLY:CA	26:Z:394:LEU:HD13	2.42	0.50
26:Z:403:ILE:HD13	26:Z:484:PHE:HD2	1.75	0.50
26:Z:415:VAL:HA	26:Z:418:MET:HE2	1.93	0.50
26:Z:424:PHE:HA	26:Z:427:TRP:CZ3	2.47	0.50
26:Z:403:ILE:CD1	26:Z:484:PHE:CD2	2.94	0.50
1:A:245:PRO:O	2:B:1114:LEU:HD12	2.12	0.49
2:B:1072:MET:HB3	2:B:1081:LEU:HD12	1.94	0.49
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.94	0.49
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.49
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.94	0.49
14:N:109:LEU:O	14:N:112:THR:N	2.45	0.49
16:P:380:ASP:O	16:P:383:HIS:C	2.50	0.49
17:Q:224:MET:HE3	17:Q:230:LEU:HD12	1.93	0.49
18:R:47:LYS:CE	18:R:47:LYS:H	2.25	0.49
21:U:83:TRP:CD1	21:U:83:TRP:N	2.80	0.49
25:Y:229:ASP:HA	25:Y:453:PHE:CB	2.31	0.49
25:Y:499:LYS:HD2	25:Y:522:TYR:CB	2.42	0.49
26:Z:335:TYR:CB	26:Z:336:PRO:HD3	2.42	0.49
26:Z:457:TYR:O	26:Z:477:LEU:HD21	2.12	0.49
26:Z:476:PHE:CE1	26:Z:487:LEU:HD11	2.46	0.49
26:Z:485:ILE:HG12	26:Z:510:LYS:HG2	1.93	0.49
26:Z:528:ASN:HA	26:Z:532:GLY:C	2.32	0.49
26:Z:618:TYR:CB	26:Z:622:MET:HE1	2.34	0.49
2:B:338:GLY:HA2	2:B:339:THR:HB	1.93	0.49
2:B:70:ILE:HG22	2:B:89:GLU:HG2	1.93	0.49
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.94	0.49
3:C:99:LEU:HB2	3:C:157:CYS:HB2	1.94	0.49
20:T:43:TYR:CE2	22:V:102:LYS:HD2	2.47	0.49
22:V:76:ILE:CD1	22:V:97:ARG:HB2	2.36	0.49
25:Y:252:LEU:CD1	25:Y:383:LEU:HG	2.42	0.49
25:Y:540:PHE:HB2	25:Y:622:MET:SD	2.52	0.49
26:Z:407:VAL:HG13	26:Z:451:GLY:CA	2.42	0.49
26:Z:406:SER:CB	26:Z:482:TRP:CE3	2.94	0.49
26:Z:723:GLN:O	26:Z:727:VAL:HG22	2.12	0.49
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.12	0.49
1:A:61:ILE:O	1:A:61:ILE:HD12	2.12	0.49
25:Y:569:ILE:HG21	25:Y:571:VAL:HG22	1.91	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:328:LYS:HE3	26:Z:329:ARG:HE	1.77	0.49
26:Z:331:GLN:NE2	26:Z:378:ARG:HD2	2.22	0.49
26:Z:474:MET:CB	26:Z:482:TRP:H	2.03	0.49
4:D:161:GLY:O	4:D:165:GLN:NE2	2.46	0.49
7:G:1:MET:CG	7:G:2:PHE:N	2.76	0.49
17:Q:87:PHE:CZ	17:Q:220:VAL:HG21	2.48	0.49
25:Y:141:ALA:O	25:Y:145:LEU:HD23	2.12	0.49
25:Y:353:SER:C	25:Y:356:PRO:HG2	2.15	0.49
25:Y:245:ILE:CG2	25:Y:439:CYS:O	2.48	0.49
25:Y:233:ILE:HA	25:Y:457:ILE:HB	1.94	0.49
25:Y:528:GLU:O	25:Y:532:ILE:CG1	2.53	0.49
25:Y:54:SER:O	25:Y:57:ILE:CG2	2.57	0.49
25:Y:681:LEU:HD21	25:Y:696:TRP:CZ3	2.46	0.49
26:Z:490:VAL:CG2	26:Z:531:ILE:HD13	2.43	0.49
1:A:89:PRO:HB2	1:A:204:THR:HB	1.94	0.49
6:F:97:ARG:NH1	7:G:15:PRO:CB	2.76	0.49
13:M:166:ILE:O	13:M:170:VAL:N	2.44	0.49
14:N:120:PRO:O	14:N:122:VAL:N	2.45	0.49
22:V:88:GLU:HA	22:V:91:THR:HG22	1.94	0.49
25:Y:129:VAL:CG1	25:Y:194:PHE:CE1	2.96	0.49
25:Y:218:ILE:CD1	25:Y:221:ARG:HH21	2.24	0.49
25:Y:357:LYS:CG	25:Y:376:PHE:CD1	2.95	0.49
25:Y:450:PHE:CZ	25:Y:475:PHE:CG	3.01	0.49
25:Y:495:MET:HG2	25:Y:686:PHE:CD1	2.44	0.49
25:Y:666:LEU:HD23	25:Y:679:MET:CB	2.42	0.49
26:Z:494:PRO:HD3	26:Z:527:LEU:HD21	1.94	0.49
2:B:35:SER:HA	2:B:811:TYR:HE1	1.76	0.49
6:F:92:ARG:HH21	7:G:63:PRO:CA	2.24	0.49
17:Q:108:ILE:O	17:Q:109:LEU:CB	2.60	0.49
20:T:100:ILE:HG13	20:T:101:ASP:H	1.77	0.49
25:Y:499:LYS:HD3	25:Y:521:ASN:CB	2.43	0.49
26:Z:609:SER:OG	26:Z:615:LEU:HD13	2.13	0.49
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.12	0.49
2:B:806:THR:HB	2:B:809:MET:HG3	1.94	0.49
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.95	0.49
7:G:18:PHE:HA	7:G:22:MET:HE3	1.95	0.49
16:P:348:TYR:O	16:P:349:LYS:CB	2.60	0.49
25:Y:273:GLU:CG	25:Y:274:VAL:N	2.76	0.49
25:Y:438:THR:HG21	25:Y:634:ILE:CG2	2.42	0.49
26:Z:474:MET:HG3	26:Z:505:ILE:CG2	2.43	0.49
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.93	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:49:LYS:O	12:L:50:ASP:CB	2.60	0.49
14:N:24:ASP:O	14:N:25:PHE:CB	2.60	0.49
20:T:46:LEU:HD12	20:T:80:LEU:HD13	1.94	0.49
25:Y:493:LEU:HD11	25:Y:666:LEU:HD21	1.94	0.49
26:Z:476:PHE:N	26:Z:485:ILE:HG22	2.28	0.49
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.12	0.49
1:A:919:ILE:HG12	1:A:983:ILE:HD13	1.94	0.49
2:B:693:ILE:HG21	2:B:701:ILE:HD13	1.95	0.49
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.41	0.49
3:C:87:PHE:HE1	18:R:120:GLN:NE2	2.11	0.49
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.33	0.49
12:L:48:CYS:SG	12:L:49:LYS:N	2.85	0.49
20:T:122:HIS:HA	23:W:130:VAL:HG13	1.51	0.49
20:T:93:ILE:HD13	22:V:122:TRP:CD2	2.47	0.49
25:Y:28:ILE:HG22	25:Y:57:ILE:HD11	1.81	0.49
25:Y:495:MET:CG	25:Y:686:PHE:CD1	2.93	0.49
26:Z:380:ARG:CB	26:Z:535:LEU:HD22	2.43	0.49
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.48	0.49
1:A:285:PRO:O	1:A:287:HIS:N	2.46	0.49
12:L:34:CYS:O	12:L:35:SER:C	2.52	0.49
18:R:178:ARG:HA	18:R:180:LYS:HE2	1.95	0.49
20:T:87:LEU:O	20:T:87:LEU:HG	2.13	0.49
20:T:94:TYR:CE2	22:V:109:GLU:CB	2.95	0.49
22:V:117:LYS:CG	22:V:121:GLU:CB	2.77	0.49
23:W:63:SER:O	23:W:67:ILE:HG13	2.13	0.49
25:Y:253:THR:HG22	25:Y:434:ILE:CB	2.42	0.49
25:Y:450:PHE:CE1	25:Y:475:PHE:CD2	3.00	0.49
26:Z:408:ILE:HG22	26:Z:484:PHE:O	2.13	0.49
26:Z:408:ILE:HG23	26:Z:485:ILE:HA	1.94	0.49
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.48
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.95	0.48
1:A:568:PRO:HG2	8:H:46:LEU:HD12	1.95	0.48
7:G:142:ARG:HB3	7:G:171:ILE:HD12	1.95	0.48
25:Y:135:ARG:CZ	25:Y:143:ARG:NE	2.53	0.48
25:Y:269:GLU:CG	25:Y:277:VAL:CG1	2.86	0.48
25:Y:421:GLU:N	25:Y:422:PRO:HD3	2.27	0.48
26:Z:447:GLN:HG3	26:Z:448:THR:H	1.78	0.48
1:A:1193:LEU:HB2	1:A:1260:LEU:CD2	2.42	0.48
1:A:216:VAL:O	1:A:220:THR:HB	2.12	0.48
2:B:574:SER:HB3	2:B:591:ARG:HE	1.77	0.48
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.96	0.48
17:Q:11:ILE:HG12	17:Q:19:LEU:CD2	2.43	0.48
17:Q:61:PRO:CG	17:Q:300:VAL:CG2	2.87	0.48
21:U:114:TYR:O	21:U:117:GLN:HB2	2.14	0.48
21:U:114:TYR:O	21:U:117:GLN:N	2.46	0.48
20:T:39:LYS:HD3	22:V:115:LEU:HA	1.95	0.48
22:V:66:ILE:N	22:V:67:PRO:HD2	2.27	0.48
25:Y:464:SER:HA	25:Y:466:LEU:HD22	1.94	0.48
25:Y:463:ILE:HD11	25:Y:469:TYR:CE1	2.48	0.48
26:Z:313:VAL:HG12	26:Z:314:HIS:CE1	2.48	0.48
26:Z:404:LYS:HA	26:Z:448:THR:HG21	1.94	0.48
26:Z:447:GLN:HG3	26:Z:448:THR:N	2.28	0.48
26:Z:516:THR:HG23	26:Z:681:ARG:HE	1.77	0.48
2:B:705:MET:H	2:B:710:LEU:HD12	1.79	0.48
2:B:542:MET:HG3	2:B:747:MET:HB3	1.95	0.48
12:L:46:VAL:CG1	12:L:56:LEU:HD12	2.43	0.48
14:N:98:LEU:HA	16:P:252:SER:HA	1.96	0.48
17:Q:232:LEU:HD21	17:Q:253:LEU:HD13	1.94	0.48
17:Q:61:PRO:CG	17:Q:300:VAL:HG21	2.38	0.48
20:T:122:HIS:CA	23:W:131:ASP:O	2.62	0.48
21:U:138:SER:O	21:U:139:ILE:HG13	2.13	0.48
22:V:82:ASN:N	22:V:86:GLN:HE22	2.10	0.48
25:Y:357:LYS:HG3	25:Y:376:PHE:CD1	2.48	0.48
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.96	0.48
1:A:52:GLY:O	1:A:56:PRO:HG3	2.13	0.48
1:A:61:ILE:HD12	1:A:61:ILE:C	2.34	0.48
1:A:1444:MET:HE3	6:F:135:ARG:CZ	2.44	0.48
18:R:29:LEU:HB3	18:R:131:ILE:O	2.13	0.48
20:T:55:LYS:HE3	20:T:62:ARG:NE	2.28	0.48
22:V:76:ILE:HD13	22:V:97:ARG:HB3	1.93	0.48
25:Y:127:THR:HG23	25:Y:361:GLN:NE2	2.28	0.48
25:Y:352:ILE:CG2	25:Y:380:ARG:CD	2.91	0.48
25:Y:230:SER:O	25:Y:455:SER:N	2.46	0.48
25:Y:492:PHE:HE2	25:Y:707:ASN:OD1	1.86	0.48
26:Z:508:HIS:CE1	26:Z:509:ALA:HB2	2.48	0.48
1:A:929:LEU:HD21	1:A:983:ILE:HG21	1.96	0.48
11:K:63:VAL:HG12	11:K:71:PHE:HB3	1.96	0.48
17:Q:13:ASP:OD1	17:Q:250:GLY:HA2	2.13	0.48
17:Q:217:THR:HB	17:Q:235:ILE:HG12	1.96	0.48
25:Y:20:GLU:O	25:Y:24:TYR:CG	2.66	0.48
25:Y:36:GLY:O	25:Y:456:VAL:HG23	2.13	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:37:ASN:CB	25:Y:456:VAL:CG1	2.83	0.48
25:Y:603:ARG:HH22	25:Y:629:TYR:HH	1.60	0.48
25:Y:631:GLU:N	25:Y:636:LYS:HE3	2.27	0.48
25:Y:495:MET:SD	25:Y:696:TRP:CZ3	3.03	0.48
26:Z:420:TRP:HB3	26:Z:424:PHE:CZ	2.48	0.48
1:A:1447:GLU:HB3	7:G:22:MET:SD	2.53	0.48
1:A:280:GLU:HG2	1:A:289:ILE:HD13	1.95	0.48
1:A:7:SER:HG	2:B:1161:HIS:CE1	2.24	0.48
2:B:351:TYR:HE1	2:B:355:ILE:HD12	1.78	0.48
25:Y:327:ARG:NH2	25:Y:330:HIS:CE1	2.81	0.48
25:Y:327:ARG:NH2	25:Y:330:HIS:NE2	2.60	0.48
25:Y:539:VAL:HG11	25:Y:623:ILE:CG1	2.44	0.48
26:Z:305:GLU:HB2	26:Z:327:LYS:CE	2.43	0.48
26:Z:474:MET:HG2	26:Z:482:TRP:O	2.13	0.48
26:Z:476:PHE:CE1	26:Z:487:LEU:CD2	2.94	0.48
26:Z:518:VAL:HG12	26:Z:519:ARG:N	2.29	0.48
2:B:345:LYS:HA	2:B:348:ARG:HD2	1.96	0.48
2:B:219:ALA:HB2	2:B:405:ARG:HG2	1.95	0.48
7:G:60:ARG:CZ	7:G:69:GLU:OE1	2.52	0.48
22:V:112:LYS:O	22:V:113:ASP:CB	2.61	0.48
25:Y:352:ILE:HG13	25:Y:380:ARG:NH2	2.26	0.48
25:Y:353:SER:OG	25:Y:381:LEU:CB	2.59	0.48
25:Y:495:MET:CB	25:Y:686:PHE:CZ	2.93	0.48
25:Y:571:VAL:HG12	25:Y:572:GLU:HB2	1.95	0.48
26:Z:394:LEU:CD1	26:Z:394:LEU:H	2.27	0.48
26:Z:522:ASP:HA	26:Z:524:ILE:HD12	1.93	0.48
1:A:1116:LEU:HG	1:A:1327:ILE:HD11	1.95	0.48
1:A:1444:MET:SD	6:F:135:ARG:HB2	2.54	0.48
1:A:36:ARG:NH2	1:A:57:ARG:HH22	2.12	0.48
2:B:1113:VAL:HG22	3:C:57:VAL:HG11	49.36	0.48
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.95	0.48
14:N:204:PHE:HA	14:N:209:GLU:O	2.13	0.48
20:T:103:ASP:O	20:T:107:LEU:HG	2.14	0.48
25:Y:108:LEU:HD12	25:Y:196:VAL:HG11	1.95	0.48
25:Y:71:TYR:CE2	25:Y:233:ILE:HD13	2.48	0.48
26:Z:348:ARG:HB3	26:Z:350:PRO:HD3	1.96	0.48
26:Z:367:GLU:HA	26:Z:367:GLU:OE1	2.14	0.48
1:A:1436:ILE:HD11	2:B:1144:ALA:HA	1.94	0.48
25:Y:273:GLU:HG2	25:Y:274:VAL:H	1.77	0.48
26:Z:407:VAL:HG22	26:Z:451:GLY:CA	2.44	0.48
26:Z:446:PHE:CA	26:Z:452:LEU:HD22	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:494:PRO:HG3	26:Z:527:LEU:HD21	1.94	0.48
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.95	0.48
1:A:67:CYS:C	1:A:68:GLN:HG3	2.34	0.48
1:A:11:LEU:HA	2:B:1193:GLN:HG2	1.95	0.48
12:L:27:LEU:N	12:L:27:LEU:HD23	2.29	0.48
17:Q:109:LEU:HG	17:Q:110:HIS:H	1.79	0.48
20:T:118:LEU:CD2	23:W:129:PHE:CB	2.58	0.48
22:V:147:LEU:O	22:V:147:LEU:HD23	2.13	0.48
25:Y:120:VAL:HG22	25:Y:121:SER:N	2.29	0.48
25:Y:571:VAL:HG12	25:Y:572:GLU:HG3	1.94	0.48
25:Y:679:MET:CE	25:Y:681:LEU:HD11	2.43	0.48
1:A:261:ASP:HB3	1:A:322:VAL:HG13	1.95	0.47
1:A:579:SER:HA	1:A:582:ILE:HG13	1.96	0.47
1:A:78:PRO:C	2:B:1201:LYS:HZ3	2.12	0.47
2:B:62:ILE:HG21	2:B:417:PHE:HD2	1.78	0.47
6:F:97:ARG:HH12	7:G:15:PRO:CB	2.26	0.47
25:Y:499:LYS:NZ	25:Y:521:ASN:O	2.45	0.47
25:Y:539:VAL:HG13	25:Y:623:ILE:HG12	1.92	0.47
26:Z:352:LEU:H	26:Z:352:LEU:CD2	2.25	0.47
26:Z:424:PHE:CE1	26:Z:451:GLY:N	2.82	0.47
26:Z:408:ILE:CG1	26:Z:475:ASP:HB3	2.21	0.47
1:A:475:THR:HG21	2:B:836:GLU:OE2	2.14	0.47
1:A:71:GLN:O	1:A:73:GLY:N	2.47	0.47
2:B:441:ASP:O	2:B:443:ASN:N	2.47	0.47
2:B:486:TYR:HB3	2:B:1096:ARG:NE	2.28	0.47
2:B:849:GLY:HA2	2:B:852:ARG:CD	2.40	0.47
18:R:46:ILE:HD13	18:R:47:LYS:HZ1	1.78	0.47
25:Y:171:LEU:CD2	25:Y:181:LEU:HD22	2.43	0.47
25:Y:200:ILE:HG13	25:Y:201:SER:N	2.29	0.47
25:Y:253:THR:HG22	25:Y:434:ILE:HG12	1.95	0.47
25:Y:288:LYS:HZ1	25:Y:336:LYS:CB	2.26	0.47
25:Y:346:MET:CA	25:Y:384:LEU:CD2	2.88	0.47
25:Y:494:PRO:HA	25:Y:697:ILE:O	2.15	0.47
25:Y:621:LEU:HG	25:Y:680:VAL:HG12	1.96	0.47
25:Y:492:PHE:HB3	25:Y:678:VAL:HG22	1.96	0.47
25:Y:693:LEU:HG	25:Y:696:TRP:CE2	2.48	0.47
26:Z:307:ASP:HB2	26:Z:323:VAL:CB	2.36	0.47
26:Z:445:MET:SD	26:Z:473:VAL:HG11	2.54	0.47
26:Z:477:LEU:HD12	26:Z:477:LEU:N	2.28	0.47
26:Z:516:THR:CG2	26:Z:681:ARG:HE	2.26	0.47
26:Z:696:ARG:CZ	26:Z:704:PHE:HZ	2.26	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:LEU:HD21	1:A:1017:LEU:HG	1.96	0.47
2:B:249:ARG:NH1	2:B:418:LYS:CD	2.76	0.47
7:G:18:PHE:HA	7:G:22:MET:CE	2.44	0.47
1:A:738:LYS:HA	8:H:19:ARG:HH12	1.79	0.47
17:Q:40:VAL:HG21	17:Q:213:PHE:CZ	2.49	0.47
21:U:132:GLU:CD	21:U:139:ILE:CD1	2.75	0.47
21:U:166:ARG:HA	21:U:169:GLN:HB3	1.97	0.47
21:U:169:GLN:HE21	23:W:5:LEU:H	1.62	0.47
25:Y:108:LEU:HA	25:Y:196:VAL:HG11	1.96	0.47
25:Y:51:SER:O	25:Y:55:LEU:HG	2.14	0.47
25:Y:631:GLU:HG2	25:Y:636:LYS:HZ3	1.80	0.47
25:Y:68:LYS:CE	25:Y:228:LYS:CE	2.87	0.47
26:Z:446:PHE:CB	26:Z:452:LEU:CD1	2.93	0.47
26:Z:487:LEU:HD21	26:Z:531:ILE:CD1	2.44	0.47
1:A:257:ARG:HB2	1:A:257:ARG:NH1	2.29	0.47
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.97	0.47
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.96	0.47
12:L:52:GLY:O	12:L:53:HIS:C	2.52	0.47
22:V:117:LYS:HZ2	22:V:121:GLU:CG	2.02	0.47
25:Y:328:ALA:CA	25:Y:417:LEU:CD2	2.72	0.47
25:Y:419:ILE:HD11	25:Y:435:MET:CE	2.41	0.47
25:Y:518:ILE:C	25:Y:522:TYR:HD2	2.12	0.47
26:Z:310:ILE:HG21	26:Z:313:VAL:CG2	2.44	0.47
26:Z:384:ILE:N	26:Z:384:ILE:HD12	2.30	0.47
26:Z:410:LEU:HD21	26:Z:457:TYR:CE2	2.48	0.47
26:Z:434:ASN:O	26:Z:452:LEU:HD12	2.15	0.47
1:A:275:SER:O	1:A:279:LEU:HD12	2.14	0.47
2:B:122:LEU:HD22	2:B:958:GLN:HG2	1.96	0.47
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.95	0.47
21:U:121:LYS:O	21:U:122:LEU:C	2.53	0.47
25:Y:350:HIS:N	25:Y:384:LEU:HG	2.29	0.47
25:Y:384:LEU:C	25:Y:384:LEU:HD13	2.35	0.47
25:Y:495:MET:HE3	25:Y:696:TRP:HB3	1.96	0.47
25:Y:571:VAL:O	25:Y:574:PRO:HD3	2.14	0.47
26:Z:372:LYS:O	26:Z:535:LEU:HD23	2.14	0.47
26:Z:519:ARG:N	26:Z:524:ILE:HG21	2.29	0.47
1:A:1444:MET:CE	6:F:135:ARG:HE	2.27	0.47
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.96	0.47
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.13	0.47
6:F:92:ARG:HE	7:G:64:THR:HA	1.73	0.47
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.95	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:904:ARG:NH1	12:L:66:GLN:O	2.42	0.47
20:T:102:LYS:HA	20:T:102:LYS:HE2	1.97	0.47
21:U:165:TYR:HE2	23:W:80:LEU:CD2	2.27	0.47
22:V:112:LYS:HD2	22:V:119:PRO:HG3	1.95	0.47
24:X:21:THR:CG2	24:X:22:ARG:N	2.77	0.47
25:Y:111:ARG:NH2	25:Y:197:ARG:HH12	2.11	0.47
1:A:132:LYS:HZ2	1:A:1415:SER:HB3	1.77	0.47
1:A:227:VAL:CG1	4:D:16:LYS:CE	2.92	0.47
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.97	0.47
2:B:756:ILE:O	2:B:759:PRO:HD3	2.15	0.47
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.95	0.47
16:P:596:ILE:O	16:P:600:ASN:CB	2.63	0.47
18:R:54:SER:OG	18:R:74:ASP:OD1	2.31	0.47
20:T:97:LEU:HD21	22:V:125:ILE:HD13	1.95	0.47
25:Y:86:LEU:HD13	25:Y:103:PHE:HZ	1.79	0.47
25:Y:162:LEU:HD13	25:Y:194:PHE:HB3	1.97	0.47
25:Y:232:VAL:CG1	25:Y:234:PHE:CE1	2.97	0.47
25:Y:248:LEU:CD1	25:Y:439:CYS:SG	3.03	0.47
26:Z:425:LEU:CB	26:Z:429:THR:HA	2.44	0.47
26:Z:436:ALA:HB2	26:Z:452:LEU:HD21	1.95	0.47
26:Z:528:ASN:ND2	26:Z:533:PRO:HA	2.30	0.47
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.96	0.47
5:E:176:PRO:O	5:E:212:ARG:HA	2.14	0.47
6:F:106:PRO:HB2	7:G:16:SER:HA	1.89	0.47
1:A:1450:LEU:CB	7:G:18:PHE:O	2.46	0.47
8:H:23:VAL:HG11	8:H:121:LEU:HD22	1.95	0.47
8:H:115:TYR:CE1	8:H:124:ARG:HG3	2.49	0.47
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.95	0.47
16:P:341:TYR:CB	16:P:353:GLY:HA2	2.44	0.47
17:Q:27:SER:HB3	17:Q:224:MET:CE	2.45	0.47
17:Q:259:VAL:HG21	17:Q:268:ILE:HD11	1.96	0.47
18:R:142:LEU:HD11	18:R:152:LEU:CD1	2.34	0.47
18:R:46:ILE:HA	18:R:47:LYS:HZ3	1.77	0.47
25:Y:134:ARG:O	25:Y:138:ASN:ND2	2.48	0.47
25:Y:440:LEU:CD1	25:Y:638:ARG:CA	2.76	0.47
25:Y:495:MET:HE3	25:Y:696:TRP:HE3	1.79	0.47
26:Z:426:GLN:NE2	26:Z:426:GLN:HA	2.30	0.47
26:Z:490:VAL:HG12	26:Z:514:THR:HB	1.97	0.47
1:A:91:PHE:CD2	1:A:179:LEU:O	2.68	0.47
2:B:563:MET:HE1	2:B:587:HIS:HB2	1.97	0.47
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:HD21	10:J:57:ILE:HD12	1.97	0.47
12:L:46:VAL:HG12	12:L:46:VAL:O	2.14	0.47
22:V:114:LEU:CD1	22:V:114:LEU:N	2.78	0.47
22:V:76:ILE:HD12	22:V:97:ARG:CD	2.42	0.47
24:X:34:ALA:HB2	24:X:78:CYS:HB3	1.97	0.47
25:Y:357:LYS:CD	25:Y:376:PHE:HD1	2.27	0.47
25:Y:248:LEU:HD12	25:Y:439:CYS:SG	2.54	0.47
25:Y:496:ILE:CG1	25:Y:682:ALA:HA	2.44	0.47
25:Y:627:PHE:HD1	25:Y:654:LEU:CD1	2.27	0.47
25:Y:68:LYS:HB2	25:Y:228:LYS:HB3	1.90	0.47
26:Z:353:ASP:HA	26:Z:447:GLN:CD	2.35	0.47
26:Z:410:LEU:HD11	26:Z:457:TYR:N	2.30	0.47
26:Z:499:ARG:HG2	26:Z:530:LEU:CD1	2.45	0.47
26:Z:622:MET:HE3	26:Z:653:PHE:CZ	2.49	0.47
2:B:291:ILE:N	2:B:291:ILE:HD12	2.30	0.47
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.97	0.47
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.55	0.47
21:U:118:GLU:O	21:U:121:LYS:N	2.48	0.47
21:U:19:TYR:CZ	24:X:22:ARG:HG3	2.50	0.47
25:Y:237:ALA:O	25:Y:240:ILE:HG12	2.15	0.47
25:Y:649:ARG:O	25:Y:653:PHE:CG	2.67	0.47
26:Z:356:LEU:HD21	26:Z:448:THR:CB	2.45	0.47
26:Z:421:ARG:NE	26:Z:430:LEU:HD21	2.29	0.47
26:Z:686:ARG:HG2	26:Z:690:ILE:HD12	1.95	0.47
26:Z:716:MET:O	26:Z:719:SER:HB2	2.15	0.47
1:A:89:PRO:HB2	1:A:204:THR:CB	2.44	0.47
3:C:100:THR:HG22	3:C:119:VAL:HG22	1.97	0.47
7:G:60:ARG:HH21	7:G:69:GLU:CD	2.18	0.47
20:T:84:VAL:HG13	20:T:85:LYS:N	2.30	0.47
21:U:162:LEU:HD23	23:W:9:GLN:CG	2.45	0.47
22:V:117:LYS:HE3	22:V:122:TRP:N	2.30	0.47
25:Y:140:GLN:HG3	25:Y:143:ARG:CZ	2.45	0.47
25:Y:218:ILE:O	25:Y:222:VAL:HG23	2.15	0.47
25:Y:46:THR:HG22	25:Y:46:THR:O	2.15	0.47
25:Y:529:PHE:CZ	25:Y:704:ALA:HB3	2.50	0.47
26:Z:397:ILE:HD11	26:Z:423:GLN:HG2	1.97	0.47
26:Z:424:PHE:HE2	26:Z:454:VAL:HG21	1.81	0.47
26:Z:477:LEU:HA	26:Z:501:VAL:CG2	2.45	0.47
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.45	0.46
6:F:96:THR:OG1	7:G:63:PRO:O	2.33	0.46
15:O:93:GLN:N	16:P:344:SER:CB	2.77	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:234:LYS:HE2	17:Q:251:PHE:CZ	2.49	0.46
17:Q:297:ASP:OD2	17:Q:299:ARG:NH1	2.48	0.46
20:T:118:LEU:O	23:W:131:ASP:N	2.36	0.46
20:T:84:VAL:CG1	22:V:70:PHE:CE2	2.95	0.46
22:V:85:ASN:O	22:V:88:GLU:HG2	2.14	0.46
21:U:166:ARG:HG3	23:W:5:LEU:HD23	1.97	0.46
26:Z:466:ARG:NE	26:Z:475:ASP:HB3	2.29	0.46
26:Z:584:ASN:CG	26:Z:586:THR:CG2	2.82	0.46
6:F:92:ARG:HE	7:G:64:THR:CB	2.25	0.46
21:U:188:GLU:O	21:U:192:ILE:HG13	2.16	0.46
23:W:12:LEU:O	23:W:12:LEU:HD23	2.16	0.46
25:Y:182:LEU:CD1	25:Y:192:PRO:HG2	2.45	0.46
25:Y:569:ILE:CG2	25:Y:571:VAL:CG2	2.87	0.46
26:Z:484:PHE:CD1	26:Z:485:ILE:N	2.83	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.80	0.46
2:B:1215:ARG:NH2	4:D:15:LEU:HD21	2.29	0.46
1:A:420:ARG:NH1	17:Q:174:ALA:HB2	2.24	0.46
17:Q:291:PRO:HG2	17:Q:296:MET:SD	2.56	0.46
20:T:55:LYS:HA	20:T:60:VAL:HG13	1.94	0.46
25:Y:206:ILE:HD11	25:Y:226:VAL:HG22	1.96	0.46
25:Y:248:LEU:HD11	25:Y:445:ALA:HB3	1.95	0.46
26:Z:400:ALA:CB	26:Z:450:SER:CA	2.94	0.46
26:Z:446:PHE:CB	26:Z:452:LEU:CD2	2.92	0.46
1:A:565:ILE:O	1:A:570:PRO:HA	2.16	0.46
2:B:662:MET:HA	2:B:665:GLU:HB2	1.97	0.46
9:I:83:ASN:HA	9:I:104:LEU:HG	1.97	0.46
17:Q:79:THR:O	17:Q:82:ASP:N	2.48	0.46
17:Q:81:MET:HE1	17:Q:92:SER:CA	2.43	0.46
20:T:39:LYS:H	22:V:113:ASP:CG	2.17	0.46
20:T:99:LYS:HE3	20:T:99:LYS:O	2.16	0.46
21:U:177:LEU:O	21:U:181:GLN:HG2	2.15	0.46
22:V:83:LEU:O	22:V:84:SER:OG	2.33	0.46
23:W:7:GLN:O	23:W:11:CYS:HB2	2.15	0.46
25:Y:140:GLN:CB	25:Y:143:ARG:HG2	2.45	0.46
25:Y:24:TYR:CE2	25:Y:482:SER:CB	2.79	0.46
25:Y:487:LEU:HD23	25:Y:490:LYS:HE3	1.96	0.46
26:Z:397:ILE:HD11	26:Z:423:GLN:CG	2.45	0.46
2:B:803:LEU:HG	10:J:52:THR:HG21	1.98	0.46
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.98	0.46
17:Q:98:ILE:CG2	17:Q:99:PRO:N	2.78	0.46
18:R:4:SER:HB3	18:R:200:LEU:HG	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:352:ILE:CB	25:Y:380:ARG:NE	2.62	0.46
26:Z:638:ASN:HD22	26:Z:638:ASN:C	2.17	0.46
1:A:11:LEU:HD13	2:B:1195:HIS:NE2	2.31	0.46
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.97	0.46
6:F:96:THR:CG2	7:G:66:GLY:CA	2.93	0.46
16:P:394:PHE:CA	16:P:407:GLY:HA2	2.36	0.46
16:P:392:ARG:H	16:P:476:ILE:HA	1.79	0.46
20:T:118:LEU:CD1	23:W:130:VAL:C	2.62	0.46
20:T:48:ARG:O	20:T:52:THR:HG23	2.16	0.46
20:T:90:TYR:CD1	22:V:112:LYS:CB	2.92	0.46
20:T:87:LEU:CD1	20:T:90:TYR:HD2	2.08	0.46
25:Y:110:SER:HB3	25:Y:212:TYR:HD1	1.81	0.46
25:Y:627:PHE:CD1	25:Y:654:LEU:CD1	2.96	0.46
1:A:883:LEU:HD23	1:A:1021:LEU:HB2	1.97	0.46
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.98	0.46
4:D:5:THR:HG21	7:G:74:TYR:OH	2.15	0.46
8:H:30:SER:HB3	8:H:36:CYS:HB3	1.98	0.46
18:R:62:PHE:HE2	18:R:201:ALA:HB1	1.65	0.46
20:T:123:ASP:OD1	23:W:132:GLY:HA3	2.16	0.46
20:T:57:VAL:O	20:T:58:GLU:HB3	2.15	0.46
25:Y:68:LYS:CB	25:Y:228:LYS:CB	2.80	0.46
25:Y:615:GLN:N	25:Y:618:ARG:HE	2.12	0.46
26:Z:449:GLU:CB	26:Z:452:LEU:HA	2.46	0.46
1:A:1074:GLU:O	1:A:1077:THR:HB	2.16	0.46
2:B:365:THR:HG21	2:B:370:PHE:CG	2.51	0.46
5:E:65:THR:O	5:E:69:ILE:HD12	2.16	0.46
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.98	0.46
16:P:387:LYS:CA	16:P:484:ASP:O	2.63	0.46
17:Q:98:ILE:HD11	17:Q:218:ILE:CD1	2.45	0.46
18:R:82:ALA:HB2	18:R:103:SER:HA	1.97	0.46
20:T:53:LEU:CD2	22:V:94:ILE:HG21	2.46	0.46
21:U:166:ARG:O	21:U:169:GLN:HB3	2.16	0.46
22:V:112:LYS:HG2	22:V:113:ASP:N	2.31	0.46
20:T:117:ILE:HD11	22:V:147:LEU:HD11	1.98	0.46
23:W:64:THR:HG23	23:W:65:ASP:N	2.31	0.46
26:Z:305:GLU:HA	26:Z:327:LYS:NZ	2.31	0.46
26:Z:327:LYS:HG3	26:Z:506:ALA:HA	1.97	0.46
26:Z:474:MET:HB2	26:Z:479:GLY:C	2.36	0.46
26:Z:476:PHE:CD2	26:Z:477:LEU:CD1	2.93	0.46
26:Z:453:VAL:CG2	26:Z:482:TRP:CZ2	2.97	0.46
1:A:180:LYS:CE	1:A:294:SER:HB3	2.46	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD22	1:A:80:HIS:O	2.16	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.97	0.46
3:C:148:ARG:N	3:C:151:GLN:HG3	2.23	0.46
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.98	0.46
2:B:902:GLY:C	12:L:65:VAL:HG11	2.31	0.46
13:M:166:ILE:CA	14:N:95:VAL:HA	2.39	0.46
18:R:203:GLN:O	18:R:204:TYR:C	2.54	0.46
21:U:161:LEU:O	21:U:162:LEU:C	2.53	0.46
20:T:93:ILE:CD1	22:V:126:ILE:HD13	2.30	0.46
25:Y:171:LEU:CB	25:Y:172:PRO:CD	2.93	0.46
25:Y:203:CYS:SG	25:Y:226:VAL:HG23	2.56	0.46
25:Y:350:HIS:O	25:Y:353:SER:OG	2.23	0.46
25:Y:231:ILE:HG22	25:Y:457:ILE:CD1	2.43	0.46
25:Y:37:ASN:C	25:Y:477:THR:OG1	2.54	0.46
26:Z:397:ILE:HD11	26:Z:423:GLN:NE2	2.30	0.46
26:Z:410:LEU:CD1	26:Z:477:LEU:HD11	2.45	0.46
26:Z:424:PHE:HB2	26:Z:435:CYS:SG	2.56	0.46
26:Z:460:VAL:C	26:Z:464:ARG:HE	2.18	0.46
26:Z:524:ILE:HD13	26:Z:524:ILE:H	1.80	0.46
2:B:86:ARG:HG2	2:B:138:GLU:HG3	1.98	0.46
17:Q:167:GLN:O	17:Q:168:ILE:HG13	2.16	0.46
22:V:84:SER:H	22:V:87:LEU:HB2	1.80	0.46
22:V:84:SER:N	22:V:87:LEU:HB2	2.31	0.46
25:Y:21:GLN:CA	25:Y:53:LEU:HD21	2.46	0.46
25:Y:342:LEU:HD23	25:Y:345:ARG:CZ	2.45	0.46
25:Y:39:ILE:HG12	25:Y:458:ILE:CB	2.39	0.46
25:Y:446:ILE:HG21	25:Y:473:LEU:CB	2.46	0.46
26:Z:305:GLU:HB2	26:Z:327:LYS:HZ1	1.81	0.46
26:Z:376:ASN:CB	26:Z:379:ALA:HB3	2.46	0.46
26:Z:516:THR:CA	26:Z:681:ARG:CZ	2.82	0.46
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.46	0.45
1:A:448:PRO:O	1:A:449:SER:CB	2.63	0.45
1:A:923:LEU:O	1:A:927:VAL:HG23	2.16	0.45
9:I:50:THR:HG22	9:I:52:ILE:H	1.82	0.45
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.81	0.45
17:Q:75:LEU:CB	17:Q:98:ILE:HD13	2.33	0.45
20:T:55:LYS:CA	20:T:60:VAL:HG12	2.39	0.45
20:T:97:LEU:HA	20:T:100:ILE:HD11	1.98	0.45
25:Y:656:PHE:HA	25:Y:659:MET:SD	2.56	0.45
26:Z:383:ILE:HD13	26:Z:383:ILE:N	2.31	0.45
26:Z:436:ALA:HB1	26:Z:444:GLU:CB	2.45	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:303:ARG:NH2	26:Z:470:SER:HB2	2.31	0.45
26:Z:659:ASP:CG	26:Z:686:ARG:HD3	2.36	0.45
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.98	0.45
2:B:900:ALA:HB1	12:L:61:THR:OG1	2.16	0.45
12:L:58:LYS:O	12:L:59:ALA:O	2.34	0.45
16:P:581:GLU:CB	16:P:618:LYS:O	2.64	0.45
21:U:26:SER:O	21:U:30:LYS:HG3	2.17	0.45
25:Y:200:ILE:HD11	25:Y:225:GLU:HB3	1.98	0.45
25:Y:229:ASP:CG	25:Y:452:ARG:O	2.55	0.45
25:Y:495:MET:CE	25:Y:696:TRP:HE3	2.30	0.45
25:Y:496:ILE:O	25:Y:686:PHE:HE2	2.00	0.45
25:Y:67:ARG:NH1	25:Y:455:SER:HG	2.09	0.45
26:Z:487:LEU:CD2	26:Z:531:ILE:CD1	2.95	0.45
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.50	0.45
2:B:846:ILE:HG23	2:B:974:PRO:HD2	1.99	0.45
9:I:72:ASP:O	9:I:81:ARG:HG2	2.16	0.45
16:P:340:GLY:O	16:P:354:ILE:CB	2.64	0.45
22:V:83:LEU:HG	22:V:87:LEU:CD1	2.29	0.45
25:Y:109:THR:HG22	25:Y:110:SER:N	2.32	0.45
25:Y:499:LYS:HZ3	25:Y:522:TYR:CA	2.07	0.45
26:Z:339:GLU:O	26:Z:340:GLU:HB2	2.16	0.45
26:Z:424:PHE:CD1	26:Z:450:SER:CB	2.93	0.45
26:Z:474:MET:CB	26:Z:481:GLU:N	2.80	0.45
26:Z:475:ASP:N	26:Z:478:THR:H	2.15	0.45
26:Z:517:LEU:HD22	26:Z:534:LYS:HB3	1.98	0.45
3:C:55:THR:HB	3:C:151:GLN:HA	1.99	0.45
4:D:31:GLN:O	4:D:34:GLN:HB2	2.17	0.45
19:S:103:GLN:O	19:S:104:ILE:C	2.54	0.45
22:V:146:LYS:CG	23:W:129:PHE:CE1	2.86	0.45
25:Y:670:LEU:C	25:Y:670:LEU:HD23	2.37	0.45
25:Y:495:MET:CG	25:Y:686:PHE:CB	2.73	0.45
26:Z:408:ILE:CG1	26:Z:466:ARG:CZ	2.95	0.45
26:Z:484:PHE:HZ	26:Z:511:LEU:CB	2.27	0.45
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.99	0.45
17:Q:89:ILE:O	17:Q:92:SER:OG	2.20	0.45
18:R:200:LEU:HD13	18:R:201:ALA:N	2.32	0.45
20:T:63:PHE:CE1	20:T:66:ASN:OD1	2.70	0.45
25:Y:462:THR:HG22	25:Y:462:THR:O	2.17	0.45
26:Z:408:ILE:CG2	26:Z:476:PHE:H	2.29	0.45
26:Z:474:MET:CG	26:Z:505:ILE:CG2	2.94	0.45
26:Z:474:MET:HG3	26:Z:479:GLY:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:476:PHE:CE1	26:Z:502:VAL:CG2	2.94	0.45
26:Z:499:ARG:CG	26:Z:530:LEU:CD1	2.95	0.45
1:A:16:GLU:CD	4:D:14:ARG:HH12	2.16	0.45
16:P:410:VAL:CB	16:P:501:ALA:C	2.84	0.45
20:T:111:THR:CG2	20:T:112:ARG:N	2.79	0.45
20:T:94:TYR:CD2	22:V:109:GLU:CB	2.98	0.45
21:U:127:LEU:O	21:U:131:LEU:HD23	2.17	0.45
25:Y:343:LYS:HA	25:Y:346:MET:HE2	1.99	0.45
25:Y:281:LYS:HE2	25:Y:345:ARG:HB3	1.98	0.45
25:Y:346:MET:CB	25:Y:384:LEU:CD2	2.91	0.45
25:Y:445:ALA:O	25:Y:448:PRO:CD	2.65	0.45
25:Y:68:LYS:NZ	25:Y:228:LYS:CE	2.80	0.45
26:Z:434:ASN:N	26:Z:434:ASN:HD22	2.15	0.45
26:Z:466:ARG:HE	26:Z:475:ASP:HB3	1.81	0.45
26:Z:476:PHE:CE1	26:Z:487:LEU:CG	3.00	0.45
13:M:140:GLY:O	13:M:151:GLN:N	2.45	0.45
16:P:618:LYS:O	16:P:619:ILE:CB	2.65	0.45
20:T:90:TYR:CE1	22:V:112:LYS:CD	2.94	0.45
25:Y:238:HIS:CE1	25:Y:239:ASN:OD1	2.69	0.45
25:Y:352:ILE:O	25:Y:356:PRO:HD2	1.98	0.45
26:Z:476:PHE:HA	26:Z:485:ILE:HG21	1.98	0.45
26:Z:484:PHE:CD1	26:Z:486:ILE:HG13	2.52	0.45
26:Z:373:MET:CE	26:Z:511:LEU:CD1	2.95	0.45
2:B:89:GLU:HB2	2:B:135:ARG:HB2	1.99	0.45
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.46	0.45
2:B:1184:GLY:C	4:D:17:LYS:NZ	2.69	0.45
7:G:98:GLY:HA3	7:G:110:VAL:O	2.17	0.45
12:L:30:ILE:HG22	12:L:31:CYS:N	2.32	0.45
13:M:189:TYR:C	13:M:191:LEU:H	2.21	0.45
18:R:4:SER:OG	18:R:200:LEU:HD23	2.17	0.45
19:S:22:ALA:O	19:S:26:ASN:CB	2.64	0.45
22:V:140:LEU:CD2	22:V:140:LEU:C	2.85	0.45
23:W:83:VAL:CG2	23:W:84:ASP:H	2.26	0.45
25:Y:467:ASP:HB3	25:Y:471:ARG:NH1	2.32	0.45
25:Y:495:MET:HG3	25:Y:681:LEU:CB	2.26	0.45
25:Y:649:ARG:HG3	25:Y:650:GLU:N	2.31	0.45
25:Y:666:LEU:C	25:Y:666:LEU:HD13	2.37	0.45
26:Z:406:SER:HA	26:Z:447:GLN:C	2.37	0.45
26:Z:408:ILE:CD1	26:Z:466:ARG:CD	2.95	0.45
26:Z:467:SER:OG	26:Z:497:MET:HG2	2.16	0.45
26:Z:474:MET:N	26:Z:480:ARG:N	2.65	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:505:ILE:CG2	26:Z:507:ALA:H	2.10	0.45
26:Z:522:ASP:O	26:Z:524:ILE:HD13	2.17	0.45
26:Z:609:SER:O	26:Z:655:SER:HA	2.16	0.45
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.65	0.45
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.99	0.45
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.99	0.45
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.97	0.45
18:R:188:SER:O	18:R:191:PRO:HD3	2.17	0.45
21:U:156:VAL:CG1	21:U:157:ASN:N	2.79	0.45
22:V:65:PHE:O	22:V:69:ILE:HG13	2.17	0.45
25:Y:229:ASP:HB3	25:Y:453:PHE:HA	1.94	0.45
25:Y:238:HIS:O	25:Y:660:ARG:NH1	2.50	0.45
25:Y:697:ILE:HG22	25:Y:698:ALA:N	2.32	0.45
26:Z:455:SER:CB	26:Z:466:ARG:HD3	2.46	0.45
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.52	0.45
1:A:1356:ILE:HG21	1:A:1363:VAL:HG23	1.99	0.45
1:A:132:LYS:NZ	1:A:1415:SER:HB3	2.30	0.45
1:A:151:ASP:HA	1:A:163:SER:HA	1.99	0.45
1:A:514:PRO:HG2	1:A:1067:LEU:HD11	1.98	0.45
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.80	0.45
2:B:1220:ARG:N	4:D:14:ARG:NH2	2.64	0.45
16:P:315:SER:CB	16:P:425:ILE:H	2.28	0.45
20:T:67:LEU:HB3	20:T:71:LYS:HE2	1.99	0.45
25:Y:337:ARG:NH1	25:Y:345:ARG:NE	2.65	0.45
25:Y:353:SER:OG	25:Y:381:LEU:CA	2.64	0.45
26:Z:303:ARG:HH21	26:Z:470:SER:HB2	1.82	0.45
26:Z:377:GLY:CA	26:Z:381:SER:HB2	2.45	0.45
26:Z:474:MET:HB3	26:Z:474:MET:HE2	1.54	0.45
26:Z:487:LEU:CD2	26:Z:531:ILE:HD13	2.47	0.45
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.99	0.44
1:A:42:ASP:O	1:A:44:THR:N	2.50	0.44
2:B:233:PRO:HG2	2:B:234:ILE:HD12	1.99	0.44
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.65	0.44
16:P:183:GLU:N	19:S:77:ARG:CB	2.80	0.44
20:T:46:LEU:CD1	20:T:80:LEU:HD13	2.47	0.44
24:X:21:THR:O	24:X:25:VAL:HG23	2.17	0.44
25:Y:83:LEU:HD13	25:Y:177:SER:HA	1.98	0.44
25:Y:537:MET:HA	25:Y:619:THR:O	2.17	0.44
25:Y:655:SER:HA	25:Y:689:LYS:NZ	2.31	0.44
26:Z:310:ILE:HG12	26:Z:313:VAL:HG23	1.97	0.44
26:Z:299:GLY:HA2	26:Z:347:HIS:N	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:356:LEU:CD2	26:Z:448:THR:CG2	2.95	0.44
26:Z:300:ASP:CG	26:Z:480:ARG:HD3	2.37	0.44
26:Z:476:PHE:CA	26:Z:485:ILE:CG2	2.95	0.44
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.99	0.44
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.44
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.82	0.44
2:B:973:ILE:HG22	2:B:974:PRO:HD2	1.99	0.44
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.99	0.44
11:K:65:HIS:HE1	11:K:67:PHE:CG	2.35	0.44
16:P:315:SER:CB	16:P:425:ILE:CA	2.96	0.44
17:Q:85:LEU:HD21	17:Q:87:PHE:HD1	1.81	0.44
24:X:21:THR:HG22	24:X:22:ARG:N	2.31	0.44
26:Z:466:ARG:HH21	26:Z:476:PHE:HB3	1.81	0.44
1:A:1393:ASN:ND2	1:A:1393:ASN:H	2.15	0.44
1:A:70:CYS:O	1:A:72:GLU:HG2	2.17	0.44
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.44
2:B:64:CYS:HA	2:B:67:SER:HB3	1.98	0.44
1:A:869:GLY:O	5:E:204:THR:HG21	2.18	0.44
6:F:92:ARG:NH1	7:G:63:PRO:HB2	2.12	0.44
13:M:137:SER:HA	13:M:153:TYR:O	2.18	0.44
16:P:238:MET:C	16:P:240:SER:N	2.71	0.44
17:Q:16:TYR:O	17:Q:20:ILE:HG12	2.18	0.44
17:Q:2:VAL:HB	18:R:100:VAL:HG11	1.99	0.44
22:V:100:LEU:HD13	22:V:100:LEU:O	2.17	0.44
22:V:133:LEU:HA	22:V:136:LYS:CE	2.42	0.44
25:Y:124:ARG:O	25:Y:128:VAL:HG23	2.16	0.44
25:Y:200:ILE:C	25:Y:226:VAL:CB	2.85	0.44
25:Y:571:VAL:HG12	25:Y:572:GLU:CG	2.47	0.44
26:Z:310:ILE:HG21	26:Z:313:VAL:HG21	2.00	0.44
26:Z:300:ASP:N	26:Z:347:HIS:HA	2.32	0.44
26:Z:478:THR:CG2	26:Z:479:GLY:H	2.21	0.44
1:A:270:LEU:HA	1:A:270:LEU:HD12	1.69	0.44
1:A:449:SER:HA	1:A:454:SER:HB3	1.98	0.44
2:B:102:VAL:HG23	2:B:112:LEU:HD22	2.00	0.44
3:C:133:ILE:HG21	3:C:236:GLY:HA3	2.00	0.44
6:F:100:GLN:CD	7:G:15:PRO:HG2	2.38	0.44
16:P:323:PHE:O	16:P:338:LYS:CA	2.65	0.44
17:Q:98:ILE:HD12	17:Q:216:LEU:CD2	2.47	0.44
17:Q:224:MET:CE	17:Q:230:LEU:HD12	2.47	0.44
17:Q:232:LEU:CD2	17:Q:253:LEU:HD13	2.47	0.44
17:Q:83:LYS:CG	17:Q:84:PRO:HD2	2.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:46:LEU:HD11	20:T:80:LEU:CD1	2.46	0.44
22:V:113:ASP:C	22:V:114:LEU:CD1	2.86	0.44
25:Y:167:VAL:HG13	25:Y:195:ILE:HG21	1.99	0.44
25:Y:453:PHE:CD2	25:Y:453:PHE:O	2.70	0.44
25:Y:57:ILE:CG2	25:Y:58:ALA:N	2.80	0.44
26:Z:455:SER:CB	26:Z:466:ARG:CG	2.93	0.44
26:Z:473:VAL:CB	26:Z:481:GLU:CG	2.95	0.44
26:Z:501:VAL:CG2	26:Z:502:VAL:N	2.81	0.44
26:Z:601:ARG:HD3	26:Z:696:ARG:HH22	1.82	0.44
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.99	0.44
1:A:743:VAL:O	1:A:747:VAL:HG23	2.16	0.44
2:B:1158:PHE:HE2	2:B:1160:VAL:HG13	1.83	0.44
1:A:11:LEU:CD1	2:B:1195:HIS:NE2	2.80	0.44
2:B:69:LEU:HD22	2:B:425:THR:HG23	2.00	0.44
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.99	0.44
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.99	0.44
1:A:1154:TYR:CE1	9:I:18:GLU:HG3	2.53	0.44
17:Q:197:ASN:HB3	17:Q:202:SER:HB3	1.99	0.44
18:R:27:SER:O	18:R:132:LEU:HD21	2.17	0.44
20:T:46:LEU:CD1	20:T:80:LEU:CD1	2.95	0.44
21:U:111:ASN:OD1	21:U:113:GLN:HG2	2.17	0.44
21:U:73:ASN:C	21:U:75:GLN:H	2.21	0.44
20:T:122:HIS:CB	23:W:130:VAL:C	2.62	0.44
23:W:18:GLN:HA	23:W:21:ALA:HB3	1.99	0.44
25:Y:378:SER:OG	25:Y:381:LEU:HB2	2.14	0.44
26:Z:424:PHE:HE2	26:Z:454:VAL:CG2	2.29	0.44
26:Z:466:ARG:NH2	26:Z:476:PHE:HB3	2.32	0.44
26:Z:535:LEU:HG	26:Z:535:LEU:O	2.18	0.44
26:Z:609:SER:OG	26:Z:615:LEU:HB2	2.18	0.44
1:A:337:ARG:NH1	2:B:1132:GLU:OE1	2.49	0.44
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.82	0.44
16:P:566:VAL:C	16:P:569:ILE:H	2.21	0.44
18:R:138:ARG:HB2	18:R:154:GLU:HB3	2.00	0.44
17:Q:196:LYS:NZ	18:R:75:ASN:HB2	2.32	0.44
21:U:166:ARG:O	21:U:169:GLN:N	2.50	0.44
25:Y:416:PHE:HE2	25:Y:440:LEU:CG	2.22	0.44
25:Y:59:TYR:CA	25:Y:62:HIS:CE1	2.76	0.44
26:Z:421:ARG:HE	26:Z:430:LEU:CD1	2.22	0.44
26:Z:434:ASN:O	26:Z:452:LEU:HG	2.18	0.44
26:Z:455:SER:HB3	26:Z:466:ARG:CG	2.48	0.44
1:A:343:LYS:NZ	2:B:1156:ASP:HB2	2.33	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:766:ARG:NH2	2:B:1020:ARG:HD3	2.33	0.44
2:B:351:TYR:OH	2:B:355:ILE:HD11	2.18	0.44
1:A:1443:VAL:CG1	6:F:132:LEU:HB3	2.48	0.44
16:P:625:GLU:O	16:P:626:HIS:CB	2.66	0.44
17:Q:256:TYR:C	17:Q:257:ILE:HG13	2.37	0.44
17:Q:259:VAL:HG21	17:Q:268:ILE:HD12	2.00	0.44
20:T:126:LYS:CB	23:W:132:GLY:O	2.66	0.44
21:U:31:LEU:HB3	21:U:32:PRO:HD3	1.99	0.44
23:W:30:HIS:O	23:W:33:GLU:N	2.50	0.44
23:W:94:ILE:HG13	23:W:95:ASP:H	1.76	0.44
25:Y:200:ILE:CD1	25:Y:226:VAL:N	2.81	0.44
25:Y:493:LEU:HB3	25:Y:696:TRP:NE1	2.33	0.44
26:Z:366:GLN:HE22	26:Z:394:LEU:HD22	1.82	0.44
26:Z:470:SER:HA	26:Z:478:THR:CB	2.48	0.44
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.44
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.44
6:F:131:PRO:CG	7:G:18:PHE:HD2	2.31	0.44
14:N:62:TRP:O	14:N:64:THR:N	2.51	0.44
16:P:451:LEU:O	16:P:453:ILE:N	2.50	0.44
25:Y:352:ILE:HB	25:Y:380:ARG:CD	2.48	0.44
25:Y:686:PHE:CD1	25:Y:687:SER:N	2.85	0.44
25:Y:708:LEU:HD23	25:Y:708:LEU:O	2.18	0.44
26:Z:299:GLY:C	26:Z:347:HIS:HB3	2.38	0.44
26:Z:456:THR:CG2	26:Z:457:TYR:H	2.30	0.44
26:Z:629:GLY:N	26:Z:657:VAL:HG11	2.33	0.44
26:Z:701:PHE:CZ	26:Z:732:ALA:CB	3.01	0.44
1:A:1436:ILE:C	1:A:1436:ILE:CD1	2.86	0.44
1:A:66:LYS:CE	1:A:68:GLN:H	2.31	0.44
1:A:22:PHE:HD2	2:B:1211:ASN:HA	1.83	0.44
10:J:36:LEU:HD11	10:J:51:LEU:HB2	1.99	0.44
14:N:194:LYS:HG3	14:N:194:LYS:O	2.18	0.44
17:Q:97:LYS:CG	17:Q:243:ASN:ND2	2.64	0.44
21:U:112:TYR:HD2	21:U:165:TYR:HD1	1.65	0.44
20:T:126:LYS:HB2	23:W:132:GLY:O	2.18	0.44
25:Y:273:GLU:O	25:Y:274:VAL:C	2.56	0.44
25:Y:533:THR:HA	25:Y:534:PRO:HD2	1.80	0.44
25:Y:539:VAL:HG12	25:Y:623:ILE:HG12	1.92	0.44
25:Y:697:ILE:HG22	25:Y:698:ALA:O	2.18	0.44
26:Z:383:ILE:C	26:Z:384:ILE:HD12	2.39	0.44
26:Z:303:ARG:CD	26:Z:504:THR:CG2	2.94	0.44
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.53	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.48	0.43
1:A:95:PHE:HE1	1:A:1414:ALA:CB	2.31	0.43
2:B:125:SER:HA	2:B:171:PRO:HA	2.00	0.43
2:B:468:GLU:HG2	2:B:469:GLN:HB2	1.99	0.43
3:C:47:ASP:C	12:L:69:ALA:HB2	2.37	0.43
20:T:55:LYS:HZ2	20:T:60:VAL:HG13	1.82	0.43
20:T:77:ASP:O	20:T:81:PHE:HD2	2.01	0.43
20:T:82:GLU:HG3	20:T:83:ASN:N	2.32	0.43
22:V:90:LEU:O	22:V:94:ILE:HG13	2.17	0.43
25:Y:127:THR:CG2	25:Y:361:GLN:OE1	2.64	0.43
25:Y:327:ARG:CB	25:Y:330:HIS:ND1	2.72	0.43
25:Y:653:PHE:CE1	25:Y:654:LEU:HB2	2.53	0.43
26:Z:335:TYR:HB3	26:Z:336:PRO:CD	2.47	0.43
26:Z:473:VAL:O	26:Z:478:THR:CB	2.63	0.43
26:Z:502:VAL:HA	26:Z:505:ILE:CG1	2.47	0.43
1:A:1025:ARG:O	1:A:1035:TYR:HE2	2.01	0.43
1:A:211:PHE:HE2	1:A:234:MET:CE	2.30	0.43
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.48	0.43
1:A:774:ARG:HH21	1:A:797:LYS:HB2	1.83	0.43
12:L:47:ARG:NH1	12:L:47:ARG:HG3	2.33	0.43
16:P:494:PRO:O	16:P:495:LYS:CB	2.66	0.43
20:T:64:LYS:H	20:T:64:LYS:CD	2.31	0.43
22:V:76:ILE:CD1	22:V:97:ARG:CD	2.95	0.43
25:Y:261:THR:HA	25:Y:282:LEU:CD1	2.48	0.43
25:Y:499:LYS:HE2	25:Y:525:MET:CB	2.47	0.43
26:Z:373:MET:CG	26:Z:381:SER:CB	2.95	0.43
26:Z:448:THR:CG2	26:Z:449:GLU:N	2.80	0.43
26:Z:466:ARG:HD2	26:Z:475:ASP:CG	2.39	0.43
26:Z:351:ASP:CB	26:Z:482:TRP:CZ3	2.93	0.43
26:Z:485:ILE:HG23	26:Z:507:ALA:HB1	1.98	0.43
26:Z:476:PHE:CZ	26:Z:493:VAL:CG1	2.97	0.43
26:Z:378:ARG:NH2	26:Z:510:LYS:HE2	2.33	0.43
26:Z:519:ARG:HB2	26:Z:521:ASP:OD1	2.17	0.43
26:Z:372:LYS:HE3	26:Z:536:TYR:CD2	2.53	0.43
26:Z:562:THR:CG2	26:Z:585:PRO:HD2	2.48	0.43
26:Z:656:LYS:CD	26:Z:656:LYS:C	2.86	0.43
1:A:1450:LEU:C	7:G:18:PHE:C	2.66	0.43
1:A:93:VAL:HA	1:A:96:ILE:HD11	2.00	0.43
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.84	0.43
6:F:96:THR:HG1	7:G:64:THR:C	2.04	0.43
7:G:1:MET:HE1	7:G:80:LYS:O	2.16	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.00	0.43
18:R:200:LEU:C	18:R:200:LEU:HD22	2.39	0.43
20:T:102:LYS:HE2	20:T:102:LYS:CA	2.48	0.43
21:U:126:LEU:HD11	23:W:19:PHE:CE2	2.53	0.43
22:V:133:LEU:CA	22:V:136:LYS:HE2	2.43	0.43
25:Y:68:LYS:NZ	25:Y:228:LYS:HE3	2.33	0.43
25:Y:233:ILE:HG12	25:Y:457:ILE:HD12	2.01	0.43
25:Y:338:LEU:HB2	25:Y:341:TYR:HD1	1.84	0.43
25:Y:526:LEU:HD12	25:Y:621:LEU:CD2	2.48	0.43
25:Y:656:PHE:HA	25:Y:659:MET:HG2	1.99	0.43
26:Z:376:ASN:HB3	26:Z:379:ALA:N	2.33	0.43
26:Z:425:LEU:HD12	26:Z:429:THR:HG23	1.96	0.43
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.00	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	2.00	0.43
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.55	0.43
1:A:534:LEU:O	1:A:574:GLY:HA3	2.17	0.43
2:B:226:PHE:HA	2:B:395:GLN:CG	2.49	0.43
5:E:181:ALA:HA	5:E:186:LEU:HD21	2.01	0.43
1:A:1444:MET:HE1	6:F:135:ARG:HE	1.83	0.43
4:D:7:THR:HG23	7:G:7:LEU:HD23	1.99	0.43
16:P:355:ALA:O	16:P:367:ASP:N	2.51	0.43
18:R:22:ASP:C	18:R:24:LEU:H	2.22	0.43
21:U:178:LEU:HB2	23:W:97:LEU:HD13	2.00	0.43
20:T:118:LEU:HD23	23:W:129:PHE:HB3	1.91	0.43
23:W:85:VAL:HG13	23:W:89:GLU:HB3	2.00	0.43
25:Y:72:CYS:SG	25:Y:210:TYR:CE1	3.03	0.43
25:Y:436:ARG:CG	25:Y:437:PHE:N	2.81	0.43
25:Y:21:GLN:CB	25:Y:53:LEU:HD21	2.48	0.43
25:Y:639:LEU:CG	25:Y:649:ARG:HB2	2.48	0.43
26:Z:410:LEU:HG	26:Z:457:TYR:CE1	2.52	0.43
1:A:497:THR:HG22	2:B:1146:PHE:CD1	2.42	0.43
2:B:980:PHE:CD1	2:B:1094:ARG:HA	2.54	0.43
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
2:B:900:ALA:CB	12:L:61:THR:OG1	2.67	0.43
1:A:1443:VAL:HG13	6:F:133:VAL:O	2.18	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HG13	2.00	0.43
8:H:4:THR:HA	8:H:60:ALA:HB2	2.00	0.43
14:N:106:HIS:C	14:N:108:SER:H	2.20	0.43
17:Q:188:THR:HG21	18:R:104:ILE:HD13	2.00	0.43
17:Q:61:PRO:O	17:Q:300:VAL:HG23	2.18	0.43
20:T:90:TYR:CD1	20:T:90:TYR:N	2.81	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:95:ASP:O	23:W:98:GLN:HB2	2.18	0.43
25:Y:657:ASP:O	25:Y:661:HIS:HD2	2.02	0.43
26:Z:438:PHE:HE1	26:Z:469:ASP:OD2	2.01	0.43
2:B:955:THR:HG22	2:B:956:THR:N	2.34	0.43
3:C:165:LYS:O	11:K:6:ARG:NH1	2.46	0.43
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.48	0.43
16:P:238:MET:O	16:P:240:SER:N	2.52	0.43
17:Q:265:ILE:H	17:Q:265:ILE:CD1	2.15	0.43
17:Q:79:THR:O	17:Q:82:ASP:CA	2.67	0.43
20:T:111:THR:HA	22:V:143:LEU:CD2	2.29	0.43
20:T:42:LEU:HD23	22:V:105:ILE:HD11	1.91	0.43
22:V:145:ARG:O	22:V:149:ARG:HG3	2.18	0.43
22:V:71:TYR:CE2	22:V:75:GLN:NE2	2.87	0.43
25:Y:212:TYR:O	25:Y:218:ILE:HG21	2.18	0.43
25:Y:568:LEU:HB2	25:Y:598:LEU:HD23	2.00	0.43
26:Z:474:MET:HG3	26:Z:505:ILE:HG22	2.01	0.43
26:Z:619:ALA:CA	26:Z:622:MET:CE	2.96	0.43
26:Z:677:TYR:HA	26:Z:678:GLY:HA2	1.51	0.43
1:A:1148:ILE:HA	9:I:49:ILE:HD12	2.00	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.53	0.43
2:B:1143:ALA:HB1	2:B:1146:PHE:HB3	2.01	0.43
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.86	0.43
13:M:138:GLY:O	13:M:153:TYR:N	2.48	0.43
17:Q:158:ASN:C	17:Q:159:GLU:HG3	2.39	0.43
18:R:120:GLN:CD	18:R:122:ILE:HD11	2.39	0.43
18:R:139:LEU:HD23	18:R:153:ILE:HG23	2.00	0.43
18:R:62:PHE:HZ	18:R:201:ALA:CA	2.32	0.43
19:S:103:GLN:C	19:S:105:GLU:N	2.72	0.43
20:T:42:LEU:CD2	22:V:105:ILE:HD12	2.26	0.43
25:Y:191:CYS:O	25:Y:195:ILE:HG13	2.18	0.43
25:Y:123:GLU:O	25:Y:376:PHE:CZ	2.71	0.43
25:Y:453:PHE:CG	25:Y:453:PHE:O	2.70	0.43
25:Y:232:VAL:O	25:Y:457:ILE:CB	2.64	0.43
25:Y:670:LEU:HD21	25:Y:672:GLY:O	2.19	0.43
26:Z:424:PHE:HD1	26:Z:450:SER:HB3	1.75	0.43
26:Z:696:ARG:NH1	26:Z:704:PHE:HE1	1.69	0.43
26:Z:675:SER:CB	26:Z:722:ARG:HH22	2.31	0.43
1:A:449:SER:HA	1:A:454:SER:CB	2.49	0.43
1:A:58:LEU:HB3	1:A:59:GLY:H	1.25	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	2.01	0.43
2:B:542:MET:HE3	2:B:636:PRO:HG2	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:43:ARG:HH21	18:R:117:MET:CE	2.17	0.43
22:V:135:ILE:CG2	22:V:136:LYS:N	2.82	0.43
22:V:76:ILE:CG2	22:V:77:ARG:N	2.82	0.43
25:Y:237:ALA:CA	25:Y:240:ILE:HG12	2.49	0.43
25:Y:289:LEU:HD22	25:Y:435:MET:HG3	2.00	0.43
25:Y:339:ILE:O	25:Y:343:LYS:HG3	2.18	0.43
25:Y:481:LYS:HD3	25:Y:483:TYR:CZ	2.51	0.43
25:Y:708:LEU:HD23	25:Y:708:LEU:C	2.39	0.43
25:Y:89:LEU:O	25:Y:101:GLU:N	2.52	0.43
26:Z:372:LYS:HE3	26:Z:536:TYR:HD2	1.83	0.43
26:Z:373:MET:SD	26:Z:511:LEU:HD13	2.59	0.43
1:A:709:THR:HB	1:A:712:GLU:H	1.83	0.43
3:C:251:LEU:O	3:C:255:VAL:HG23	2.19	0.43
1:A:358:ASN:HB2	11:K:65:HIS:HD2	1.84	0.43
20:T:79:ALA:HA	20:T:82:GLU:HG2	2.00	0.43
25:Y:639:LEU:HD23	25:Y:639:LEU:C	2.39	0.43
25:Y:656:PHE:CA	25:Y:659:MET:HE3	2.48	0.43
1:A:306:ASN:O	1:A:313:GLN:HG2	2.19	0.43
1:A:33:ALA:HB2	1:A:57:ARG:HB2	2.01	0.43
17:Q:61:PRO:HG2	17:Q:300:VAL:HG23	1.94	0.43
21:U:144:TYR:OH	23:W:26:ILE:CG2	2.67	0.43
20:T:94:TYR:CD2	22:V:109:GLU:HB3	2.53	0.43
25:Y:244:CYS:O	25:Y:248:LEU:HG	2.18	0.43
25:Y:639:LEU:CD1	25:Y:649:ARG:HH11	2.20	0.43
25:Y:67:ARG:HD2	25:Y:230:SER:CA	2.49	0.43
25:Y:71:TYR:CZ	25:Y:233:ILE:CG2	3.02	0.43
26:Z:303:ARG:NE	26:Z:471:GLN:HG3	2.34	0.43
26:Z:320:ASN:HD22	26:Z:321:GLU:H	1.65	0.43
26:Z:356:LEU:HB3	26:Z:427:TRP:HD1	1.82	0.43
26:Z:421:ARG:CZ	26:Z:430:LEU:HD21	2.49	0.43
26:Z:429:THR:CG2	26:Z:430:LEU:N	2.81	0.43
26:Z:407:VAL:CB	26:Z:451:GLY:HA2	2.48	0.43
26:Z:457:TYR:O	26:Z:458:SER:HB3	2.19	0.43
1:A:11:LEU:HD21	2:B:1195:HIS:HD2	1.84	0.42
1:A:22:PHE:HB2	2:B:1211:ASN:O	2.18	0.42
2:B:171:PRO:HG2	2:B:461:LEU:HD12	2.01	0.42
2:B:1217:TYR:HH	4:D:15:LEU:HA	1.79	0.42
7:G:93:SER:OG	7:G:100:GLU:HB2	2.18	0.42
13:M:188:LEU:C	13:M:190:ASP:N	2.72	0.42
17:Q:83:LYS:HG3	17:Q:84:PRO:CD	2.46	0.42
25:Y:383:LEU:HD23	25:Y:383:LEU:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:625:ILE:CG2	25:Y:626:PRO:HD2	2.49	0.42
25:Y:486:THR:HG21	25:Y:670:LEU:HD21	2.00	0.42
26:Z:427:TRP:CH2	26:Z:450:SER:CB	2.95	0.42
26:Z:474:MET:HB2	26:Z:481:GLU:N	2.34	0.42
26:Z:562:THR:OG1	26:Z:565:PHE:CD1	2.72	0.42
1:A:541:ILE:HG21	1:A:549:MET:CE	2.49	0.42
1:A:729:ALA:HA	1:A:732:LEU:HD12	2.01	0.42
2:B:935:ARG:HD2	2:B:935:ARG:H	1.84	0.42
3:C:148:ARG:HG3	3:C:151:GLN:HG3	2.01	0.42
17:Q:78:GLU:HG2	17:Q:80:MET:N	2.35	0.42
21:U:147:LYS:HA	21:U:147:LYS:HD3	1.61	0.42
21:U:162:LEU:HG	23:W:8:LEU:HD23	2.00	0.42
22:V:112:LYS:CE	22:V:119:PRO:HG3	2.49	0.42
22:V:132:GLU:HA	22:V:135:ILE:HG22	2.02	0.42
23:W:99:LYS:C	23:W:101:LEU:N	2.72	0.42
25:Y:140:GLN:OE1	25:Y:140:GLN:HA	2.19	0.42
25:Y:61:MET:HB2	25:Y:231:ILE:HD11	2.01	0.42
25:Y:660:ARG:O	25:Y:664:GLN:HG2	2.18	0.42
26:Z:378:ARG:N	26:Z:381:SER:CB	2.82	0.42
26:Z:456:THR:CG2	26:Z:457:TYR:N	2.81	0.42
26:Z:477:LEU:CD1	26:Z:477:LEU:N	2.82	0.42
26:Z:327:LYS:CG	26:Z:506:ALA:N	2.82	0.42
1:A:867:ILE:HD13	1:A:1000:LEU:HD11	2.01	0.42
3:C:184:ASN:ND2	3:C:189:THR:O	2.52	0.42
5:E:10:SER:O	5:E:14:ARG:HG3	2.19	0.42
17:Q:287:GLU:HG3	17:Q:287:GLU:O	2.19	0.42
21:U:203:LEU:HA	21:U:203:LEU:HD12	1.92	0.42
25:Y:218:ILE:CG2	25:Y:219:ALA:N	2.82	0.42
26:Z:393:THR:O	26:Z:397:ILE:HG13	2.19	0.42
26:Z:459:MET:HB2	26:Z:464:ARG:CZ	2.49	0.42
26:Z:475:ASP:CA	26:Z:478:THR:H	2.33	0.42
26:Z:562:THR:OG1	26:Z:565:PHE:HB2	2.19	0.42
1:A:332:LYS:HA	1:A:337:ARG:HB2	2.00	0.42
2:B:341:LEU:HD11	2:B:343:ILE:HB	2.02	0.42
2:B:65:GLU:HG3	2:B:66:ASP:H	1.84	0.42
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.85	0.42
8:H:16:ASP:HA	8:H:17:PRO:HD3	1.92	0.42
17:Q:212:GLU:HG2	17:Q:213:PHE:HD1	1.85	0.42
17:Q:236:TRP:NE1	17:Q:245:GLN:HB2	2.33	0.42
17:Q:82:ASP:CG	17:Q:83:LYS:H	2.22	0.42
18:R:48:ASN:HA	18:R:48:ASN:HD22	1.63	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:184:TYR:CE1	25:Y:190:LEU:HD21	2.54	0.42
25:Y:184:TYR:HE1	25:Y:190:LEU:HD21	1.85	0.42
25:Y:288:LYS:HZ2	25:Y:334:PHE:C	2.01	0.42
25:Y:54:SER:C	25:Y:57:ILE:HG22	2.37	0.42
25:Y:75:THR:O	25:Y:79:ILE:HG13	2.19	0.42
26:Z:335:TYR:HD1	26:Z:336:PRO:CD	2.23	0.42
1:A:1447:GLU:HG2	7:G:22:MET:HE3	1.88	0.42
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.84	0.42
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.37	0.42
1:A:1438:THR:HB	2:B:1142:GLY:O	2.19	0.42
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.02	0.42
2:B:169:ARG:HB2	2:B:454:THR:HG23	2.01	0.42
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.84	0.42
17:Q:189:ILE:HG12	18:R:87:ILE:HG23	2.02	0.42
20:T:44:GLU:HA	20:T:44:GLU:OE1	2.19	0.42
25:Y:349:LEU:CD1	25:Y:380:ARG:CD	2.91	0.42
25:Y:252:LEU:C	25:Y:434:ILE:HG23	2.39	0.42
25:Y:515:ASP:HB3	25:Y:516:PRO:HD2	2.01	0.42
25:Y:639:LEU:HD21	25:Y:649:ARG:NH1	2.34	0.42
26:Z:403:ILE:O	26:Z:404:LYS:HD2	2.19	0.42
26:Z:474:MET:O	26:Z:482:TRP:CG	2.73	0.42
26:Z:636:ARG:HE	26:Z:636:ARG:HB2	1.61	0.42
21:U:65:LEU:N	21:U:65:LEU:HD23	2.35	0.42
23:W:92:ARG:O	23:W:93:LYS:C	2.58	0.42
24:X:35:ASN:OD1	24:X:35:ASN:C	2.58	0.42
26:Z:313:VAL:CG1	26:Z:314:HIS:CE1	3.02	0.42
26:Z:397:ILE:HD13	26:Z:423:GLN:HE21	1.83	0.42
26:Z:429:THR:HG22	26:Z:431:GLN:H	1.85	0.42
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.77	0.42
1:A:332:LYS:O	1:A:333:GLU:HB2	2.19	0.42
2:B:915:THR:O	2:B:917:PRO:HD3	2.19	0.42
6:F:82:THR:HG22	6:F:83:PRO:HD2	2.01	0.42
18:R:53:VAL:HG12	18:R:54:SER:N	2.32	0.42
20:T:43:TYR:CE1	22:V:105:ILE:CD1	3.02	0.42
20:T:74:ILE:CG2	20:T:75:ARG:N	2.83	0.42
21:U:113:GLN:OE1	23:W:83:VAL:O	2.38	0.42
23:W:92:ARG:HG3	23:W:93:LYS:N	2.35	0.42
25:Y:108:LEU:HD13	25:Y:196:VAL:HG12	2.02	0.42
25:Y:203:CYS:HG	25:Y:226:VAL:HG23	1.84	0.42
25:Y:335:LEU:N	25:Y:335:LEU:HD13	2.29	0.42
26:Z:383:ILE:HD13	26:Z:533:PRO:C	2.40	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:417:VAL:HG13	26:Z:454:VAL:HG12	1.98	0.42
26:Z:427:TRP:CZ3	26:Z:450:SER:HB2	2.52	0.42
1:A:260:ASP:OD1	1:A:328:ARG:NH2	2.42	0.42
1:A:420:ARG:HH12	17:Q:174:ALA:CB	2.25	0.42
1:A:562:THR:O	1:A:576:GLN:NE2	2.53	0.42
2:B:279:ASP:OD1	2:B:279:ASP:N	2.53	0.42
2:B:841:MET:HG2	2:B:1010:LEU:HD12	2.01	0.42
3:C:99:LEU:HB3	3:C:118:LEU:HD22	2.02	0.42
17:Q:268:ILE:HD12	17:Q:268:ILE:HA	1.84	0.42
18:R:72:ILE:HD11	18:R:202:TYR:HB2	1.84	0.42
20:T:92:ASN:O	20:T:95:ARG:HB2	2.19	0.42
21:U:124:LYS:CG	21:U:125:SER:N	2.83	0.42
21:U:146:ARG:O	21:U:149:GLU:HB3	2.20	0.42
20:T:39:LYS:HZ3	22:V:115:LEU:HA	1.83	0.42
25:Y:499:LYS:HE2	25:Y:525:MET:HB2	2.01	0.42
26:Z:349:ASN:O	26:Z:481:GLU:HA	2.19	0.42
26:Z:638:ASN:O	26:Z:638:ASN:ND2	2.49	0.42
26:Z:717:TYR:C	26:Z:717:TYR:CD1	2.92	0.42
2:B:383:ASN:O	2:B:387:LEU:HB2	2.19	0.42
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.78	0.42
12:L:54:ARG:HG3	12:L:54:ARG:H	1.56	0.42
17:Q:166:LEU:HD23	17:Q:166:LEU:C	2.41	0.42
17:Q:31:PRO:HG3	17:Q:87:PHE:HE1	1.83	0.42
17:Q:81:MET:HG3	17:Q:88:ARG:CZ	2.50	0.42
17:Q:94:THR:HA	17:Q:245:GLN:HE22	1.85	0.42
20:T:63:PHE:CD1	20:T:66:ASN:OD1	2.73	0.42
20:T:97:LEU:HA	20:T:100:ILE:CG1	2.50	0.42
21:U:146:ARG:HD2	21:U:149:GLU:OE1	2.20	0.42
21:U:202:LYS:HA	21:U:202:LYS:HD2	1.91	0.42
21:U:73:ASN:HD22	21:U:75:GLN:CG	2.32	0.42
25:Y:90:MET:CE	25:Y:175:VAL:CG2	2.98	0.42
25:Y:353:SER:OG	25:Y:381:LEU:HD13	2.20	0.42
25:Y:62:HIS:CD2	25:Y:69:ILE:CG1	3.03	0.42
26:Z:407:VAL:CG2	26:Z:408:ILE:N	2.82	0.42
26:Z:427:TRP:HE3	26:Z:427:TRP:H	1.65	0.42
26:Z:424:PHE:CB	26:Z:435:CYS:SG	3.07	0.42
26:Z:481:GLU:O	26:Z:482:TRP:CE3	2.73	0.42
26:Z:327:LYS:HB3	26:Z:504:THR:C	2.39	0.42
26:Z:583:MET:O	26:Z:584:ASN:C	2.57	0.42
1:A:469:ARG:NH2	2:B:991:GLY:O	2.53	0.42
3:C:88:CYS:HB2	3:C:89:GLU:H	1.70	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.02	0.42
16:P:308:TYR:HA	16:P:362:GLU:CB	2.50	0.42
20:T:42:LEU:CD1	20:T:80:LEU:CD1	2.94	0.42
21:U:12:LEU:O	21:U:12:LEU:HG	2.19	0.42
23:W:31:GLY:HA2	23:W:34:ARG:HG2	2.02	0.42
23:W:92:ARG:O	23:W:95:ASP:N	2.53	0.42
25:Y:446:ILE:C	25:Y:448:PRO:HD2	2.41	0.42
25:Y:481:LYS:CD	25:Y:483:TYR:CD2	2.97	0.42
25:Y:59:TYR:CG	25:Y:62:HIS:NE2	2.87	0.42
26:Z:425:LEU:HA	26:Z:429:THR:CA	2.49	0.42
26:Z:473:VAL:H	26:Z:478:THR:HG21	1.80	0.42
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	2.01	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.01	0.41
2:B:986:GLN:OE1	2:B:1016:ALA:HB1	2.20	0.41
2:B:1221:SER:N	4:D:14:ARG:CZ	2.83	0.41
7:G:60:ARG:O	7:G:68:ALA:HA	2.19	0.41
21:U:182:LEU:O	21:U:186:ARG:HG3	2.20	0.41
23:W:13:ASP:O	23:W:14:GLN:C	2.58	0.41
25:Y:131:GLU:OE2	25:Y:361:GLN:NE2	2.49	0.41
25:Y:625:ILE:HG23	25:Y:626:PRO:HD2	2.02	0.41
26:Z:326:VAL:CG1	26:Z:327:LYS:N	2.83	0.41
26:Z:522:ASP:CA	26:Z:524:ILE:CD1	2.95	0.41
2:B:216:GLU:OE2	2:B:404:LYS:HD2	2.20	0.41
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.84	0.41
12:L:61:THR:HG22	12:L:63:ARG:HG2	2.01	0.41
17:Q:55:ARG:O	17:Q:56:ASN:C	2.59	0.41
18:R:22:ASP:C	18:R:24:LEU:N	2.74	0.41
23:W:109:ILE:HG22	23:W:110:GLU:N	2.35	0.41
25:Y:142:LYS:HG2	25:Y:145:LEU:HD21	2.02	0.41
25:Y:168:GLU:HG2	25:Y:199:MET:SD	2.59	0.41
25:Y:494:PRO:O	25:Y:680:VAL:HA	2.20	0.41
26:Z:356:LEU:CD2	26:Z:356:LEU:N	2.83	0.41
26:Z:426:GLN:CA	26:Z:426:GLN:HE21	2.33	0.41
26:Z:448:THR:HG22	26:Z:449:GLU:H	1.83	0.41
1:A:133:LYS:HE3	1:A:1391:ARG:HH12	1.85	0.41
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.01	0.41
2:B:190:TYR:CE2	2:B:196:PRO:HG3	2.55	0.41
2:B:509:ALA:O	2:B:511:PRO:HD3	2.20	0.41
6:F:92:ARG:NH1	7:G:63:PRO:HB3	2.32	0.41
16:P:392:ARG:N	16:P:476:ILE:HA	2.34	0.41
17:Q:187:GLU:HG2	17:Q:188:THR:N	2.34	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:84:VAL:CG1	20:T:85:LYS:N	2.83	0.41
22:V:99:LYS:HZ2	22:V:99:LYS:HB3	1.84	0.41
25:Y:169:ASP:O	25:Y:173:LYS:HB2	2.19	0.41
25:Y:472:MET:HG2	25:Y:642:MET:CE	2.50	0.41
25:Y:639:LEU:CB	25:Y:653:PHE:HE2	2.01	0.41
26:Z:356:LEU:HD21	26:Z:448:THR:CG2	2.50	0.41
26:Z:420:TRP:O	26:Z:424:PHE:CD2	2.73	0.41
26:Z:487:LEU:CD1	26:Z:487:LEU:N	2.82	0.41
26:Z:505:ILE:HD12	26:Z:510:LYS:HZ2	1.83	0.41
26:Z:518:VAL:CG1	26:Z:519:ARG:N	2.83	0.41
1:A:1390:ASN:O	1:A:1399:ARG:HD2	2.20	0.41
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.19	0.41
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.03	0.41
2:B:1166:CYS:O	2:B:1168:LEU:N	2.42	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
2:B:848:ARG:HD2	10:J:8:PHE:O	2.20	0.41
3:C:125:MET:HB2	3:C:127:ARG:NE	2.36	0.41
16:P:238:MET:C	16:P:240:SER:H	2.24	0.41
17:Q:44:ASN:HA	17:Q:210:VAL:CG2	2.51	0.41
17:Q:94:THR:O	17:Q:95:ASN:HB2	2.20	0.41
17:Q:188:THR:HB	18:R:107:ILE:HD12	2.03	0.41
21:U:166:ARG:O	21:U:167:PRO:C	2.57	0.41
20:T:100:ILE:HD11	22:V:129:ARG:HG3	1.99	0.41
22:V:91:THR:HA	22:V:94:ILE:HD12	2.02	0.41
23:W:74:ASN:O	23:W:75:LYS:C	2.59	0.41
25:Y:161:ASN:O	25:Y:167:VAL:CG2	2.65	0.41
25:Y:458:ILE:HG21	25:Y:469:TYR:CZ	2.55	0.41
26:Z:356:LEU:H	26:Z:356:LEU:HD22	1.84	0.41
26:Z:457:TYR:CE2	26:Z:492:VAL:HB	2.56	0.41
26:Z:638:ASN:ND2	26:Z:638:ASN:C	2.73	0.41
1:A:1404:GLU:HB3	1:A:1408:ILE:HG13	2.02	0.41
1:A:270:LEU:O	1:A:274:ILE:HG13	2.19	0.41
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.36	0.41
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.86	0.41
20:T:97:LEU:CA	20:T:100:ILE:HG12	2.50	0.41
22:V:147:LEU:C	22:V:147:LEU:HD23	2.41	0.41
23:W:22:THR:O	23:W:24:ASN:N	2.53	0.41
25:Y:335:LEU:HD23	25:Y:335:LEU:O	2.20	0.41
25:Y:419:ILE:CD1	25:Y:435:MET:HE2	2.44	0.41
25:Y:37:ASN:C	25:Y:477:THR:HG1	2.24	0.41
25:Y:496:ILE:CG2	25:Y:704:ALA:HB2	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:296:VAL:HG12	26:Z:297:ILE:N	2.34	0.41
26:Z:316:PHE:HZ	26:Z:321:GLU:HG2	1.86	0.41
26:Z:300:ASP:H	26:Z:347:HIS:HA	1.85	0.41
26:Z:415:VAL:CG1	26:Z:416:SER:N	2.83	0.41
26:Z:474:MET:H	26:Z:480:ARG:N	2.18	0.41
26:Z:328:LYS:HA	26:Z:505:ILE:O	2.21	0.41
26:Z:328:LYS:CD	26:Z:530:LEU:HD23	2.50	0.41
26:Z:698:ASP:O	26:Z:699:GLU:CB	2.68	0.41
1:A:1094:VAL:HG22	1:A:1113:THR:HB	2.03	0.41
1:A:262:LEU:HG	1:A:328:ARG:NH2	2.35	0.41
1:A:497:THR:CG2	2:B:1146:PHE:CD1	3.03	0.41
1:A:11:LEU:HA	2:B:1193:GLN:O	2.19	0.41
1:A:11:LEU:HD21	2:B:1195:HIS:CD2	2.55	0.41
1:A:1444:MET:CG	7:G:61:ILE:O	2.68	0.41
20:T:43:TYR:CD2	22:V:102:LYS:CD	3.03	0.41
20:T:89:GLU:CD	20:T:89:GLU:H	2.24	0.41
20:T:94:TYR:HE2	20:T:98:GLN:HE21	1.67	0.41
21:U:73:ASN:HD22	21:U:75:GLN:HG3	1.85	0.41
25:Y:67:ARG:CD	25:Y:230:SER:HB2	2.50	0.41
25:Y:335:LEU:HD21	25:Y:342:LEU:HG	2.02	0.41
26:Z:344:ARG:NE	26:Z:344:ARG:HA	2.34	0.41
26:Z:354:ILE:CG2	26:Z:355:ASP:N	2.82	0.41
26:Z:403:ILE:O	26:Z:404:LYS:HG3	2.21	0.41
26:Z:452:LEU:CD2	26:Z:452:LEU:C	2.88	0.41
1:A:10:PRO:HG2	2:B:1192:TYR:HD1	1.85	0.41
1:A:340:LEU:CD2	2:B:1199:ALA:HB3	2.50	0.41
1:A:34:LYS:HG2	1:A:36:ARG:NH1	2.36	0.41
2:B:311:LEU:HB3	9:I:4:PHE:HE2	1.85	0.41
2:B:904:ARG:HG3	2:B:948:ILE:HG13	2.02	0.41
4:D:194:LEU:O	4:D:196:PRO:HD3	2.21	0.41
6:F:92:ARG:NH2	7:G:63:PRO:C	2.73	0.41
16:P:425:ILE:HA	16:P:428:GLN:CB	2.50	0.41
17:Q:97:LYS:CE	17:Q:237:GLN:O	2.68	0.41
17:Q:78:GLU:CD	17:Q:80:MET:HB3	2.41	0.41
18:R:46:ILE:CD1	18:R:47:LYS:HZ1	2.33	0.41
18:R:52:ASP:OD1	18:R:53:VAL:N	2.53	0.41
21:U:118:GLU:O	21:U:119:LEU:C	2.59	0.41
21:U:121:LYS:O	21:U:124:LYS:N	2.53	0.41
25:Y:257:LEU:HD23	25:Y:257:LEU:HA	1.90	0.41
25:Y:353:SER:HB2	25:Y:381:LEU:H	1.85	0.41
25:Y:546:TYR:O	25:Y:550:ILE:HG12	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:57:ILE:O	25:Y:57:ILE:HD13	2.21	0.41
1:A:332:LYS:HA	1:A:337:ARG:CB	2.50	0.41
1:A:567:LYS:HA	1:A:568:PRO:C	2.41	0.41
2:B:642:ASP:HA	2:B:649:LYS:HA	2.02	0.41
2:B:789:MET:HG3	2:B:953:LEU:HD21	2.02	0.41
2:B:1111:MET:O	3:C:57:VAL:HG12	46.11	0.41
10:J:22:LEU:O	10:J:26:GLN:HG2	2.20	0.41
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.03	0.41
13:M:178:SER:O	16:P:214:ALA:CB	2.69	0.41
20:T:93:ILE:HD13	22:V:122:TRP:CG	2.54	0.41
25:Y:103:PHE:CD1	25:Y:205:ILE:CD1	2.86	0.41
25:Y:327:ARG:CB	25:Y:330:HIS:HD1	2.31	0.41
25:Y:420:ILE:HG13	25:Y:633:ARG:NH1	2.21	0.41
25:Y:231:ILE:HG23	25:Y:457:ILE:HD11	1.93	0.41
26:Z:478:THR:CG2	26:Z:479:GLY:N	2.81	0.41
26:Z:519:ARG:CG	26:Z:524:ILE:CG2	2.95	0.41
2:B:1082:MET:HA	3:C:189:THR:HA	2.03	0.41
20:T:77:ASP:O	20:T:81:PHE:CD2	2.74	0.41
21:U:70:MET:SD	24:X:23:PHE:CE2	3.09	0.41
23:W:22:THR:C	23:W:24:ASN:N	2.74	0.41
25:Y:622:MET:CG	25:Y:679:MET:HE2	2.50	0.41
26:Z:316:PHE:CE2	26:Z:317:GLU:O	2.74	0.41
26:Z:326:VAL:HG12	26:Z:327:LYS:H	1.84	0.41
26:Z:434:ASN:O	26:Z:452:LEU:CG	2.69	0.41
26:Z:475:ASP:OD1	26:Z:482:TRP:CD1	2.73	0.41
26:Z:528:ASN:CG	26:Z:533:PRO:HB3	2.41	0.41
1:A:369:SER:HB3	11:K:2:ASN:OD1	2.21	0.41
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.94	0.41
1:A:354:SER:O	1:A:469:ARG:HA	2.21	0.41
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.83	0.41
2:B:199:MET:N	2:B:199:MET:SD	2.90	0.41
2:B:856:PHE:CE2	2:B:969:ARG:HG3	2.55	0.41
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.03	0.41
6:F:131:PRO:HG2	7:G:18:PHE:HD2	1.86	0.41
10:J:28:ASP:C	10:J:30:LEU:H	2.24	0.41
17:Q:86:ASN:C	17:Q:89:ILE:HG12	2.41	0.41
20:T:60:VAL:CG2	20:T:61:ASP:N	2.83	0.41
22:V:66:ILE:O	22:V:70:PHE:HD1	2.03	0.41
25:Y:123:GLU:O	25:Y:376:PHE:HZ	2.04	0.41
25:Y:529:PHE:HD1	25:Y:529:PHE:N	2.19	0.41
25:Y:631:GLU:HG2	25:Y:636:LYS:NZ	2.36	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:328:LYS:HG3	26:Z:329:ARG:N	2.35	0.41
26:Z:435:CYS:HA	26:Z:452:LEU:HG	2.01	0.41
26:Z:449:GLU:HB3	26:Z:451:GLY:C	2.41	0.41
26:Z:484:PHE:HE1	26:Z:486:ILE:CG1	2.29	0.41
26:Z:484:PHE:CE1	26:Z:485:ILE:O	2.74	0.41
26:Z:474:MET:CG	26:Z:505:ILE:HG22	2.51	0.41
26:Z:524:ILE:CD1	26:Z:524:ILE:H	2.33	0.41
1:A:243:PRO:HB2	1:A:245:PRO:HD2	2.02	0.41
1:A:36:ARG:NH2	1:A:57:ARG:NH2	2.69	0.41
1:A:227:VAL:HG11	4:D:16:LYS:HE3	2.02	0.41
4:D:43:GLU:HG3	4:D:43:GLU:H	1.70	0.41
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.56	0.41
11:K:39:ASP:OD1	11:K:41:THR:HB	2.21	0.41
16:P:479:LEU:C	16:P:481:LEU:N	2.74	0.41
21:U:144:TYR:OH	23:W:26:ILE:HG22	2.21	0.41
24:X:37:GLN:O	24:X:40:THR:HB	2.20	0.41
25:Y:537:MET:SD	25:Y:621:LEU:CD1	2.89	0.41
25:Y:603:ARG:NH2	25:Y:629:TYR:HH	2.13	0.41
26:Z:485:ILE:CG1	26:Z:510:LYS:HA	2.50	0.41
1:A:1447:GLU:CB	7:G:22:MET:SD	3.07	0.40
1:A:36:ARG:NH2	1:A:57:ARG:CZ	2.81	0.40
1:A:441:PRO:HD2	1:A:498:ARG:CZ	2.51	0.40
2:B:979:LYS:HD3	2:B:1095:LEU:HD13	2.03	0.40
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.03	0.40
5:E:178:ILE:HG12	5:E:185:ALA:HB2	2.03	0.40
9:I:8:ARG:O	9:I:9:ASP:CB	2.69	0.40
13:M:167:PHE:HA	13:M:170:VAL:CB	2.50	0.40
17:Q:236:TRP:CD1	17:Q:245:GLN:HB2	2.56	0.40
18:R:79:VAL:HG21	18:R:198:CYS:SG	2.61	0.40
20:T:97:LEU:O	20:T:100:ILE:HG12	2.20	0.40
20:T:121:CYS:SG	20:T:122:HIS:N	2.94	0.40
22:V:125:ILE:CG2	22:V:126:ILE:HD12	2.39	0.40
22:V:143:LEU:HD12	22:V:144:TYR:CA	2.50	0.40
24:X:84:LEU:HD23	24:X:84:LEU:HA	1.76	0.40
25:Y:106:LEU:HD13	25:Y:107:GLY:O	2.22	0.40
25:Y:216:PRO:O	25:Y:220:GLU:HG2	2.22	0.40
25:Y:274:VAL:CG1	25:Y:275:ARG:N	2.73	0.40
25:Y:666:LEU:HD13	25:Y:666:LEU:O	2.21	0.40
26:Z:429:THR:HB	26:Z:432:PRO:CG	2.51	0.40
26:Z:519:ARG:N	26:Z:524:ILE:CG2	2.84	0.40
1:A:1196:GLU:HA	1:A:1236:LEU:O	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.36	0.40
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.56	0.40
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.86	0.40
2:B:681:TRP:HA	2:B:684:LEU:HD12	2.03	0.40
13:M:138:GLY:O	13:M:152:ASP:CB	2.69	0.40
16:P:196:THR:CB	16:P:200:PHE:H	2.33	0.40
14:N:100:LYS:CB	16:P:251:PRO:CB	2.99	0.40
21:U:182:LEU:HG	21:U:186:ARG:NH1	2.36	0.40
20:T:126:LYS:HG3	23:W:133:ILE:HB	2.03	0.40
25:Y:259:ARG:CB	25:Y:379:GLU:OE2	2.60	0.40
25:Y:418:LEU:HD12	25:Y:438:THR:HG1	1.72	0.40
25:Y:515:ASP:HB2	25:Y:518:ILE:HG13	2.03	0.40
26:Z:335:TYR:CZ	26:Z:339:GLU:OE2	2.74	0.40
26:Z:387:PRO:HD2	26:Z:390:ALA:HB2	2.03	0.40
1:A:346:ASP:OD1	2:B:1106:ARG:NH2	2.54	0.40
2:B:344:LYS:HB3	2:B:347:LYS:HB2	2.04	0.40
6:F:97:ARG:HA	6:F:97:ARG:HD2	1.82	0.40
2:B:622:LYS:HE3	9:I:59:VAL:HG22	2.02	0.40
3:C:69:LEU:HD23	10:J:6:ARG:HB2	2.04	0.40
13:M:113:THR:N	13:M:120:VAL:O	2.50	0.40
16:P:323:PHE:O	16:P:338:LYS:HA	2.21	0.40
20:T:123:ASP:OD1	23:W:132:GLY:HA2	2.20	0.40
20:T:86:LEU:O	20:T:90:TYR:CE2	2.74	0.40
21:U:194:GLN:O	21:U:197:LYS:N	2.53	0.40
22:V:112:LYS:CG	22:V:113:ASP:H	2.35	0.40
22:V:71:TYR:HE2	22:V:75:GLN:NE2	2.19	0.40
25:Y:622:MET:CG	25:Y:679:MET:CE	3.00	0.40
26:Z:500:ARG:HA	26:Z:500:ARG:NE	2.30	0.40
26:Z:610:ASP:OD2	26:Z:674:SER:OG	2.39	0.40
2:B:758:PHE:CE2	2:B:1027:ILE:HG22	2.56	0.40
2:B:1219:ASP:O	4:D:14:ARG:NH2	2.54	0.40
2:B:406:LEU:HD12	2:B:633:VAL:HG22	2.03	0.40
2:B:831:SER:HG	2:B:994:TYR:HE2	1.64	0.40
2:B:871:THR:HG22	2:B:872:GLU:O	2.21	0.40
3:C:258:ILE:HG13	11:K:42:LEU:HD21	2.03	0.40
4:D:10:THR:HG22	4:D:12:ARG:HH22	1.87	0.40
8:H:104:PHE:CE1	8:H:136:LYS:HG3	2.57	0.40
14:N:85:HIS:O	14:N:88:GLU:N	2.44	0.40
20:T:55:LYS:CA	20:T:60:VAL:CG1	2.94	0.40
20:T:94:TYR:O	20:T:98:GLN:HG2	2.22	0.40
21:U:161:LEU:O	21:U:164:GLU:N	2.55	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:213:LEU:O	25:Y:219:ALA:HB2	2.21	0.40
25:Y:619:THR:HA	25:Y:678:VAL:O	2.22	0.40
26:Z:305:GLU:HB2	26:Z:327:LYS:HE3	2.03	0.40
26:Z:343:PHE:CD2	26:Z:343:PHE:C	2.95	0.40
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.85	0.40
1:A:886:ILE:HD13	1:A:944:ARG:HG2	2.04	0.40
3:C:18:VAL:CG2	3:C:240:VAL:HB	2.49	0.40
3:C:99:LEU:HD12	3:C:118:LEU:HB3	2.02	0.40
6:F:89:GLU:C	6:F:93:ILE:HD12	2.42	0.40
7:G:83:LYS:HD3	7:G:149:GLY:HA2	2.04	0.40
18:R:47:LYS:HZ3	18:R:47:LYS:N	2.14	0.40
21:U:134:ILE:HD13	21:U:134:ILE:HG21	1.88	0.40
21:U:143:MET:O	21:U:144:TYR:C	2.60	0.40
25:Y:185:CYS:CB	25:Y:190:LEU:O	2.63	0.40
25:Y:338:LEU:HB2	25:Y:341:TYR:HB2	2.02	0.40
25:Y:499:LYS:HD3	25:Y:521:ASN:HB3	2.03	0.40
25:Y:631:GLU:CA	25:Y:636:LYS:HZ1	2.32	0.40
25:Y:493:LEU:HD22	25:Y:696:TRP:NE1	2.23	0.40
26:Z:410:LEU:CD2	26:Z:457:TYR:CD2	2.96	0.40
26:Z:474:MET:SD	26:Z:507:ALA:N	2.95	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 PDB entries followed by that with respect to all EM entries.

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	1414/1733 (82%)	1254 (89%)	112 (8%)	48 (3%)	5	40
2	B	1142/1224 (93%)	1022 (90%)	84 (7%)	36 (3%)	5	41
3	C	264/318 (83%)	242 (92%)	20 (8%)	2 (1%)	24	69
4	D	174/221 (79%)	149 (86%)	17 (10%)	8 (5%)	3	33

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/215 (99%)	195 (92%)	13 (6%)	4 (2%)	10	52
6	F	82/155 (53%)	75 (92%)	7 (8%)	0	100	100
7	G	169/171 (99%)	157 (93%)	9 (5%)	3 (2%)	11	53
8	H	129/146 (88%)	106 (82%)	14 (11%)	9 (7%)	1	22
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	7	45
10	J	63/70 (90%)	51 (81%)	9 (14%)	3 (5%)	3	32
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0	2
13	M	152/295 (52%)	115 (76%)	20 (13%)	17 (11%)	0	11
14	N	164/223 (74%)	133 (81%)	16 (10%)	15 (9%)	1	17
15	O	99/115 (86%)	92 (93%)	4 (4%)	3 (3%)	5	42
16	P	479/687 (70%)	385 (80%)	61 (13%)	33 (7%)	1	23
17	Q	249/307 (81%)	217 (87%)	25 (10%)	7 (3%)	6	44
18	R	207/210 (99%)	190 (92%)	12 (6%)	5 (2%)	7	47
19	S	105/121 (87%)	91 (87%)	7 (7%)	7 (7%)	1	24
20	T	89/284 (31%)	69 (78%)	20 (22%)	0	100	100
21	U	150/222 (68%)	127 (85%)	22 (15%)	1 (1%)	26	71
22	V	83/149 (56%)	73 (88%)	5 (6%)	5 (6%)	2	26
23	W	115/140 (82%)	95 (83%)	18 (16%)	2 (2%)	11	55
24	X	90/127 (71%)	86 (96%)	4 (4%)	0	100	100
25	Y	534/778 (69%)	503 (94%)	23 (4%)	8 (2%)	13	57
26	Z	461/843 (55%)	430 (93%)	26 (6%)	5 (1%)	17	63
27	a	60/513 (12%)	60 (100%)	0	0	100	100
28	b	61/72 (85%)	58 (95%)	3 (5%)	0	100	100
29	c	185/345 (54%)	164 (89%)	19 (10%)	2 (1%)	17	63
30	d	110/286 (38%)	103 (94%)	7 (6%)	0	100	100
31	e	97/122 (80%)	93 (96%)	4 (4%)	0	100	100
32	f	143/735 (20%)	130 (91%)	9 (6%)	4 (3%)	6	44
33	g	164/400 (41%)	148 (90%)	12 (7%)	4 (2%)	7	47
34	h	112/482 (23%)	100 (89%)	10 (9%)	2 (2%)	11	53
35	i	114/328 (35%)	102 (90%)	9 (8%)	3 (3%)	7	45

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	j	178/240 (74%)	170 (96%)	5 (3%)	3 (2%)	11	55
37	k	23/25 (92%)	9 (39%)	6 (26%)	8 (35%)	0	0
All	All	8147/12614 (65%)	7220 (89%)	666 (8%)	261 (3%)	8	41

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	MET
1	A	189	ARG
1	A	195	ASP
1	A	286	HIS
1	A	317	LYS
1	A	449	SER
1	A	628	GLY
1	A	1377	THR
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	344	LYS
2	B	442	PHE
2	B	466	TRP
2	B	473	MET
2	B	531	GLN
2	B	772	ALA
2	B	1046	PRO
2	B	1181	GLU
4	D	18	VAL
4	D	53	SER
4	D	199	ASN
9	I	9	ASP
9	I	95	THR
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
13	M	5	PRO
13	M	7	ASP
13	M	13	SER
13	M	23	ARG
13	M	35	PRO
13	M	98	PRO
13	M	123	PRO

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
13	M	164	PRO
13	M	173	ARG
14	N	25	PHE
14	N	29	PRO
14	N	99	PRO
14	N	109	LEU
14	N	121	GLU
14	N	135	VAL
14	N	140	LEU
15	O	94	ASP
16	P	231	SER
16	P	251	PRO
16	P	252	SER
16	P	349	LYS
16	P	369	ILE
16	P	370	PRO
16	P	381	PHE
16	P	476	ILE
16	P	487	VAL
16	P	494	PRO
16	P	495	LYS
16	P	544	PRO
16	P	615	ARG
16	P	619	ILE
16	P	622	PRO
16	P	626	HIS
17	Q	56	ASN
17	Q	108	ILE
17	Q	177	ASN
17	Q	299	ARG
18	R	204	TYR
19	S	19	VAL
19	S	47	GLU
19	S	102	LYS
19	S	104	ILE
22	V	84	SER
25	Y	494	PRO
25	Y	534	PRO
25	Y	572	GLU
26	Z	447	GLN
26	Z	458	SER
26	Z	699	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	c	200	THR
32	f	136	PRO
32	f	349	PRO
33	g	129	VAL
34	h	149	CYS
35	i	232	VAL
36	j	154	ASP
37	k	4	SER
37	k	14	SER
37	k	21	SER
1	A	40	THR
1	A	44	THR
1	A	51	GLY
1	A	52	GLY
1	A	66	LYS
1	A	68	GLN
1	A	167	CYS
1	A	178	GLY
1	A	193	ASP
1	A	224	PHE
1	A	252	PHE
1	A	254	GLU
1	A	330	LYS
1	A	672	ASP
1	A	1175	SER
1	A	1281	ARG
1	A	1437	GLY
2	B	262	GLU
2	B	282	ILE
2	B	339	THR
2	B	341	LEU
2	B	707	PRO
2	B	731	VAL
2	B	792	MET
2	B	1175	LEU
2	B	1176	ASN
4	D	16	LYS
4	D	52	LEU
4	D	169	SER
5	E	36	GLU
7	G	2	PHE
8	H	17	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
8	H	81	PRO
8	H	82	PRO
8	H	83	GLN
8	H	90	ALA
10	J	6	ARG
12	L	35	SER
13	M	19	VAL
13	M	95	PHE
13	M	131	GLN
13	M	149	PRO
13	M	189	TYR
14	N	137	THR
14	N	138	ALA
15	O	42	GLU
16	P	420	ALA
16	P	457	VAL
16	P	472	GLU
16	P	493	LEU
16	P	585	PRO
16	P	638	PRO
17	Q	109	LEU
17	Q	261	ARG
18	R	187	ASP
22	V	110	ASP
25	Y	268	ASP
26	Z	378	ARG
26	Z	449	GLU
34	h	153	ASP
36	j	78	CYS
37	k	10	TYR
37	k	15	PRO
37	k	19	PRO
37	k	20	THR
1	A	54	ASN
1	A	975	HIS
1	A	1173	HIS
2	B	340	ALA
2	B	343	ILE
2	B	711	GLU
2	B	1155	SER
2	B	1156	ASP
2	B	1157	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1167	GLY
4	D	22	GLU
5	E	45	LYS
5	E	48	ASP
7	G	154	VAL
8	H	18	GLY
12	L	40	LEU
12	L	54	ARG
13	M	160	ILE
14	N	63	TYR
14	N	139	LEU
16	P	239	SER
16	P	392	ARG
16	P	403	TYR
16	P	478	LEU
16	P	627	LYS
18	R	56	LEU
25	Y	230	SER
25	Y	274	VAL
25	Y	483	TYR
32	f	114	MET
32	f	135	LEU
35	i	204	GLY
37	k	9	SER
1	A	69	THR
1	A	72	GLU
1	A	465	TYR
1	A	569	LYS
1	A	846	GLU
1	A	958	VAL
1	A	1255	GLU
1	A	1438	THR
2	B	441	ASP
2	B	648	HIS
2	B	1108	ARG
3	C	88	CYS
9	I	91	ARG
10	J	29	GLU
12	L	43	THR
12	L	56	LEU
12	L	60	ARG
13	M	168	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
14	N	136	THR
16	P	192	GLU
16	P	247	LYS
16	P	248	VAL
16	P	452	LEU
16	P	574	SER
18	R	189	LEU
33	g	60	ASP
35	i	161	GLU
36	j	110	LYS
1	A	156	ASP
1	A	567	LYS
1	A	1171	GLN
1	A	1366	ARG
2	B	251	ILE
2	B	462	ALA
2	B	469	GLN
2	B	1223	ASP
4	D	21	GLU
8	H	60	ALA
8	H	128	ASN
10	J	2	ILE
14	N	123	ASP
15	O	100	GLU
16	P	551	PHE
18	R	135	LEU
19	S	32	ASP
19	S	100	ASP
22	V	111	THR
22	V	118	SER
22	V	119	PRO
33	g	345	TYR
1	A	35	ILE
1	A	155	GLU
1	A	885	THR
3	C	214	ASN
12	L	28	LYS
12	L	46	VAL
21	U	111	ASN
23	W	132	GLY
29	c	164	LYS
1	A	196	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1388	GLY
5	E	90	VAL
7	G	63	PRO
2	B	364	ILE
13	M	122	GLU
23	W	83	VAL
1	A	192	GLY
1	A	448	PRO
2	B	1121	GLY
14	N	28	VAL
14	N	97	PRO
25	Y	533	THR
2	B	1214	PRO
8	H	59	ILE
19	S	58	VAL
17	Q	83	LYS
33	g	343	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1240/1520 (82%)	1071 (86%)	169 (14%)	5	27
2	B	985/1061 (93%)	868 (88%)	117 (12%)	6	31
3	C	234/274 (85%)	206 (88%)	28 (12%)	6	31
4	D	160/200 (80%)	129 (81%)	31 (19%)	2	12
5	E	196/197 (100%)	175 (89%)	21 (11%)	8	36
6	F	74/137 (54%)	67 (90%)	7 (10%)	11	41
7	G	152/152 (100%)	137 (90%)	15 (10%)	10	39
8	H	117/128 (91%)	103 (88%)	14 (12%)	6	31
9	I	113/116 (97%)	106 (94%)	7 (6%)	23	60
10	J	60/65 (92%)	49 (82%)	11 (18%)	2	14
11	K	99/102 (97%)	87 (88%)	12 (12%)	6	31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	40/57 (70%)	37 (92%)	3 (8%)	17	53
13	M	1/259 (0%)	1 (100%)	0	100	100
14	N	16/207 (8%)	14 (88%)	2 (12%)	6	30
17	Q	226/280 (81%)	206 (91%)	20 (9%)	12	45
18	R	177/178 (99%)	162 (92%)	15 (8%)	13	48
20	T	87/258 (34%)	81 (93%)	6 (7%)	19	56
21	U	149/208 (72%)	142 (95%)	7 (5%)	32	68
22	V	84/144 (58%)	80 (95%)	4 (5%)	31	67
23	W	113/132 (86%)	108 (96%)	5 (4%)	35	69
24	X	87/117 (74%)	84 (97%)	3 (3%)	44	75
25	Y	512/707 (72%)	504 (98%)	8 (2%)	70	88
26	Z	412/737 (56%)	375 (91%)	37 (9%)	12	44
27	a	57/468 (12%)	57 (100%)	0	100	100
28	b	57/66 (86%)	57 (100%)	0	100	100
29	c	136/299 (46%)	118 (87%)	18 (13%)	5	28
30	d	107/260 (41%)	104 (97%)	3 (3%)	51	78
31	e	91/108 (84%)	83 (91%)	8 (9%)	12	45
32	f	136/641 (21%)	135 (99%)	1 (1%)	88	94
33	g	162/363 (45%)	157 (97%)	5 (3%)	47	77
34	h	108/429 (25%)	91 (84%)	17 (16%)	3	21
35	i	113/295 (38%)	86 (76%)	27 (24%)	1	7
36	j	152/205 (74%)	143 (94%)	9 (6%)	24	61
37	k	25/25 (100%)	25 (100%)	0	100	100
All	All	6478/10395 (62%)	5848 (90%)	630 (10%)	15	40

All (630) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	15	LYS
1	A	22	PHE
1	A	41	MET
1	A	42	ASP
1	A	53	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	54	ASN
1	A	64	ASN
1	A	66	LYS
1	A	68	GLN
1	A	74	MET
1	A	80	HIS
1	A	93	VAL
1	A	106	VAL
1	A	131	SER
1	A	134	ARG
1	A	147	VAL
1	A	157	ASP
1	A	173	THR
1	A	174	ILE
1	A	175	ARG
1	A	176	LYS
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	219	PHE
1	A	220	THR
1	A	222	LEU
1	A	249	SER
1	A	257	ARG
1	A	265	LYS
1	A	277	GLU
1	A	279	LEU
1	A	307	ASP
1	A	311	GLN
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	398	GLU
1	A	408	ASP
1	A	411	ASP
1	A	412	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	424	ILE
1	A	425	GLN
1	A	434	ARG
1	A	436	ILE
1	A	438	ASP
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	489	LEU
1	A	498	ARG
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	532	ARG
1	A	544	ASP
1	A	566	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	596	THR
1	A	602	ASP
1	A	603	ASN
1	A	618	GLU
1	A	629	LEU
1	A	634	THR
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	691	LEU
1	A	702	LEU
1	A	738	LYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	797	LYS
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	827	THR
1	A	831	THR
1	A	834	THR
1	A	839	ARG
1	A	849	MET
1	A	886	ILE
1	A	896	ARG
1	A	919	ILE
1	A	920	LEU
1	A	948	VAL
1	A	949	ASP
1	A	964	ILE
1	A	973	ILE
1	A	976	THR
1	A	998	LEU
1	A	1009	ASN
1	A	1015	VAL
1	A	1029	ARG
1	A	1030	ARG
1	A	1047	SER
1	A	1058	VAL
1	A	1062	GLU
1	A	1067	LEU
1	A	1078	GLN
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1142	THR
1	A	1173	HIS
1	A	1176	LEU
1	A	1195	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1273	LEU
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1317	MET
1	A	1325	THR
1	A	1327	ILE
1	A	1336	MET
1	A	1341	ILE
1	A	1355	VAL
1	A	1366	ARG
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1405	THR
1	A	1406	VAL
1	A	1426	GLU
1	A	1433	MET
1	A	1438	THR
1	A	1453	TYR
1	A	1454	MET
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	69	LEU
2	B	72	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	73	GLN
2	B	103	ASN
2	B	104	GLU
2	B	110	HIS
2	B	169	ARG
2	B	175	ARG
2	B	178	ASN
2	B	183	GLU
2	B	211	VAL
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	279	ASP
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	337	ARG
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	348	ARG
2	B	357	GLN
2	B	365	THR
2	B	393	LYS
2	B	408	LEU
2	B	419	THR
2	B	440	HIS
2	B	442	PHE
2	B	470	LYS
2	B	476	ARG
2	B	482	VAL
2	B	485	ARG
2	B	487	THR
2	B	529	GLU
2	B	531	GLN
2	B	547	VAL
2	B	552	MET
2	B	563	MET
2	B	570	VAL
2	B	574	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	595	ARG
2	B	596	LEU
2	B	601	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	646	LEU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	680	THR
2	B	696	GLU
2	B	708	GLU
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	771	SER
2	B	776	GLN
2	B	786	ASN
2	B	790	ASP
2	B	791	THR
2	B	801	LYS
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	860	MET
2	B	879	ARG
2	B	933	SER
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	956	THR
2	B	959	ASP
2	B	967	ARG
2	B	975	GLN
2	B	986	GLN
2	B	997	GLU
2	B	999	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	1007	VAL
2	B	1028	GLU
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1084	GLN
2	B	1094	ARG
2	B	1106	ARG
2	B	1123	SER
2	B	1129	ARG
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1193	GLN
2	B	1201	LYS
2	B	1202	LEU
2	B	1210	MET
2	B	1220	ARG
2	B	1223	ASP
3	C	3	GLU
3	C	12	GLU
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	81	GLU
3	C	84	ARG
3	C	100	THR
3	C	101	LEU
3	C	119	VAL
3	C	121	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	124	LEU
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	147	LEU
3	C	148	ARG
3	C	215	GLU
3	C	224	GLN
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	12	ARG
4	D	13	ARG
4	D	17	LYS
4	D	18	VAL
4	D	27	LEU
4	D	32	GLU
4	D	34	GLN
4	D	35	LEU
4	D	40	HIS
4	D	47	LEU
4	D	52	LEU
4	D	53	SER
4	D	65	GLU
4	D	118	THR
4	D	126	ILE
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	153	ARG
4	D	156	ASP
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	201	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	215	SER
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	31	THR
5	E	37	LEU
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	84	ASP
5	E	92	THR
5	E	104	ASN
5	E	131	THR
5	E	140	LEU
5	E	146	HIS
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	178	ILE
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
5	E	204	THR
6	F	72	LYS
6	F	79	ARG
6	F	82	THR
6	F	86	THR
6	F	90	ARG
6	F	110	ASP
6	F	133	VAL
7	G	2	PHE
7	G	13	LEU
7	G	24	GLN
7	G	26	LEU
7	G	64	THR
7	G	96	GLN
7	G	106	MET
7	G	112	LYS
7	G	133	SER
7	G	138	THR
7	G	143	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
7	G	145	VAL
7	G	155	SER
7	G	162	SER
7	G	171	ILE
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	34	ASP
8	H	76	THR
8	H	77	ARG
8	H	83	GLN
8	H	89	LEU
8	H	91	ASP
8	H	92	ASP
8	H	103	LYS
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	74	GLU
9	I	94	ASP
9	I	106	CYS
9	I	111	THR
10	J	1	MET
10	J	2	ILE
10	J	3	VAL
10	J	7	CYS
10	J	12	LYS
10	J	13	VAL
10	J	22	LEU
10	J	29	GLU
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
11	K	18	LYS
11	K	20	LYS
11	K	25	THR
11	K	29	ASN
11	K	31	VAL
11	K	37	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	70	ARG
11	K	101	LEU
11	K	107	THR
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG
14	N	194	LYS
14	N	210	LYS
17	Q	50	GLU
17	Q	55	ARG
17	Q	58	LEU
17	Q	79	THR
17	Q	81	MET
17	Q	86	ASN
17	Q	88	ARG
17	Q	96	ASP
17	Q	108	ILE
17	Q	110	HIS
17	Q	159	GLU
17	Q	176	ASN
17	Q	180	VAL
17	Q	217	THR
17	Q	246	ILE
17	Q	260	SER
17	Q	268	ILE
17	Q	275	LEU
17	Q	280	LYS
17	Q	287	GLU
18	R	26	ASN
18	R	47	LYS
18	R	49	LEU
18	R	64	HIS
18	R	67	ARG
18	R	121	LEU
18	R	153	ILE
18	R	158	ASP
18	R	181	GLU
18	R	188	SER
18	R	189	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	R	192	ASP
18	R	193	THR
18	R	199	ASP
18	R	200	LEU
20	T	55	LYS
20	T	99	LYS
20	T	102	LYS
20	T	118	LEU
20	T	120	GLU
20	T	124	GLU
21	U	83	TRP
21	U	131	LEU
21	U	140	ASN
21	U	152	ARG
21	U	156	VAL
21	U	159	HIS
21	U	161	LEU
22	V	99	LYS
22	V	135	ILE
22	V	137	ARG
22	V	141	ASP
23	W	11	CYS
23	W	13	ASP
23	W	16	THR
23	W	63	SER
23	W	80	LEU
24	X	46	GLN
24	X	97	ASP
24	X	99	LEU
25	Y	57	ILE
25	Y	80	GLU
25	Y	179	GLU
25	Y	335	LEU
25	Y	479	LEU
25	Y	578	GLU
25	Y	587	ARG
25	Y	653	PHE
26	Z	320	ASN
26	Z	327	LYS
26	Z	333	ILE
26	Z	349	ASN
26	Z	383	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
26	Z	404	LYS
26	Z	407	VAL
26	Z	442	ASN
26	Z	524	ILE
26	Z	549	ILE
26	Z	570	LEU
26	Z	573	THR
26	Z	582	ILE
26	Z	621	LYS
26	Z	622	MET
26	Z	628	TYR
26	Z	630	SER
26	Z	634	GLN
26	Z	638	ASN
26	Z	647	ASP
26	Z	656	LYS
26	Z	660	THR
26	Z	664	LEU
26	Z	668	THR
26	Z	669	CYS
26	Z	674	SER
26	Z	677	TYR
26	Z	680	ARG
26	Z	681	ARG
26	Z	711	LYS
26	Z	714	GLN
26	Z	717	TYR
26	Z	720	THR
26	Z	740	HIS
26	Z	747	ASN
26	Z	756	ARG
26	Z	757	ARG
29	c	35	VAL
29	c	39	SER
29	c	52	LEU
29	c	59	THR
29	c	62	GLU
29	c	64	ARG
29	c	78	ARG
29	c	81	GLU
29	c	86	LEU
29	c	101	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	c	114	GLN
29	c	142	LEU
29	c	145	ILE
29	c	168	MET
29	c	171	ILE
29	c	182	ARG
29	c	198	VAL
29	c	209	ILE
30	d	14	VAL
30	d	247	LEU
30	d	262	LEU
31	e	19	LEU
31	e	23	LEU
31	e	29	ASP
31	e	39	ARG
31	e	41	LEU
31	e	66	LEU
31	e	111	LEU
31	e	117	ASN
32	f	340	LYS
33	g	55	GLU
33	g	127	LYS
33	g	293	ARG
33	g	349	TYR
33	g	356	LYS
34	h	67	ILE
34	h	71	LYS
34	h	123	MET
34	h	129	THR
34	h	130	LYS
34	h	132	THR
34	h	133	GLN
34	h	142	PHE
34	h	144	ARG
34	h	145	THR
34	h	146	GLU
34	h	148	LEU
34	h	150	SER
34	h	151	LEU
34	h	152	CYS
34	h	154	GLU
34	h	156	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
35	i	127	LYS
35	i	135	ILE
35	i	137	LYS
35	i	140	LYS
35	i	149	ASP
35	i	154	LYS
35	i	159	VAL
35	i	161	GLU
35	i	162	LEU
35	i	164	LYS
35	i	165	LYS
35	i	166	LEU
35	i	167	ASP
35	i	171	PHE
35	i	179	LYS
35	i	196	LEU
35	i	207	CYS
35	i	208	LYS
35	i	209	ASP
35	i	219	GLU
35	i	220	THR
35	i	221	ILE
35	i	225	GLU
35	i	228	SER
35	i	232	VAL
35	i	233	LEU
35	i	238	ASP
36	j	68	GLN
36	j	78	CYS
36	j	87	LEU
36	j	141	ARG
36	j	145	LYS
36	j	151	LYS
36	j	211	LYS
36	j	233	VAL
36	j	234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	545	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	548	ASN
1	A	603	ASN
1	A	966	ASN
1	A	994	GLN
1	A	1106	ASN
1	A	1140	HIS
1	A	1173	HIS
1	A	1270	ASN
1	A	1393	ASN
2	B	110	HIS
2	B	300	HIS
2	B	325	GLN
2	B	350	GLN
2	B	357	GLN
2	B	449	ASN
2	B	842	ASN
2	B	975	GLN
2	B	1025	HIS
2	B	1193	GLN
2	B	1195	HIS
3	C	184	ASN
4	D	37	GLN
4	D	143	ASN
4	D	165	GLN
5	E	3	GLN
7	G	71	ASN
7	G	102	GLN
8	H	35	GLN
8	H	83	GLN
9	I	83	ASN
9	I	89	GLN
9	I	108	HIS
17	Q	4	GLN
17	Q	53	ASN
17	Q	57	GLN
17	Q	86	ASN
17	Q	176	ASN
17	Q	205	ASN
17	Q	243	ASN
17	Q	258	ASN
17	Q	269	ASN
18	R	26	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
18	R	68	GLN
18	R	118	GLN
20	T	66	ASN
21	U	74	GLN
21	U	75	GLN
21	U	168	HIS
21	U	169	GLN
21	U	198	GLN
22	V	108	ASN
23	W	74	ASN
24	X	95	ASN
25	Y	60	GLN
25	Y	62	HIS
25	Y	138	ASN
25	Y	242	ASN
25	Y	362	HIS
25	Y	628	GLN
25	Y	661	HIS
25	Y	707	ASN
26	Z	320	ASN
26	Z	331	GLN
26	Z	349	ASN
26	Z	361	GLN
26	Z	366	GLN
26	Z	423	GLN
26	Z	426	GLN
26	Z	434	ASN
26	Z	447	GLN
26	Z	471	GLN
26	Z	491	HIS
26	Z	508	HIS
26	Z	528	ASN
26	Z	551	ASN
26	Z	589	GLN
26	Z	596	GLN
26	Z	638	ASN
26	Z	648	GLN
26	Z	676	HIS
26	Z	738	HIS
26	Z	740	HIS
26	Z	747	ASN
26	Z	761	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
28	b	11	GLN
28	b	22	GLN
29	c	208	ASN
30	d	3	ASN
30	d	40	ASN
30	d	43	GLN
30	d	59	GLN
30	d	270	ASN
30	d	272	ASN
31	e	57	GLN
31	e	84	GLN
31	e	117	ASN
33	g	86	ASN
33	g	98	ASN
33	g	118	HIS
33	g	131	ASN
33	g	220	HIS
33	g	328	HIS
34	h	50	ASN
34	h	133	GLN
34	h	141	ASN
35	i	199	GLN
35	i	216	GLN
36	j	68	GLN
36	j	88	HIS
36	j	144	GLN
36	j	158	GLN
36	j	219	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.