Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 12:44 AM JST

PDB ID	:	7Y18
Title	:	Crystal structure of ribosomal ITS2 pre-rRNA processing complex from Saccharomyces cerevisiae
Authors	:	Chen, J.; Liu, L.
Deposited on	:	2022-06-07
Resolution	:	3.69 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

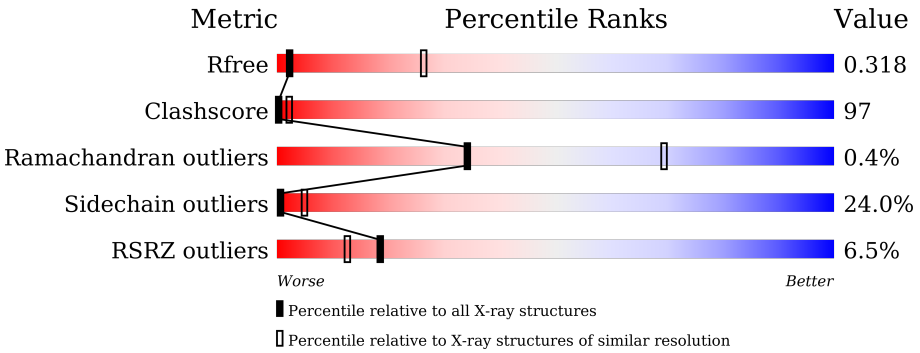
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.69 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	632	2% 18% 43% 22% 16%
1	B	632	4% 23% 42% 17% • 16%
1	E	632	2% 22% 43% 17% • 17%
2	C	502	8% 31% 40% 14% 14%
2	D	502	7% 34% 39% 11% • 15%
2	F	502	12% 33% 34% 11% • 21%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23039 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Polynucleotide 5'-hydroxyl-kinase GRC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4122	2649	693	771	9			
1	B	528	Total	C	N	O	S	0	0	0
			4069	2607	693	759	10			
1	E	527	Total	C	N	O	S	0	0	0
			4076	2614	691	761	10			

- Molecule 2 is a protein called Protein LAS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	430	Total	C	N	O	S	0	0	0
			3614	2324	629	652	9			
2	D	429	Total	C	N	O	S	0	0	0
			3614	2325	628	652	9			
2	F	397	Total	C	N	O	S	0	0	0
			3364	2176	584	595	9			

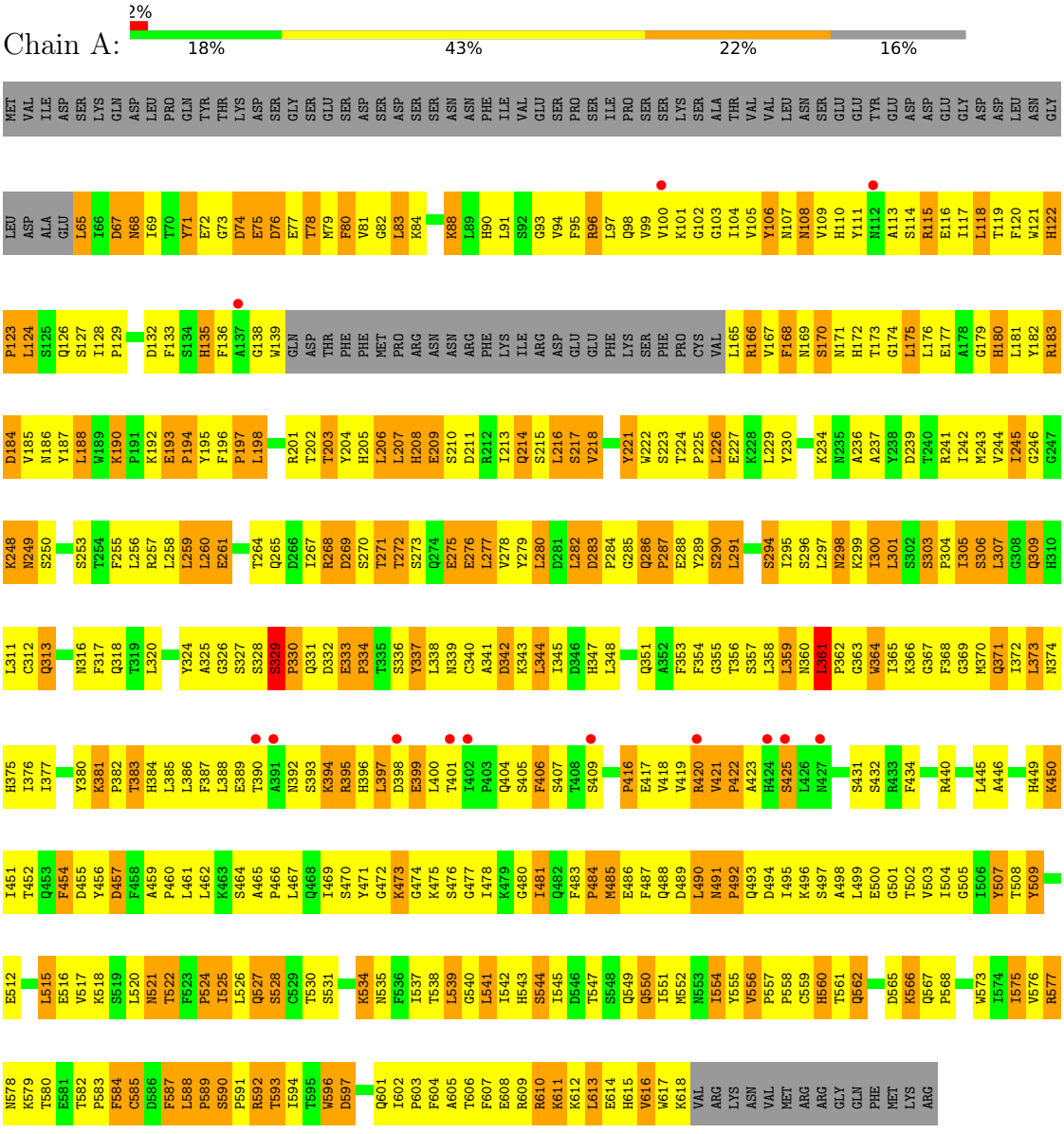
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	C	31	Total	O	0	0
			31	31		
3	D	21	Total	O	0	0
			21	21		
3	B	30	Total	O	0	0
			30	30		
3	E	43	Total	O	0	0
			43	43		
3	F	19	Total	O	0	0
			19	19		

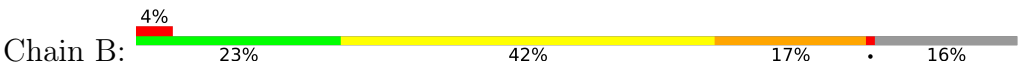
3 Residue-property plots (i)

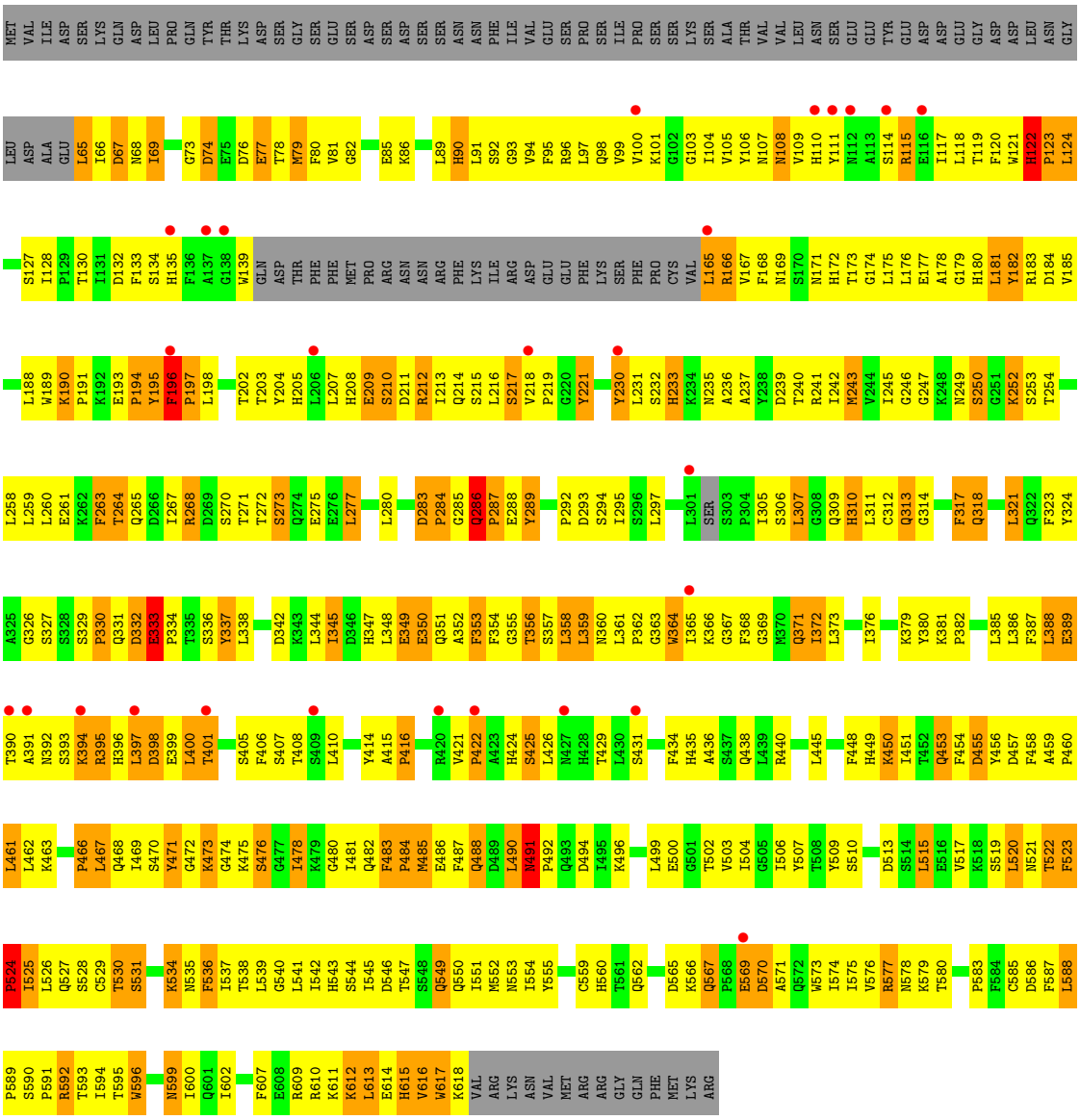
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Polynucleotide 5'-hydroxyl-kinase GRC3

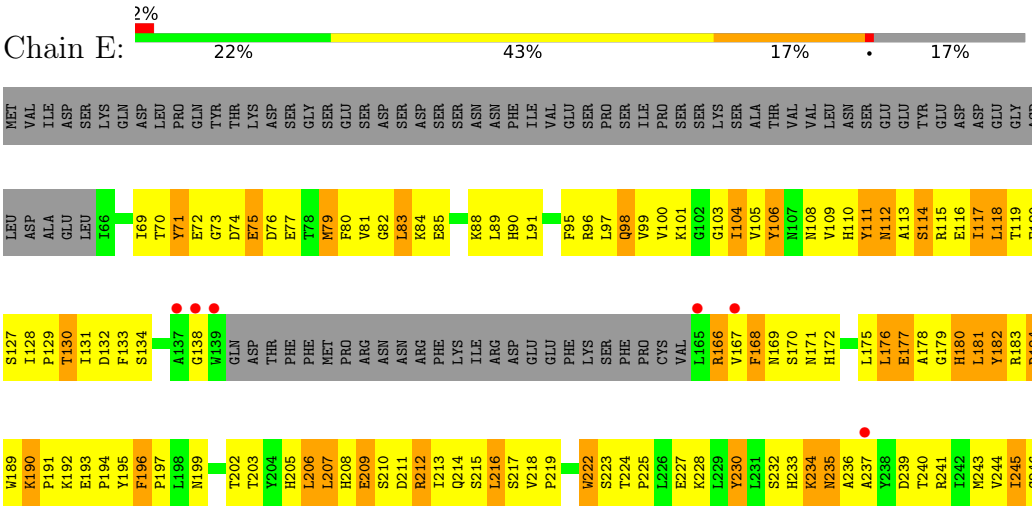


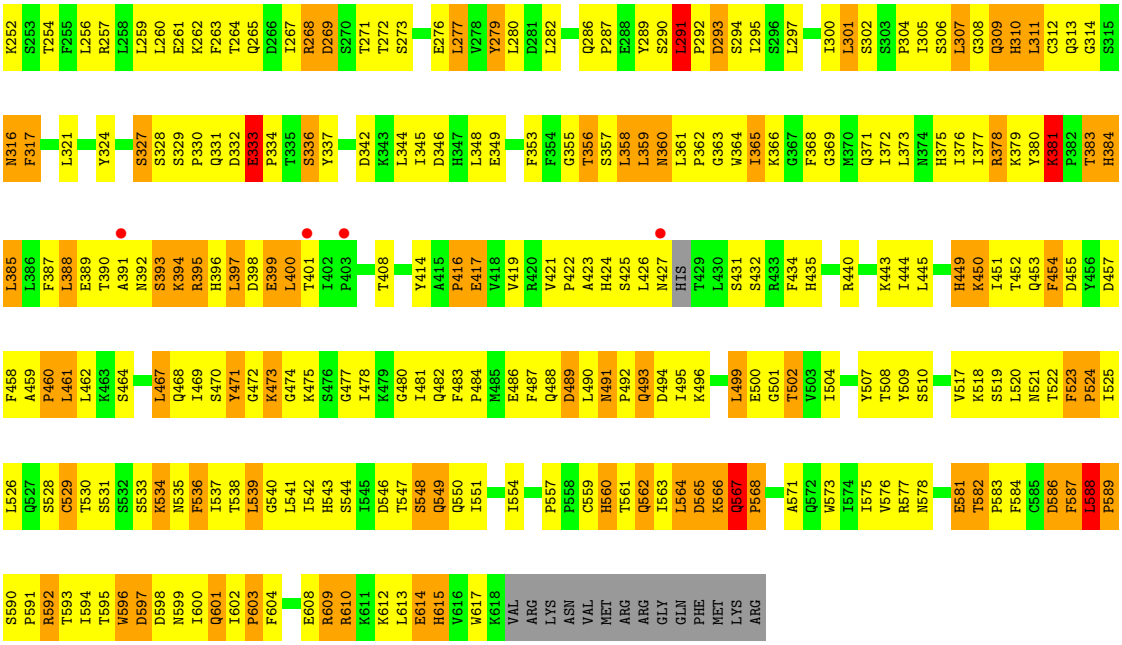
• Molecule 1: Polynucleotide 5'-hydroxyl-kinase GRC3





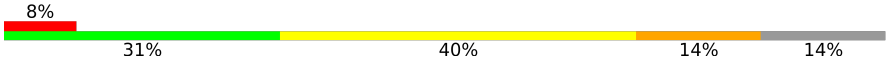
• Molecule 1: Polynucleotide 5'-hydroxyl-kinase GRC3

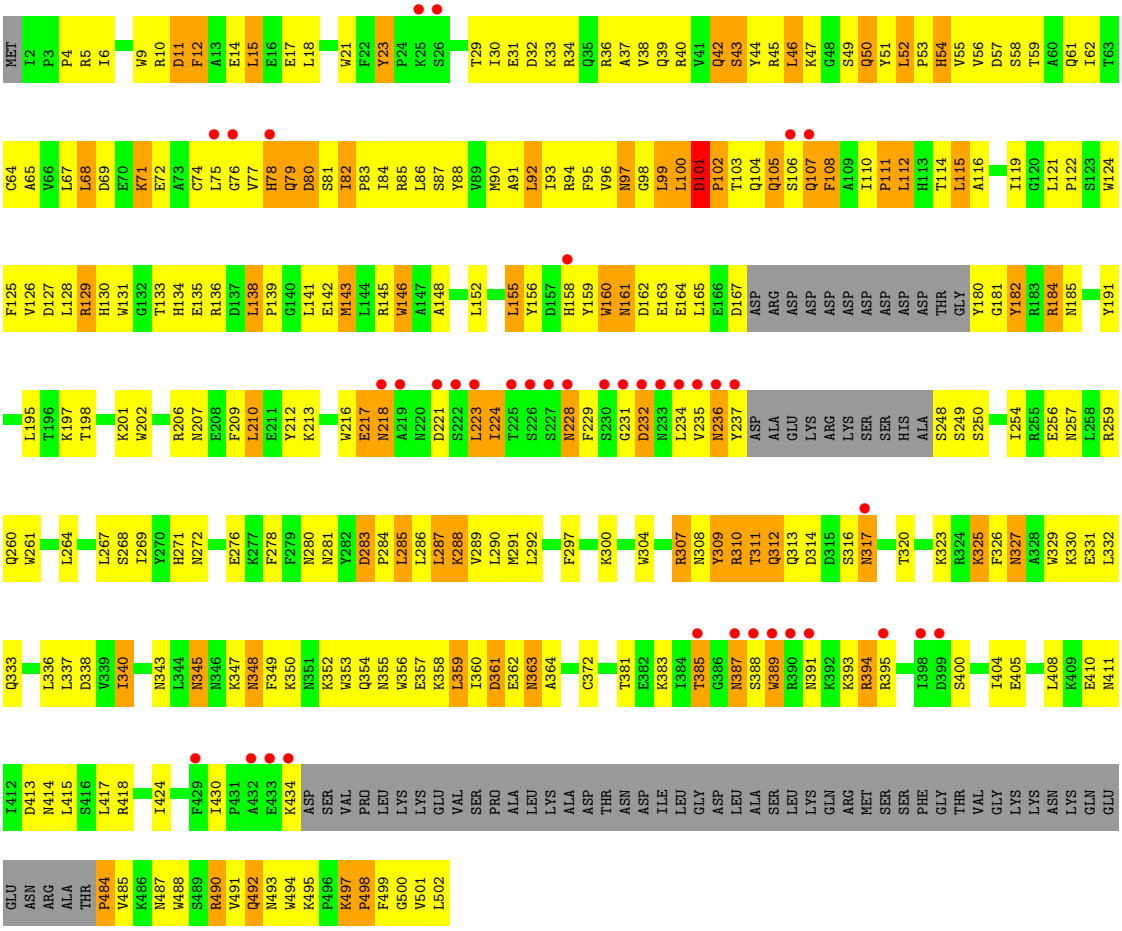




• Molecule 2: Protein LAS1

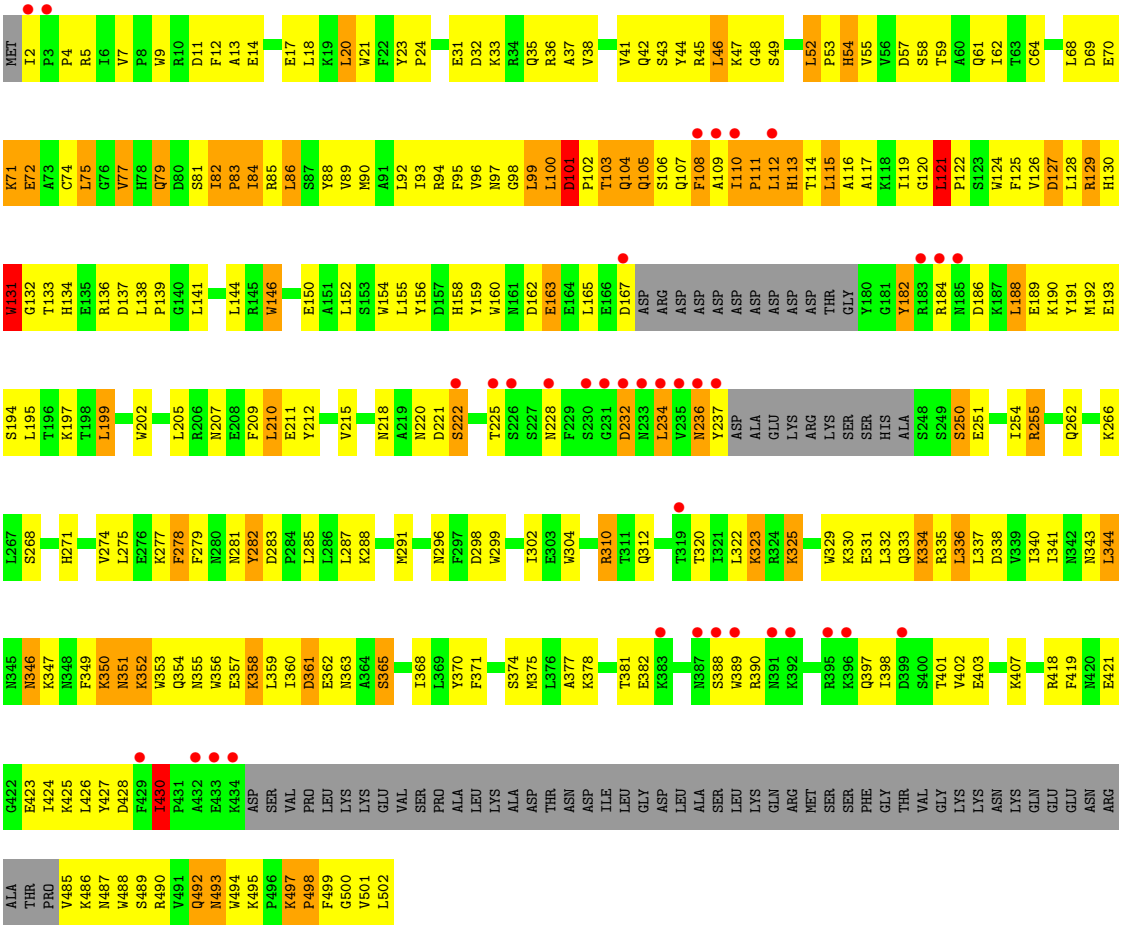
Chain C:





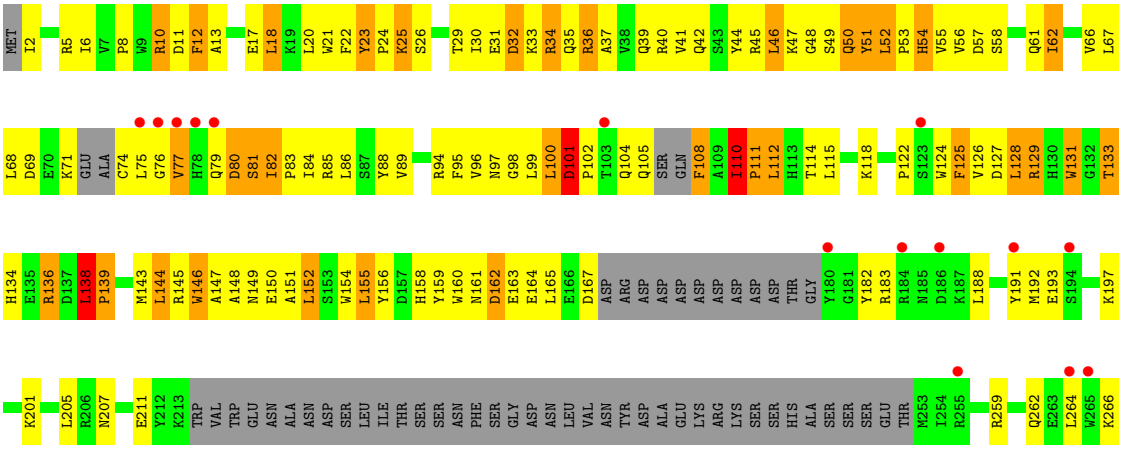
• Molecule 2: Protein LAS1

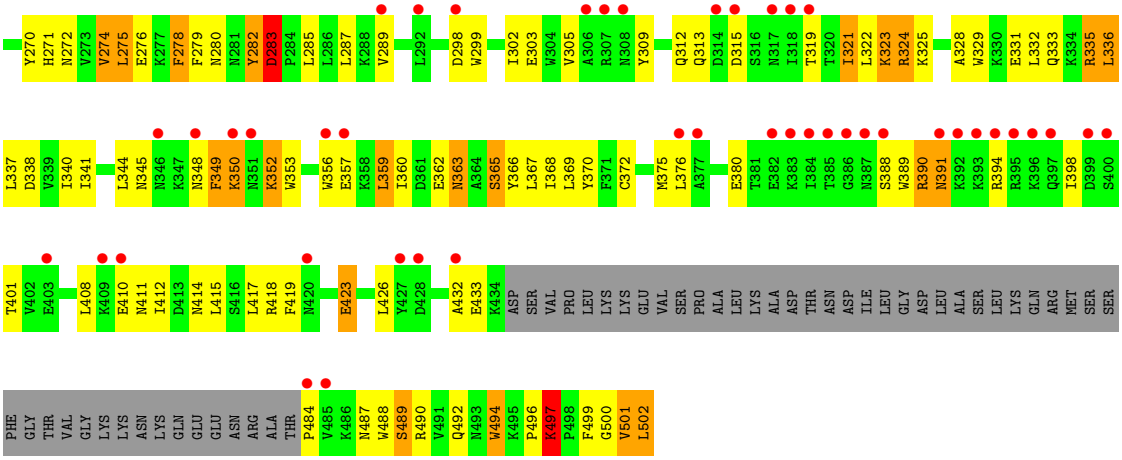
Chain D:



• Molecule 2: Protein LAS1

Chain F:




Y270 H271 N272 V273 V274 L275 E276 K277 F278 F279 N280 N281 Y282 D283 P284 L285 L286 L287 K288 V289 L292 D298 W299 I302 E303 W304 V305 A306 R307 N308 Y309 Q312 Q313 D314 D315 S316 N317 I318 T319 T320 I321 L322 K323 R324 K325 A328 W329 K330 E331 L332 Q333 K334 R335 L336
L337 D338 V339 I340 I341 L344 N345 N346 K347 N348 F349 K350 N351 K352 W353 W356 E357 K358 L359 I360 D361 E362 N363 A364 S365 Y366 L367 I368 L369 Y370 F371 G372 M375 L376 A377 E380 T381 E382 K383 I384 T385 G386 N387 S388 W389 R390 N391 K392 K393 R394 R395 K396 Q397 I398 D399 S400
T401 V402 E403 L408 K409 E410 N411 I412 D413 N414 L415 S416 L417 R418 F419 N420 E423 L426 Y427 D428 A432 E433 K434 ASP SER VAL PRO LEU LYS LYS GLU VAL SER PRO ALA LEU LYS ALA ASP THR ASN ASP ILE LEU GLY ASP LEU ALA SER LEU LYS GLN ARG MET SER SER
PHE GLY THR VAL GLY LYS LYS ASN LYS GLN GLU GLU ASN ARG ALA THR P484 V485 K486 N487 W488 S489 R490 V491 Q492 N493 W494 K495 P496 K497 P498 F499 G500 V501 L502

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	233.56Å 116.14Å 159.31Å 90.00° 96.41° 90.00°	Depositor
Resolution (Å)	48.63 – 3.69 48.63 – 3.69	Depositor EDS
% Data completeness (in resolution range)	80.1 (48.63-3.69) 80.2 (48.63-3.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.03 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.278 , 0.318 0.278 , 0.318	Depositor DCC
R_{free} test set	1824 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 63.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	23039	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.56	15/4230 (0.4%)	0.72	19/5764 (0.3%)
1	B	0.46	10/4169 (0.2%)	0.73	22/5676 (0.4%)
1	E	0.49	14/4179 (0.3%)	0.67	15/5690 (0.3%)
2	C	0.42	5/3703 (0.1%)	0.57	7/5016 (0.1%)
2	D	0.42	4/3704 (0.1%)	0.56	7/5017 (0.1%)
2	F	0.43	4/3445 (0.1%)	0.59	8/4658 (0.2%)
All	All	0.47	52/23430 (0.2%)	0.65	78/31821 (0.2%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	304	PRO	N-CD	5.72	1.55	1.47
1	A	304	PRO	N-CD	5.55	1.55	1.47
1	B	191	PRO	N-CD	5.38	1.55	1.47
1	B	194	PRO	N-CD	5.38	1.55	1.47
1	B	123	PRO	N-CD	5.38	1.55	1.47
2	C	102	PRO	N-CD	5.35	1.55	1.47
2	D	24	PRO	N-CD	5.32	1.55	1.47
2	F	139	PRO	N-CD	5.32	1.55	1.47
1	A	589	PRO	N-CD	5.29	1.55	1.47
2	D	498	PRO	N-CD	5.28	1.55	1.47
1	A	197	PRO	N-CD	5.26	1.55	1.47
1	A	382	PRO	N-CD	5.25	1.55	1.47
1	A	123	PRO	N-CD	5.25	1.55	1.47
1	B	484	PRO	N-CD	5.25	1.55	1.47
1	E	191	PRO	N-CD	5.25	1.55	1.47
2	C	139	PRO	N-CD	5.24	1.55	1.47
1	E	568	PRO	N-CD	5.24	1.55	1.47
1	A	334	PRO	N-CD	5.23	1.55	1.47
2	C	498	PRO	N-CD	5.22	1.55	1.47
1	E	603	PRO	N-CD	5.21	1.55	1.47
1	E	492	PRO	N-CD	5.20	1.55	1.47
1	A	330	PRO	N-CD	5.18	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	330	PRO	N-CD	5.18	1.55	1.47
1	A	287	PRO	N-CD	5.16	1.55	1.47
2	C	111	PRO	N-CD	5.16	1.55	1.47
1	A	591	PRO	N-CD	5.16	1.55	1.47
1	B	524	PRO	N-CD	5.16	1.55	1.47
1	B	287	PRO	N-CD	5.16	1.55	1.47
1	B	197	PRO	N-CD	5.15	1.55	1.47
1	E	292	PRO	N-CD	5.14	1.55	1.47
1	E	484	PRO	N-CD	5.13	1.55	1.47
1	A	484	PRO	N-CD	5.13	1.55	1.47
1	E	589	PRO	N-CD	5.13	1.55	1.47
2	D	111	PRO	N-CD	5.12	1.55	1.47
1	B	284	PRO	N-CD	5.12	1.55	1.47
1	B	492	PRO	N-CD	5.11	1.55	1.47
1	A	492	PRO	N-CD	5.11	1.54	1.47
1	E	460	PRO	N-CD	5.09	1.54	1.47
1	E	591	PRO	N-CD	5.09	1.54	1.47
1	A	568	PRO	N-CD	5.07	1.54	1.47
2	F	111	PRO	N-CD	5.07	1.54	1.47
2	F	24	PRO	N-CD	5.07	1.54	1.47
2	F	496	PRO	N-CD	5.06	1.54	1.47
1	E	219	PRO	N-CD	5.03	1.54	1.47
1	A	524	PRO	N-CD	5.03	1.54	1.47
1	E	334	PRO	N-CD	5.03	1.54	1.47
2	D	83	PRO	N-CD	5.03	1.54	1.47
1	A	422	PRO	N-CD	5.02	1.54	1.47
2	C	284	PRO	N-CD	5.02	1.54	1.47
1	E	524	PRO	N-CD	5.02	1.54	1.47
1	B	330	PRO	N-CD	5.01	1.54	1.47
1	A	558	PRO	N-CD	5.00	1.54	1.47

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	197	PRO	N-CA-C	-13.72	76.42	112.10
1	B	618	LYS	N-CA-C	-10.92	81.53	111.00
1	B	198	LEU	N-CA-CB	-9.77	90.87	110.40
1	B	617	TRP	CB-CA-C	-8.25	93.90	110.40
1	B	617	TRP	N-CA-C	-7.62	90.42	111.00
1	B	197	PRO	CB-CA-C	-7.37	93.57	112.00
1	A	193	GLU	C-N-CD	6.48	142.00	128.40
1	A	283	ASP	C-N-CD	6.25	141.53	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	497	LYS	C-N-CD	6.13	141.28	128.40
1	A	416	PRO	N-CA-CB	6.11	110.63	103.30
2	C	484	PRO	N-CA-CB	6.05	110.57	103.30
1	A	218	VAL	C-N-CD	6.03	141.05	128.40
1	E	416	PRO	N-CA-CB	5.99	110.49	103.30
1	A	602	ILE	C-N-CD	5.98	140.95	128.40
2	D	101	ASP	C-N-CD	5.96	140.91	128.40
2	F	484	PRO	N-CA-CB	5.93	110.42	103.30
1	B	567	GLN	C-N-CD	5.93	140.85	128.40
1	E	523	PHE	C-N-CD	5.91	140.80	128.40
1	A	556	VAL	C-N-CD	5.90	140.79	128.40
2	D	121	LEU	C-N-CD	5.89	140.78	128.40
1	B	459	ALA	C-N-CD	5.87	140.74	128.40
2	D	52	LEU	C-N-CD	5.87	140.72	128.40
2	C	82	ILE	C-N-CD	5.87	140.72	128.40
1	B	333	GLU	C-N-CD	5.86	140.71	128.40
1	A	361	LEU	C-N-CD	5.84	140.66	128.40
2	D	430	ILE	C-N-CD	5.83	140.63	128.40
1	E	582	THR	C-N-CD	5.82	140.62	128.40
1	E	459	ALA	C-N-CD	5.82	140.62	128.40
2	C	23	TYR	C-N-CD	5.81	140.61	128.40
1	B	523	PHE	C-N-CD	5.81	140.59	128.40
1	A	459	ALA	C-N-CD	5.80	140.59	128.40
1	B	416	PRO	N-CA-CB	5.80	110.26	103.30
2	F	283	ASP	C-N-CD	5.80	140.58	128.40
1	A	557	PRO	C-N-CD	5.80	140.57	128.40
1	B	286	GLN	C-N-CD	5.79	140.57	128.40
1	E	381	LYS	C-N-CD	5.78	140.54	128.40
1	A	590	SER	C-N-CD	5.78	140.53	128.40
2	C	283	ASP	C-N-CD	5.78	140.54	128.40
1	E	333	GLU	C-N-CD	5.78	140.53	128.40
2	F	82	ILE	C-N-CD	5.78	140.53	128.40
2	F	101	ASP	C-N-CD	5.76	140.51	128.40
2	F	23	TYR	C-N-CD	5.76	140.50	128.40
1	E	491	ASN	C-N-CD	5.76	140.49	128.40
1	E	291	LEU	C-N-CD	5.75	140.47	128.40
2	F	110	ILE	C-N-CD	5.75	140.47	128.40
1	B	329	SER	C-N-CD	5.75	140.47	128.40
1	E	588	LEU	C-N-CD	5.74	140.46	128.40
1	E	483	PHE	C-N-CD	5.74	140.45	128.40
1	A	421	VAL	C-N-CD	5.74	140.45	128.40
1	A	491	ASN	C-N-CD	5.73	140.43	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	82	ILE	C-N-CD	5.73	140.43	128.40
2	D	110	ILE	C-N-CD	5.73	140.43	128.40
1	A	122	HIS	C-N-CD	5.72	140.41	128.40
1	B	196	PHE	C-N-CD	5.72	140.41	128.40
1	E	218	VAL	C-N-CD	5.72	140.41	128.40
2	D	497	LYS	C-N-CD	5.71	140.40	128.40
1	B	283	ASP	C-N-CD	5.70	140.37	128.40
1	A	286	GLN	C-N-CD	5.68	140.34	128.40
1	B	491	ASN	C-N-CD	5.68	140.33	128.40
1	A	483	PHE	C-N-CD	5.67	140.31	128.40
1	E	602	ILE	C-N-CD	5.67	140.31	128.40
1	A	588	LEU	C-N-CD	5.66	140.28	128.40
2	C	497	LYS	C-N-CD	5.66	140.28	128.40
1	E	329	SER	C-N-CD	5.65	140.27	128.40
2	C	138	LEU	C-N-CD	5.65	140.26	128.40
1	B	483	PHE	C-N-CD	5.64	140.24	128.40
2	F	138	LEU	C-N-CD	5.63	140.23	128.40
1	E	190	LYS	C-N-CD	5.63	140.22	128.40
1	A	333	GLU	C-N-CD	5.62	140.20	128.40
1	E	567	GLN	C-N-CD	5.60	140.16	128.40
1	A	329	SER	C-N-CD	5.59	140.15	128.40
1	B	193	GLU	C-N-CD	5.59	140.14	128.40
2	C	101	ASP	C-N-CD	5.57	140.09	128.40
1	A	381	LYS	C-N-CD	5.55	140.06	128.40
1	B	122	HIS	C-N-CD	5.46	139.86	128.40
1	B	190	LYS	C-N-CD	5.43	139.81	128.40
1	B	422	PRO	N-CA-CB	5.36	109.74	103.30
1	B	466	PRO	N-CA-CB	5.33	109.69	103.30

There are no chirality outliers.

There are no planarity outliers.

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	4122	0	3931	1015	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4069	0	3873	963	0
1	E	4076	0	3880	878	3
2	C	3614	0	3553	694	0
2	D	3614	0	3551	665	0
2	F	3364	0	3350	537	6
3	A	36	0	0	4	0
3	B	30	0	0	2	0
3	C	31	0	0	3	0
3	D	21	0	0	1	0
3	E	43	0	0	8	0
3	F	19	0	0	1	0
All	All	23039	0	22138	4373	6

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 97.

All (4373) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:CB	1:A:139:TRP:CD1	1.77	1.65
2:C:202:TRP:CZ3	2:C:209:PHE:CE1	1.77	1.62
2:D:4:PRO:HB3	1:B:607:PHE:CE1	1.10	1.62
1:E:331:GLN:HG3	1:E:364:TRP:CZ2	1.21	1.62
1:A:607:PHE:CE1	2:C:4:PRO:CB	1.82	1.62
1:B:366:LYS:HB3	1:B:396:HIS:CD2	1.38	1.58
2:D:69:ASP:CA	2:D:77:VAL:HG21	1.26	1.58
1:B:79:MET:CA	1:B:167:VAL:HG21	1.32	1.57
2:D:202:TRP:CZ3	2:D:209:PHE:CE2	1.92	1.56
1:A:331:GLN:CG	1:A:364:TRP:HZ2	1.09	1.56
1:A:504:ILE:HD12	1:A:575:ILE:CG2	1.13	1.56
2:D:4:PRO:CB	1:B:607:PHE:CE1	1.86	1.56
1:E:331:GLN:CG	1:E:364:TRP:HZ2	1.12	1.55
1:B:90:HIS:CE1	1:B:128:ILE:HD11	1.42	1.55
1:E:96:ARG:HG3	1:E:168:PHE:CE2	1.06	1.55
1:A:365:ILE:HA	1:A:397:LEU:CD2	1.36	1.54
2:D:202:TRP:HZ3	2:D:209:PHE:CE2	1.24	1.53
2:D:69:ASP:HA	2:D:77:VAL:CG2	1.33	1.53
2:C:278:PHE:CE2	2:C:286:LEU:HD23	1.37	1.52
1:E:469:ILE:HG21	1:E:478:ILE:CD1	1.09	1.52
1:B:177:GLU:HG2	1:B:458:PHE:CD2	1.45	1.52
1:E:96:ARG:CG	1:E:168:PHE:CE2	1.90	1.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:PHE:CE1	2:C:4:PRO:CD	1.88	1.50
1:B:79:MET:N	1:B:167:VAL:CG2	1.70	1.50
2:C:202:TRP:HZ3	2:C:209:PHE:CE1	1.09	1.50
2:C:23:TYR:CD2	2:C:156:TYR:HD2	1.26	1.49
2:D:5:ARG:CD	1:B:610:ARG:HE	1.23	1.47
1:A:504:ILE:CD1	1:A:575:ILE:CG2	1.91	1.47
2:C:202:TRP:CZ3	2:C:209:PHE:HE1	1.17	1.46
2:F:128:LEU:HB2	2:F:131:TRP:CZ3	1.48	1.46
2:D:312:GLN:NE2	2:D:323:LYS:HG3	1.20	1.46
1:A:538:THR:HB	1:A:560:HIS:CD2	1.47	1.46
1:A:607:PHE:CZ	2:C:4:PRO:CG	1.99	1.45
1:B:172:HIS:CD2	1:B:454:PHE:HA	1.52	1.45
1:B:504:ILE:HD12	1:B:575:ILE:CG2	1.47	1.45
2:F:68:LEU:HD22	2:F:84:ILE:CD1	1.46	1.44
1:E:614:GLU:OE2	2:F:159:TYR:CE1	1.68	1.43
1:A:331:GLN:CG	1:A:364:TRP:CZ2	1.98	1.43
1:B:96:ARG:NH2	1:B:171:ASN:HD21	1.01	1.43
1:B:366:LYS:HG2	1:B:396:HIS:CB	1.48	1.43
1:E:301:LEU:CD1	1:E:316:ASN:O	1.67	1.42
1:B:366:LYS:HA	1:B:396:HIS:CE1	1.52	1.42
2:D:202:TRP:CZ3	2:D:209:PHE:CD2	2.04	1.42
2:D:329:TRP:CE2	2:D:424:ILE:CD1	2.02	1.42
1:A:326:GLY:HA3	1:A:578:ASN:ND2	1.10	1.42
1:A:538:THR:CB	1:A:560:HIS:HD2	1.29	1.41
1:B:471:TYR:HE1	1:B:550:GLN:CA	1.32	1.41
2:C:206:ARG:O	2:C:210:LEU:CD1	1.66	1.41
2:D:202:TRP:HZ3	2:D:209:PHE:CZ	1.38	1.41
2:D:329:TRP:CD2	2:D:424:ILE:CD1	2.00	1.41
1:A:98:GLN:NE2	1:A:115:ARG:CG	1.83	1.41
1:A:488:GLN:NE2	1:A:527:GLN:HE22	0.98	1.41
1:A:589:PRO:HD2	1:A:596:TRP:CH2	1.56	1.41
1:A:105:VAL:CB	1:A:132:ASP:HB2	1.49	1.40
1:B:174:GLY:O	1:B:458:PHE:CE2	1.71	1.40
1:A:502:THR:HB	1:A:577:ARG:NH2	1.34	1.40
1:A:366:LYS:CE	1:A:395:ARG:HH22	1.35	1.39
1:A:368:PHE:HE1	2:D:146:TRP:NE1	1.15	1.39
1:A:488:GLN:NE2	1:A:527:GLN:NE2	1.68	1.39
1:A:366:LYS:CE	1:A:395:ARG:NH2	1.86	1.39
1:A:105:VAL:HB	1:A:132:ASP:CB	1.51	1.39
2:D:146:TRP:CH2	2:D:150:GLU:OE1	1.75	1.39
2:D:146:TRP:CZ3	2:D:150:GLU:HB2	1.57	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:18:LEU:CD2	2:F:22:PHE:CE2	2.05	1.38
1:A:607:PHE:CE1	2:C:4:PRO:CA	2.06	1.38
2:C:80:ASP:OD1	2:C:82:ILE:CG2	1.69	1.38
2:D:312:GLN:HE22	2:D:323:LYS:CG	1.35	1.37
1:E:169:ASN:OD1	1:E:203:THR:CG2	1.71	1.37
2:C:202:TRP:CZ3	2:C:209:PHE:CD1	2.10	1.37
1:B:366:LYS:CB	1:B:396:HIS:CD2	2.05	1.37
2:D:23:TYR:CD2	2:D:156:TYR:HD2	1.42	1.36
1:A:607:PHE:HE1	2:C:4:PRO:N	1.20	1.36
2:D:4:PRO:HB3	1:B:607:PHE:CZ	1.60	1.36
2:D:23:TYR:CD2	2:D:156:TYR:CD2	2.12	1.36
1:A:589:PRO:CD	1:A:596:TRP:HH2	1.38	1.36
1:E:469:ILE:CG2	1:E:478:ILE:CD1	2.04	1.35
1:B:366:LYS:HA	1:B:396:HIS:ND1	1.41	1.35
1:A:607:PHE:CZ	2:C:4:PRO:HB3	1.61	1.35
2:F:272:ASN:HA	2:F:275:LEU:CD1	1.52	1.34
1:A:84:LYS:CB	1:A:139:TRP:CG	2.09	1.34
2:F:272:ASN:CA	2:F:275:LEU:CD1	2.05	1.34
1:A:216:LEU:CD1	1:A:425:SER:OG	1.72	1.34
2:D:84:ILE:HD11	2:D:88:TYR:CE2	1.61	1.34
2:C:23:TYR:CD2	2:C:156:TYR:CD2	2.16	1.34
1:A:84:LYS:CB	1:A:139:TRP:HB3	1.57	1.33
1:E:182:TYR:HE1	1:E:184:ASP:CG	0.93	1.33
1:A:592:ARG:NH2	2:C:184:ARG:NH2	1.74	1.33
1:E:364:TRP:HD1	1:E:369:GLY:N	1.20	1.33
1:B:239:ASP:CB	1:B:355:GLY:H	1.39	1.33
1:A:388:LEU:O	1:A:423:ALA:CB	1.75	1.32
1:A:607:PHE:HE1	2:C:4:PRO:CD	1.27	1.32
1:E:469:ILE:CG2	1:E:478:ILE:HD11	1.55	1.32
1:B:230:TYR:CE1	1:B:263:PHE:HE1	1.44	1.32
2:F:272:ASN:CA	2:F:275:LEU:HD13	1.60	1.32
1:A:607:PHE:CE1	2:C:4:PRO:HD3	1.57	1.32
2:F:350:LYS:NZ	2:F:401:THR:HG22	1.41	1.32
2:D:23:TYR:CE2	2:D:156:TYR:HD2	1.48	1.31
1:B:122:HIS:CE1	1:B:128:ILE:HB	1.62	1.31
1:B:230:TYR:CE1	1:B:263:PHE:CE1	2.17	1.31
1:B:177:GLU:CG	1:B:458:PHE:HD2	1.42	1.31
1:E:187:TYR:CE1	1:E:192:LYS:CB	2.13	1.31
1:E:109:VAL:HG23	1:E:111:TYR:CE1	1.65	1.30
2:F:312:GLN:OE1	2:F:323:LYS:CE	1.78	1.30
1:A:488:GLN:HE21	1:A:527:GLN:NE2	1.23	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:HIS:NE2	2:C:98:GLY:HA3	1.45	1.30
2:D:5:ARG:HD2	1:B:610:ARG:NE	1.42	1.30
2:D:77:VAL:CG1	2:D:84:ILE:HG12	1.61	1.30
1:E:519:SER:O	1:E:520:LEU:HD23	1.18	1.30
2:C:497:LYS:HD2	2:C:502:LEU:O	1.15	1.30
1:A:181:LEU:CD1	1:A:585:CYS:SG	2.18	1.29
2:C:180:TYR:O	2:C:184:ARG:HG2	1.17	1.29
2:D:146:TRP:CH2	2:D:150:GLU:HB2	1.66	1.29
1:A:607:PHE:CE1	2:C:4:PRO:CG	2.14	1.29
1:A:507:TYR:HD1	1:A:535:ASN:O	1.08	1.29
1:B:79:MET:O	1:B:167:VAL:CG2	1.81	1.29
1:B:90:HIS:CE1	1:B:128:ILE:CD1	2.13	1.29
1:A:84:LYS:CB	1:A:139:TRP:CB	2.11	1.29
1:A:366:LYS:HE3	1:A:395:ARG:NH2	1.43	1.29
1:B:366:LYS:HA	1:B:396:HIS:CG	1.66	1.29
2:F:312:GLN:NE2	2:F:323:LYS:HD2	1.44	1.29
1:B:361:LEU:CD2	1:B:376:ILE:HD12	1.59	1.28
1:A:607:PHE:CZ	2:C:4:PRO:CB	2.10	1.28
2:C:278:PHE:HE2	2:C:286:LEU:CD2	1.44	1.28
1:B:471:TYR:CE1	1:B:550:GLN:HA	1.66	1.28
2:F:98:GLY:O	2:F:102:PRO:HD3	1.33	1.28
1:B:219:PRO:HB3	1:B:221:TYR:CE2	1.69	1.28
1:E:83:LEU:HD13	1:E:101:LYS:O	1.34	1.28
2:F:58:SER:O	2:F:62:ILE:CG1	1.81	1.28
1:A:387:PHE:O	1:A:421:VAL:HG22	1.21	1.28
1:A:607:PHE:CE1	2:C:4:PRO:HB3	1.53	1.28
1:A:589:PRO:CD	1:A:596:TRP:CH2	2.15	1.28
1:A:96:ARG:O	1:A:168:PHE:CE1	1.86	1.27
1:A:226:LEU:HD11	1:A:230:TYR:OH	1.16	1.27
2:C:85:ARG:HD3	1:B:486:GLU:OE2	1.22	1.27
1:B:96:ARG:NH2	1:B:171:ASN:ND2	1.82	1.27
1:E:487:PHE:O	1:E:490:LEU:HD11	1.13	1.27
2:C:64:CYS:SG	2:D:82:ILE:HG21	1.73	1.27
2:F:58:SER:O	2:F:62:ILE:HG13	1.10	1.27
2:F:131:TRP:HE1	2:F:139:PRO:CG	1.46	1.26
1:E:96:ARG:CG	1:E:168:PHE:HE2	1.31	1.26
2:C:206:ARG:O	2:C:210:LEU:HD11	1.08	1.26
1:E:609:ARG:O	2:F:5:ARG:NH1	1.66	1.25
2:D:23:TYR:CE2	2:D:156:TYR:CD2	2.25	1.25
1:E:538:THR:OG1	1:E:560:HIS:HD2	1.20	1.25
1:E:222:TRP:NE1	1:E:422:PRO:O	1.67	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:HIS:CE1	1:B:213:ILE:HD11	1.72	1.24
2:F:68:LEU:CD2	2:F:84:ILE:HD13	1.65	1.24
1:A:246:GLY:O	1:A:363:GLY:HA3	1.33	1.24
2:F:97:ASN:OD1	2:F:129:ARG:NH2	1.71	1.24
1:A:365:ILE:HG22	1:A:397:LEU:CD2	1.68	1.24
2:D:146:TRP:HH2	2:D:150:GLU:OE1	1.06	1.24
1:E:487:PHE:O	1:E:490:LEU:CD1	1.84	1.24
1:A:326:GLY:CA	1:A:578:ASN:ND2	1.99	1.23
1:B:96:ARG:CZ	1:B:171:ASN:HD21	1.51	1.23
2:F:18:LEU:HD23	2:F:22:PHE:CE2	1.66	1.23
1:A:366:LYS:HG3	1:A:396:HIS:CB	1.65	1.23
1:A:216:LEU:HD12	1:A:425:SER:OG	1.19	1.23
1:A:365:ILE:CA	1:A:397:LEU:CD2	2.15	1.23
2:C:288:LYS:HE2	2:C:343:ASN:OD1	1.31	1.23
1:B:174:GLY:O	1:B:458:PHE:HE2	0.89	1.23
2:D:98:GLY:O	2:D:102:PRO:HD3	1.37	1.23
1:E:614:GLU:OE2	2:F:159:TYR:CZ	1.90	1.23
1:A:98:GLN:NE2	1:A:115:ARG:CA	2.02	1.23
2:D:23:TYR:CE2	2:D:156:TYR:HB2	1.73	1.23
1:B:166:ARG:O	1:B:167:VAL:HG22	1.37	1.22
1:B:297:LEU:CB	1:B:344:LEU:HD11	1.67	1.22
2:D:69:ASP:C	2:D:77:VAL:HG21	1.58	1.22
1:A:592:ARG:HH21	2:C:184:ARG:NH2	1.34	1.22
2:C:86:LEU:CD2	2:C:138:LEU:HD11	1.70	1.22
2:C:119:ILE:HD11	2:C:121:LEU:CB	1.70	1.22
1:A:96:ARG:HG3	1:A:168:PHE:CE1	1.75	1.21
1:A:607:PHE:CZ	2:C:4:PRO:HG3	1.69	1.21
1:B:79:MET:C	1:B:167:VAL:HG21	1.60	1.21
1:E:289:TYR:HD1	1:E:317:PHE:CD2	1.57	1.21
1:A:359:LEU:HD12	1:A:360:ASN:N	1.56	1.21
1:E:289:TYR:HB3	1:E:317:PHE:CE2	1.73	1.21
1:A:366:LYS:HG2	1:A:395:ARG:NH1	1.55	1.21
2:C:86:LEU:CD2	2:C:138:LEU:CD1	2.19	1.21
1:A:226:LEU:HD11	1:A:230:TYR:CZ	1.75	1.21
2:C:119:ILE:CD1	2:C:121:LEU:HB2	1.69	1.21
1:B:270:SER:OG	1:B:273:SER:OG	1.56	1.21
1:E:169:ASN:OD1	1:E:203:THR:HG23	1.25	1.21
1:A:98:GLN:NE2	1:A:115:ARG:HA	1.53	1.21
1:A:464:SER:O	2:C:494:TRP:CZ3	1.92	1.20
1:E:97:LEU:HD21	1:E:120:PHE:CE1	1.74	1.20
2:D:279:PHE:CE1	2:D:304:TRP:CZ3	2.28	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:CD	1:A:115:ARG:HA	1.59	1.20
2:C:80:ASP:OD1	2:C:82:ILE:HG22	1.29	1.20
2:F:17:GLU:OE2	2:F:21:TRP:CH2	1.93	1.20
2:F:18:LEU:CD2	2:F:22:PHE:CZ	2.24	1.20
2:F:365:SER:CA	2:F:419:PHE:HE1	1.55	1.20
2:C:497:LYS:HD2	2:C:502:LEU:C	1.59	1.19
1:B:172:HIS:HD2	1:B:454:PHE:CA	1.54	1.19
1:E:331:GLN:CG	1:E:364:TRP:CZ2	1.98	1.19
2:D:329:TRP:CE2	2:D:424:ILE:HD11	1.70	1.19
1:B:172:HIS:HA	1:B:454:PHE:O	1.40	1.19
1:B:367:GLY:H	1:B:396:HIS:CE1	1.59	1.19
1:A:84:LYS:CB	1:A:139:TRP:HD1	1.25	1.19
1:A:492:PRO:O	1:A:495:ILE:HG13	1.38	1.19
2:D:159:TYR:CE1	1:B:614:GLU:HG2	1.78	1.19
1:E:246:GLY:O	1:E:363:GLY:HA2	1.40	1.19
2:F:313:GLN:NE2	2:F:423:GLU:OE1	1.74	1.19
2:D:362:GLU:OE1	2:D:490:ARG:CD	1.91	1.18
2:F:128:LEU:HB2	2:F:131:TRP:CE3	1.76	1.18
1:E:369:GLY:HA2	1:E:372:ILE:HG22	1.18	1.18
1:A:331:GLN:HG3	1:A:364:TRP:CZ2	1.65	1.18
2:C:32:ASP:OD1	2:C:34:ARG:NE	1.74	1.18
2:C:86:LEU:HD23	2:C:138:LEU:CD1	1.72	1.18
2:D:36:ARG:HD3	1:B:491:ASN:OD1	1.44	1.18
1:B:79:MET:N	1:B:167:VAL:HG23	1.41	1.18
1:E:182:TYR:CE1	1:E:184:ASP:CG	1.77	1.18
2:F:151:ALA:O	2:F:155:LEU:CD1	1.91	1.18
2:C:23:TYR:CE2	2:C:156:TYR:HD2	1.61	1.18
1:E:232:SER:O	1:E:236:ALA:HB2	1.38	1.18
2:F:365:SER:HA	2:F:419:PHE:CE1	1.78	1.18
1:A:98:GLN:NE2	1:A:115:ARG:CB	2.06	1.18
1:A:98:GLN:HE22	1:A:115:ARG:HG3	1.04	1.18
1:A:367:GLY:N	1:A:396:HIS:CE1	2.12	1.18
2:C:110:ILE:CG2	2:C:114:THR:HB	1.74	1.18
2:D:96:VAL:O	2:D:100:LEU:HB2	1.38	1.17
2:F:75:LEU:O	2:F:77:VAL:HG22	1.39	1.17
1:A:365:ILE:CA	1:A:397:LEU:HD22	1.71	1.17
2:C:291:MET:CE	2:C:340:ILE:HG22	1.74	1.17
2:F:126:VAL:O	2:F:129:ARG:CG	1.91	1.17
1:A:538:THR:CB	1:A:560:HIS:CD2	2.13	1.17
1:A:469:ILE:CD1	2:C:488:TRP:CH2	2.27	1.17
1:B:321:LEU:HD21	1:B:344:LEU:CD1	1.74	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:LEU:CD2	1:E:120:PHE:CE1	2.27	1.17
1:E:246:GLY:O	1:E:363:GLY:CA	1.92	1.17
1:E:469:ILE:HG21	1:E:478:ILE:HD12	1.26	1.17
2:F:350:LYS:NZ	2:F:401:THR:CG2	2.07	1.17
2:C:52:LEU:HD12	2:C:53:PRO:CD	1.73	1.16
1:E:190:LYS:NZ	1:E:202:THR:OG1	1.77	1.16
2:F:74:CYS:HB3	2:F:75:LEU:HB2	1.23	1.16
1:B:504:ILE:CD1	1:B:575:ILE:HG21	1.75	1.16
1:B:366:LYS:CA	1:B:396:HIS:CD2	2.28	1.16
1:A:469:ILE:HD13	2:C:488:TRP:CH2	1.79	1.16
2:D:329:TRP:CE3	2:D:424:ILE:HD13	1.81	1.16
2:D:329:TRP:CZ2	2:D:424:ILE:HD11	1.79	1.16
1:E:121:TRP:CB	1:E:309:GLN:O	1.93	1.16
1:A:181:LEU:HD13	1:A:585:CYS:SG	1.83	1.16
2:C:52:LEU:HD12	2:C:53:PRO:N	1.61	1.16
2:D:489:SER:O	1:B:467:LEU:HB2	1.43	1.16
1:B:510:SER:HB3	1:B:535:ASN:OD1	1.43	1.16
1:E:364:TRP:CD1	1:E:369:GLY:N	2.13	1.16
1:A:181:LEU:HD11	1:A:585:CYS:SG	1.78	1.15
1:B:80:PHE:HE1	1:B:166:ARG:N	1.44	1.15
1:A:491:ASN:OD1	1:A:494:ASP:OD1	1.61	1.15
2:D:159:TYR:HE1	1:B:614:GLU:CG	1.59	1.15
1:B:311:LEU:O	1:B:313:GLN:OE1	1.63	1.15
1:B:471:TYR:CD1	1:B:550:GLN:O	1.99	1.15
1:E:118:LEU:CD1	1:E:305:ILE:HG21	1.77	1.15
1:A:368:PHE:CE1	2:D:146:TRP:NE1	2.06	1.15
2:D:423:GLU:HA	2:D:426:LEU:HG	1.18	1.15
1:E:96:ARG:HG3	1:E:168:PHE:CD2	1.81	1.15
1:A:469:ILE:CG2	2:C:488:TRP:H	1.60	1.14
1:A:615:HIS:HD2	2:C:102:PRO:CG	1.60	1.14
1:E:187:TYR:CZ	1:E:192:LYS:CB	2.30	1.14
2:F:126:VAL:O	2:F:129:ARG:HG2	1.45	1.14
1:A:607:PHE:HE1	2:C:4:PRO:CA	1.51	1.14
1:B:471:TYR:CE1	1:B:550:GLN:CA	2.24	1.14
1:A:507:TYR:CD1	1:A:535:ASN:O	2.01	1.14
2:C:278:PHE:CE2	2:C:286:LEU:CD2	2.21	1.14
1:B:79:MET:CA	1:B:167:VAL:CG2	2.17	1.14
1:E:118:LEU:HB3	1:E:305:ILE:HB	1.27	1.14
2:F:280:ASN:O	2:F:325:LYS:NZ	1.80	1.14
1:E:301:LEU:HD12	1:E:316:ASN:O	1.27	1.14
1:E:369:GLY:HA2	1:E:372:ILE:CG2	1.77	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:491:ASN:ND2	2:F:36:ARG:NE	1.94	1.14
2:F:55:VAL:HG11	2:F:159:TYR:CD1	1.83	1.14
2:D:362:GLU:OE1	2:D:490:ARG:HD3	0.96	1.13
2:D:329:TRP:CD2	2:D:424:ILE:HD13	1.75	1.13
1:E:98:GLN:HG3	1:E:117:ILE:HG23	1.19	1.13
1:A:98:GLN:HE21	1:A:115:ARG:CG	1.53	1.13
1:A:366:LYS:CG	1:A:395:ARG:HH12	1.61	1.13
2:C:52:LEU:HD11	2:C:56:VAL:HB	1.27	1.13
1:A:74:ASP:OD1	1:A:75:GLU:N	1.82	1.12
1:A:528:SER:OG	3:A:701:HOH:O	1.58	1.12
2:C:136:ARG:O	2:D:94:ARG:NH2	1.80	1.12
2:D:296:ASN:OD1	2:D:352:LYS:NZ	1.81	1.12
1:B:364:TRP:HB3	1:B:369:GLY:HA3	1.16	1.13
1:B:366:LYS:CA	1:B:396:HIS:CG	2.32	1.12
1:E:188:LEU:CD1	1:E:434:PHE:CZ	2.32	1.13
1:E:188:LEU:HD12	1:E:434:PHE:CZ	1.83	1.13
2:F:333:GLN:HG3	2:F:337:LEU:HD21	1.19	1.13
2:D:159:TYR:CE1	1:B:614:GLU:CG	2.32	1.12
1:B:366:LYS:CG	1:B:396:HIS:HB2	1.80	1.12
1:B:230:TYR:HE1	1:B:263:PHE:CE1	1.57	1.12
1:E:121:TRP:HB3	1:E:309:GLN:O	1.44	1.12
2:C:52:LEU:CD1	2:C:53:PRO:HD2	1.79	1.12
1:B:175:LEU:HB2	1:B:456:TYR:CD2	1.83	1.12
1:A:555:TYR:OH	2:C:494:TRP:HH2	1.31	1.11
2:D:329:TRP:CD2	2:D:424:ILE:HD12	1.76	1.11
2:D:356:TRP:O	2:D:360:ILE:HG13	1.49	1.11
1:E:590:SER:OG	1:E:593:THR:OG1	1.67	1.11
1:A:331:GLN:CD	1:A:364:TRP:HZ2	1.50	1.11
2:D:36:ARG:CD	1:B:491:ASN:OD1	1.98	1.11
2:D:146:TRP:CE3	2:D:146:TRP:O	2.02	1.11
1:E:324:TYR:HB2	1:E:536:PHE:CE2	1.84	1.11
2:D:5:ARG:CD	1:B:610:ARG:NE	2.03	1.11
2:D:46:LEU:HD11	1:B:483:PHE:CE1	1.83	1.11
1:B:80:PHE:CE1	1:B:166:ARG:N	2.17	1.11
1:B:366:LYS:CB	1:B:396:HIS:CG	2.34	1.11
2:F:52:LEU:HD21	2:F:57:ASP:HB2	1.31	1.11
1:A:96:ARG:O	1:A:168:PHE:CD1	2.03	1.11
2:D:96:VAL:O	2:D:100:LEU:CB	1.98	1.11
1:E:96:ARG:CG	1:E:168:PHE:CD2	2.32	1.11
1:E:364:TRP:HB3	1:E:369:GLY:HA3	1.14	1.11
1:E:431:SER:OG	1:E:434:PHE:N	1.84	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:PRO:CB	1:B:607:PHE:HE1	1.34	1.11
1:B:611:LYS:HB2	1:B:614:GLU:OE2	1.49	1.11
1:E:491:ASN:ND2	2:F:36:ARG:CD	2.14	1.11
2:F:139:PRO:HG2	2:F:144:LEU:HD11	1.28	1.11
2:F:350:LYS:HZ2	2:F:401:THR:CG2	1.62	1.11
1:A:365:ILE:CG2	1:A:397:LEU:HD23	1.81	1.10
2:C:23:TYR:CE2	2:C:156:TYR:HB2	1.86	1.10
2:C:102:PRO:HA	2:C:104:GLN:OE1	1.48	1.10
1:B:449:HIS:HB3	1:B:457:ASP:O	1.49	1.10
1:B:321:LEU:HD21	1:B:344:LEU:HD12	1.24	1.10
1:B:367:GLY:N	1:B:396:HIS:NE2	1.97	1.10
1:E:468:GLN:O	2:F:487:ASN:O	1.69	1.10
1:A:466:PRO:O	2:C:491:VAL:HG23	1.48	1.10
2:D:77:VAL:HG12	2:D:84:ILE:HG21	1.22	1.10
2:D:312:GLN:OE1	2:D:430:ILE:HG13	1.48	1.10
1:B:589:PRO:HD2	1:B:596:TRP:CH2	1.85	1.10
1:E:109:VAL:CG2	1:E:111:TYR:CE1	2.34	1.10
1:A:226:LEU:CD1	1:A:230:TYR:CZ	2.34	1.10
1:A:367:GLY:H	1:A:396:HIS:CE1	1.70	1.10
1:A:372:ILE:HG23	1:A:373:LEU:HD23	1.24	1.10
2:C:202:TRP:CH2	2:C:209:PHE:HD1	1.69	1.10
1:E:589:PRO:HD2	1:E:596:TRP:CH2	1.86	1.10
2:F:152:LEU:HA	2:F:155:LEU:CD1	1.82	1.10
1:A:331:GLN:CD	1:A:364:TRP:CZ2	2.23	1.09
1:A:388:LEU:O	1:A:423:ALA:HB2	0.93	1.09
2:C:210:LEU:HD12	2:C:210:LEU:H	1.16	1.09
2:D:358:LYS:HA	2:D:361:ASP:OD2	1.52	1.09
1:E:109:VAL:CG2	1:E:111:TYR:HE1	1.64	1.09
1:A:98:GLN:HE21	1:A:115:ARG:CA	1.63	1.09
2:C:78:HIS:HB2	2:D:35:GLN:NE2	1.64	1.09
2:D:485:VAL:CG2	1:B:470:SER:HB3	1.82	1.09
1:B:252:LYS:NZ	1:B:361:LEU:O	1.84	1.09
1:B:361:LEU:HD21	1:B:376:ILE:HD12	1.31	1.09
2:C:291:MET:HE1	2:C:340:ILE:HG22	1.14	1.09
1:B:79:MET:O	1:B:167:VAL:CG1	2.01	1.09
1:B:485:MET:SD	1:B:486:GLU:N	2.24	1.09
1:A:336:SER:OG	1:A:340:CYS:SG	2.09	1.09
1:A:388:LEU:C	1:A:423:ALA:HB2	1.73	1.09
2:D:77:VAL:CG1	2:D:84:ILE:CG1	2.28	1.09
1:B:366:LYS:CG	1:B:396:HIS:CB	2.29	1.09
1:B:450:LYS:CD	1:B:456:TYR:OH	2.00	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:VAL:HG11	2:D:84:ILE:CG1	1.81	1.09
2:D:329:TRP:CE2	2:D:424:ILE:HD12	1.79	1.09
1:B:99:VAL:CG2	1:B:166:ARG:NH2	2.17	1.08
1:A:98:GLN:CG	1:A:115:ARG:HA	1.83	1.08
1:A:226:LEU:CD1	1:A:230:TYR:OH	2.00	1.08
2:D:95:PHE:CE1	2:D:155:LEU:HD21	1.89	1.08
2:C:136:ARG:HD3	1:B:617:TRP:O	1.50	1.08
2:C:224:ILE:HB	2:C:229:PHE:HE2	1.19	1.08
1:B:239:ASP:CB	1:B:355:GLY:N	2.16	1.08
1:B:366:LYS:HG2	1:B:396:HIS:HB2	1.30	1.08
1:B:366:LYS:HA	1:B:396:HIS:CD2	1.86	1.08
1:E:524:PRO:C	1:E:525:ILE:HD13	1.74	1.08
1:A:502:THR:CB	1:A:577:ARG:NH2	2.17	1.08
1:A:566:LYS:HZ3	1:A:566:LYS:HA	1.18	1.08
2:D:95:PHE:HE1	2:D:155:LEU:HD21	1.15	1.08
1:A:338:LEU:HD21	1:A:372:ILE:HG13	1.35	1.08
1:A:469:ILE:HG22	2:C:488:TRP:N	1.67	1.08
2:C:80:ASP:OD1	2:C:82:ILE:HG21	1.48	1.08
1:B:277:LEU:HD23	1:B:277:LEU:H	1.16	1.08
1:B:366:LYS:CA	1:B:396:HIS:CE1	2.36	1.08
1:A:589:PRO:HG3	1:A:594:ILE:HD12	1.27	1.07
2:C:96:VAL:HG21	2:C:128:LEU:HD21	1.30	1.07
2:C:497:LYS:CD	2:C:502:LEU:O	2.02	1.07
1:B:99:VAL:CG2	1:B:166:ARG:HH21	1.66	1.07
1:B:395:ARG:NH1	1:B:396:HIS:HD2	1.50	1.07
1:E:589:PRO:HD2	1:E:596:TRP:HH2	1.06	1.07
1:A:480:GLY:HA2	1:A:524:PRO:O	1.54	1.07
1:E:289:TYR:CD1	1:E:317:PHE:CD2	2.42	1.07
1:E:567:GLN:HE21	1:E:567:GLN:HA	1.17	1.07
1:A:75:GLU:HA	2:C:259:ARG:HH21	1.18	1.07
1:A:265:GLN:OE1	1:A:268:ARG:NH1	1.88	1.07
1:A:365:ILE:HA	1:A:397:LEU:HD22	1.23	1.07
1:B:80:PHE:CZ	1:B:165:LEU:HA	1.89	1.07
1:E:548:SER:OG	1:E:549:GLN:NE2	1.88	1.07
2:F:18:LEU:HD22	2:F:22:PHE:CE2	1.87	1.07
1:A:246:GLY:O	1:A:363:GLY:CA	2.03	1.07
1:A:504:ILE:HD12	1:A:575:ILE:HG23	1.14	1.07
2:C:52:LEU:CD1	2:C:53:PRO:CD	2.32	1.07
2:C:312:GLN:OE1	2:C:323:LYS:HD2	1.53	1.07
2:D:251:GLU:OE1	2:D:255:ARG:NH2	1.88	1.07
1:B:79:MET:C	1:B:167:VAL:CG2	2.19	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:LEU:HD11	1:B:353:PHE:CD1	1.89	1.07
1:B:496:LYS:NZ	1:B:500:GLU:OE2	1.88	1.07
2:F:338:ASP:HA	2:F:341:ILE:HD12	1.10	1.07
1:A:169:ASN:OD1	1:A:204:TYR:HE1	1.36	1.06
1:A:388:LEU:HA	1:A:421:VAL:HG23	1.22	1.06
1:A:116:GLU:OE1	1:A:116:GLU:N	1.89	1.06
1:A:496:LYS:NZ	1:A:500:GLU:OE2	1.88	1.06
2:C:86:LEU:HD21	2:C:138:LEU:HD11	1.35	1.06
2:D:358:LYS:HD3	2:D:490:ARG:HH21	1.17	1.06
1:B:469:ILE:HD13	1:B:554:ILE:HG21	1.09	1.06
1:E:510:SER:HB2	1:E:533:SER:O	1.52	1.06
2:F:98:GLY:O	2:F:102:PRO:CD	2.03	1.06
1:A:592:ARG:HH21	2:C:184:ARG:CZ	1.67	1.06
2:D:202:TRP:CZ3	2:D:209:PHE:CZ	2.30	1.06
1:B:210:SER:O	1:B:212:ARG:NH2	1.88	1.06
1:B:230:TYR:CD1	1:B:263:PHE:CE1	2.41	1.06
1:E:210:SER:O	1:E:212:ARG:NH2	1.87	1.06
2:F:312:GLN:CD	2:F:323:LYS:CD	2.24	1.06
2:D:46:LEU:HD11	1:B:483:PHE:HE1	1.00	1.06
1:E:301:LEU:HD11	1:E:316:ASN:O	1.54	1.06
1:A:107:ASN:O	1:A:108:ASN:ND2	1.88	1.06
2:D:77:VAL:CG1	2:D:84:ILE:CB	2.33	1.06
2:D:120:GLY:O	2:D:158:HIS:HE1	1.38	1.06
1:B:179:GLY:O	1:B:182:TYR:O	1.72	1.06
1:E:471:TYR:O	1:E:550:GLN:O	1.74	1.06
2:F:128:LEU:CB	2:F:131:TRP:CZ3	2.37	1.06
1:A:98:GLN:HE21	1:A:115:ARG:HG2	1.20	1.05
1:B:310:HIS:CD2	1:B:314:GLY:HA3	1.90	1.05
1:E:188:LEU:CD1	1:E:434:PHE:CE1	2.38	1.05
2:F:152:LEU:CA	2:F:155:LEU:CD1	2.32	1.05
1:A:366:LYS:HG3	1:A:396:HIS:HB2	1.37	1.05
1:A:469:ILE:CD1	2:C:488:TRP:CZ2	2.39	1.05
2:C:136:ARG:HG3	1:B:617:TRP:HB3	1.36	1.05
1:B:509:TYR:CE2	1:B:513:ASP:HB2	1.91	1.05
2:F:88:TYR:HB3	2:F:144:LEU:HD23	1.37	1.05
2:F:145:ARG:O	2:F:149:ASN:ND2	1.88	1.05
1:B:107:ASN:O	1:B:108:ASN:ND2	1.89	1.05
1:E:397:LEU:HD12	1:E:397:LEU:H	1.22	1.05
1:A:469:ILE:HD13	2:C:488:TRP:CZ3	1.92	1.05
1:E:118:LEU:HD13	1:E:305:ILE:HG21	1.34	1.05
2:C:202:TRP:CE3	2:C:209:PHE:HE1	1.75	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:23:TYR:HD2	2:D:156:TYR:CD2	1.59	1.05
1:B:197:PRO:O	1:B:197:PRO:CG	2.02	1.05
2:F:350:LYS:NZ	2:F:401:THR:CB	2.19	1.05
2:D:96:VAL:HG13	2:D:100:LEU:HG	1.35	1.04
2:D:202:TRP:CE3	2:D:209:PHE:CE2	2.45	1.04
1:B:175:LEU:HB2	1:B:456:TYR:HD2	0.91	1.04
2:C:307:ARG:HB2	2:C:307:ARG:HH11	1.19	1.04
2:D:485:VAL:HG23	1:B:470:SER:HB3	1.07	1.04
1:E:469:ILE:HD13	1:E:478:ILE:HD11	1.36	1.04
1:B:366:LYS:HG2	1:B:396:HIS:HB3	1.34	1.04
1:E:289:TYR:CB	1:E:317:PHE:CE2	2.41	1.04
1:A:245:ILE:CD1	1:A:363:GLY:HA2	1.86	1.04
1:A:615:HIS:CD2	2:C:102:PRO:HG3	1.91	1.04
1:A:616:VAL:HG23	1:A:618:LYS:HE2	1.35	1.04
2:C:202:TRP:CH2	2:C:209:PHE:CD1	2.44	1.04
2:D:279:PHE:CE1	2:D:304:TRP:HZ3	1.71	1.04
1:B:367:GLY:N	1:B:396:HIS:CE1	2.24	1.04
2:F:312:GLN:CD	2:F:323:LYS:HD2	1.78	1.04
2:C:23:TYR:CE2	2:C:156:TYR:CD2	2.41	1.04
2:D:209:PHE:CZ	2:D:254:ILE:HG23	1.93	1.04
1:B:309:GLN:OE1	1:B:311:LEU:N	1.88	1.04
1:A:226:LEU:CD1	1:A:230:TYR:CE1	2.40	1.03
1:A:336:SER:O	1:A:340:CYS:N	1.90	1.03
1:E:241:ARG:N	1:E:383:THR:OG1	1.91	1.03
2:F:275:LEU:H	2:F:275:LEU:HD12	1.19	1.03
1:A:615:HIS:CD2	2:C:102:PRO:CG	2.40	1.03
2:C:95:PHE:CE1	2:C:155:LEU:HD11	1.92	1.03
2:D:279:PHE:CD1	2:D:304:TRP:CZ3	2.46	1.03
2:D:69:ASP:CA	2:D:77:VAL:CG2	2.07	1.03
2:D:278:PHE:CD1	2:D:279:PHE:HD2	1.77	1.03
2:F:365:SER:HA	2:F:419:PHE:HE1	0.89	1.03
1:A:127:SER:OG	1:A:216:LEU:HD22	1.56	1.03
1:E:364:TRP:HB3	1:E:369:GLY:CA	1.88	1.03
1:E:538:THR:OG1	1:E:560:HIS:CD2	2.12	1.03
1:A:607:PHE:CZ	2:C:4:PRO:HD3	1.92	1.03
1:E:524:PRO:O	1:E:525:ILE:HD13	1.59	1.03
1:A:290:SER:OG	1:A:296:SER:OG	1.73	1.02
1:B:397:LEU:HG	1:B:400:LEU:HD21	1.06	1.02
2:F:131:TRP:HE1	2:F:139:PRO:CD	1.70	1.02
2:D:69:ASP:O	2:D:77:VAL:CG2	2.07	1.02
1:B:247:GLY:N	1:B:365:ILE:HG23	1.72	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:ARG:NH2	2:C:314:ASP:OD1	1.93	1.02
2:D:329:TRP:CG	2:D:424:ILE:HD12	1.93	1.02
1:E:389:GLU:CG	1:E:394:LYS:HA	1.90	1.02
2:F:139:PRO:HG2	2:F:144:LEU:CD1	1.89	1.02
2:F:270:TYR:O	2:F:274:VAL:HG23	1.59	1.02
1:A:607:PHE:HZ	2:C:4:PRO:HG3	0.85	1.02
2:D:77:VAL:HG13	2:D:84:ILE:HB	1.35	1.02
1:B:197:PRO:O	1:B:197:PRO:HG2	1.54	1.02
1:B:515:LEU:HD23	1:B:515:LEU:H	1.23	1.02
1:E:245:ILE:HD13	1:E:373:LEU:HD13	1.40	1.02
2:C:99:LEU:HD22	2:C:99:LEU:H	1.22	1.02
2:D:77:VAL:HG12	2:D:84:ILE:CG2	1.88	1.02
1:B:79:MET:O	1:B:167:VAL:HG22	1.56	1.02
1:B:297:LEU:HB2	1:B:344:LEU:CD1	1.88	1.02
2:F:18:LEU:HD23	2:F:22:PHE:CZ	1.91	1.02
2:F:22:PHE:CE1	2:F:37:ALA:HB1	1.95	1.02
1:A:364:TRP:HD1	1:A:369:GLY:CA	1.73	1.01
1:B:509:TYR:HE2	1:B:513:ASP:HB2	1.20	1.01
1:B:589:PRO:CD	1:B:596:TRP:CH2	2.42	1.01
1:E:83:LEU:CD1	1:E:101:LYS:O	2.07	1.01
1:E:359:LEU:HD11	1:E:361:LEU:HG	1.35	1.01
1:E:369:GLY:CA	1:E:372:ILE:HG22	1.89	1.01
1:E:614:GLU:OE2	2:F:159:TYR:OH	1.78	1.01
2:C:97:ASN:ND2	2:C:129:ARG:CD	2.23	1.01
2:D:357:GLU:O	2:D:361:ASP:OD2	1.75	1.01
1:B:166:ARG:O	1:B:167:VAL:CG2	2.08	1.01
2:F:128:LEU:HA	2:F:131:TRP:HE3	1.26	1.01
1:A:365:ILE:HA	1:A:397:LEU:HD21	1.03	1.01
1:A:387:PHE:O	1:A:421:VAL:CG2	2.08	1.01
1:A:504:ILE:CD1	1:A:575:ILE:HG21	1.88	1.01
1:A:607:PHE:HZ	2:C:4:PRO:CG	1.50	1.01
2:C:125:PHE:HA	2:C:128:LEU:HD23	1.39	1.01
1:A:99:VAL:HG21	1:A:104:ILE:HD11	1.40	1.01
1:A:592:ARG:NH2	2:C:184:ARG:HH21	1.42	1.01
2:C:434:LYS:HE2	3:C:612:HOH:O	1.60	1.01
2:D:46:LEU:HD21	1:B:577:ARG:HD3	1.43	1.01
1:B:214:GLN:OE1	1:B:426:LEU:CB	2.09	1.01
1:E:213:ILE:HD11	1:E:215:SER:HB3	1.42	1.01
1:A:365:ILE:CG2	1:A:397:LEU:CD2	2.34	1.01
2:D:84:ILE:CD1	2:D:88:TYR:HE2	1.72	1.01
2:D:358:LYS:HB3	2:D:490:ARG:HE	1.22	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:482:GLN:HB3	1:E:576:VAL:HG22	1.41	1.01
2:F:270:TYR:O	2:F:274:VAL:CG2	2.07	1.01
1:A:290:SER:OG	1:A:296:SER:CB	2.09	1.00
1:A:366:LYS:CG	1:A:395:ARG:NH1	2.21	1.00
1:B:79:MET:N	1:B:167:VAL:HG21	1.47	1.00
1:E:199:ASN:HB3	1:E:202:THR:HG23	1.43	1.00
2:F:151:ALA:O	2:F:155:LEU:HD11	1.59	1.00
1:A:368:PHE:CE1	2:D:146:TRP:CD1	2.49	1.00
2:D:125:PHE:O	2:D:128:LEU:HB3	1.61	1.00
2:D:495:LYS:O	2:D:497:LYS:HG3	1.61	1.00
1:E:241:ARG:NE	1:E:381:LYS:HD3	1.75	1.00
1:B:219:PRO:CB	1:B:221:TYR:CE2	2.43	1.00
1:E:450:LYS:HE3	1:E:453:GLN:HA	1.39	1.00
2:D:84:ILE:CD1	2:D:88:TYR:CE2	2.43	1.00
1:E:364:TRP:CD1	1:E:369:GLY:CA	2.44	1.00
1:A:348:LEU:HD11	1:A:353:PHE:HB3	1.37	1.00
2:C:180:TYR:O	2:C:184:ARG:CG	2.08	1.00
1:B:330:PRO:HB3	1:B:337:TYR:CD1	1.96	1.00
1:B:361:LEU:HD22	1:B:376:ILE:HD12	1.40	1.00
1:A:481:ILE:CG2	1:A:575:ILE:HB	1.92	1.00
2:C:138:LEU:HD21	2:D:94:ARG:HD2	1.43	1.00
1:B:175:LEU:CB	1:B:456:TYR:HD2	1.75	1.00
1:B:369:GLY:HA2	1:B:372:ILE:HG22	1.44	1.00
1:E:612:LYS:CD	2:F:164:GLU:CD	2.30	1.00
1:A:98:GLN:NE2	1:A:115:ARG:HG3	1.64	0.99
1:E:97:LEU:CD2	1:E:120:PHE:HE1	1.69	0.99
2:F:131:TRP:NE1	2:F:139:PRO:CG	2.25	0.99
1:A:331:GLN:HG2	1:A:364:TRP:CZ2	1.97	0.99
2:D:358:LYS:CA	2:D:361:ASP:OD2	2.10	0.99
1:B:469:ILE:HD13	1:B:554:ILE:CG2	1.91	0.99
1:E:610:ARG:HD2	2:F:167:ASP:CB	1.92	0.99
2:D:430:ILE:H	2:D:430:ILE:HD13	1.23	0.99
2:F:151:ALA:O	2:F:155:LEU:HD12	1.60	0.99
2:D:485:VAL:HG23	1:B:470:SER:CB	1.93	0.99
2:D:487:ASN:CG	2:D:488:TRP:H	1.62	0.99
1:B:387:PHE:CE2	1:B:397:LEU:HD21	1.97	0.99
1:B:327:SER:CB	1:B:332:ASP:OD2	2.09	0.99
1:A:469:ILE:HD13	2:C:488:TRP:CZ2	1.97	0.99
2:C:202:TRP:CE3	2:C:209:PHE:CE1	2.49	0.99
2:D:184:ARG:HB3	1:B:592:ARG:CD	1.92	0.99
1:B:366:LYS:CD	1:B:396:HIS:HB2	1.92	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ASN:OD1	1:B:579:LYS:N	1.96	0.99
2:F:312:GLN:OE1	2:F:323:LYS:HE2	1.58	0.99
2:C:304:TRP:CD2	2:C:308:ASN:ND2	2.30	0.99
1:E:97:LEU:HD21	1:E:120:PHE:HE1	1.23	0.99
1:E:106:TYR:OH	1:E:122:HIS:NE2	1.95	0.99
2:C:209:PHE:CE2	2:C:254:ILE:HG23	1.98	0.98
1:E:293:ASP:OD2	1:E:327:SER:C	2.02	0.98
2:C:17:GLU:OE2	2:C:40:ARG:NH1	1.94	0.98
1:B:365:ILE:CD1	1:B:366:LYS:HG3	1.92	0.98
1:B:589:PRO:CD	1:B:596:TRP:HH2	1.76	0.98
1:E:491:ASN:ND2	2:F:36:ARG:HD2	1.79	0.98
2:F:338:ASP:HA	2:F:341:ILE:CD1	1.93	0.98
2:C:224:ILE:HB	2:C:229:PHE:CE2	1.97	0.98
1:E:431:SER:OG	1:E:434:PHE:C	2.02	0.98
1:A:469:ILE:HG22	2:C:488:TRP:H	0.82	0.98
2:C:345:ASN:OD1	2:C:348:ASN:N	1.96	0.98
2:F:312:GLN:OE1	2:F:323:LYS:NZ	1.96	0.98
2:D:336:LEU:HD11	2:D:340:ILE:HD11	1.43	0.98
1:E:169:ASN:CG	1:E:203:THR:HG23	1.84	0.98
1:A:169:ASN:OD1	1:A:204:TYR:CE1	2.17	0.98
1:E:450:LYS:CE	1:E:453:GLN:HA	1.92	0.98
1:B:366:LYS:HA	1:B:396:HIS:NE2	1.77	0.98
1:E:182:TYR:HE1	1:E:184:ASP:OD1	1.46	0.98
2:F:18:LEU:HD22	2:F:22:PHE:HE2	1.23	0.98
2:D:146:TRP:CZ3	2:D:150:GLU:CB	2.46	0.98
2:D:202:TRP:CZ3	2:D:209:PHE:CG	2.51	0.98
1:B:589:PRO:HG2	1:B:596:TRP:CH2	1.99	0.98
1:B:348:LEU:CD1	1:B:353:PHE:HB3	1.93	0.98
1:B:390:THR:HG23	1:B:391:ALA:H	1.26	0.98
1:E:301:LEU:HD11	1:E:316:ASN:C	1.83	0.98
1:A:616:VAL:HG11	2:C:50:GLN:O	1.64	0.97
1:B:86:LYS:HA	1:B:133:PHE:HB3	1.45	0.97
1:B:471:TYR:HE1	1:B:550:GLN:HA	0.82	0.97
1:A:216:LEU:HD12	1:A:425:SER:HG	1.16	0.97
1:A:245:ILE:HD12	1:A:246:GLY:N	1.79	0.97
1:E:289:TYR:HB3	1:E:317:PHE:HE2	1.19	0.97
1:A:616:VAL:HG23	1:A:618:LYS:CE	1.93	0.97
2:D:4:PRO:CG	1:B:607:PHE:HE1	1.76	0.97
2:D:202:TRP:CH2	2:D:209:PHE:CG	2.53	0.97
1:A:592:ARG:HD2	2:C:184:ARG:HE	1.29	0.97
2:F:280:ASN:HA	2:F:325:LYS:HE3	1.46	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:TRP:HD1	1:A:369:GLY:HA2	1.26	0.97
2:D:278:PHE:HD1	2:D:279:PHE:HD2	1.09	0.97
1:E:364:TRP:HD1	1:E:369:GLY:CA	1.76	0.97
2:F:312:GLN:OE1	2:F:323:LYS:CD	2.11	0.97
2:F:333:GLN:CG	2:F:337:LEU:HD21	1.94	0.97
1:E:241:ARG:CZ	1:E:381:LYS:HD3	1.95	0.97
1:E:491:ASN:HD21	2:F:36:ARG:HD2	1.28	0.96
2:F:104:GLN:OE1	2:F:105:GLN:N	1.98	0.96
1:A:399:GLU:OE2	1:A:400:LEU:N	1.98	0.96
2:D:4:PRO:CA	1:B:607:PHE:CE1	2.46	0.96
1:B:99:VAL:HG22	1:B:166:ARG:NH2	1.80	0.96
1:B:105:VAL:HG21	1:B:134:SER:OG	1.64	0.96
1:E:175:LEU:HD22	1:E:189:TRP:NE1	1.79	0.96
1:A:370:MET:CB	1:A:400:LEU:CB	2.44	0.96
1:E:175:LEU:CD2	1:E:189:TRP:HE1	1.77	0.96
2:F:350:LYS:HZ3	2:F:401:THR:HG22	1.25	0.96
1:A:603:PRO:O	2:C:10:ARG:O	1.82	0.96
2:C:206:ARG:O	2:C:210:LEU:HD12	1.66	0.96
2:D:97:ASN:O	2:D:101:ASP:N	1.98	0.96
2:F:52:LEU:CD2	2:F:57:ASP:HB2	1.94	0.96
1:B:366:LYS:HD3	1:B:395:ARG:HE	1.29	0.96
1:A:365:ILE:CB	1:A:397:LEU:CD2	2.42	0.96
1:A:590:SER:OG	2:C:184:ARG:NE	1.98	0.96
2:D:69:ASP:HA	2:D:77:VAL:HG22	1.45	0.96
1:B:79:MET:CB	1:B:167:VAL:HG21	1.94	0.96
1:B:366:LYS:HB3	1:B:396:HIS:HD2	1.15	0.96
2:C:288:LYS:CE	2:C:343:ASN:OD1	2.13	0.96
2:C:133:THR:HG22	2:D:97:ASN:ND2	1.81	0.96
2:C:234:LEU:O	2:C:235:VAL:HG23	1.64	0.96
1:B:96:ARG:CZ	1:B:171:ASN:ND2	2.22	0.96
1:A:367:GLY:N	1:A:396:HIS:HE1	1.54	0.96
2:D:5:ARG:CZ	1:B:610:ARG:HG2	1.96	0.96
1:E:99:VAL:O	1:E:113:ALA:O	1.78	0.96
2:F:55:VAL:HG21	2:F:159:TYR:CB	1.95	0.96
1:B:247:GLY:N	1:B:365:ILE:CG2	2.30	0.95
2:D:485:VAL:CG2	1:B:470:SER:CB	2.44	0.95
1:B:219:PRO:HB3	1:B:221:TYR:HE2	1.01	0.95
1:B:361:LEU:CD2	1:B:376:ILE:CD1	2.44	0.95
1:B:365:ILE:HD12	1:B:366:LYS:HG3	1.47	0.95
1:B:348:LEU:HD12	1:B:353:PHE:HB3	1.48	0.95
1:B:361:LEU:HD22	1:B:376:ILE:CD1	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LYS:CA	1:B:396:HIS:NE2	2.30	0.95
1:E:496:LYS:NZ	3:E:701:HOH:O	1.93	0.95
2:D:497:LYS:O	1:B:543:HIS:NE2	2.00	0.95
1:B:89:LEU:HD13	1:B:90:HIS:N	1.82	0.95
1:A:98:GLN:NE2	1:A:115:ARG:HG2	1.76	0.95
1:A:616:VAL:CG1	2:C:50:GLN:O	2.15	0.95
1:B:397:LEU:CG	1:B:400:LEU:HD21	1.95	0.95
2:F:282:TYR:HE2	2:F:287:LEU:HD22	1.30	0.95
1:A:96:ARG:O	1:A:168:PHE:HE1	1.49	0.95
1:A:331:GLN:HG3	1:A:364:TRP:CH2	2.02	0.95
1:B:208:HIS:ND1	1:B:209:GLU:HG2	1.80	0.95
1:B:249:ASN:OD1	1:B:424:HIS:NE2	1.99	0.95
1:B:397:LEU:HD12	1:B:400:LEU:HD11	1.45	0.95
2:F:88:TYR:HB3	2:F:144:LEU:CD2	1.96	0.95
1:A:326:GLY:CA	1:A:578:ASN:HD22	1.69	0.94
1:A:504:ILE:HD12	1:A:575:ILE:HG22	0.97	0.94
1:A:607:PHE:CZ	2:C:4:PRO:CD	2.30	0.94
1:B:100:VAL:HB	3:B:708:HOH:O	1.65	0.94
1:B:243:MET:SD	1:B:361:LEU:HD11	2.07	0.94
1:A:311:LEU:O	1:A:313:GLN:NE2	1.99	0.94
1:E:519:SER:O	1:E:520:LEU:CD2	2.13	0.94
1:A:331:GLN:HE21	1:A:364:TRP:HE1	1.14	0.94
2:D:154:TRP:CE3	2:D:155:LEU:HD23	2.02	0.94
2:F:18:LEU:HD21	2:F:22:PHE:CZ	2.01	0.94
1:B:471:TYR:CE1	1:B:550:GLN:C	2.40	0.94
1:E:103:GLY:HA3	1:E:134:SER:O	1.68	0.94
1:E:469:ILE:CD1	1:E:478:ILE:HD11	1.95	0.94
1:B:541:LEU:HD12	1:B:542:ILE:N	1.83	0.94
2:F:128:LEU:CB	2:F:131:TRP:CE3	2.49	0.94
2:C:138:LEU:CD2	2:D:94:ARG:NH1	2.29	0.94
1:B:366:LYS:HD3	1:B:396:HIS:HB2	1.46	0.94
1:A:589:PRO:CG	1:A:594:ILE:HD12	1.98	0.94
1:E:452:THR:OG1	1:E:455:ASP:OD2	1.85	0.94
2:F:350:LYS:HZ1	2:F:401:THR:CB	1.81	0.94
1:A:366:LYS:HE2	1:A:395:ARG:NH2	1.58	0.94
1:A:502:THR:HB	1:A:577:ARG:HH21	1.15	0.94
1:A:604:PHE:HE2	2:C:10:ARG:NH1	1.66	0.94
2:C:97:ASN:HD21	2:C:129:ARG:CD	1.81	0.94
1:B:330:PRO:HD2	1:B:364:TRP:CZ2	2.03	0.94
2:F:32:ASP:OD2	2:F:34:ARG:NE	2.01	0.94
2:F:272:ASN:HA	2:F:275:LEU:HD13	0.95	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:HG2	1:A:395:ARG:HH12	0.78	0.94
1:A:406:PHE:HD1	1:A:407:SER:H	1.15	0.94
2:C:79:GLN:O	2:C:79:GLN:NE2	2.00	0.94
2:D:489:SER:O	1:B:467:LEU:CB	2.15	0.94
1:E:499:LEU:O	1:E:502:THR:OG1	1.85	0.94
2:F:338:ASP:CA	2:F:341:ILE:HD12	1.97	0.94
1:A:226:LEU:HD12	1:A:230:TYR:CE1	2.02	0.94
1:A:368:PHE:CE2	1:A:372:ILE:HB	2.03	0.94
2:C:105:GLN:HA	2:C:105:GLN:NE2	1.83	0.94
2:D:96:VAL:CG1	2:D:100:LEU:HG	1.98	0.94
1:B:288:GLU:HG2	1:B:289:TYR:CE2	2.03	0.94
1:B:449:HIS:NE2	1:B:461:LEU:HG	1.82	0.94
2:D:154:TRP:CZ2	2:D:158:HIS:ND1	2.36	0.93
2:D:209:PHE:CE1	2:D:254:ILE:CG2	2.51	0.93
1:B:395:ARG:NH1	1:B:396:HIS:CD2	2.35	0.93
1:A:592:ARG:NH2	2:C:184:ARG:CZ	2.27	0.93
2:D:329:TRP:CD1	2:D:424:ILE:HD12	2.04	0.93
1:B:389:GLU:O	1:B:390:THR:HG22	1.68	0.93
2:C:138:LEU:HD23	2:D:94:ARG:NH1	1.83	0.93
1:B:388:LEU:HA	1:B:421:VAL:O	1.67	0.93
1:A:365:ILE:HG22	1:A:397:LEU:HD23	0.95	0.93
1:A:395:ARG:NH1	1:A:396:HIS:HB2	1.83	0.93
2:C:23:TYR:CZ	2:C:156:TYR:HB2	2.02	0.93
2:D:358:LYS:HB3	2:D:490:ARG:NE	1.82	0.93
1:A:100:VAL:HG12	3:A:704:HOH:O	1.68	0.93
1:A:507:TYR:HD1	1:A:535:ASN:C	1.71	0.93
2:C:133:THR:HG23	2:D:93:ILE:CG2	1.98	0.93
2:C:307:ARG:O	2:C:311:THR:OG1	1.85	0.93
1:B:115:ARG:HB2	1:B:115:ARG:NH2	1.84	0.93
1:E:491:ASN:CG	2:F:36:ARG:CD	2.36	0.93
2:D:312:GLN:OE1	2:D:427:TYR:CD2	2.21	0.93
1:A:467:LEU:CD2	1:A:556:VAL:HG22	1.99	0.93
1:A:589:PRO:HD2	1:A:596:TRP:CZ3	2.03	0.93
1:B:588:LEU:H	1:B:588:LEU:HD12	1.31	0.93
1:E:100:VAL:HG12	1:E:101:LYS:HG2	1.49	0.93
1:A:366:LYS:HE2	1:A:395:ARG:HH22	0.77	0.93
2:D:122:PRO:HB2	2:D:125:PHE:HD2	1.30	0.93
1:E:289:TYR:HB3	1:E:317:PHE:CD2	2.04	0.93
1:E:610:ARG:HD2	2:F:167:ASP:HB2	1.49	0.93
1:A:471:TYR:HD1	1:A:552:MET:HG3	1.30	0.93
2:C:359:LEU:O	2:C:363:ASN:ND2	2.02	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ASP:C	2:D:77:VAL:CG2	2.30	0.93
1:A:99:VAL:HB	1:A:113:ALA:HA	1.48	0.93
1:E:610:ARG:HG2	1:E:610:ARG:HH11	1.34	0.93
2:C:312:GLN:OE1	2:C:323:LYS:CD	2.17	0.92
2:D:23:TYR:HE2	2:D:156:TYR:HB2	1.35	0.92
1:B:247:GLY:O	1:B:250:SER:OG	1.85	0.92
1:A:169:ASN:CG	1:A:203:THR:HG23	1.90	0.92
1:E:289:TYR:CB	1:E:317:PHE:HE2	1.80	0.92
1:A:365:ILE:HD12	1:A:366:LYS:H	1.31	0.92
2:D:84:ILE:HD11	2:D:88:TYR:HE2	0.79	0.92
2:D:209:PHE:CZ	2:D:254:ILE:CG2	2.52	0.92
1:B:541:LEU:HD12	1:B:542:ILE:H	1.33	0.92
1:E:467:LEU:CD1	2:F:488:TRP:HB3	1.98	0.92
1:A:126:GLN:HE22	1:A:257:ARG:NH1	1.67	0.92
1:B:310:HIS:HD2	1:B:314:GLY:HA3	1.24	0.92
2:F:131:TRP:NE1	2:F:139:PRO:HG3	1.83	0.92
1:A:96:ARG:NH2	1:A:171:ASN:OD1	2.02	0.92
2:D:358:LYS:O	2:D:362:GLU:N	2.01	0.92
1:B:471:TYR:CE1	1:B:550:GLN:O	2.21	0.92
1:E:612:LYS:HD2	2:F:164:GLU:OE2	1.69	0.92
1:A:365:ILE:CA	1:A:397:LEU:HD21	1.89	0.92
1:A:368:PHE:HE1	2:D:146:TRP:CD1	1.86	0.92
1:A:538:THR:OG1	1:A:560:HIS:CD2	2.22	0.92
1:E:175:LEU:HD22	1:E:189:TRP:HE1	1.30	0.92
2:F:126:VAL:O	2:F:129:ARG:HG3	1.69	0.92
1:A:291:LEU:O	1:A:294:SER:HB3	1.67	0.92
2:D:278:PHE:CD1	2:D:279:PHE:CD2	2.58	0.92
1:B:268:ARG:NH1	1:B:305:ILE:HD12	1.84	0.92
1:B:327:SER:HB2	1:B:332:ASP:OD2	1.69	0.92
1:E:169:ASN:OD1	1:E:203:THR:HG21	1.67	0.92
1:E:615:HIS:ND1	1:E:615:HIS:O	2.03	0.92
1:E:615:HIS:CE1	2:F:102:PRO:HG3	2.05	0.92
2:F:126:VAL:HG13	2:F:129:ARG:HD3	1.52	0.92
2:F:131:TRP:HE1	2:F:139:PRO:HG3	1.31	0.92
2:D:418:ARG:HB2	2:D:419:PHE:CD2	2.04	0.91
2:D:423:GLU:CA	2:D:426:LEU:HG	1.99	0.91
1:E:383:THR:HB	1:E:384:HIS:HD2	1.34	0.91
1:A:98:GLN:HE21	1:A:115:ARG:CB	1.73	0.91
1:A:326:GLY:HA3	1:A:578:ASN:CG	1.89	0.91
2:D:23:TYR:CE2	2:D:156:TYR:CB	2.52	0.91
1:A:250:SER:O	1:A:423:ALA:O	1.87	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLY:HA2	1:A:372:ILE:CG2	2.00	0.91
1:A:469:ILE:HD11	2:C:488:TRP:CH2	2.02	0.91
1:B:450:LYS:HD3	1:B:456:TYR:HH	1.20	0.91
1:B:546:ASP:HB3	1:B:549:GLN:HG3	1.52	0.91
1:E:301:LEU:HD12	1:E:301:LEU:H	1.31	0.91
1:B:297:LEU:HB2	1:B:344:LEU:HD11	0.94	0.91
1:E:182:TYR:CE1	1:E:184:ASP:CB	2.52	0.91
1:E:357:SER:HG	1:E:380:TYR:HH	1.04	0.91
1:E:83:LEU:HD23	1:E:83:LEU:H	1.31	0.91
1:A:207:LEU:HD12	1:A:213:ILE:HG12	1.50	0.91
2:D:122:PRO:HB2	2:D:125:PHE:CD2	2.06	0.91
1:E:612:LYS:HD2	2:F:164:GLU:CD	1.90	0.91
2:F:152:LEU:C	2:F:155:LEU:CD1	2.39	0.91
1:A:196:PHE:HB3	1:A:205:HIS:HE1	1.33	0.91
1:B:591:PRO:O	1:B:592:ARG:HB3	1.69	0.91
1:A:451:ILE:HG22	1:A:452:THR:HG23	1.51	0.91
1:A:464:SER:O	2:C:494:TRP:HZ3	1.36	0.91
2:C:95:PHE:O	2:C:99:LEU:CD2	2.19	0.91
2:C:97:ASN:ND2	2:C:129:ARG:HD3	1.85	0.91
2:D:54:HIS:CD2	2:D:98:GLY:HA3	2.05	0.91
1:E:109:VAL:HG23	1:E:111:TYR:HE1	1.06	0.91
1:E:310:HIS:CD2	1:E:314:GLY:HA3	2.04	0.91
1:A:206:LEU:C	1:A:207:LEU:HD23	1.91	0.91
2:C:383:LYS:NZ	2:C:405:GLU:OE1	2.04	0.91
2:D:487:ASN:ND2	2:D:488:TRP:N	2.18	0.91
1:B:239:ASP:CB	1:B:355:GLY:O	2.20	0.91
1:B:324:TYR:HB2	1:B:536:PHE:CE2	2.04	0.91
2:F:365:SER:CA	2:F:419:PHE:CE1	2.46	0.91
1:A:282:LEU:HD12	1:A:359:LEU:CD1	2.01	0.90
2:C:23:TYR:HD2	2:C:156:TYR:CD2	1.86	0.90
2:D:82:ILE:HG22	2:D:83:PRO:HD3	1.50	0.90
2:D:159:TYR:CZ	1:B:614:GLU:HG2	2.06	0.90
2:D:487:ASN:ND2	2:D:488:TRP:H	1.69	0.90
1:E:121:TRP:HB2	1:E:309:GLN:O	1.69	0.90
1:A:365:ILE:O	1:A:396:HIS:CE1	2.25	0.90
1:A:368:PHE:HE2	1:A:372:ILE:HB	1.34	0.90
1:A:245:ILE:HD11	1:A:363:GLY:HA2	1.53	0.90
1:B:321:LEU:HD13	1:B:347:HIS:HD1	1.36	0.90
1:E:71:TYR:CD1	1:E:80:PHE:CE2	2.59	0.90
1:E:118:LEU:CB	1:E:305:ILE:HB	2.01	0.90
1:E:206:LEU:C	1:E:207:LEU:HD23	1.91	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:152:LEU:HA	2:F:155:LEU:HD13	1.49	0.90
1:A:366:LYS:HG3	1:A:396:HIS:CG	1.95	0.90
1:E:389:GLU:HG2	1:E:394:LYS:HA	1.50	0.90
1:A:566:LYS:HA	1:A:566:LYS:NZ	1.86	0.90
1:A:589:PRO:HD2	1:A:596:TRP:HH2	0.93	0.90
2:C:10:ARG:HG2	2:C:10:ARG:HH11	1.36	0.90
2:D:96:VAL:O	2:D:100:LEU:N	2.05	0.90
2:D:418:ARG:HB2	2:D:419:PHE:CE2	2.06	0.90
1:A:604:PHE:HE2	2:C:10:ARG:HH12	1.18	0.90
1:B:397:LEU:HD12	1:B:400:LEU:CD1	2.01	0.90
1:E:612:LYS:HD3	2:F:164:GLU:CD	1.89	0.90
2:D:358:LYS:O	2:D:362:GLU:HB2	1.71	0.90
1:E:245:ILE:CD1	1:E:373:LEU:HD13	2.01	0.90
1:A:398:ASP:OD2	1:A:399:GLU:N	2.05	0.90
2:C:85:ARG:CD	1:B:486:GLU:OE2	2.18	0.90
2:D:423:GLU:HA	2:D:426:LEU:CG	2.01	0.90
1:B:366:LYS:HG2	1:B:396:HIS:CG	2.06	0.90
1:A:126:GLN:HE22	1:A:257:ARG:NH2	1.70	0.90
2:D:44:TYR:O	2:D:48:GLY:N	2.04	0.90
2:D:312:GLN:OE1	2:D:427:TYR:HD2	1.55	0.90
1:B:219:PRO:HB2	1:B:221:TYR:CD2	2.06	0.90
1:E:96:ARG:HG2	1:E:168:PHE:CD2	2.04	0.90
1:A:325:ALA:O	1:A:578:ASN:ND2	2.05	0.89
2:C:304:TRP:CE2	2:C:308:ASN:ND2	2.39	0.89
2:C:362:GLU:HG3	2:C:490:ARG:HG2	1.53	0.89
2:D:120:GLY:O	2:D:158:HIS:CE1	2.25	0.89
1:B:197:PRO:O	1:B:197:PRO:CD	2.09	0.89
1:B:219:PRO:CB	1:B:221:TYR:CD2	2.55	0.89
2:F:359:LEU:HD23	2:F:360:ILE:N	1.85	0.89
1:B:246:GLY:O	1:B:363:GLY:CA	2.19	0.89
1:E:98:GLN:HG3	1:E:117:ILE:CG2	2.01	0.89
2:F:152:LEU:HA	2:F:155:LEU:HD11	1.51	0.89
2:F:272:ASN:C	2:F:275:LEU:HD13	1.93	0.89
1:A:282:LEU:O	1:A:337:TYR:OH	1.90	0.89
1:A:365:ILE:CB	1:A:397:LEU:HD22	2.02	0.89
1:A:615:HIS:CD2	2:C:102:PRO:HG2	2.07	0.89
2:D:156:TYR:HA	2:D:160:TRP:HD1	1.36	0.89
2:D:349:PHE:HE2	2:D:356:TRP:CD2	1.89	0.89
1:B:246:GLY:O	1:B:363:GLY:HA3	1.73	0.89
1:E:364:TRP:CB	1:E:369:GLY:HA3	2.01	0.89
1:A:170:SER:OG	1:A:172:HIS:ND1	2.05	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:THR:CG2	2:D:93:ILE:CG2	2.51	0.89
2:D:77:VAL:CG1	2:D:84:ILE:HB	1.99	0.89
1:B:175:LEU:HD13	1:B:456:TYR:CD2	2.07	0.89
1:A:381:LYS:CB	1:A:409:SER:CB	2.50	0.89
2:D:154:TRP:CZ3	2:D:155:LEU:HD23	2.08	0.89
2:F:20:LEU:O	2:F:23:TYR:O	1.89	0.89
1:A:475:LYS:CB	1:A:478:ILE:O	2.20	0.89
1:A:592:ARG:CD	2:C:184:ARG:HE	1.85	0.89
1:A:615:HIS:HD2	2:C:102:PRO:HG3	1.30	0.89
2:C:209:PHE:HE2	2:C:254:ILE:HG23	1.36	0.89
1:B:259:LEU:O	1:B:263:PHE:CD1	2.26	0.89
1:E:491:ASN:ND2	2:F:39:GLN:HB3	1.88	0.89
2:C:138:LEU:HD21	2:D:94:ARG:CD	2.02	0.89
1:B:177:GLU:CG	1:B:458:PHE:CD2	2.30	0.89
1:B:365:ILE:HD12	1:B:366:LYS:N	1.88	0.89
2:F:272:ASN:C	2:F:275:LEU:CD1	2.39	0.89
1:A:465:ALA:HA	2:C:494:TRP:CE3	2.07	0.89
2:D:69:ASP:O	2:D:77:VAL:HG23	1.72	0.89
1:E:449:HIS:HB3	1:E:457:ASP:O	1.72	0.89
1:A:477:GLY:O	1:A:573:TRP:HB2	1.73	0.89
1:E:241:ARG:HD3	1:E:381:LYS:O	1.72	0.89
2:F:131:TRP:HE1	2:F:139:PRO:CB	1.86	0.89
2:F:155:LEU:HD12	2:F:155:LEU:H	1.37	0.89
2:F:272:ASN:CA	2:F:275:LEU:HD11	1.89	0.89
1:A:222:TRP:O	1:A:225:PRO:HD2	1.73	0.88
1:A:181:LEU:HD13	1:A:585:CYS:HG	1.33	0.88
2:C:291:MET:CE	2:C:340:ILE:CG2	2.50	0.88
2:D:4:PRO:CD	1:B:607:PHE:HE1	1.87	0.88
2:D:23:TYR:HE2	2:D:156:TYR:CD2	1.89	0.88
1:B:233:HIS:CE1	1:B:275:GLU:OE1	2.27	0.88
1:B:247:GLY:CA	1:B:365:ILE:HG23	2.03	0.88
1:E:77:GLU:OE2	1:E:169:ASN:ND2	2.05	0.88
1:B:366:LYS:HB3	1:B:395:ARG:HH11	1.38	0.88
1:E:383:THR:HB	1:E:384:HIS:CD2	2.08	0.88
2:C:95:PHE:O	2:C:99:LEU:HD21	1.73	0.88
2:C:100:LEU:HG	2:C:101:ASP:OD1	1.74	0.88
1:B:92:SER:HB2	1:B:207:LEU:HD11	1.52	0.88
1:B:366:LYS:CG	1:B:396:HIS:CG	2.57	0.88
2:F:389:TRP:NE1	2:F:390:ARG:HD2	1.89	0.88
1:A:614:GLU:OE2	2:C:159:TYR:OH	1.91	0.88
2:D:69:ASP:O	2:D:77:VAL:HG21	1.69	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:HIS:HE1	1:B:128:ILE:CD1	1.81	0.88
1:E:529:CYS:O	1:E:530:THR:OG1	1.92	0.88
2:C:310:ARG:NE	2:C:314:ASP:OD2	2.06	0.88
1:E:172:HIS:HA	1:E:454:PHE:O	1.74	0.88
1:E:194:PRO:HB2	1:E:205:HIS:CE1	2.09	0.88
1:E:245:ILE:CD1	1:E:373:LEU:CD1	2.52	0.88
1:E:592:ARG:HH21	1:E:592:ARG:HG3	1.39	0.88
1:A:77:GLU:O	1:A:204:TYR:OH	1.91	0.88
1:A:84:LYS:CA	1:A:139:TRP:HB3	2.04	0.88
1:A:357:SER:HG	1:A:380:TYR:HH	1.08	0.88
1:B:180:HIS:HB3	1:B:592:ARG:HH12	1.39	0.88
1:B:589:PRO:CG	1:B:596:TRP:CH2	2.57	0.88
1:A:504:ILE:CD1	1:A:575:ILE:HG23	1.79	0.88
2:D:77:VAL:HG11	2:D:84:ILE:HG12	0.90	0.88
1:A:98:GLN:HE22	1:A:115:ARG:CG	1.64	0.87
1:A:589:PRO:CG	1:A:596:TRP:CH2	2.57	0.87
1:A:369:GLY:HA2	1:A:372:ILE:HG22	1.53	0.87
1:B:90:HIS:ND1	1:B:128:ILE:CD1	2.37	0.87
2:F:128:LEU:HA	2:F:131:TRP:CE3	2.09	0.87
1:B:99:VAL:HG21	1:B:166:ARG:NH2	1.87	0.87
1:B:504:ILE:CD1	1:B:575:ILE:CG2	2.43	0.87
1:E:246:GLY:O	1:E:363:GLY:HA3	1.71	0.87
1:A:273:SER:HB3	1:A:275:GLU:OE1	1.74	0.87
1:B:178:ALA:N	1:B:458:PHE:CD2	2.43	0.87
1:E:213:ILE:CD1	1:E:215:SER:HB3	2.05	0.87
1:A:126:GLN:HE22	1:A:257:ARG:CZ	1.86	0.87
1:A:477:GLY:O	1:A:478:ILE:HD13	1.74	0.87
1:A:592:ARG:HH22	2:C:184:ARG:NH2	1.68	0.87
2:C:86:LEU:HD23	2:C:138:LEU:HD13	1.55	0.87
1:B:504:ILE:HD12	1:B:575:ILE:HG21	0.87	0.87
1:E:123:PRO:HG3	1:E:309:GLN:HG2	1.55	0.87
1:A:282:LEU:HD11	1:A:359:LEU:HD22	1.55	0.87
1:A:491:ASN:HD21	2:C:36:ARG:CZ	1.87	0.87
1:A:541:LEU:HD12	1:A:542:ILE:N	1.90	0.87
2:C:362:GLU:CG	2:C:490:ARG:HG2	2.04	0.87
1:E:96:ARG:CD	1:E:168:PHE:CE2	2.57	0.87
1:A:401:THR:O	1:A:405:SER:N	2.06	0.87
1:B:80:PHE:HZ	1:B:165:LEU:HA	1.31	0.87
1:E:128:ILE:O	1:E:215:SER:HB2	1.74	0.87
1:E:232:SER:O	1:E:236:ALA:CB	2.23	0.87
2:F:17:GLU:OE2	2:F:21:TRP:CZ2	2.27	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:LEU:HA	1:A:421:VAL:CG2	2.05	0.87
2:D:279:PHE:HE1	2:D:304:TRP:HZ3	1.23	0.87
1:B:571:ALA:O	1:B:573:TRP:NE1	2.07	0.87
1:E:504:ILE:O	1:E:540:GLY:N	2.08	0.87
1:E:590:SER:OG	1:E:592:ARG:NH2	2.08	0.87
1:A:99:VAL:O	1:A:113:ALA:O	1.92	0.86
1:A:615:HIS:HD2	2:C:102:PRO:HG2	1.37	0.86
1:B:469:ILE:CD1	1:B:554:ILE:HG21	2.00	0.86
1:B:589:PRO:HD2	1:B:596:TRP:CZ2	2.09	0.86
2:C:136:ARG:CG	1:B:617:TRP:HB3	2.05	0.86
1:A:96:ARG:CG	1:A:168:PHE:CE1	2.57	0.86
1:A:282:LEU:HD12	1:A:359:LEU:HD13	1.56	0.86
1:B:366:LYS:HD3	1:B:395:ARG:NE	1.90	0.86
1:B:369:GLY:CA	1:B:372:ILE:HG22	2.05	0.86
1:E:103:GLY:CA	1:E:134:SER:O	2.23	0.86
1:A:105:VAL:CG1	1:A:132:ASP:HB2	2.06	0.86
1:B:172:HIS:CA	1:B:454:PHE:O	2.24	0.86
1:B:369:GLY:HA2	1:B:372:ILE:CG2	2.05	0.86
1:B:611:LYS:HB2	1:B:614:GLU:CD	1.95	0.86
1:A:348:LEU:CD1	1:A:353:PHE:HB3	2.06	0.86
2:C:96:VAL:HG11	2:C:128:LEU:HD11	1.57	0.86
2:C:110:ILE:HG22	2:C:114:THR:HB	1.57	0.86
1:B:91:LEU:HD11	1:B:204:TYR:HB2	1.56	0.86
1:B:357:SER:C	1:B:358:LEU:HD13	1.96	0.86
1:B:364:TRP:HB3	1:B:369:GLY:CA	2.04	0.86
1:E:365:ILE:O	1:E:396:HIS:CB	2.23	0.86
1:A:290:SER:OG	1:A:296:SER:HB3	1.74	0.86
1:B:390:THR:HG23	1:B:391:ALA:N	1.91	0.86
1:A:390:THR:OG1	1:A:421:VAL:O	1.93	0.86
2:D:184:ARG:HB3	1:B:592:ARG:HD3	1.56	0.86
1:E:118:LEU:HD23	1:E:118:LEU:H	1.40	0.86
2:F:128:LEU:HB2	2:F:131:TRP:HZ3	1.32	0.86
1:A:216:LEU:HD23	1:A:217:SER:N	1.91	0.86
1:A:471:TYR:HA	1:A:478:ILE:HB	1.57	0.86
1:A:492:PRO:HA	1:A:495:ILE:HD11	1.56	0.86
1:B:105:VAL:CG2	1:B:134:SER:OG	2.23	0.86
1:E:85:GLU:O	1:E:133:PHE:HD1	1.57	0.86
1:E:222:TRP:HE1	1:E:422:PRO:C	1.79	0.86
1:E:469:ILE:CG2	1:E:478:ILE:HD12	1.89	0.86
1:E:614:GLU:OE2	2:F:159:TYR:HE1	1.27	0.86
1:A:73:GLY:HA3	1:A:78:THR:HG23	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TYR:CE2	1:A:192:LYS:CB	2.59	0.86
1:A:226:LEU:HD11	1:A:230:TYR:HH	0.96	0.86
1:A:383:THR:HB	1:A:384:HIS:ND1	1.91	0.86
1:A:75:GLU:CA	2:C:259:ARG:HH21	1.88	0.85
1:B:90:HIS:ND1	1:B:128:ILE:HD11	1.90	0.85
1:B:105:VAL:HA	1:B:109:VAL:O	1.75	0.85
2:F:58:SER:OG	2:F:62:ILE:HD11	1.75	0.85
2:F:163:GLU:O	2:F:165:LEU:HD22	1.76	0.85
2:C:307:ARG:HH11	2:C:307:ARG:CB	1.88	0.85
1:B:364:TRP:CB	1:B:369:GLY:HA3	2.04	0.85
2:C:54:HIS:CD2	2:C:98:GLY:HA3	2.10	0.85
2:F:152:LEU:CA	2:F:155:LEU:HD11	2.03	0.85
1:A:96:ARG:C	1:A:168:PHE:HE1	1.80	0.85
1:A:105:VAL:HB	1:A:132:ASP:HB2	0.85	0.85
1:A:124:LEU:HB2	1:A:188:LEU:O	1.76	0.85
2:C:93:ILE:O	2:C:97:ASN:HB2	1.76	0.85
2:C:358:LYS:CB	2:C:490:ARG:NH1	2.40	0.85
1:B:338:LEU:HD21	1:B:372:ILE:HD12	1.57	0.85
1:A:331:GLN:HG2	1:A:364:TRP:HZ2	1.28	0.85
2:D:99:LEU:HD12	2:D:99:LEU:H	1.41	0.85
1:B:321:LEU:O	1:B:321:LEU:HD23	1.77	0.85
1:B:387:PHE:CZ	1:B:401:THR:HG23	2.11	0.85
1:B:589:PRO:HD2	1:B:596:TRP:HH2	1.30	0.85
1:E:487:PHE:CE2	2:F:46:LEU:HA	2.12	0.85
2:F:337:LEU:HD22	2:F:370:TYR:CD1	2.09	0.85
1:A:488:GLN:HE22	1:A:527:GLN:NE2	1.75	0.85
1:B:450:LYS:HD3	1:B:456:TYR:OH	1.03	0.85
1:E:245:ILE:HD11	1:E:373:LEU:CD1	2.04	0.85
1:E:349:GLU:OE2	1:E:381:LYS:NZ	2.08	0.85
2:C:82:ILE:CG2	2:D:64:CYS:SG	2.64	0.85
2:D:202:TRP:HZ3	2:D:209:PHE:CE1	1.95	0.85
2:D:288:LYS:HG3	2:D:343:ASN:ND2	1.92	0.85
2:F:389:TRP:HE1	2:F:390:ARG:HD2	1.40	0.85
1:E:469:ILE:HG21	1:E:478:ILE:CG1	2.07	0.85
2:D:68:LEU:O	2:D:71:LYS:HG3	1.76	0.85
1:B:327:SER:OG	1:B:332:ASP:OD2	1.93	0.85
1:E:267:ILE:HD11	1:E:302:SER:HB3	1.58	0.85
2:F:25:LYS:HE2	2:F:25:LYS:O	1.76	0.85
1:A:226:LEU:HD11	1:A:230:TYR:CE1	2.08	0.85
1:B:261:GLU:HA	1:B:264:THR:OG1	1.77	0.85
1:E:493:GLN:NE2	2:F:36:ARG:NH2	2.23	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ILE:O	1:A:396:HIS:ND1	1.98	0.84
2:C:125:PHE:O	2:C:128:LEU:HG	1.77	0.84
2:D:159:TYR:HE1	1:B:614:GLU:HG3	1.40	0.84
1:B:207:LEU:HD13	1:B:213:ILE:HD13	1.59	0.84
2:F:312:GLN:NE2	2:F:323:LYS:CD	2.33	0.84
1:A:126:GLN:NE2	1:A:257:ARG:HH12	1.74	0.84
1:B:174:GLY:C	1:B:458:PHE:HE2	1.81	0.84
2:C:125:PHE:O	2:C:128:LEU:N	2.09	0.84
2:D:207:ASN:O	2:D:211:GLU:HG3	1.78	0.84
2:D:323:LYS:CG	2:D:427:TYR:HE2	1.90	0.84
1:B:90:HIS:HE1	1:B:128:ILE:CG1	1.90	0.84
1:B:400:LEU:HD23	1:B:401:THR:N	1.92	0.84
2:F:17:GLU:OE2	2:F:21:TRP:HH2	1.60	0.84
1:A:366:LYS:CG	1:A:396:HIS:CB	2.53	0.84
1:A:481:ILE:HG22	1:A:575:ILE:HB	1.59	0.84
1:A:282:LEU:HA	1:A:295:ILE:HG23	1.59	0.84
1:A:545:ILE:HG12	1:A:552:MET:HG2	1.60	0.84
2:C:68:LEU:O	2:C:68:LEU:HD12	1.78	0.84
2:D:46:LEU:CD2	1:B:577:ARG:HD3	2.07	0.84
2:D:69:ASP:CG	2:D:88:TYR:OH	2.16	0.84
2:D:79:GLN:NE2	2:D:79:GLN:HA	1.92	0.84
2:F:152:LEU:O	2:F:155:LEU:HD13	1.77	0.84
2:C:32:ASP:OD1	2:C:34:ARG:CZ	2.25	0.84
2:D:146:TRP:CH2	2:D:150:GLU:CB	2.59	0.84
1:B:80:PHE:HE1	1:B:165:LEU:C	1.80	0.84
2:F:52:LEU:HD21	2:F:57:ASP:CB	2.07	0.84
2:F:283:ASP:OD1	2:F:285:LEU:N	2.11	0.84
2:F:302:ILE:HD11	2:F:340:ILE:HG21	1.58	0.84
2:D:5:ARG:HD3	1:B:610:ARG:NE	1.91	0.84
2:D:71:LYS:NZ	2:D:71:LYS:HB3	1.91	0.84
1:B:365:ILE:O	1:B:396:HIS:ND1	2.11	0.84
1:E:615:HIS:NE2	2:F:102:PRO:HG3	1.92	0.84
2:C:95:PHE:CE1	2:C:155:LEU:CD1	2.60	0.83
1:B:99:VAL:HG22	1:B:166:ARG:CZ	2.08	0.83
1:B:105:VAL:HG23	1:B:134:SER:HB2	1.60	0.83
1:B:357:SER:O	1:B:358:LEU:HD13	1.78	0.83
2:C:278:PHE:HZ	2:C:287:LEU:HD13	1.44	0.83
2:D:121:LEU:HD12	2:D:122:PRO:CD	2.08	0.83
2:D:156:TYR:HA	2:D:160:TRP:CD1	2.13	0.83
2:D:312:GLN:NE2	2:D:323:LYS:CG	2.09	0.83
1:B:448:PHE:HB3	1:B:461:LEU:CD2	2.07	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:350:LYS:HZ1	2:F:401:THR:CA	1.90	0.83
1:A:364:TRP:CD1	1:A:369:GLY:CA	2.61	0.83
1:A:471:TYR:CD1	1:A:552:MET:HG3	2.13	0.83
1:B:99:VAL:CG1	1:B:166:ARG:HH21	1.91	0.83
2:F:350:LYS:HZ1	2:F:401:THR:HA	1.44	0.83
1:A:216:LEU:HD13	1:A:425:SER:OG	1.79	0.83
2:D:146:TRP:O	2:D:146:TRP:HE3	1.61	0.83
2:D:188:LEU:HD12	2:D:188:LEU:O	1.77	0.83
1:B:615:HIS:ND1	1:B:615:HIS:O	2.11	0.83
1:E:369:GLY:O	1:E:373:LEU:HG	1.77	0.83
2:F:98:GLY:O	2:F:102:PRO:CG	2.27	0.83
1:A:388:LEU:O	1:A:423:ALA:CA	2.26	0.83
2:C:291:MET:HE1	2:C:340:ILE:CG2	2.05	0.83
2:D:358:LYS:HD3	2:D:490:ARG:NH2	1.92	0.83
2:C:278:PHE:CZ	2:C:287:LEU:CD1	2.62	0.83
1:E:71:TYR:CE1	1:E:80:PHE:CE2	2.66	0.83
1:A:381:LYS:HB3	1:A:409:SER:CB	2.09	0.83
1:A:460:PRO:HB2	1:A:594:ILE:HD11	1.61	0.83
2:D:4:PRO:CG	1:B:607:PHE:CE1	2.57	0.83
1:E:491:ASN:ND2	2:F:36:ARG:HE	1.74	0.83
2:C:125:PHE:HD1	2:C:128:LEU:CD2	1.92	0.83
2:D:53:PRO:HB3	1:B:614:GLU:O	1.77	0.83
2:D:278:PHE:HD1	2:D:279:PHE:CD2	1.94	0.83
2:F:350:LYS:HZ2	2:F:401:THR:HG22	1.07	0.83
1:A:181:LEU:HD13	1:A:181:LEU:O	1.78	0.83
2:C:54:HIS:NE2	2:C:98:GLY:CA	2.36	0.83
2:D:86:LEU:HD12	2:D:138:LEU:CD2	2.09	0.83
2:D:336:LEU:HD12	2:D:340:ILE:HG13	1.61	0.83
2:C:217:GLU:HB3	2:C:218:ASN:OD1	1.79	0.82
1:B:284:PRO:O	1:B:287:PRO:HD3	1.79	0.82
1:E:118:LEU:HD12	1:E:305:ILE:HG21	1.58	0.82
1:A:451:ILE:HG22	1:A:452:THR:CG2	2.08	0.82
1:A:504:ILE:CD1	1:A:575:ILE:HG22	1.81	0.82
2:F:85:ARG:HB3	2:F:138:LEU:HD22	1.59	0.82
2:F:131:TRP:NE1	2:F:139:PRO:HB3	1.93	0.82
2:C:62:ILE:HG21	2:C:152:LEU:HD21	1.60	0.82
1:B:247:GLY:H	1:B:365:ILE:CG2	1.91	0.82
1:E:471:TYR:OH	1:E:523:PHE:CE1	2.32	0.82
2:F:312:GLN:HE22	2:F:323:LYS:HD2	1.39	0.82
2:F:492:GLN:NE2	2:F:492:GLN:H	1.78	0.82
1:A:249:ASN:O	1:A:249:ASN:ND2	2.13	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:THR:OG1	2:C:155:LEU:HD22	1.78	0.82
2:C:75:LEU:HD23	2:C:76:GLY:O	1.78	0.82
2:D:356:TRP:O	2:D:360:ILE:CG1	2.26	0.82
1:B:306:SER:C	1:B:307:LEU:HD23	1.98	0.82
2:C:96:VAL:HG21	2:C:128:LEU:CD2	2.07	0.82
1:E:360:ASN:ND2	1:E:360:ASN:O	2.12	0.82
1:E:487:PHE:HE2	2:F:46:LEU:HA	1.44	0.82
1:E:537:ILE:HD12	1:E:573:TRP:HZ3	1.42	0.82
1:A:270:SER:HB2	1:A:273:SER:OG	1.79	0.82
2:C:78:HIS:HB2	2:D:35:GLN:HE22	1.41	0.82
2:C:276:GLU:O	2:C:280:ASN:ND2	2.12	0.82
2:D:52:LEU:O	1:B:616:VAL:HG13	1.77	0.82
1:B:331:GLN:O	1:B:334:PRO:HD3	1.80	0.82
1:B:467:LEU:O	1:B:467:LEU:HD23	1.79	0.82
1:B:473:LYS:HE2	1:B:474:GLY:H	1.42	0.82
1:E:89:LEU:HB3	1:E:131:ILE:HB	1.62	0.82
2:F:55:VAL:HG21	2:F:159:TYR:CG	2.15	0.82
2:C:156:TYR:HA	2:C:160:TRP:HB2	1.61	0.82
2:D:279:PHE:CD1	2:D:304:TRP:CH2	2.67	0.82
1:B:210:SER:O	1:B:212:ARG:HD3	1.80	0.82
1:B:517:VAL:HG12	1:B:526:LEU:HD12	1.61	0.82
2:F:152:LEU:O	2:F:155:LEU:CD1	2.27	0.82
1:A:388:LEU:CA	1:A:421:VAL:HG23	2.08	0.82
1:A:608:GLU:N	1:A:608:GLU:OE2	2.13	0.82
2:D:352:LYS:O	2:D:355:ASN:HB2	1.80	0.82
1:B:219:PRO:HB2	1:B:221:TYR:HD2	1.42	0.82
1:B:288:GLU:HG2	1:B:289:TYR:HE2	1.42	0.82
1:E:310:HIS:HB2	1:E:314:GLY:N	1.94	0.82
2:F:80:ASP:O	2:F:83:PRO:HD2	1.80	0.82
2:C:357:GLU:O	2:C:361:ASP:N	2.13	0.81
2:D:358:LYS:O	2:D:362:GLU:CB	2.27	0.81
1:B:400:LEU:HD23	1:B:401:THR:H	1.43	0.81
1:A:69:ILE:HG21	1:A:80:PHE:HB3	1.62	0.81
2:C:61:GLN:OE1	2:D:138:LEU:HD11	1.80	0.81
2:C:125:PHE:CA	2:C:128:LEU:HD23	2.10	0.81
2:D:54:HIS:CD2	2:D:99:LEU:HD12	2.15	0.81
1:E:188:LEU:HD11	1:E:434:PHE:CE1	2.14	0.81
2:F:111:PRO:HG2	2:F:114:THR:CB	2.10	0.81
1:A:491:ASN:ND2	2:C:36:ARG:NE	2.28	0.81
2:C:96:VAL:CB	2:C:128:LEU:HD11	2.09	0.81
2:D:199:LEU:CD1	2:D:281:ASN:OD1	2.29	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:LEU:HD11	2:F:488:TRP:HB3	1.61	0.81
2:F:54:HIS:CE1	2:F:58:SER:HB2	2.14	0.81
2:F:74:CYS:HB3	2:F:75:LEU:CB	2.10	0.81
2:F:151:ALA:C	2:F:155:LEU:HD11	2.00	0.81
1:A:79:MET:SD	1:A:80:PHE:N	2.54	0.81
1:A:607:PHE:CE1	2:C:4:PRO:HA	2.15	0.81
2:C:393:LYS:HE2	2:C:393:LYS:HA	1.62	0.81
2:C:59:THR:OG1	2:C:155:LEU:CD2	2.28	0.81
1:A:226:LEU:HD12	1:A:226:LEU:O	1.80	0.81
2:C:23:TYR:CE2	2:C:156:TYR:CB	2.63	0.81
2:D:98:GLY:O	2:D:102:PRO:CD	2.26	0.81
2:D:131:TRP:HA	2:D:131:TRP:CE3	2.16	0.81
1:A:381:LYS:HA	1:A:409:SER:CB	2.11	0.81
2:C:97:ASN:ND2	2:C:129:ARG:NE	2.28	0.81
2:C:133:THR:HG23	2:D:93:ILE:HG21	1.61	0.81
2:F:88:TYR:CB	2:F:144:LEU:CD2	2.58	0.81
2:C:101:ASP:HA	2:C:105:GLN:HG2	1.63	0.81
2:C:136:ARG:HA	1:B:617:TRP:CD2	2.15	0.81
1:B:90:HIS:HE1	1:B:213:ILE:HD11	1.44	0.81
1:B:172:HIS:HD2	1:B:454:PHE:HA	0.78	0.81
1:B:309:GLN:OE1	1:B:310:HIS:N	2.13	0.81
1:B:364:TRP:CD1	1:B:372:ILE:HG21	2.16	0.81
2:C:136:ARG:HG3	1:B:617:TRP:CB	2.10	0.81
2:C:352:LYS:HB3	2:C:355:ASN:HD22	1.44	0.81
2:D:336:LEU:HD12	2:D:336:LEU:O	1.81	0.81
1:B:397:LEU:HG	1:B:400:LEU:CD2	2.01	0.81
1:E:537:ILE:HD12	1:E:573:TRP:CZ3	2.14	0.81
2:D:96:VAL:C	2:D:100:LEU:HB2	2.01	0.81
1:B:337:TYR:OH	1:B:362:PRO:HG2	1.81	0.81
1:E:385:LEU:H	1:E:417:GLU:HB3	1.44	0.81
2:C:234:LEU:O	2:C:235:VAL:CG2	2.29	0.80
1:B:96:ARG:HH22	1:B:171:ASN:HD21	1.26	0.80
2:F:372:CYS:O	2:F:412:ILE:HD11	1.80	0.80
1:A:256:LEU:HD12	1:A:279:TYR:OH	1.82	0.80
1:A:306:SER:OG	1:A:316:ASN:ND2	2.14	0.80
2:C:182:TYR:CE1	2:F:183:ARG:HG3	2.17	0.80
1:B:488:GLN:NE2	1:B:488:GLN:HA	1.95	0.80
2:F:350:LYS:NZ	2:F:401:THR:CA	2.44	0.80
2:F:353:TRP:NE1	2:F:357:GLU:OE2	2.13	0.80
1:A:99:VAL:HG21	1:A:104:ILE:CD1	2.11	0.80
1:A:290:SER:HG	1:A:296:SER:CB	1.88	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:CYS:SG	2:D:82:ILE:CG2	2.64	0.80
2:C:353:TRP:HH2	2:C:408:LEU:CD2	1.94	0.80
2:D:323:LYS:HG3	2:D:427:TYR:HE2	1.45	0.80
1:A:280:LEU:CD1	1:A:297:LEU:HD12	2.10	0.80
2:C:96:VAL:CG1	2:C:128:LEU:HD11	2.12	0.80
1:B:123:PRO:HG3	1:B:309:GLN:HG3	1.61	0.80
2:F:125:PHE:HA	2:F:128:LEU:HD23	1.64	0.80
2:D:4:PRO:CA	1:B:607:PHE:HE1	1.90	0.80
1:B:79:MET:O	1:B:167:VAL:CB	2.30	0.80
1:E:359:LEU:HD12	1:E:360:ASN:N	1.97	0.80
2:F:328:ALA:HB3	2:F:331:GLU:HG3	1.61	0.80
1:A:616:VAL:O	1:A:618:LYS:HG3	1.82	0.80
2:D:126:VAL:O	2:D:129:ARG:HG3	1.80	0.80
2:F:319:THR:HG21	2:F:433:GLU:H	1.47	0.80
2:D:349:PHE:HE2	2:D:356:TRP:CE2	1.99	0.80
2:D:96:VAL:HG13	2:D:100:LEU:CG	2.12	0.80
2:D:146:TRP:CZ2	2:D:150:GLU:OE1	2.35	0.80
1:B:79:MET:O	1:B:167:VAL:HG13	1.79	0.80
1:B:590:SER:O	1:B:593:THR:OG1	2.00	0.80
1:A:467:LEU:HD22	1:A:556:VAL:HG22	1.62	0.80
2:C:288:LYS:O	2:C:292:LEU:HG	1.82	0.80
2:D:86:LEU:CD1	2:D:138:LEU:CD2	2.60	0.80
1:B:359:LEU:HD12	1:B:360:ASN:N	1.97	0.80
2:F:55:VAL:HG21	2:F:159:TYR:HB3	1.62	0.80
2:F:128:LEU:HD12	2:F:128:LEU:O	1.82	0.80
2:F:372:CYS:C	2:F:412:ILE:HD11	2.01	0.80
1:A:372:ILE:HG23	1:A:373:LEU:CD2	2.11	0.80
2:D:122:PRO:HG2	2:D:125:PHE:CE2	2.16	0.80
1:B:90:HIS:CE1	1:B:213:ILE:CD1	2.62	0.80
1:B:544:SER:OG	1:B:553:ASN:OD1	1.99	0.80
1:E:118:LEU:CD1	1:E:305:ILE:CG2	2.58	0.80
1:E:549:GLN:HB2	1:E:551:ILE:HG23	1.62	0.80
1:E:589:PRO:CD	1:E:596:TRP:CH2	2.65	0.80
1:A:222:TRP:NE1	1:A:422:PRO:O	2.13	0.79
1:A:324:TYR:HH	1:A:580:THR:HG1	1.26	0.79
1:A:607:PHE:CD1	2:C:4:PRO:CA	2.66	0.79
2:D:350:LYS:NZ	2:D:401:THR:HG22	1.96	0.79
2:C:53:PRO:HD2	2:C:56:VAL:CG2	2.12	0.79
2:C:388:SER:O	2:C:391:ASN:ND2	2.16	0.79
2:F:54:HIS:HE1	2:F:58:SER:HB2	1.47	0.79
2:F:131:TRP:HE1	2:F:139:PRO:HD3	1.44	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:ARG:HH21	1:E:212:ARG:HG3	1.48	0.79
1:E:395:ARG:HH21	1:E:395:ARG:HG3	1.46	0.79
1:A:102:GLY:O	1:A:113:ALA:HB2	1.83	0.79
1:A:196:PHE:HB3	1:A:205:HIS:CE1	2.17	0.79
1:E:245:ILE:CD1	1:E:373:LEU:HD22	2.12	0.79
1:A:282:LEU:CD1	1:A:359:LEU:CD2	2.61	0.79
1:A:589:PRO:HD3	1:A:596:TRP:HH2	1.43	0.79
2:D:487:ASN:CG	2:D:488:TRP:N	2.34	0.79
1:E:79:MET:O	1:E:166:ARG:O	2.00	0.79
1:A:105:VAL:HG12	1:A:132:ASP:OD2	1.82	0.79
1:A:327:SER:OG	1:A:329:SER:O	1.99	0.79
2:C:52:LEU:HD12	2:C:53:PRO:HD2	1.47	0.79
2:C:133:THR:CG2	2:D:93:ILE:HG21	2.13	0.79
1:B:331:GLN:HA	1:B:334:PRO:HG3	1.63	0.79
1:B:571:ALA:O	1:B:573:TRP:CD1	2.35	0.79
2:C:103:THR:N	2:C:104:GLN:HA	1.95	0.79
1:B:330:PRO:HB3	1:B:337:TYR:CE1	2.18	0.79
1:B:590:SER:N	1:B:593:THR:OG1	2.15	0.79
2:D:5:ARG:HD2	1:B:610:ARG:HE	0.62	0.79
2:D:349:PHE:CE2	2:D:356:TRP:CE2	2.71	0.79
1:B:408:THR:CB	1:B:414:TYR:HA	2.13	0.79
1:E:601:GLN:NE2	1:E:601:GLN:HA	1.98	0.79
1:A:174:GLY:HA2	1:A:177:GLU:OE1	1.83	0.79
1:A:394:LYS:O	1:A:394:LYS:HD2	1.82	0.79
1:B:387:PHE:CE2	1:B:397:LEU:CD2	2.66	0.79
1:B:387:PHE:CE1	1:B:401:THR:CG2	2.66	0.79
1:B:559:CYS:SG	1:B:560:HIS:ND1	2.56	0.79
1:E:289:TYR:CA	1:E:317:PHE:CE2	2.66	0.79
1:E:471:TYR:CE1	1:E:550:GLN:HA	2.18	0.79
1:A:555:TYR:OH	2:C:494:TRP:CH2	2.14	0.79
2:C:156:TYR:CZ	2:C:161:ASN:ND2	2.51	0.79
2:C:207:ASN:HA	2:C:210:LEU:HD13	1.65	0.79
2:D:84:ILE:HD12	2:D:84:ILE:O	1.81	0.79
1:E:106:TYR:HE2	1:E:120:PHE:CD2	2.01	0.79
1:A:207:LEU:CD1	1:A:213:ILE:HG12	2.12	0.78
2:C:46:LEU:O	2:C:46:LEU:HD22	1.84	0.78
2:D:74:CYS:O	2:D:75:LEU:HD13	1.82	0.78
2:D:312:GLN:OE1	2:D:430:ILE:CG1	2.28	0.78
1:B:348:LEU:HD11	1:B:353:PHE:CG	2.17	0.78
2:F:131:TRP:NE1	2:F:139:PRO:HD3	1.98	0.78
1:A:331:GLN:NE2	1:A:364:TRP:NE1	2.32	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:O	1:A:208:HIS:ND1	2.15	0.78
2:C:231:GLY:HA3	2:C:234:LEU:HD21	1.66	0.78
1:B:181:LEU:HD21	1:B:460:PRO:HG3	1.65	0.78
1:B:249:ASN:OD1	1:B:424:HIS:CD2	2.36	0.78
1:E:245:ILE:CD1	1:E:373:LEU:CD2	2.61	0.78
2:F:68:LEU:CD2	2:F:84:ILE:CD1	2.42	0.78
2:F:128:LEU:CA	2:F:131:TRP:HE3	1.96	0.78
1:A:301:LEU:CD2	1:A:318:GLN:HE21	1.95	0.78
2:C:156:TYR:CE1	2:C:161:ASN:ND2	2.48	0.78
1:E:176:LEU:HD22	1:E:176:LEU:H	1.47	0.78
2:F:111:PRO:HG2	2:F:114:THR:OG1	1.84	0.78
2:F:337:LEU:HD12	2:F:338:ASP:N	1.99	0.78
1:A:221:TYR:HB2	1:A:422:PRO:HG2	1.65	0.78
2:C:97:ASN:HD21	2:C:129:ARG:NE	1.82	0.78
1:B:105:VAL:HG23	1:B:134:SER:CB	2.14	0.78
1:B:387:PHE:CZ	1:B:401:THR:CG2	2.66	0.78
1:A:105:VAL:HB	1:A:132:ASP:HB3	1.65	0.78
1:B:388:LEU:H	1:B:388:LEU:HD12	1.48	0.78
1:A:607:PHE:CE1	2:C:4:PRO:N	2.11	0.78
2:D:329:TRP:NE1	2:D:424:ILE:HD12	1.96	0.78
1:B:177:GLU:HG2	1:B:458:PHE:CE2	2.16	0.78
1:B:219:PRO:CB	1:B:221:TYR:HE2	1.87	0.78
1:B:425:SER:HA	1:B:426:LEU:C	2.03	0.78
2:F:17:GLU:CG	2:F:21:TRP:CZ2	2.67	0.78
2:F:88:TYR:CB	2:F:144:LEU:HD22	2.13	0.78
1:A:527:GLN:NE2	1:A:527:GLN:O	2.17	0.78
2:F:152:LEU:CA	2:F:155:LEU:HD13	2.08	0.78
1:A:480:GLY:H	1:A:524:PRO:HG2	1.46	0.78
1:A:607:PHE:CD1	2:C:4:PRO:HA	2.18	0.78
1:B:172:HIS:CD2	1:B:454:PHE:CA	2.42	0.78
1:E:309:GLN:OE1	1:E:311:LEU:HD13	1.84	0.78
2:C:138:LEU:HD21	2:D:94:ARG:CZ	2.14	0.78
2:C:138:LEU:CD2	2:D:94:ARG:CZ	2.62	0.78
2:C:278:PHE:CZ	2:C:287:LEU:HD13	2.19	0.78
1:E:470:SER:O	1:E:477:GLY:HA3	1.84	0.78
2:F:88:TYR:HB2	2:F:144:LEU:HD22	1.63	0.78
1:A:395:ARG:CZ	1:A:396:HIS:HB2	2.13	0.77
1:A:489:ASP:HB2	2:D:79:GLN:O	1.84	0.77
2:C:133:THR:HG23	2:D:93:ILE:HG22	1.65	0.77
2:D:58:SER:HA	2:D:61:GLN:HB2	1.65	0.77
1:E:188:LEU:HD13	1:E:434:PHE:CE1	2.17	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:384:HIS:HA	1:E:417:GLU:CB	2.15	0.77
2:F:350:LYS:HZ1	2:F:401:THR:HB	1.49	0.77
1:A:606:THR:CG2	2:C:5:ARG:NH1	2.47	0.77
2:C:34:ARG:HG3	2:C:67:LEU:HD11	1.66	0.77
2:D:128:LEU:O	2:D:128:LEU:HD23	1.84	0.77
2:D:212:TYR:CE2	2:D:250:SER:CB	2.68	0.77
1:B:529:CYS:O	1:B:530:THR:OG1	2.02	0.77
2:F:359:LEU:HD21	2:F:368:ILE:HD13	1.64	0.77
1:A:282:LEU:CD1	1:A:359:LEU:HD22	2.14	0.77
1:A:371:GLN:NE2	1:A:371:GLN:O	2.17	0.77
1:B:216:LEU:HD23	1:B:217:SER:N	2.00	0.77
2:F:270:TYR:O	2:F:274:VAL:HG22	1.83	0.77
2:C:130:HIS:HB2	2:C:134:HIS:ND1	1.99	0.77
2:D:489:SER:O	1:B:467:LEU:CA	2.33	0.77
2:F:497:LYS:HE2	2:F:502:LEU:O	1.84	0.77
1:A:305:ILE:HG22	1:A:307:LEU:HD11	1.65	0.77
1:A:507:TYR:CD1	1:A:535:ASN:C	2.51	0.77
2:C:53:PRO:HB2	2:C:56:VAL:HG23	1.65	0.77
1:B:321:LEU:CD2	1:B:344:LEU:CD1	2.60	0.77
1:E:241:ARG:CZ	1:E:381:LYS:CD	2.62	0.77
2:F:131:TRP:NE1	2:F:139:PRO:CB	2.45	0.77
1:A:256:LEU:HD11	1:A:360:ASN:HB3	1.65	0.77
1:A:366:LYS:CG	1:A:396:HIS:HB2	2.14	0.77
2:C:336:LEU:HD12	2:C:336:LEU:O	1.84	0.77
1:B:175:LEU:HD13	1:B:456:TYR:CE2	2.20	0.77
1:B:369:GLY:O	1:B:372:ILE:HG22	1.85	0.77
2:D:190:LYS:NZ	3:D:601:HOH:O	2.16	0.77
1:E:289:TYR:CA	1:E:317:PHE:HE2	1.98	0.77
2:F:129:ARG:HB3	2:F:129:ARG:HH21	1.50	0.77
2:F:280:ASN:CA	2:F:325:LYS:HE3	2.15	0.77
1:A:83:LEU:HD23	1:A:166:ARG:NH1	2.00	0.77
1:A:467:LEU:HD21	1:A:556:VAL:HG22	1.65	0.77
2:D:23:TYR:CZ	2:D:156:TYR:HB2	2.19	0.77
2:D:202:TRP:CH2	2:D:209:PHE:CD1	2.73	0.77
1:B:395:ARG:HH11	1:B:396:HIS:CD2	1.97	0.77
2:C:410:GLU:O	2:C:414:ASN:ND2	2.18	0.77
2:F:22:PHE:CD1	2:F:37:ALA:HB1	2.20	0.77
2:F:271:HIS:CA	2:F:274:VAL:HG23	2.15	0.77
1:A:196:PHE:CG	1:A:197:PRO:HD2	2.20	0.77
1:A:592:ARG:HH21	2:C:184:ARG:NE	1.82	0.77
2:D:105:GLN:HG2	1:B:615:HIS:CD2	2.19	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:C	1:B:242:ILE:HD12	2.05	0.77
2:C:111:PRO:HG2	2:C:114:THR:OG1	1.85	0.76
2:D:23:TYR:HD2	2:D:156:TYR:CE2	2.02	0.76
2:F:131:TRP:CE2	2:F:139:PRO:HG3	2.20	0.76
2:C:82:ILE:O	2:C:86:LEU:HG	1.85	0.76
1:E:214:GLN:OE1	1:E:427:ASN:N	2.17	0.76
1:E:301:LEU:HD13	1:E:301:LEU:O	1.85	0.76
1:E:399:GLU:OE2	1:E:400:LEU:N	2.18	0.76
1:E:469:ILE:HG22	1:E:470:SER:H	1.48	0.76
2:F:271:HIS:HA	2:F:274:VAL:HG23	1.66	0.76
1:A:313:GLN:HG3	1:A:456:TYR:OH	1.85	0.76
1:A:592:ARG:HD2	2:C:184:ARG:NE	1.98	0.76
1:A:270:SER:CB	1:A:273:SER:OG	2.32	0.76
1:A:280:LEU:O	1:A:359:LEU:HD13	1.84	0.76
1:A:502:THR:CB	1:A:577:ARG:HH21	1.85	0.76
2:C:82:ILE:HG23	2:D:64:CYS:SG	2.23	0.76
2:D:154:TRP:CE2	2:D:158:HIS:ND1	2.51	0.76
1:B:261:GLU:CA	1:B:264:THR:OG1	2.32	0.76
2:F:362:GLU:C	2:F:363:ASN:HD22	1.88	0.76
1:A:555:TYR:HH	2:C:494:TRP:HH2	0.81	0.76
1:B:175:LEU:HA	1:B:458:PHE:CZ	2.20	0.76
1:B:311:LEU:N	1:B:311:LEU:HD22	2.01	0.76
1:B:389:GLU:O	1:B:390:THR:CG2	2.33	0.76
1:A:381:LYS:HD3	1:A:409:SER:CB	2.13	0.76
2:C:99:LEU:HD22	2:C:99:LEU:N	2.00	0.76
2:D:125:PHE:O	2:D:128:LEU:CB	2.34	0.76
2:D:184:ARG:HB3	1:B:592:ARG:HD2	1.65	0.76
1:B:245:ILE:HD13	1:B:361:LEU:HB2	1.66	0.76
2:F:350:LYS:NZ	2:F:401:THR:HA	1.99	0.76
1:A:488:GLN:NE2	1:A:527:GLN:CD	2.38	0.76
2:C:40:ARG:HD3	2:C:44:TYR:OH	1.85	0.76
1:E:106:TYR:HE2	1:E:120:PHE:HD2	1.34	0.76
2:F:55:VAL:HG11	2:F:159:TYR:CE1	2.21	0.76
2:F:332:LEU:HD23	2:F:332:LEU:O	1.86	0.76
1:A:226:LEU:HD12	1:A:230:TYR:CZ	2.16	0.76
1:A:469:ILE:HD13	2:C:488:TRP:CE3	2.21	0.76
2:C:79:GLN:N	2:C:79:GLN:HE21	1.82	0.76
2:C:209:PHE:CE2	2:C:254:ILE:HG12	2.20	0.76
2:D:113:HIS:ND1	2:D:126:VAL:HG11	2.00	0.76
2:D:354:GLN:O	2:D:358:LYS:HG2	1.86	0.76
1:E:364:TRP:HD1	1:E:369:GLY:H	1.32	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:TRP:CD2	3:E:705:HOH:O	2.38	0.76
1:A:331:GLN:NE2	1:A:364:TRP:CZ2	2.53	0.76
2:C:62:ILE:CG2	2:C:152:LEU:HD21	2.16	0.76
2:C:363:ASN:HA	2:C:492:GLN:O	1.85	0.76
2:D:23:TYR:CE2	2:D:156:TYR:CG	2.73	0.76
1:A:280:LEU:HD11	1:A:297:LEU:HD12	1.66	0.75
1:A:469:ILE:HD13	2:C:488:TRP:CE2	2.20	0.75
1:A:614:GLU:HB3	2:C:159:TYR:CE1	2.21	0.75
2:D:349:PHE:HE2	2:D:356:TRP:CG	2.04	0.75
1:E:245:ILE:HD11	1:E:373:LEU:HD11	1.66	0.75
1:B:364:TRP:CD1	1:B:369:GLY:HA2	2.21	0.75
1:B:469:ILE:CG1	1:B:552:MET:HB3	2.17	0.75
1:B:588:LEU:HD12	1:B:588:LEU:N	2.01	0.75
2:F:100:LEU:N	2:F:100:LEU:HD23	2.02	0.75
1:A:307:LEU:HD12	1:A:307:LEU:N	2.01	0.75
2:D:278:PHE:CE1	2:D:279:PHE:CD2	2.74	0.75
1:E:519:SER:C	1:E:520:LEU:HD23	2.04	0.75
2:F:128:LEU:CA	2:F:131:TRP:CE3	2.67	0.75
1:A:179:GLY:HA2	1:A:182:TYR:O	1.86	0.75
1:A:361:LEU:HD11	1:A:376:ILE:HD11	1.68	0.75
1:A:539:LEU:N	1:A:539:LEU:HD23	2.02	0.75
2:D:113:HIS:CE1	2:D:126:VAL:HG11	2.21	0.75
2:D:212:TYR:CE2	2:D:250:SER:HB2	2.20	0.75
1:E:103:GLY:O	1:E:134:SER:N	2.17	0.75
1:A:118:LEU:N	1:A:118:LEU:HD23	2.02	0.75
2:C:133:THR:CG2	2:D:93:ILE:HG22	2.16	0.75
1:B:106:TYR:O	1:B:109:VAL:HG22	1.86	0.75
2:F:101:ASP:HB2	2:F:105:GLN:HB2	1.66	0.75
1:B:243:MET:HE3	1:B:380:TYR:HD2	1.50	0.75
1:B:577:ARG:NH2	1:B:578:ASN:O	2.19	0.75
1:E:307:LEU:N	1:E:307:LEU:HD12	2.02	0.75
1:B:165:LEU:HD12	1:B:165:LEU:N	2.02	0.75
2:F:58:SER:O	2:F:62:ILE:HG12	1.85	0.75
2:F:131:TRP:NE1	2:F:139:PRO:CD	2.49	0.75
1:A:126:GLN:HE22	1:A:257:ARG:HH22	1.32	0.75
2:C:64:CYS:HG	2:D:82:ILE:HG21	1.51	0.75
1:E:199:ASN:CB	1:E:202:THR:HG23	2.16	0.75
1:E:567:GLN:HA	1:E:567:GLN:NE2	1.99	0.75
1:A:471:TYR:OH	1:A:547:THR:HA	1.87	0.74
2:C:10:ARG:HB2	2:C:11:ASP:OD2	1.87	0.74
1:B:68:ASN:CB	1:B:82:GLY:H	2.00	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:411:ASN:O	2:F:415:LEU:N	2.20	0.74
2:C:206:ARG:C	2:C:210:LEU:HD11	2.05	0.74
2:D:88:TYR:HB2	2:D:144:LEU:HD13	1.69	0.74
1:B:590:SER:CA	1:B:593:THR:OG1	2.35	0.74
1:E:472:GLY:O	1:E:475:LYS:CB	2.35	0.74
2:D:68:LEU:O	2:D:77:VAL:HG22	1.86	0.74
1:E:212:ARG:NH2	1:E:212:ARG:HG3	2.01	0.74
2:C:119:ILE:HD11	2:C:121:LEU:HB2	0.81	0.74
2:D:333:GLN:NE2	2:D:370:TYR:CE2	2.56	0.74
1:B:230:TYR:HE1	1:B:263:PHE:HE1	0.81	0.74
1:E:175:LEU:O	1:E:175:LEU:HD23	1.87	0.74
2:C:100:LEU:HB2	2:C:115:LEU:HD13	1.70	0.74
2:D:184:ARG:CB	1:B:592:ARG:HD2	2.17	0.74
2:D:312:GLN:HE22	2:D:427:TYR:HE2	1.33	0.74
1:B:103:GLY:O	1:B:134:SER:HB2	1.87	0.74
1:B:306:SER:O	1:B:307:LEU:HD23	1.87	0.74
1:B:395:ARG:HE	1:B:396:HIS:HB2	1.52	0.74
1:E:98:GLN:CG	1:E:117:ILE:HG23	2.08	0.74
1:A:604:PHE:CE2	2:C:10:ARG:NH1	2.54	0.74
2:C:75:LEU:CD2	2:C:76:GLY:O	2.36	0.74
2:D:36:ARG:NE	1:B:491:ASN:OD1	2.19	0.74
1:B:366:LYS:C	1:B:396:HIS:NE2	2.40	0.74
2:F:125:PHE:O	2:F:128:LEU:HG	1.87	0.74
1:A:288:GLU:HG2	1:A:289:TYR:HD2	1.51	0.74
2:D:5:ARG:HD2	1:B:610:ARG:CZ	2.18	0.74
1:B:358:LEU:HD22	1:B:358:LEU:N	2.02	0.74
1:E:76:ASP:O	1:E:77:GLU:HG2	1.88	0.74
1:A:517:VAL:HG23	1:A:524:PRO:HB2	1.69	0.74
2:C:231:GLY:CA	2:C:234:LEU:HD21	2.18	0.74
2:D:77:VAL:HG13	2:D:84:ILE:CB	2.03	0.74
2:D:112:LEU:O	2:D:116:ALA:N	2.21	0.74
1:B:80:PHE:CZ	1:B:165:LEU:CA	2.68	0.74
1:B:268:ARG:NH1	1:B:305:ILE:CD1	2.51	0.74
1:A:213:ILE:O	1:A:213:ILE:HD12	1.88	0.74
2:C:52:LEU:CD1	2:C:56:VAL:HB	2.13	0.74
2:C:92:LEU:N	2:C:92:LEU:HD23	2.02	0.74
1:B:178:ALA:N	1:B:458:PHE:CE2	2.56	0.74
1:E:177:GLU:O	1:E:180:HIS:HB2	1.88	0.74
1:E:331:GLN:CG	1:E:364:TRP:CE2	2.70	0.74
2:F:17:GLU:CD	2:F:21:TRP:CZ2	2.60	0.74
2:F:111:PRO:HG2	2:F:114:THR:HB	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:HD23	1:A:83:LEU:N	2.03	0.74
1:A:126:GLN:HE22	1:A:257:ARG:HH12	1.28	0.74
1:A:616:VAL:O	1:A:618:LYS:HE2	1.87	0.74
2:C:90:MET:HB3	2:D:86:LEU:HG	1.70	0.74
2:D:159:TYR:CE1	1:B:614:GLU:HG3	2.17	0.74
2:D:362:GLU:CD	2:D:490:ARG:HD3	2.04	0.74
1:B:297:LEU:HB3	1:B:321:LEU:CD2	2.18	0.74
1:B:574:ILE:C	1:B:575:ILE:HD13	2.08	0.74
1:E:469:ILE:HG22	1:E:470:SER:N	2.03	0.74
2:F:152:LEU:C	2:F:155:LEU:HD12	2.07	0.74
2:F:280:ASN:O	2:F:325:LYS:CE	2.34	0.74
1:A:207:LEU:HD23	1:A:207:LEU:N	2.02	0.73
1:A:301:LEU:HD21	1:A:318:GLN:HE21	1.51	0.73
2:C:278:PHE:CD2	2:C:286:LEU:CD2	2.70	0.73
1:E:609:ARG:O	2:F:5:ARG:CZ	2.36	0.73
2:F:23:TYR:OH	2:F:152:LEU:O	2.06	0.73
2:D:329:TRP:CE3	2:D:424:ILE:CD1	2.54	0.73
2:D:336:LEU:HD11	2:D:340:ILE:CD1	2.16	0.73
1:A:65:LEU:HD12	1:A:65:LEU:N	2.03	0.73
2:D:112:LEU:HD23	2:D:112:LEU:N	2.02	0.73
2:D:310:ARG:NH2	2:D:495:LYS:HE3	2.04	0.73
1:B:525:ILE:HD13	1:B:525:ILE:N	2.04	0.73
1:B:611:LYS:HD3	1:B:614:GLU:OE2	1.87	0.73
1:E:194:PRO:HB2	1:E:205:HIS:HE1	1.53	0.73
1:A:94:VAL:O	1:A:203:THR:OG1	2.05	0.73
1:A:353:PHE:HE1	1:A:355:GLY:C	1.92	0.73
1:B:175:LEU:O	1:B:458:PHE:CZ	2.41	0.73
1:B:181:LEU:CD2	1:B:460:PRO:HG3	2.18	0.73
1:A:245:ILE:HD12	1:A:363:GLY:HA2	1.71	0.73
2:D:333:GLN:NE2	2:D:370:TYR:CZ	2.55	0.73
1:B:365:ILE:HD13	1:B:366:LYS:HG3	1.70	0.73
1:E:118:LEU:HB3	1:E:305:ILE:CB	2.15	0.73
1:E:324:TYR:HB3	1:E:507:TYR:OH	1.88	0.73
1:E:384:HIS:HA	1:E:417:GLU:HB2	1.70	0.73
2:F:98:GLY:C	2:F:102:PRO:HD3	2.09	0.73
1:A:337:TYR:HA	1:A:340:CYS:HB2	1.70	0.73
1:A:471:TYR:HE1	1:A:545:ILE:HG23	1.53	0.73
2:D:4:PRO:HA	1:B:607:PHE:CD1	2.23	0.73
2:D:346:ASN:ND2	2:D:382:GLU:OE1	2.21	0.73
1:E:400:LEU:N	1:E:400:LEU:HD12	2.03	0.73
1:A:390:THR:OG1	1:A:422:PRO:HA	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:THR:HG22	2:D:97:ASN:HD21	1.54	0.73
1:B:366:LYS:CA	1:B:396:HIS:ND1	2.35	0.73
1:E:97:LEU:HD21	1:E:120:PHE:CZ	2.24	0.73
1:E:469:ILE:HD13	1:E:478:ILE:CD1	2.14	0.73
1:E:491:ASN:CG	2:F:36:ARG:HD3	2.08	0.73
1:E:577:ARG:HD2	1:E:578:ASN:N	2.02	0.73
1:A:331:GLN:NE2	1:A:364:TRP:HE1	1.86	0.73
2:C:77:VAL:HB	2:C:79:GLN:HG3	1.69	0.73
2:D:184:ARG:CB	1:B:592:ARG:CD	2.66	0.73
1:B:90:HIS:HE1	1:B:128:ILE:HG12	1.53	0.73
1:B:263:PHE:O	1:B:267:ILE:HG23	1.89	0.73
1:E:118:LEU:HD12	1:E:305:ILE:CG2	2.18	0.73
1:A:126:GLN:NE2	1:A:257:ARG:HH22	1.87	0.73
2:D:356:TRP:O	2:D:360:ILE:N	2.18	0.73
1:B:124:LEU:HB3	1:B:434:PHE:HE2	1.54	0.73
1:B:241:ARG:HB3	1:B:380:TYR:CZ	2.24	0.73
1:E:83:LEU:HD23	1:E:83:LEU:N	2.03	0.73
1:E:259:LEU:O	1:E:263:PHE:HD1	1.72	0.73
1:E:365:ILE:CD1	1:E:366:LYS:H	2.02	0.73
1:A:98:GLN:CG	1:A:115:ARG:CA	2.65	0.73
2:C:312:GLN:HE22	2:C:323:LYS:HB2	1.53	0.73
2:D:113:HIS:HA	2:D:116:ALA:HB3	1.71	0.73
1:B:174:GLY:HA3	1:B:177:GLU:OE2	1.89	0.73
1:E:469:ILE:CD1	1:E:478:ILE:CD1	2.65	0.73
1:A:303:SER:O	3:A:702:HOH:O	2.06	0.72
1:A:480:GLY:H	1:A:524:PRO:CG	2.01	0.72
2:C:10:ARG:NH1	2:C:10:ARG:HG2	2.02	0.72
2:C:105:GLN:HA	2:C:105:GLN:HE21	1.50	0.72
2:D:350:LYS:HZ3	2:D:401:THR:HG22	1.52	0.72
1:B:478:ILE:HD13	1:B:478:ILE:N	2.03	0.72
1:B:559:CYS:HG	1:B:560:HIS:HD1	1.36	0.72
1:E:473:LYS:HD2	1:E:473:LYS:N	2.03	0.72
1:E:491:ASN:OD1	2:F:36:ARG:HD3	1.88	0.72
1:E:610:ARG:HG2	1:E:610:ARG:NH1	1.98	0.72
2:F:76:GLY:O	2:F:77:VAL:HG13	1.89	0.72
2:F:282:TYR:CE2	2:F:287:LEU:HD22	2.21	0.72
1:A:90:HIS:NE2	1:A:213:ILE:HD11	2.04	0.72
1:A:99:VAL:HB	1:A:113:ALA:CA	2.19	0.72
1:A:276:GLU:N	1:A:276:GLU:OE2	2.22	0.72
1:A:326:GLY:HA3	1:A:578:ASN:HD22	0.91	0.72
1:B:330:PRO:HB3	1:B:337:TYR:HD1	1.50	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:CD2	1:B:397:LEU:CD2	2.73	0.72
1:E:289:TYR:O	1:E:317:PHE:CE2	2.42	0.72
2:C:86:LEU:HD21	2:C:138:LEU:CD1	2.03	0.72
1:B:174:GLY:O	1:B:458:PHE:CD2	2.39	0.72
1:E:358:LEU:HD23	1:E:358:LEU:H	1.53	0.72
1:A:288:GLU:HG2	1:A:289:TYR:CD2	2.23	0.72
2:C:54:HIS:CD2	2:C:98:GLY:CA	2.72	0.72
2:C:85:ARG:NE	2:C:138:LEU:HB2	2.05	0.72
2:D:2:ILE:HG12	1:B:609:ARG:HE	1.55	0.72
2:D:98:GLY:C	2:D:102:PRO:HD3	2.08	0.72
2:D:121:LEU:HD12	2:D:122:PRO:HD2	1.69	0.72
2:D:202:TRP:CZ3	2:D:209:PHE:CE1	2.71	0.72
1:B:124:LEU:HB3	1:B:434:PHE:CE2	2.24	0.72
1:A:105:VAL:N	1:A:132:ASP:O	2.20	0.72
1:A:466:PRO:O	2:C:491:VAL:CG2	2.34	0.72
1:B:99:VAL:HG22	1:B:166:ARG:NE	2.04	0.72
1:E:362:PRO:HB2	3:E:705:HOH:O	1.88	0.72
2:C:138:LEU:HD21	2:D:94:ARG:NH1	2.05	0.72
2:C:400:SER:O	2:C:404:ILE:HG13	1.89	0.72
2:D:88:TYR:O	2:D:92:LEU:HG	1.90	0.72
2:D:278:PHE:CE1	2:D:279:PHE:CE2	2.78	0.72
2:D:357:GLU:O	2:D:361:ASP:CG	2.27	0.72
1:E:169:ASN:CG	1:E:203:THR:CG2	2.52	0.72
1:E:331:GLN:HG2	1:E:364:TRP:CZ2	2.18	0.72
1:A:538:THR:HB	1:A:560:HIS:HD2	0.57	0.72
2:C:112:LEU:N	2:C:112:LEU:HD23	2.03	0.72
2:C:350:LYS:HG2	2:C:404:ILE:HD12	1.70	0.72
1:B:261:GLU:C	1:B:264:THR:OG1	2.28	0.72
1:B:392:ASN:N	1:B:393:SER:HA	2.04	0.72
1:A:267:ILE:HD11	1:A:277:LEU:CD2	2.20	0.72
1:B:277:LEU:HD23	1:B:277:LEU:N	2.00	0.72
1:B:388:LEU:HD12	1:B:388:LEU:N	2.03	0.72
1:E:365:ILE:N	1:E:365:ILE:HD12	2.04	0.72
1:A:206:LEU:HD22	1:A:207:LEU:N	2.05	0.72
1:A:471:TYR:HE1	1:A:545:ILE:CG2	2.03	0.72
2:C:158:HIS:O	2:C:162:ASP:HB3	1.89	0.72
1:E:310:HIS:CB	1:E:314:GLY:CA	2.68	0.72
1:E:480:GLY:H	1:E:524:PRO:CG	2.02	0.72
2:F:54:HIS:CD2	2:F:98:GLY:HA3	2.25	0.72
1:A:84:LYS:N	1:A:139:TRP:HB3	2.05	0.71
1:A:347:HIS:NE2	1:A:351:GLN:OE1	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HD23	1:A:373:LEU:N	2.05	0.71
2:C:52:LEU:HD13	2:C:53:PRO:CD	2.18	0.71
2:C:159:TYR:HE2	2:C:160:TRP:CZ3	2.08	0.71
1:B:80:PHE:CD1	1:B:166:ARG:HB2	2.24	0.71
1:B:347:HIS:CD2	1:B:351:GLN:HG2	2.25	0.71
1:E:397:LEU:HD12	1:E:397:LEU:N	2.01	0.71
1:E:599:ASN:OD1	1:E:600:ILE:N	2.23	0.71
1:A:105:VAL:O	1:A:132:ASP:HB2	1.89	0.71
1:A:502:THR:CG2	1:A:577:ARG:NH2	2.52	0.71
2:C:45:ARG:NH2	2:C:57:ASP:OD1	2.23	0.71
2:C:68:LEU:O	2:C:71:LYS:HD2	1.90	0.71
1:B:321:LEU:HD13	1:B:347:HIS:ND1	2.05	0.71
1:B:408:THR:CB	1:B:415:ALA:N	2.53	0.71
2:F:89:VAL:HG23	2:F:144:LEU:HD21	1.71	0.71
1:A:369:GLY:CA	1:A:372:ILE:HG22	2.20	0.71
1:A:395:ARG:O	1:A:398:ASP:OD1	2.09	0.71
2:D:99:LEU:HD12	2:D:99:LEU:N	2.05	0.71
1:B:451:ILE:HD13	1:B:451:ILE:N	2.04	0.71
1:E:97:LEU:HD22	1:E:120:PHE:CE1	2.23	0.71
1:E:116:GLU:OE1	1:E:116:GLU:N	2.23	0.71
1:A:466:PRO:HB2	1:A:554:ILE:O	1.91	0.71
1:B:324:TYR:HB2	1:B:536:PHE:CD2	2.24	0.71
1:E:199:ASN:O	1:E:202:THR:OG1	2.08	0.71
2:F:68:LEU:HD22	2:F:84:ILE:HD13	0.76	0.71
1:A:364:TRP:CD1	1:A:369:GLY:HA2	2.17	0.71
1:B:79:MET:O	1:B:167:VAL:HG11	1.89	0.71
1:E:118:LEU:HD23	1:E:118:LEU:N	2.04	0.71
2:F:305:VAL:HG21	2:F:336:LEU:HD21	1.72	0.71
2:F:389:TRP:CD1	2:F:390:ARG:HD2	2.25	0.71
1:A:98:GLN:HG3	1:A:115:ARG:C	2.11	0.71
1:A:126:GLN:NE2	1:A:257:ARG:NH1	2.34	0.71
2:D:46:LEU:CD1	1:B:483:PHE:CE1	2.71	0.71
1:B:337:TYR:OH	1:B:362:PRO:CG	2.38	0.71
1:B:364:TRP:HD1	1:B:369:GLY:HA2	1.55	0.71
1:B:521:ASN:O	1:B:522:THR:HG22	1.90	0.71
1:B:575:ILE:HD13	1:B:575:ILE:N	2.04	0.71
1:E:166:ARG:HG2	1:E:166:ARG:NH1	2.04	0.71
1:A:245:ILE:HD11	1:A:363:GLY:O	1.89	0.71
1:A:359:LEU:HD12	1:A:360:ASN:H	1.55	0.71
1:A:521:ASN:O	1:A:522:THR:HG22	1.91	0.71
2:C:102:PRO:CA	2:C:104:GLN:OE1	2.35	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:PHE:HE2	2:C:254:ILE:CG2	2.04	0.71
2:C:224:ILE:HG21	2:C:229:PHE:HZ	1.54	0.71
2:D:88:TYR:CB	2:D:144:LEU:HD13	2.20	0.71
2:D:363:ASN:O	2:D:368:ILE:HD12	1.90	0.71
1:B:366:LYS:HB3	1:B:395:ARG:NH1	2.05	0.71
1:B:480:GLY:HA2	1:B:524:PRO:O	1.91	0.71
1:E:387:PHE:CE1	1:E:401:THR:CG2	2.74	0.71
1:B:612:LYS:O	1:B:613:LEU:HD12	1.90	0.71
2:C:23:TYR:CE2	2:C:160:TRP:HD1	2.09	0.71
1:B:474:GLY:N	1:B:475:LYS:HA	2.06	0.71
1:E:166:ARG:HG2	1:E:166:ARG:HH11	1.56	0.71
2:F:131:TRP:CZ2	2:F:139:PRO:HG3	2.26	0.71
1:A:75:GLU:HA	2:C:259:ARG:NH2	2.01	0.71
2:D:130:HIS:O	2:D:132:GLY:N	2.23	0.71
1:B:259:LEU:O	1:B:263:PHE:HD1	1.71	0.71
1:B:503:VAL:CG1	1:B:539:LEU:HD22	2.21	0.71
1:A:420:ARG:HG2	1:A:420:ARG:HH21	1.56	0.70
2:C:106:SER:OG	2:C:108:PHE:O	2.07	0.70
1:B:348:LEU:HD11	1:B:353:PHE:HB3	1.69	0.70
1:E:390:THR:OG1	1:E:423:ALA:N	2.24	0.70
2:F:54:HIS:NE2	2:F:98:GLY:HA3	2.06	0.70
2:F:278:PHE:O	2:F:282:TYR:N	2.24	0.70
1:A:196:PHE:CD2	1:A:197:PRO:HD2	2.26	0.70
1:A:223:SER:O	1:A:227:GLU:N	2.20	0.70
2:D:69:ASP:HA	2:D:77:VAL:CB	2.20	0.70
1:A:440:ARG:NH1	3:A:703:HOH:O	2.22	0.70
2:D:23:TYR:HE2	2:D:156:TYR:CB	1.97	0.70
1:E:123:PRO:HG3	1:E:309:GLN:CG	2.22	0.70
2:F:68:LEU:HB3	2:F:84:ILE:HD11	1.72	0.70
1:A:469:ILE:CG2	2:C:488:TRP:N	2.38	0.70
2:C:80:ASP:CG	2:C:82:ILE:HG22	2.10	0.70
2:C:210:LEU:HD12	2:C:210:LEU:N	2.01	0.70
2:C:309:TYR:HE1	2:C:313:GLN:NE2	1.89	0.70
1:B:515:LEU:HD23	1:B:515:LEU:N	2.03	0.70
1:B:544:SER:OG	1:B:553:ASN:HB2	1.92	0.70
2:F:58:SER:C	2:F:62:ILE:HG13	2.07	0.70
1:A:245:ILE:HD12	1:A:246:GLY:H	1.56	0.70
1:A:381:LYS:CA	1:A:409:SER:CB	2.69	0.70
1:B:90:HIS:ND1	1:B:128:ILE:HD13	2.05	0.70
1:B:123:PRO:HG3	1:B:309:GLN:CG	2.21	0.70
1:B:517:VAL:HB	1:B:525:ILE:O	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:395:ARG:HG3	1:E:395:ARG:NH2	2.00	0.70
1:E:397:LEU:H	1:E:397:LEU:CD1	2.03	0.70
1:E:450:LYS:HE3	1:E:453:GLN:CA	2.19	0.70
2:F:333:GLN:HA	2:F:337:LEU:HD23	1.72	0.70
1:A:91:LEU:HD21	1:A:167:VAL:HG11	1.72	0.70
1:A:214:GLN:HG2	1:A:214:GLN:O	1.92	0.70
1:A:305:ILE:CG2	1:A:307:LEU:HD11	2.21	0.70
1:B:473:LYS:CE	1:B:474:GLY:H	2.04	0.70
1:E:241:ARG:NH1	1:E:381:LYS:CD	2.54	0.70
1:E:293:ASP:OD2	1:E:328:SER:N	2.25	0.70
1:E:450:LYS:HE2	1:E:453:GLN:HA	1.72	0.70
1:E:469:ILE:HG21	1:E:478:ILE:HD11	0.71	0.70
2:F:99:LEU:O	2:F:102:PRO:HD2	1.91	0.70
1:A:331:GLN:NE2	1:A:364:TRP:CE2	2.59	0.70
1:A:616:VAL:HG12	2:C:50:GLN:O	1.92	0.70
2:C:53:PRO:HD2	2:C:56:VAL:HG21	1.74	0.70
2:C:110:ILE:CG2	2:C:114:THR:CB	2.64	0.70
2:C:110:ILE:HG21	2:C:114:THR:HB	1.72	0.70
1:B:99:VAL:HG22	1:B:166:ARG:HH21	1.41	0.70
1:B:471:TYR:HD1	1:B:550:GLN:O	1.71	0.70
2:F:271:HIS:HA	2:F:274:VAL:CG2	2.21	0.70
1:A:105:VAL:CB	1:A:132:ASP:CB	2.34	0.70
2:C:182:TYR:OH	2:F:183:ARG:HG3	1.92	0.70
2:D:288:LYS:HG3	2:D:343:ASN:HD22	1.56	0.70
1:B:243:MET:SD	1:B:361:LEU:CD1	2.80	0.70
1:A:365:ILE:O	1:A:396:HIS:CG	2.45	0.70
1:A:491:ASN:HD21	2:C:36:ARG:NE	1.88	0.70
2:D:72:GLU:OE1	2:D:72:GLU:HA	1.91	0.70
2:D:96:VAL:CG1	2:D:100:LEU:CG	2.70	0.70
1:B:348:LEU:HD11	1:B:353:PHE:HD1	1.56	0.70
1:B:387:PHE:CD2	1:B:397:LEU:HD21	2.27	0.70
1:E:105:VAL:HA	1:E:109:VAL:O	1.91	0.70
1:E:577:ARG:HD2	1:E:578:ASN:H	1.57	0.70
1:A:590:SER:OG	2:C:184:ARG:CD	2.39	0.70
2:D:86:LEU:CD1	2:D:138:LEU:HD21	2.22	0.70
1:B:246:GLY:O	1:B:363:GLY:HA2	1.91	0.70
1:A:105:VAL:O	1:A:132:ASP:CB	2.39	0.69
1:E:85:GLU:O	1:E:133:PHE:CD1	2.43	0.69
1:E:109:VAL:HG21	1:E:111:TYR:CE1	2.26	0.69
1:E:179:GLY:HA2	1:E:185:VAL:HG13	1.74	0.69
1:A:104:ILE:HD12	1:A:104:ILE:N	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:VAL:HG11	2:C:64:CYS:SG	2.31	0.69
1:B:91:LEU:HD11	1:B:204:TYR:CB	2.22	0.69
1:E:431:SER:OG	1:E:434:PHE:CA	2.40	0.69
1:B:79:MET:C	1:B:167:VAL:HG22	2.04	0.69
1:E:213:ILE:HD12	1:E:213:ILE:O	1.92	0.69
1:E:451:ILE:O	1:E:452:THR:OG1	2.10	0.69
1:A:504:ILE:HD13	1:A:575:ILE:HG21	1.71	0.69
1:B:398:ASP:OD2	1:B:398:ASP:N	2.24	0.69
1:B:599:ASN:ND2	1:B:600:ILE:HD13	2.08	0.69
1:E:230:TYR:HB3	1:E:262:LYS:NZ	2.07	0.69
1:E:241:ARG:HB2	1:E:383:THR:H	1.56	0.69
2:F:79:GLN:HA	2:F:83:PRO:HG2	1.73	0.69
1:A:480:GLY:N	1:A:524:PRO:HG2	2.07	0.69
2:D:202:TRP:CH2	2:D:209:PHE:CD2	2.73	0.69
2:F:68:LEU:HD23	2:F:68:LEU:C	2.13	0.69
2:C:125:PHE:CD1	2:C:128:LEU:CD2	2.75	0.69
2:D:202:TRP:CZ3	2:D:209:PHE:CD1	2.81	0.69
1:B:400:LEU:HD22	1:B:400:LEU:H	1.56	0.69
1:E:89:LEU:O	1:E:130:THR:HG22	1.93	0.69
1:E:493:GLN:HE21	2:F:36:ARG:HH22	1.39	0.69
1:A:106:TYR:O	1:A:109:VAL:HG13	1.93	0.69
1:A:353:PHE:CE1	1:A:355:GLY:N	2.60	0.69
2:D:139:PRO:HG2	2:D:144:LEU:HD21	1.75	0.69
1:B:69:ILE:O	1:B:69:ILE:HD13	1.93	0.69
1:B:96:ARG:CZ	1:B:171:ASN:OD1	2.40	0.69
1:B:230:TYR:CE1	1:B:263:PHE:CD1	2.80	0.69
1:B:366:LYS:CD	1:B:395:ARG:HH11	2.06	0.69
1:B:389:GLU:HG3	1:B:393:SER:O	1.91	0.69
1:B:578:ASN:OD1	1:B:579:LYS:HG2	1.91	0.69
1:E:613:LEU:O	2:F:159:TYR:HD1	1.75	0.69
2:F:322:LEU:HD21	2:F:332:LEU:HD11	1.75	0.69
1:A:106:TYR:O	1:A:109:VAL:HG22	1.92	0.69
2:C:54:HIS:CD2	2:C:98:GLY:C	2.66	0.69
2:C:349:PHE:CZ	2:C:353:TRP:CZ3	2.81	0.69
1:B:92:SER:CB	1:B:207:LEU:HD11	2.22	0.69
1:B:471:TYR:HA	1:B:478:ILE:HG12	1.74	0.69
1:B:506:ILE:HD11	1:B:540:GLY:HA3	1.72	0.69
1:B:546:ASP:HB3	1:B:549:GLN:CG	2.22	0.69
1:E:96:ARG:HG2	1:E:168:PHE:HD2	1.57	0.69
1:E:245:ILE:HD11	1:E:373:LEU:CD2	2.22	0.69
1:E:477:GLY:O	1:E:478:ILE:HG13	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:548:SER:CB	1:E:549:GLN:HE21	2.05	0.69
2:F:278:PHE:CE2	2:F:282:TYR:HA	2.28	0.69
2:F:366:TYR:N	2:F:419:PHE:CD1	2.60	0.69
1:A:165:LEU:N	1:A:165:LEU:HD12	2.07	0.69
1:A:245:ILE:HD11	1:A:363:GLY:CA	2.23	0.69
1:B:243:MET:CE	1:B:380:TYR:CD2	2.76	0.69
1:E:205:HIS:O	1:E:207:LEU:CD2	2.40	0.69
1:E:240:THR:OG1	1:E:356:THR:HG22	1.93	0.69
1:E:561:THR:HG23	1:E:562:GLN:HA	1.75	0.69
1:A:180:HIS:HB2	2:C:269:ILE:HD12	1.74	0.69
2:C:353:TRP:HH2	2:C:408:LEU:HD21	1.57	0.69
1:B:122:HIS:HE1	1:B:128:ILE:HB	1.48	0.69
1:E:181:LEU:O	1:E:181:LEU:HD13	1.93	0.69
1:E:390:THR:HG22	1:E:391:ALA:H	1.56	0.69
1:E:489:ASP:OD1	1:E:489:ASP:N	2.25	0.69
1:A:105:VAL:CA	1:A:132:ASP:HB2	2.24	0.68
1:A:174:GLY:CA	1:A:177:GLU:OE1	2.41	0.68
2:C:101:ASP:O	2:C:105:GLN:N	2.26	0.68
2:D:86:LEU:HD11	2:D:138:LEU:HD21	1.75	0.68
2:D:349:PHE:CE2	2:D:356:TRP:CD1	2.82	0.68
1:B:480:GLY:HA2	1:B:524:PRO:HG2	1.75	0.68
1:E:100:VAL:C	1:E:101:LYS:HG2	2.13	0.68
1:E:169:ASN:ND2	1:E:203:THR:HG23	2.07	0.68
1:E:389:GLU:OE1	1:E:389:GLU:HA	1.93	0.68
1:A:507:TYR:CD2	1:A:576:VAL:HG21	2.28	0.68
2:C:353:TRP:CH2	2:C:408:LEU:HD21	2.27	0.68
1:B:510:SER:CB	1:B:535:ASN:OD1	2.34	0.68
1:A:265:GLN:HA	1:A:268:ARG:HH11	1.57	0.68
1:A:617:TRP:HD1	1:A:618:LYS:N	1.91	0.68
2:C:357:GLU:O	2:C:361:ASP:HB2	1.93	0.68
2:D:323:LYS:CG	2:D:427:TYR:CE2	2.74	0.68
1:E:103:GLY:N	1:E:134:SER:O	2.26	0.68
1:E:222:TRP:CD1	1:E:422:PRO:HB2	2.28	0.68
1:A:392:ASN:N	1:A:393:SER:HA	2.09	0.68
1:A:469:ILE:HG21	2:C:488:TRP:CD2	2.29	0.68
1:A:488:GLN:HE21	1:A:527:GLN:CD	1.96	0.68
1:B:211:ASP:O	1:B:212:ARG:HB2	1.94	0.68
1:E:79:MET:HG2	1:E:80:PHE:N	2.07	0.68
1:E:521:ASN:O	1:E:522:THR:HG22	1.92	0.68
1:A:77:GLU:HG3	1:A:201:ARG:O	1.94	0.68
1:A:93:GLY:H	1:A:122:HIS:HB2	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PHE:CE1	1:A:355:GLY:CA	2.77	0.68
2:D:138:LEU:HD12	2:D:138:LEU:H	1.58	0.68
1:B:265:GLN:HA	1:B:268:ARG:HH21	1.57	0.68
2:C:95:PHE:O	2:C:99:LEU:HD22	1.93	0.68
2:D:99:LEU:O	2:D:102:PRO:HD2	1.93	0.68
1:B:455:ASP:OD1	1:B:455:ASP:N	2.27	0.68
1:E:289:TYR:O	1:E:317:PHE:HE2	1.76	0.68
1:E:310:HIS:HB2	1:E:314:GLY:CA	2.22	0.68
1:A:377:ILE:HD13	1:A:385:LEU:HD11	1.76	0.68
1:A:507:TYR:HA	1:A:535:ASN:O	1.93	0.68
1:B:364:TRP:HD1	1:B:372:ILE:CG2	2.06	0.68
2:F:366:TYR:N	2:F:419:PHE:HD1	1.91	0.68
1:A:83:LEU:HD23	1:A:83:LEU:H	1.59	0.68
1:A:381:LYS:CD	1:A:409:SER:CB	2.72	0.68
1:A:420:ARG:HG2	1:A:420:ARG:NH2	2.08	0.68
2:D:359:LEU:HD23	2:D:359:LEU:C	2.14	0.68
1:B:507:TYR:HB2	1:B:574:ILE:O	1.94	0.68
1:E:88:LYS:HG2	1:E:132:ASP:OD1	1.94	0.68
1:A:374:ASN:OD1	1:A:404:GLN:CB	2.42	0.68
1:A:507:TYR:HD2	1:A:576:VAL:HG21	1.58	0.68
2:C:332:LEU:HD23	2:C:332:LEU:C	2.14	0.68
2:D:4:PRO:CD	1:B:607:PHE:CE1	2.75	0.68
2:D:84:ILE:CD1	2:D:88:TYR:CD2	2.76	0.68
1:E:592:ARG:HD2	1:E:592:ARG:C	2.14	0.68
1:A:313:GLN:N	1:A:313:GLN:HE21	1.92	0.68
1:A:502:THR:HB	1:A:577:ARG:HH22	1.54	0.68
2:D:212:TYR:CZ	2:D:250:SER:CB	2.77	0.68
2:D:500:GLY:O	2:D:501:VAL:HG22	1.93	0.68
1:E:592:ARG:HG3	1:E:592:ARG:NH2	2.01	0.68
2:F:272:ASN:HA	2:F:275:LEU:HD11	1.55	0.68
1:A:541:LEU:O	1:A:554:ILE:HG13	1.93	0.67
2:F:338:ASP:OD1	2:F:370:TYR:OH	2.12	0.67
2:F:350:LYS:NZ	2:F:401:THR:HB	2.03	0.67
1:A:541:LEU:HD12	1:A:541:LEU:C	2.14	0.67
1:A:597:ASP:N	1:A:597:ASP:OD1	2.27	0.67
2:D:99:LEU:H	2:D:99:LEU:CD1	2.05	0.67
2:D:119:ILE:HD11	2:D:121:LEU:HD22	1.76	0.67
1:B:321:LEU:HD23	1:B:321:LEU:C	2.15	0.67
1:B:400:LEU:HD22	1:B:400:LEU:N	2.08	0.67
1:E:106:TYR:CE2	1:E:120:PHE:CD2	2.82	0.67
2:F:80:ASP:OD1	2:F:83:PRO:HD3	1.93	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:337:LEU:HD12	2:F:337:LEU:C	2.15	0.67
1:A:267:ILE:HD11	1:A:277:LEU:HD23	1.75	0.67
1:A:365:ILE:HD12	1:A:366:LYS:N	2.08	0.67
2:C:82:ILE:CG2	2:D:64:CYS:HG	2.07	0.67
2:C:97:ASN:ND2	2:C:129:ARG:HE	1.92	0.67
2:C:102:PRO:C	2:C:104:GLN:HA	2.13	0.67
2:C:182:TYR:CZ	2:F:183:ARG:HG3	2.29	0.67
2:D:495:LYS:O	2:D:497:LYS:CG	2.41	0.67
1:B:67:ASP:OD2	1:B:67:ASP:N	2.27	0.67
2:F:333:GLN:O	2:F:337:LEU:HG	1.94	0.67
1:A:226:LEU:HD12	1:A:226:LEU:C	2.15	0.67
1:A:481:ILE:HG23	1:A:575:ILE:HB	1.73	0.67
2:D:357:GLU:C	2:D:361:ASP:OD2	2.31	0.67
2:D:430:ILE:HD13	2:D:430:ILE:N	2.04	0.67
1:B:239:ASP:CB	1:B:355:GLY:CA	2.71	0.67
1:E:75:GLU:OE1	1:E:76:ASP:N	2.27	0.67
1:E:207:LEU:HD23	1:E:207:LEU:N	2.09	0.67
2:F:418:ARG:O	2:F:419:PHE:HD2	1.78	0.67
1:A:264:THR:O	1:A:268:ARG:HD3	1.93	0.67
1:A:589:PRO:CB	1:A:594:ILE:HD12	2.24	0.67
2:C:11:ASP:OD2	2:C:11:ASP:N	2.26	0.67
2:D:45:ARG:NH2	2:D:57:ASP:OD2	2.27	0.67
2:D:5:ARG:NE	1:B:610:ARG:CG	2.58	0.67
1:B:97:LEU:HB2	1:B:120:PHE:HE1	1.59	0.67
1:E:346:ASP:OD1	1:E:379:LYS:NZ	2.27	0.67
1:E:385:LEU:O	1:E:419:VAL:CG2	2.43	0.67
1:E:493:GLN:HE21	2:F:36:ARG:NH2	1.91	0.67
1:B:549:GLN:O	1:B:550:GLN:HB2	1.95	0.67
1:E:88:LYS:HB3	1:E:130:THR:HG21	1.75	0.67
1:E:324:TYR:HB2	1:E:536:PHE:CD2	2.28	0.67
1:E:368:PHE:O	1:E:372:ILE:N	2.27	0.67
1:E:390:THR:HG22	1:E:391:ALA:N	2.10	0.67
1:E:536:PHE:HD1	1:E:537:ILE:N	1.92	0.67
1:E:592:ARG:HH21	1:E:593:THR:N	1.93	0.67
2:F:331:GLU:O	2:F:335:ARG:HB2	1.94	0.67
1:B:115:ARG:HB2	1:B:115:ARG:CZ	2.24	0.67
2:C:75:LEU:HD23	2:C:75:LEU:C	2.14	0.67
2:C:100:LEU:C	2:C:100:LEU:HD12	2.15	0.67
2:C:349:PHE:CZ	2:C:353:TRP:HZ3	2.12	0.67
2:D:486:LYS:O	2:D:486:LYS:HD3	1.93	0.67
1:B:172:HIS:HD2	1:B:454:PHE:C	1.97	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:LEU:HD12	1:B:491:ASN:N	2.10	0.67
2:C:86:LEU:HD23	2:C:138:LEU:HD12	1.75	0.67
1:B:326:GLY:O	1:B:578:ASN:OD1	2.12	0.67
1:B:471:TYR:OH	1:B:547:THR:HA	1.94	0.67
1:E:538:THR:HG22	1:E:539:LEU:O	1.95	0.67
3:E:701:HOH:O	2:F:502:LEU:CD2	2.43	0.67
2:F:22:PHE:CE1	2:F:37:ALA:CB	2.75	0.67
2:F:501:VAL:O	2:F:502:LEU:HD12	1.94	0.67
1:A:359:LEU:HD12	1:A:359:LEU:C	2.15	0.66
1:A:471:TYR:HD1	1:A:552:MET:CG	2.04	0.66
1:A:590:SER:HB3	1:A:593:THR:OG1	1.95	0.66
2:C:210:LEU:CD1	2:C:210:LEU:H	1.96	0.66
2:D:54:HIS:NE2	2:D:99:LEU:HD12	2.10	0.66
2:D:62:ILE:HG21	2:D:152:LEU:HD21	1.77	0.66
2:D:77:VAL:HG12	2:D:84:ILE:CB	2.11	0.66
1:B:96:ARG:CZ	1:B:171:ASN:CG	2.63	0.66
1:B:230:TYR:HD1	1:B:263:PHE:CE1	2.07	0.66
1:B:450:LYS:HB3	1:B:450:LYS:NZ	2.10	0.66
1:E:110:HIS:C	1:E:111:TYR:HD1	1.98	0.66
1:E:369:GLY:HA2	1:E:372:ILE:HG21	1.71	0.66
2:F:128:LEU:CB	2:F:131:TRP:HZ3	1.94	0.66
1:A:106:TYR:HD2	1:A:120:PHE:HE2	1.40	0.66
1:A:216:LEU:HD23	1:A:217:SER:H	1.59	0.66
1:A:381:LYS:CG	1:A:409:SER:CB	2.72	0.66
2:D:209:PHE:CE1	2:D:254:ILE:HG23	2.24	0.66
1:B:365:ILE:HD12	1:B:366:LYS:CG	2.23	0.66
1:B:470:SER:HA	1:B:551:ILE:HA	1.76	0.66
1:E:103:GLY:C	1:E:104:ILE:HD12	2.15	0.66
1:E:257:ARG:HD2	1:E:308:GLY:O	1.96	0.66
1:E:310:HIS:HD2	1:E:314:GLY:HA3	1.57	0.66
1:E:331:GLN:CD	1:E:364:TRP:CZ2	2.66	0.66
2:F:333:GLN:HA	2:F:337:LEU:CD2	2.25	0.66
2:F:359:LEU:HD23	2:F:359:LEU:C	2.15	0.66
1:A:261:GLU:HG2	1:A:307:LEU:HD23	1.76	0.66
1:A:299:LYS:C	1:A:300:ILE:HD12	2.16	0.66
1:B:261:GLU:O	1:B:264:THR:OG1	2.14	0.66
2:F:48:GLY:HA2	2:F:50:GLN:O	1.95	0.66
1:A:331:GLN:O	1:A:334:PRO:HD3	1.94	0.66
2:D:322:LEU:HD23	2:D:322:LEU:C	2.15	0.66
1:E:205:HIS:O	1:E:207:LEU:HD21	1.95	0.66
1:E:230:TYR:HB3	1:E:262:LYS:HZ3	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:473:LYS:HD2	1:E:474:GLY:H	1.60	0.66
1:A:229:LEU:HD12	1:A:259:LEU:HD21	1.77	0.66
1:A:589:PRO:HG3	1:A:594:ILE:CD1	2.16	0.66
2:C:95:PHE:CZ	2:C:155:LEU:HD12	2.29	0.66
2:C:138:LEU:HD21	2:D:94:ARG:NE	2.09	0.66
2:C:337:LEU:O	2:C:337:LEU:HD23	1.96	0.66
2:D:128:LEU:HD23	2:D:128:LEU:C	2.16	0.66
1:B:364:TRP:HD1	1:B:372:ILE:HG21	1.59	0.66
1:B:599:ASN:HD21	1:B:600:ILE:CD1	2.07	0.66
1:E:364:TRP:CD1	1:E:369:GLY:HA2	2.29	0.66
1:B:599:ASN:HD21	1:B:600:ILE:HD13	1.61	0.66
1:B:288:GLU:HG2	1:B:289:TYR:CD2	2.30	0.66
1:B:348:LEU:HD11	1:B:353:PHE:CB	2.25	0.66
1:E:289:TYR:HD1	1:E:317:PHE:CG	2.12	0.66
2:F:500:GLY:C	2:F:501:VAL:HG23	2.16	0.66
1:A:107:ASN:ND2	1:A:258:LEU:HD21	2.10	0.66
1:A:504:ILE:HD13	1:A:575:ILE:CG2	2.15	0.66
2:D:96:VAL:O	2:D:100:LEU:CA	2.43	0.66
2:D:202:TRP:HH2	2:D:209:PHE:CD1	2.14	0.66
1:B:65:LEU:C	1:B:65:LEU:HD12	2.15	0.66
1:B:359:LEU:HD12	1:B:359:LEU:C	2.15	0.66
1:B:366:LYS:C	1:B:396:HIS:CE1	2.68	0.66
1:E:562:GLN:O	1:E:565:ASP:N	2.29	0.66
2:D:108:PHE:H	2:D:108:PHE:HD2	1.44	0.66
2:D:133:THR:HB	2:D:134:HIS:CD2	2.31	0.66
1:E:260:LEU:O	1:E:264:THR:OG1	2.09	0.66
1:E:306:SER:O	1:E:307:LEU:HG	1.95	0.66
1:E:359:LEU:HD12	1:E:359:LEU:C	2.15	0.66
1:E:364:TRP:CB	1:E:369:GLY:CA	2.67	0.66
1:E:561:THR:HA	1:E:564:LEU:HD12	1.76	0.66
1:A:614:GLU:HB3	2:C:159:TYR:HE1	1.57	0.66
2:C:182:TYR:OH	2:F:183:ARG:CG	2.44	0.66
1:B:471:TYR:CE1	1:B:550:GLN:CB	2.79	0.66
1:E:324:TYR:HB2	1:E:536:PHE:HE2	1.52	0.66
1:E:390:THR:O	1:E:394:LYS:HG3	1.95	0.66
1:E:546:ASP:OD1	1:E:549:GLN:NE2	2.29	0.66
1:E:612:LYS:HD3	2:F:164:GLU:OE1	1.96	0.66
2:F:372:CYS:C	2:F:412:ILE:CD1	2.63	0.66
2:C:52:LEU:HD12	2:C:52:LEU:C	2.15	0.65
2:C:207:ASN:CA	2:C:210:LEU:HD13	2.26	0.65
2:D:46:LEU:CD1	1:B:483:PHE:HE1	1.92	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:LYS:HG3	2:D:427:TYR:CE2	2.29	0.65
1:B:515:LEU:H	1:B:515:LEU:CD2	1.97	0.65
2:C:100:LEU:HD13	2:C:115:LEU:HD12	1.77	0.65
1:B:80:PHE:CE1	1:B:165:LEU:HA	2.29	0.65
1:E:83:LEU:CD1	1:E:101:LYS:C	2.63	0.65
1:A:81:VAL:H	1:A:166:ARG:HG2	1.62	0.65
1:A:366:LYS:HG3	1:A:395:ARG:NH1	2.09	0.65
1:B:80:PHE:CE1	1:B:165:LEU:C	2.64	0.65
1:B:110:HIS:O	1:B:111:TYR:HD1	1.79	0.65
1:B:277:LEU:H	1:B:277:LEU:CD2	1.97	0.65
1:E:188:LEU:HD12	1:E:434:PHE:CE2	2.32	0.65
1:E:213:ILE:HD12	1:E:213:ILE:C	2.16	0.65
1:E:333:GLU:OE1	1:E:336:SER:HB2	1.95	0.65
2:F:53:PRO:HB2	2:F:56:VAL:HG23	1.78	0.65
2:F:66:VAL:HA	2:F:88:TYR:OH	1.97	0.65
1:A:90:HIS:O	1:A:206:LEU:HD23	1.96	0.65
2:C:381:THR:O	2:C:385:THR:OG1	2.13	0.65
1:B:107:ASN:O	1:B:109:VAL:HG13	1.96	0.65
1:E:233:HIS:HB2	1:E:263:PHE:HE2	1.60	0.65
1:E:584:PHE:CE1	1:E:588:LEU:HD12	2.31	0.65
1:A:366:LYS:HE3	1:A:395:ARG:CZ	2.20	0.65
1:A:386:LEU:HD23	1:A:419:VAL:HG23	1.76	0.65
1:A:607:PHE:CD1	2:C:4:PRO:HB3	2.27	0.65
2:C:387:ASN:N	2:C:387:ASN:OD1	2.30	0.65
2:D:2:ILE:CG1	1:B:609:ARG:HE	2.10	0.65
2:D:349:PHE:CE2	2:D:356:TRP:CD2	2.80	0.65
1:B:297:LEU:CB	1:B:344:LEU:CD1	2.61	0.65
2:F:25:LYS:HE2	2:F:25:LYS:C	2.16	0.65
1:E:310:HIS:CG	1:E:314:GLY:HA3	2.30	0.65
1:A:618:LYS:C	2:C:104:GLN:HE22	2.00	0.65
2:C:40:ARG:O	2:C:43:SER:N	2.28	0.65
2:D:70:GLU:HG3	2:D:70:GLU:O	1.96	0.65
2:D:184:ARG:HD3	1:B:592:ARG:HD3	1.79	0.65
1:B:166:ARG:C	1:B:167:VAL:HG22	2.15	0.65
1:E:491:ASN:CG	2:F:36:ARG:NE	2.45	0.65
1:A:368:PHE:HE1	2:D:146:TRP:HE1	0.66	0.65
1:A:406:PHE:HD1	1:A:407:SER:N	1.90	0.65
2:D:493:ASN:HD22	2:D:493:ASN:N	1.94	0.65
1:B:98:GLN:OE1	1:B:165:LEU:HD11	1.96	0.65
1:B:471:TYR:HE1	1:B:550:GLN:CB	2.08	0.65
1:E:293:ASP:OD2	1:E:327:SER:O	2.14	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:306:SER:C	1:E:307:LEU:HD12	2.17	0.65
2:F:82:ILE:HG22	2:F:83:PRO:HD3	1.78	0.65
1:A:105:VAL:CG1	1:A:132:ASP:CB	2.70	0.65
2:D:31:GLU:HA	2:D:31:GLU:OE1	1.97	0.65
2:D:218:ASN:ND2	2:D:221:ASP:OD2	2.30	0.65
2:D:337:LEU:O	2:D:341:ILE:HG13	1.95	0.65
2:D:349:PHE:HE2	2:D:356:TRP:CD1	2.15	0.65
1:B:114:SER:C	1:B:115:ARG:HG3	2.15	0.65
1:B:590:SER:C	1:B:593:THR:OG1	2.36	0.65
1:E:257:ARG:CD	1:E:308:GLY:O	2.45	0.65
2:F:17:GLU:OE2	2:F:40:ARG:NH1	2.30	0.65
2:F:337:LEU:CD2	2:F:370:TYR:CZ	2.72	0.65
2:F:345:ASN:HB3	2:F:348:ASN:HB2	1.78	0.65
2:D:336:LEU:HD12	2:D:336:LEU:C	2.15	0.65
1:A:353:PHE:CE1	1:A:355:GLY:C	2.70	0.64
1:B:397:LEU:CD1	1:B:400:LEU:HD11	2.22	0.64
1:E:241:ARG:H	1:E:383:THR:HG1	1.40	0.64
1:E:615:HIS:NE2	2:F:102:PRO:CG	2.60	0.64
2:F:332:LEU:HD23	2:F:332:LEU:C	2.17	0.64
2:D:46:LEU:CD2	1:B:577:ARG:CD	2.75	0.64
1:A:106:TYR:CD2	1:A:120:PHE:HE2	2.15	0.64
1:A:348:LEU:HD11	1:A:353:PHE:CB	2.22	0.64
2:D:312:GLN:NE2	2:D:427:TYR:HE2	1.96	0.64
1:E:613:LEU:O	2:F:159:TYR:CD1	2.51	0.64
1:A:196:PHE:CD1	1:A:197:PRO:HD2	2.32	0.64
1:A:592:ARG:HH21	2:C:184:ARG:HH21	1.02	0.64
1:B:185:VAL:HG23	1:B:188:LEU:HD12	1.79	0.64
1:A:301:LEU:CD2	1:A:318:GLN:NE2	2.60	0.64
1:A:371:GLN:HE21	1:A:371:GLN:HA	1.63	0.64
2:C:75:LEU:HD23	2:C:76:GLY:N	2.12	0.64
2:C:231:GLY:O	2:C:234:LEU:HG	1.98	0.64
2:D:62:ILE:CG2	2:D:152:LEU:HD21	2.28	0.64
2:D:68:LEU:O	2:D:71:LYS:CG	2.45	0.64
1:B:469:ILE:HG12	1:B:552:MET:O	1.98	0.64
1:B:469:ILE:HG13	1:B:552:MET:HB3	1.79	0.64
1:B:538:THR:HG22	1:B:539:LEU:O	1.98	0.64
1:E:256:LEU:HD22	1:E:358:LEU:HD12	1.80	0.64
1:E:491:ASN:ND2	2:F:39:GLN:CB	2.59	0.64
2:F:11:ASP:OD2	2:F:13:ALA:HB3	1.97	0.64
1:A:491:ASN:ND2	2:C:36:ARG:CZ	2.59	0.64
1:A:492:PRO:HA	1:A:495:ILE:CD1	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:307:ARG:HB2	2:C:307:ARG:NH1	2.02	0.64
1:E:106:TYR:CD2	1:E:120:PHE:HE2	2.15	0.64
1:A:265:GLN:OE1	1:A:265:GLN:HA	1.96	0.64
1:A:395:ARG:HG3	1:A:396:HIS:N	2.12	0.64
1:A:590:SER:CB	2:C:184:ARG:CZ	2.75	0.64
2:C:80:ASP:O	2:C:81:SER:OG	2.08	0.64
1:B:242:ILE:HD12	1:B:242:ILE:N	2.12	0.64
1:E:471:TYR:OH	1:E:523:PHE:CD1	2.47	0.64
2:C:6:ILE:HG21	2:C:51:TYR:CE1	2.33	0.64
2:C:55:VAL:HG23	2:C:155:LEU:CD2	2.27	0.64
2:D:312:GLN:NE2	2:D:427:TYR:CE2	2.66	0.64
1:E:123:PRO:CG	1:E:309:GLN:HG2	2.27	0.64
1:E:269:ASP:N	1:E:269:ASP:OD2	2.28	0.64
2:F:418:ARG:C	2:F:419:PHE:HD2	2.01	0.64
2:C:104:GLN:OE1	2:C:104:GLN:HA	1.98	0.64
2:C:130:HIS:HB2	2:C:134:HIS:CE1	2.33	0.64
1:B:207:LEU:HD13	1:B:213:ILE:CD1	2.28	0.64
1:B:408:THR:CB	1:B:414:TYR:CA	2.75	0.64
1:E:71:TYR:HD1	1:E:80:PHE:CD2	2.16	0.64
1:E:241:ARG:O	1:E:383:THR:N	2.31	0.64
2:F:34:ARG:O	2:F:37:ALA:N	2.30	0.64
2:F:365:SER:C	2:F:419:PHE:CE1	2.71	0.64
1:A:299:LYS:O	1:A:300:ILE:HD12	1.97	0.64
1:A:469:ILE:CD1	2:C:488:TRP:CZ3	2.70	0.64
2:D:131:TRP:HA	2:D:131:TRP:HE3	1.60	0.64
2:D:350:LYS:NZ	2:D:401:THR:CG2	2.61	0.64
1:E:385:LEU:N	1:E:417:GLU:HB3	2.13	0.64
1:E:567:GLN:HE21	1:E:567:GLN:CA	2.01	0.64
1:E:615:HIS:CE1	2:F:102:PRO:CG	2.80	0.64
2:F:30:ILE:C	2:F:30:ILE:HD12	2.17	0.64
2:F:352:LYS:O	2:F:356:TRP:HD1	1.81	0.64
1:A:590:SER:OG	2:C:184:ARG:CZ	2.46	0.63
2:C:12:PHE:O	2:C:12:PHE:HD1	1.80	0.63
2:D:82:ILE:CG2	2:D:83:PRO:HD3	2.25	0.63
1:B:338:LEU:HD21	1:B:372:ILE:CD1	2.27	0.63
1:B:359:LEU:HD12	1:B:360:ASN:C	2.18	0.63
1:E:358:LEU:HD23	1:E:358:LEU:N	2.13	0.63
1:A:489:ASP:CB	2:D:79:GLN:O	2.46	0.63
2:C:125:PHE:C	2:C:128:LEU:HG	2.18	0.63
2:D:188:LEU:HD12	2:D:188:LEU:C	2.18	0.63
1:B:108:ASN:C	1:B:108:ASN:HD22	2.01	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:LEU:HD12	1:E:400:LEU:H	1.63	0.63
1:A:516:GLU:O	1:A:516:GLU:HG2	1.97	0.63
2:C:156:TYR:OH	2:C:161:ASN:ND2	2.31	0.63
2:C:352:LYS:HB3	2:C:355:ASN:ND2	2.13	0.63
2:C:362:GLU:HG2	2:C:490:ARG:HG2	1.80	0.63
1:B:450:LYS:O	1:B:559:CYS:HB3	1.97	0.63
1:E:295:ILE:HD11	1:E:337:TYR:CD2	2.33	0.63
1:E:472:GLY:C	1:E:475:LYS:CB	2.67	0.63
1:A:96:ARG:C	1:A:168:PHE:CE1	2.59	0.63
1:A:127:SER:HG	1:A:216:LEU:HD22	1.63	0.63
2:D:202:TRP:CE3	2:D:209:PHE:CD2	2.75	0.63
2:D:329:TRP:CH2	2:D:424:ILE:HD11	2.31	0.63
1:B:128:ILE:HG12	1:B:213:ILE:HD12	1.81	0.63
1:B:469:ILE:CD1	1:B:554:ILE:CG2	2.71	0.63
1:A:71:TYR:HD2	1:A:72:GLU:N	1.96	0.63
1:A:103:GLY:C	1:A:104:ILE:HD12	2.18	0.63
1:A:105:VAL:O	1:A:132:ASP:CG	2.37	0.63
1:A:286:GLN:HG3	1:A:286:GLN:O	1.97	0.63
1:A:301:LEU:HD23	1:A:318:GLN:NE2	2.13	0.63
2:C:78:HIS:HB2	2:D:35:GLN:CD	2.18	0.63
2:C:95:PHE:HE1	2:C:155:LEU:HD11	1.61	0.63
2:C:181:GLY:O	2:C:185:ASN:HB2	1.99	0.63
1:B:174:GLY:O	1:B:177:GLU:HG2	1.99	0.63
1:B:365:ILE:HD12	1:B:366:LYS:H	1.60	0.63
2:F:75:LEU:O	2:F:77:VAL:CG2	2.32	0.63
1:A:96:ARG:HG3	1:A:168:PHE:CD1	2.33	0.63
2:C:79:GLN:NE2	3:C:601:HOH:O	2.30	0.63
2:D:5:ARG:NE	1:B:610:ARG:HG2	2.14	0.63
1:B:105:VAL:CG2	1:B:134:SER:CB	2.76	0.63
1:B:545:ILE:HD11	1:B:552:MET:HE2	1.80	0.63
1:A:126:GLN:NE2	1:A:257:ARG:NH2	2.43	0.63
2:C:52:LEU:HD13	2:C:53:PRO:HD2	1.73	0.63
2:C:99:LEU:H	2:C:99:LEU:CD2	2.02	0.63
2:C:290:LEU:HD12	2:C:297:PHE:CZ	2.34	0.63
1:B:194:PRO:HG3	1:B:205:HIS:NE2	2.13	0.63
1:B:233:HIS:HE1	1:B:275:GLU:OE1	1.79	0.63
1:E:83:LEU:HD12	1:E:138:GLY:HA3	1.81	0.63
2:F:411:ASN:HA	2:F:414:ASN:HB3	1.80	0.63
2:C:304:TRP:O	2:C:308:ASN:ND2	2.30	0.63
1:E:71:TYR:CD1	1:E:80:PHE:CD2	2.86	0.63
2:F:328:ALA:HB3	2:F:331:GLU:CG	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:369:LEU:HA	2:F:415:LEU:HD12	1.81	0.63
1:A:123:PRO:HG3	1:A:309:GLN:HG2	1.80	0.63
1:A:182:TYR:HB3	1:A:185:VAL:HG12	1.81	0.63
1:A:366:LYS:HG3	1:A:396:HIS:HB3	1.71	0.63
1:A:386:LEU:HD23	1:A:419:VAL:CG2	2.28	0.63
1:A:181:LEU:HD13	1:A:181:LEU:C	2.19	0.62
1:A:507:TYR:HD2	1:A:576:VAL:CG2	2.12	0.62
1:B:297:LEU:HB3	1:B:344:LEU:HD11	1.76	0.62
1:B:364:TRP:HA	1:B:364:TRP:CE3	2.33	0.62
1:B:387:PHE:CD2	1:B:397:LEU:HD22	2.34	0.62
1:B:546:ASP:CB	1:B:549:GLN:HG3	2.28	0.62
1:A:469:ILE:HD13	2:C:488:TRP:CD2	2.34	0.62
1:B:252:LYS:HD2	1:B:360:ASN:HB2	1.80	0.62
1:B:594:ILE:HG22	1:B:596:TRP:H	1.64	0.62
1:E:301:LEU:CD1	1:E:301:LEU:H	2.08	0.62
1:E:562:GLN:CA	1:E:565:ASP:HB2	2.29	0.62
2:F:126:VAL:C	2:F:129:ARG:HG2	2.19	0.62
2:C:119:ILE:CG1	2:C:121:LEU:H	2.12	0.62
2:D:341:ILE:HD13	2:D:374:SER:CB	2.29	0.62
1:B:387:PHE:HE2	1:B:397:LEU:HD11	1.64	0.62
1:E:471:TYR:CZ	1:E:523:PHE:CE1	2.88	0.62
1:E:491:ASN:OD1	2:F:36:ARG:CD	2.47	0.62
2:F:312:GLN:CD	2:F:323:LYS:CE	2.59	0.62
1:A:108:ASN:HD22	1:A:108:ASN:C	2.01	0.62
2:D:69:ASP:HB3	2:D:84:ILE:HD11	1.82	0.62
2:D:184:ARG:CB	1:B:592:ARG:HD3	2.29	0.62
2:D:310:ARG:CZ	2:D:495:LYS:HE3	2.30	0.62
1:B:120:PHE:HA	1:B:307:LEU:O	1.99	0.62
1:E:100:VAL:HG12	1:E:101:LYS:HE2	1.81	0.62
1:E:169:ASN:OD1	1:E:203:THR:CB	2.46	0.62
1:E:522:THR:OG1	1:E:550:GLN:NE2	2.31	0.62
1:E:577:ARG:NE	1:E:578:ASN:O	2.29	0.62
1:A:206:LEU:HD21	1:A:208:HIS:CE1	2.34	0.62
1:A:342:ASP:OD1	1:A:375:HIS:NE2	2.31	0.62
2:C:96:VAL:HB	2:C:128:LEU:HD11	1.80	0.62
1:B:96:ARG:NE	1:B:171:ASN:OD1	2.32	0.62
1:B:128:ILE:HG12	1:B:213:ILE:CD1	2.29	0.62
1:B:333:GLU:OE2	1:B:336:SER:N	2.22	0.62
1:E:106:TYR:HH	1:E:122:HIS:CD2	2.14	0.62
1:A:617:TRP:O	2:D:136:ARG:HD3	1.99	0.62
1:E:71:TYR:CE2	1:E:73:GLY:HA3	2.35	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:507:TYR:CD1	1:E:536:PHE:HA	2.33	0.62
2:F:128:LEU:HD12	2:F:128:LEU:C	2.20	0.62
2:C:129:ARG:NH1	2:C:129:ARG:HG2	2.15	0.62
2:D:278:PHE:HE1	2:D:279:PHE:CE2	2.16	0.62
1:B:359:LEU:HD11	1:B:361:LEU:HG	1.82	0.62
1:E:106:TYR:O	1:E:109:VAL:HG22	1.99	0.62
1:A:69:ILE:HB	1:A:80:PHE:O	2.00	0.62
1:A:365:ILE:HB	1:A:397:LEU:HD22	1.82	0.62
2:C:209:PHE:CE2	2:C:254:ILE:CG2	2.77	0.62
2:C:234:LEU:C	2:C:235:VAL:HG23	2.20	0.62
2:D:492:GLN:HB2	2:D:493:ASN:ND2	2.15	0.62
1:B:91:LEU:CD1	1:B:204:TYR:HB2	2.28	0.62
1:B:121:TRP:N	1:B:307:LEU:O	2.30	0.62
1:E:118:LEU:HB2	1:E:305:ILE:HG22	1.81	0.62
1:E:245:ILE:HD12	1:E:373:LEU:HD22	1.81	0.62
1:E:471:TYR:OH	1:E:523:PHE:HE1	1.81	0.62
2:F:129:ARG:NH2	2:F:129:ARG:HB3	2.15	0.62
2:F:148:ALA:O	2:F:152:LEU:HB2	2.00	0.62
1:A:366:LYS:HD2	1:A:396:HIS:HB3	1.82	0.62
1:B:86:LYS:CA	1:B:133:PHE:HB3	2.24	0.62
1:A:472:GLY:HA2	1:A:550:GLN:HE21	1.65	0.62
2:C:98:GLY:O	2:C:102:PRO:HD3	2.00	0.62
2:D:86:LEU:CD1	2:D:138:LEU:HD22	2.29	0.62
2:D:333:GLN:HG2	2:D:338:ASP:OD2	2.00	0.62
1:E:280:LEU:HG	1:E:297:LEU:HD12	1.81	0.62
1:E:471:TYR:HH	1:E:523:PHE:HD1	1.45	0.62
2:F:151:ALA:C	2:F:155:LEU:CD1	2.65	0.62
2:F:158:HIS:O	2:F:162:ASP:OD2	2.18	0.62
1:A:395:ARG:HH21	1:A:395:ARG:CG	2.13	0.61
2:C:59:THR:HG21	2:C:160:TRP:HE1	1.63	0.61
2:C:191:TYR:OH	2:C:264:LEU:O	2.18	0.61
1:B:80:PHE:CE1	1:B:165:LEU:CA	2.82	0.61
1:B:240:THR:OG1	1:B:242:ILE:HD11	1.99	0.61
1:B:260:LEU:O	1:B:264:THR:OG1	2.05	0.61
1:E:106:TYR:OH	1:E:122:HIS:CD2	2.53	0.61
1:E:287:PRO:O	1:E:443:LYS:NZ	2.33	0.61
1:E:603:PRO:O	1:E:604:PHE:HB2	2.00	0.61
1:A:471:TYR:CE1	1:A:545:ILE:HG23	2.35	0.61
2:C:316:SER:OG	2:C:317:ASN:OD1	2.18	0.61
2:D:146:TRP:CE3	2:D:146:TRP:C	2.73	0.61
1:E:387:PHE:CE1	1:E:401:THR:HG21	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:387:PHE:HE1	1:E:401:THR:CG2	2.13	0.61
1:A:543:HIS:HE1	2:C:502:LEU:C	2.03	0.61
2:D:105:GLN:HG2	1:B:615:HIS:HD2	1.65	0.61
2:D:494:TRP:HH2	2:D:497:LYS:HB2	1.66	0.61
2:D:501:VAL:O	2:D:501:VAL:HG23	2.00	0.61
1:B:449:HIS:CB	1:B:457:ASP:O	2.39	0.61
1:B:461:LEU:HD12	1:B:461:LEU:H	1.65	0.61
1:E:376:ILE:O	1:E:380:TYR:N	2.28	0.61
1:E:469:ILE:HD11	2:F:488:TRP:CH2	2.34	0.61
2:D:430:ILE:H	2:D:430:ILE:CD1	1.97	0.61
1:B:369:GLY:C	1:B:372:ILE:HG22	2.20	0.61
1:B:408:THR:CB	1:B:414:TYR:C	2.69	0.61
1:E:272:THR:HG22	3:E:707:HOH:O	1.99	0.61
1:E:364:TRP:CG	1:E:369:GLY:CA	2.83	0.61
1:E:507:TYR:HD1	1:E:536:PHE:HA	1.65	0.61
1:A:282:LEU:HD12	1:A:359:LEU:HD11	1.83	0.61
1:A:481:ILE:HG22	1:A:575:ILE:O	2.01	0.61
2:C:202:TRP:CE2	2:C:286:LEU:HD12	2.35	0.61
2:D:336:LEU:CD1	2:D:340:ILE:HG13	2.31	0.61
1:B:79:MET:O	1:B:79:MET:HE3	1.99	0.61
1:B:247:GLY:H	1:B:365:ILE:HG21	1.65	0.61
1:B:529:CYS:C	1:B:530:THR:OG1	2.38	0.61
1:A:185:VAL:HG22	1:A:185:VAL:O	2.00	0.61
1:A:333:GLU:OE2	1:A:333:GLU:HA	2.00	0.61
1:A:589:PRO:CD	1:A:596:TRP:CZ3	2.75	0.61
2:D:323:LYS:HG2	2:D:427:TYR:CE2	2.36	0.61
1:B:243:MET:CE	1:B:380:TYR:HD2	2.13	0.61
1:B:347:HIS:HD2	1:B:351:GLN:HG2	1.66	0.61
1:B:366:LYS:CB	1:B:395:ARG:HH11	2.10	0.61
1:E:230:TYR:CG	1:E:262:LYS:NZ	2.68	0.61
1:E:549:GLN:HB2	1:E:551:ILE:CG2	2.30	0.61
1:A:603:PRO:HB2	1:A:604:PHE:HD2	1.66	0.61
2:C:278:PHE:HZ	2:C:287:LEU:CD1	2.07	0.61
2:D:485:VAL:HG21	1:B:470:SER:CB	2.29	0.61
1:B:321:LEU:CD2	1:B:344:LEU:HD12	2.17	0.61
1:E:110:HIS:HD2	1:E:111:TYR:N	1.98	0.61
1:E:185:VAL:O	1:E:185:VAL:HG22	2.00	0.61
1:E:507:TYR:HE1	1:E:536:PHE:HB2	1.65	0.61
1:E:610:ARG:CD	2:F:167:ASP:CG	2.69	0.61
2:F:8:PRO:HD3	2:F:51:TYR:O	2.00	0.61
2:F:275:LEU:CD1	2:F:275:LEU:H	1.94	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASP:OD2	1:A:78:THR:HG22	2.01	0.61
1:B:527:GLN:O	1:B:528:SER:OG	2.15	0.61
1:E:71:TYR:CE1	1:E:80:PHE:HE2	2.13	0.61
1:E:365:ILE:HD12	1:E:365:ILE:H	1.66	0.61
1:E:480:GLY:H	1:E:524:PRO:CB	2.14	0.61
1:E:531:SER:O	1:E:534:LYS:HE2	2.00	0.61
1:A:110:HIS:O	1:A:111:TYR:HD1	1.83	0.61
2:C:280:ASN:O	2:C:281:ASN:OD1	2.19	0.61
2:D:188:LEU:HD11	2:D:192:MET:HG3	1.83	0.61
2:D:494:TRP:CH2	2:D:497:LYS:HB2	2.35	0.61
2:D:499:PHE:HD1	1:B:543:HIS:HA	1.66	0.61
1:E:482:GLN:CB	1:E:576:VAL:HG22	2.25	0.61
1:A:374:ASN:CG	1:A:404:GLN:CB	2.69	0.61
1:A:522:THR:OG1	1:A:550:GLN:OE1	2.19	0.61
2:C:80:ASP:OD1	2:D:64:CYS:SG	2.56	0.61
2:D:485:VAL:HG13	2:D:485:VAL:O	2.01	0.61
1:B:90:HIS:CE1	1:B:128:ILE:CG1	2.71	0.61
1:A:97:LEU:O	1:A:118:LEU:HD23	2.01	0.60
2:D:71:LYS:HB3	2:D:71:LYS:HZ3	1.66	0.60
1:B:566:LYS:O	1:B:567:GLN:HG2	2.00	0.60
2:F:335:ARG:HH11	2:F:335:ARG:CG	2.13	0.60
1:A:79:MET:SD	1:A:81:VAL:HG23	2.41	0.60
1:A:177:GLU:HG2	2:C:267:LEU:CD2	2.30	0.60
1:A:589:PRO:CG	1:A:596:TRP:CZ3	2.83	0.60
2:C:64:CYS:CB	2:D:82:ILE:HG21	2.31	0.60
2:C:159:TYR:CE2	2:C:160:TRP:CZ3	2.89	0.60
2:C:310:ARG:HH11	2:C:310:ARG:CG	2.14	0.60
1:B:123:PRO:HB3	1:B:311:LEU:HD21	1.82	0.60
1:B:562:GLN:O	1:B:566:LYS:N	2.33	0.60
1:A:107:ASN:HD22	1:A:258:LEU:CD2	2.14	0.60
2:C:141:LEU:HD23	2:C:145:ARG:NH2	2.16	0.60
2:C:345:ASN:HB3	2:C:348:ASN:HB2	1.83	0.60
2:D:188:LEU:HD11	2:D:192:MET:CG	2.31	0.60
1:B:90:HIS:CD2	1:B:207:LEU:O	2.54	0.60
1:E:185:VAL:HG23	1:E:188:LEU:HD22	1.82	0.60
1:E:187:TYR:CD1	1:E:192:LYS:CB	2.81	0.60
2:F:408:LEU:O	2:F:412:ILE:HG13	2.02	0.60
2:F:501:VAL:C	2:F:502:LEU:HG	2.22	0.60
1:A:284:PRO:O	1:A:287:PRO:HD3	2.00	0.60
2:C:110:ILE:HG23	2:C:114:THR:HB	1.77	0.60
2:D:212:TYR:CZ	2:D:250:SER:OG	2.53	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ARG:HB2	1:B:115:ARG:HH21	1.61	0.60
1:B:473:LYS:HG2	1:B:474:GLY:N	2.15	0.60
2:F:152:LEU:C	2:F:155:LEU:HD13	2.11	0.60
2:F:154:TRP:CE3	2:F:155:LEU:HA	2.36	0.60
1:A:241:ARG:HB3	1:A:380:TYR:CZ	2.37	0.60
1:A:467:LEU:HD21	1:A:556:VAL:CG2	2.31	0.60
1:A:588:LEU:HD11	2:C:6:ILE:HD13	1.82	0.60
2:C:125:PHE:HB3	2:C:128:LEU:HD21	1.82	0.60
2:C:394:ARG:HH11	2:C:394:ARG:CG	2.15	0.60
1:B:80:PHE:HD1	1:B:166:ARG:CB	2.15	0.60
1:B:103:GLY:N	1:B:134:SER:O	2.23	0.60
1:B:347:HIS:NE2	1:B:351:GLN:CD	2.55	0.60
1:E:262:LYS:HD2	1:E:262:LYS:O	2.01	0.60
2:F:275:LEU:HD12	2:F:275:LEU:N	2.04	0.60
1:A:172:HIS:HA	1:A:454:PHE:O	1.99	0.60
2:C:100:LEU:HD12	2:C:100:LEU:O	2.02	0.60
2:D:101:ASP:O	2:D:103:THR:OG1	2.17	0.60
2:D:105:GLN:OE1	2:D:105:GLN:N	2.34	0.60
2:D:124:TRP:HA	2:D:127:ASP:OD1	2.02	0.60
1:B:99:VAL:CB	1:B:166:ARG:HH21	2.13	0.60
1:E:525:ILE:HD13	1:E:525:ILE:N	2.15	0.60
2:F:50:GLN:HB2	2:F:51:TYR:CD2	2.37	0.60
2:F:312:GLN:CD	2:F:323:LYS:HD3	2.21	0.60
2:D:199:LEU:HD11	2:D:281:ASN:CB	2.30	0.60
2:D:209:PHE:CE2	2:D:254:ILE:HG23	2.35	0.60
1:B:509:TYR:O	1:B:510:SER:OG	2.10	0.60
1:E:91:LEU:O	1:E:122:HIS:ND1	2.28	0.60
1:E:359:LEU:HD12	1:E:360:ASN:C	2.22	0.60
1:E:522:THR:HG23	1:E:522:THR:O	2.01	0.60
2:F:99:LEU:C	2:F:102:PRO:HD2	2.22	0.60
2:F:278:PHE:CE2	2:F:282:TYR:HB2	2.37	0.60
1:A:121:TRP:N	1:A:307:LEU:O	2.25	0.60
1:A:339:ASN:O	1:A:343:LYS:HG3	2.01	0.60
1:A:366:LYS:CD	1:A:396:HIS:HB3	2.31	0.60
2:D:38:VAL:HG11	2:D:64:CYS:HB2	1.84	0.60
2:D:489:SER:O	1:B:467:LEU:HA	2.00	0.60
1:B:167:VAL:O	1:B:204:TYR:CE1	2.54	0.60
2:F:126:VAL:CG1	2:F:129:ARG:HD3	2.30	0.60
2:F:312:GLN:CD	2:F:323:LYS:NZ	2.54	0.60
1:A:75:GLU:O	1:A:76:ASP:OD2	2.18	0.60
1:A:96:ARG:CB	1:A:168:PHE:HE1	2.15	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:345:ASN:OD1	2:C:347:LYS:N	2.34	0.60
2:C:349:PHE:HZ	2:C:353:TRP:HZ3	1.50	0.60
2:D:99:LEU:C	2:D:102:PRO:HD2	2.21	0.60
1:B:590:SER:HB2	1:B:593:THR:OG1	2.02	0.60
1:E:70:THR:HG22	1:E:70:THR:O	2.02	0.60
1:A:121:TRP:HB3	1:A:309:GLN:O	2.02	0.60
1:A:174:GLY:O	1:A:177:GLU:OE1	2.20	0.60
1:A:509:TYR:CZ	1:A:512:GLU:CB	2.85	0.60
2:D:36:ARG:NH1	1:B:494:ASP:OD1	2.34	0.60
2:D:69:ASP:OD1	2:D:88:TYR:OH	2.20	0.60
1:B:80:PHE:HZ	1:B:165:LEU:CA	2.06	0.60
1:B:174:GLY:HA3	1:B:456:TYR:O	2.02	0.60
1:B:175:LEU:CD1	1:B:456:TYR:CD2	2.83	0.60
1:E:166:ARG:HH11	1:E:166:ARG:CG	2.15	0.60
2:C:501:VAL:O	2:C:501:VAL:HG12	2.02	0.59
2:D:322:LEU:HD23	2:D:323:LYS:N	2.17	0.59
1:B:121:TRP:HB3	1:B:309:GLN:O	2.02	0.59
1:B:389:GLU:C	1:B:390:THR:HG22	2.22	0.59
1:B:397:LEU:HD12	1:B:400:LEU:CG	2.32	0.59
1:E:118:LEU:HB2	1:E:305:ILE:CG2	2.32	0.59
1:E:212:ARG:HH21	1:E:212:ARG:CG	2.14	0.59
2:F:349:PHE:CE1	2:F:375:MET:HE2	2.37	0.59
1:A:190:LYS:HD3	1:A:205:HIS:HB2	1.84	0.59
1:A:206:LEU:HD22	1:A:207:LEU:H	1.67	0.59
1:B:445:LEU:HD11	1:B:586:ASP:HB2	1.84	0.59
1:B:559:CYS:SG	1:B:560:HIS:N	2.74	0.59
1:A:246:GLY:C	1:A:363:GLY:HA3	2.18	0.59
1:A:465:ALA:HA	2:C:494:TRP:CZ3	2.37	0.59
1:B:175:LEU:HA	1:B:458:PHE:HZ	1.67	0.59
1:B:207:LEU:HA	1:B:211:ASP:OD1	2.01	0.59
1:B:283:ASP:OD1	1:B:285:GLY:N	2.34	0.59
1:E:216:LEU:HG	1:E:217:SER:O	2.02	0.59
1:E:268:ARG:HH11	1:E:268:ARG:CG	2.14	0.59
1:E:369:GLY:C	1:E:372:ILE:HG22	2.22	0.59
1:E:493:GLN:NE2	2:F:36:ARG:HH22	1.96	0.59
2:F:102:PRO:O	2:F:104:GLN:HG2	2.02	0.59
2:F:275:LEU:O	2:F:279:PHE:HD2	1.85	0.59
1:A:509:TYR:CE2	1:A:512:GLU:CB	2.86	0.59
2:C:314:ASP:HB3	2:C:495:LYS:NZ	2.17	0.59
2:D:54:HIS:NE2	2:D:98:GLY:HA3	2.17	0.59
2:D:84:ILE:HD12	2:D:88:TYR:CD2	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:GLN:OE1	2:D:427:TYR:CE2	2.55	0.59
2:D:492:GLN:HB2	2:D:493:ASN:HD22	1.67	0.59
1:B:104:ILE:HD11	1:B:166:ARG:HH22	1.67	0.59
1:B:169:ASN:OD1	1:B:203:THR:N	2.33	0.59
1:B:390:THR:O	1:B:394:LYS:HB3	2.02	0.59
1:E:233:HIS:HB2	1:E:263:PHE:CE2	2.37	0.59
1:A:234:LYS:CE	1:A:270:SER:OG	2.50	0.59
1:A:256:LEU:O	1:A:260:LEU:N	2.34	0.59
1:A:395:ARG:HG3	1:A:396:HIS:H	1.66	0.59
2:C:82:ILE:HG21	2:D:64:CYS:SG	2.43	0.59
1:B:231:LEU:O	1:B:235:ASN:ND2	2.35	0.59
1:B:364:TRP:CD1	1:B:369:GLY:CA	2.86	0.59
1:E:71:TYR:CE2	1:E:73:GLY:CA	2.85	0.59
1:E:584:PHE:CZ	1:E:588:LEU:CD1	2.86	0.59
2:F:337:LEU:HD21	2:F:370:TYR:CZ	2.37	0.59
1:A:67:ASP:N	1:A:67:ASP:OD2	2.35	0.59
1:A:185:VAL:CG2	1:A:188:LEU:HD12	2.32	0.59
2:C:129:ARG:CG	2:C:129:ARG:HH11	2.15	0.59
2:C:224:ILE:CG2	2:C:229:PHE:HZ	2.16	0.59
2:D:133:THR:CB	2:D:134:HIS:CD2	2.85	0.59
1:B:448:PHE:HB3	1:B:461:LEU:HD21	1.85	0.59
1:E:100:VAL:HG12	1:E:101:LYS:CG	2.26	0.59
2:F:66:VAL:HA	2:F:88:TYR:CE1	2.37	0.59
1:A:69:ILE:HG22	1:A:69:ILE:O	2.02	0.59
2:D:359:LEU:HA	2:D:362:GLU:HB3	1.84	0.59
2:D:426:LEU:N	2:D:426:LEU:HD23	2.17	0.59
1:B:177:GLU:HG2	1:B:458:PHE:HD2	0.68	0.59
1:B:288:GLU:C	1:B:289:TYR:HD2	2.06	0.59
1:B:461:LEU:O	1:B:555:TYR:CE2	2.55	0.59
1:E:98:GLN:CG	1:E:117:ILE:CG2	2.74	0.59
1:E:408:THR:CB	1:E:414:TYR:CB	2.81	0.59
1:E:538:THR:HG22	1:E:539:LEU:N	2.18	0.59
2:F:262:GLN:O	2:F:266:LYS:HG3	2.03	0.59
1:A:183:ARG:HH21	1:A:183:ARG:CG	2.14	0.59
2:D:336:LEU:O	2:D:340:ILE:HG13	2.01	0.59
1:B:478:ILE:HG23	1:B:575:ILE:HD11	1.85	0.59
1:E:365:ILE:HD12	1:E:366:LYS:H	1.67	0.59
2:F:329:TRP:O	2:F:333:GLN:N	2.31	0.59
1:A:183:ARG:NH2	1:A:183:ARG:HG2	2.16	0.59
1:A:353:PHE:HE1	1:A:355:GLY:CA	2.15	0.59
1:A:406:PHE:CD1	1:A:407:SER:N	2.68	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:353:TRP:HA	2:D:356:TRP:HD1	1.65	0.59
1:B:105:VAL:O	1:B:132:ASP:HB2	2.03	0.59
1:B:395:ARG:HD2	1:B:395:ARG:C	2.23	0.59
1:E:248:LYS:O	1:E:249:ASN:HB3	2.01	0.59
1:E:496:LYS:O	1:E:500:GLU:HG3	2.03	0.59
1:A:353:PHE:HE1	1:A:355:GLY:O	1.85	0.59
2:C:304:TRP:CE3	2:C:308:ASN:ND2	2.71	0.59
2:C:314:ASP:CB	2:C:495:LYS:NZ	2.66	0.59
2:D:23:TYR:HE2	2:D:156:TYR:CG	2.16	0.59
1:B:280:LEU:O	1:B:359:LEU:HB2	2.03	0.59
1:B:389:GLU:HB3	1:B:394:LYS:HA	1.85	0.59
1:A:90:HIS:HE2	1:A:213:ILE:CD1	2.17	0.58
2:D:122:PRO:CG	2:D:125:PHE:CE2	2.86	0.58
1:B:80:PHE:CD1	1:B:166:ARG:CB	2.85	0.58
1:E:310:HIS:CB	1:E:314:GLY:HA3	2.32	0.58
1:A:288:GLU:O	1:A:289:TYR:HB2	2.01	0.58
1:B:247:GLY:CA	1:B:365:ILE:CG2	2.75	0.58
1:B:359:LEU:HD12	1:B:360:ASN:CA	2.32	0.58
1:B:448:PHE:HB3	1:B:461:LEU:HD23	1.83	0.58
1:E:233:HIS:CG	1:E:263:PHE:CE2	2.91	0.58
1:A:489:ASP:OD1	2:D:79:GLN:O	2.21	0.58
2:C:23:TYR:CE2	2:C:156:TYR:CG	2.89	0.58
2:C:307:ARG:HH11	2:C:307:ARG:CG	2.15	0.58
2:D:113:HIS:CE1	2:D:126:VAL:CG1	2.86	0.58
1:B:243:MET:HE3	1:B:382:PRO:HB3	1.85	0.58
1:E:241:ARG:CA	1:E:383:THR:OG1	2.50	0.58
1:A:502:THR:CB	1:A:577:ARG:HH22	2.12	0.58
2:C:207:ASN:HA	2:C:210:LEU:CD1	2.33	0.58
2:C:336:LEU:HD12	2:C:336:LEU:C	2.22	0.58
2:D:184:ARG:HE	1:B:183:ARG:HH12	1.49	0.58
1:B:98:GLN:HB3	1:B:165:LEU:CD1	2.32	0.58
1:B:389:GLU:HB3	1:B:394:LYS:CB	2.33	0.58
1:B:499:LEU:O	1:B:502:THR:OG1	2.21	0.58
1:E:96:ARG:HD3	1:E:169:ASN:O	2.03	0.58
1:E:193:GLU:N	1:E:194:PRO:HD3	2.18	0.58
1:E:259:LEU:O	1:E:263:PHE:CD1	2.54	0.58
1:E:276:GLU:O	1:E:353:PHE:HZ	1.87	0.58
1:A:83:LEU:CD2	1:A:166:ARG:NH1	2.66	0.58
1:A:489:ASP:CG	2:D:79:GLN:O	2.41	0.58
1:A:562:GLN:CB	1:A:565:ASP:HB2	2.33	0.58
2:D:354:GLN:O	2:D:358:LYS:CG	2.50	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLY:O	1:B:134:SER:N	2.36	0.58
1:B:239:ASP:CB	1:B:355:GLY:C	2.71	0.58
1:B:275:GLU:HG3	1:B:275:GLU:O	2.04	0.58
1:E:549:GLN:CB	1:E:551:ILE:HG23	2.33	0.58
2:F:89:VAL:CG2	2:F:144:LEU:HD21	2.32	0.58
1:A:327:SER:OG	1:A:332:ASP:OD2	2.17	0.58
2:C:191:TYR:CE2	2:C:264:LEU:HD22	2.38	0.58
2:D:159:TYR:OH	1:B:614:GLU:HG2	2.04	0.58
2:D:499:PHE:HE2	1:B:587:PHE:HA	1.68	0.58
1:B:128:ILE:O	1:B:128:ILE:HD12	2.03	0.58
1:E:259:LEU:HG	1:E:263:PHE:HE1	1.68	0.58
1:E:365:ILE:HD13	1:E:366:LYS:H	1.67	0.58
1:E:461:LEU:HB2	1:E:586:ASP:OD2	2.03	0.58
1:A:83:LEU:CD2	1:A:166:ARG:CZ	2.82	0.58
1:A:98:GLN:HE21	1:A:115:ARG:C	2.05	0.58
1:A:543:HIS:HE1	2:C:502:LEU:CA	2.17	0.58
2:C:95:PHE:CZ	2:C:155:LEU:CD1	2.86	0.58
2:C:119:ILE:HG13	2:C:121:LEU:N	2.18	0.58
2:D:54:HIS:CD2	2:D:98:GLY:CA	2.84	0.58
1:B:243:MET:HE3	1:B:380:TYR:CD2	2.34	0.58
1:E:188:LEU:HD13	1:E:434:PHE:CZ	2.35	0.58
1:E:230:TYR:CB	1:E:262:LYS:NZ	2.66	0.58
2:F:55:VAL:HG11	2:F:159:TYR:CG	2.35	0.58
2:F:272:ASN:O	2:F:275:LEU:HD13	2.03	0.58
1:A:198:LEU:CD2	1:A:205:HIS:CD2	2.86	0.58
1:A:480:GLY:CA	1:A:524:PRO:HG2	2.33	0.58
1:A:517:VAL:CG2	1:A:524:PRO:HB2	2.32	0.58
2:C:97:ASN:HD22	2:C:129:ARG:HD3	1.67	0.58
2:C:103:THR:N	2:C:104:GLN:CA	2.64	0.58
2:C:136:ARG:CD	1:B:617:TRP:O	2.39	0.58
1:B:515:LEU:O	1:B:517:VAL:HG13	2.04	0.58
1:E:186:ASN:C	1:E:186:ASN:HD22	2.05	0.58
1:E:268:ARG:HG3	1:E:268:ARG:NH1	2.17	0.58
1:E:301:LEU:HD11	1:E:316:ASN:CA	2.34	0.58
1:E:614:GLU:CD	2:F:159:TYR:OH	2.41	0.58
2:F:66:VAL:O	2:F:69:ASP:OD1	2.21	0.58
2:F:115:LEU:O	2:F:115:LEU:HD23	2.03	0.58
2:F:372:CYS:O	2:F:412:ILE:CD1	2.50	0.58
2:C:72:GLU:OE1	2:C:72:GLU:HA	2.04	0.58
2:C:80:ASP:CG	2:D:64:CYS:HG	2.06	0.58
2:D:111:PRO:HG2	2:D:114:THR:OG1	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:LEU:CB	1:E:305:ILE:CB	2.77	0.58
1:E:609:ARG:HD2	2:F:2:ILE:HG12	1.85	0.58
1:A:221:TYR:CB	1:A:422:PRO:HG2	2.34	0.58
1:E:289:TYR:HA	1:E:317:PHE:CE2	2.38	0.58
2:F:66:VAL:HA	2:F:88:TYR:HH	1.67	0.58
1:B:79:MET:HB3	1:B:167:VAL:HG21	1.81	0.57
1:B:209:GLU:N	1:B:209:GLU:OE2	2.37	0.57
1:E:193:GLU:N	1:E:194:PRO:CD	2.67	0.57
1:E:467:LEU:HD12	2:F:488:TRP:HB3	1.85	0.57
2:F:133:THR:HB	2:F:134:HIS:ND1	2.20	0.57
2:F:278:PHE:HE2	2:F:282:TYR:HA	1.68	0.57
2:F:337:LEU:HD12	2:F:341:ILE:HD11	1.86	0.57
1:A:98:GLN:HG3	1:A:116:GLU:N	2.19	0.57
2:C:23:TYR:CE2	2:C:160:TRP:CD1	2.90	0.57
2:D:4:PRO:CA	1:B:607:PHE:CD1	2.81	0.57
2:D:69:ASP:HA	2:D:77:VAL:CG1	2.34	0.57
2:D:349:PHE:CE2	2:D:356:TRP:CG	2.90	0.57
1:B:231:LEU:O	1:B:235:ASN:OD1	2.22	0.57
1:E:71:TYR:HD1	1:E:80:PHE:CE2	2.19	0.57
2:F:18:LEU:HD21	2:F:22:PHE:HZ	1.58	0.57
2:F:152:LEU:O	2:F:155:LEU:HD12	2.01	0.57
1:A:96:ARG:CB	1:A:168:PHE:CE1	2.87	0.57
2:D:127:ASP:OD2	2:D:127:ASP:N	2.36	0.57
2:D:363:ASN:O	2:D:368:ILE:CD1	2.52	0.57
1:B:260:LEU:C	1:B:264:THR:HG1	2.05	0.57
1:E:451:ILE:HG22	1:E:452:THR:HG23	1.86	0.57
2:F:410:GLU:O	2:F:414:ASN:HB2	2.04	0.57
1:A:90:HIS:NE2	1:A:213:ILE:CD1	2.67	0.57
2:C:43:SER:O	2:C:46:LEU:N	2.38	0.57
2:C:314:ASP:OD2	2:C:495:LYS:HE3	2.04	0.57
2:C:387:ASN:HA	2:C:391:ASN:HD21	1.68	0.57
1:B:122:HIS:CE1	1:B:128:ILE:CB	2.59	0.57
1:E:97:LEU:H	1:E:97:LEU:HD23	1.70	0.57
2:F:298:ASP:CG	2:F:356:TRP:HZ2	2.07	0.57
1:A:96:ARG:HG3	1:A:168:PHE:CZ	2.36	0.57
1:A:196:PHE:CB	1:A:205:HIS:HE1	2.14	0.57
1:A:486:GLU:O	1:A:487:PHE:CB	2.52	0.57
1:A:488:GLN:OE1	1:A:488:GLN:HA	2.05	0.57
1:B:538:THR:HG22	1:B:539:LEU:N	2.19	0.57
1:E:301:LEU:HD12	1:E:301:LEU:N	2.11	0.57
1:E:510:SER:CB	1:E:533:SER:O	2.41	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:617:TRP:HD1	1:E:617:TRP:O	1.88	0.57
2:F:75:LEU:HG	2:F:76:GLY:N	2.19	0.57
1:A:365:ILE:C	1:A:397:LEU:HD22	2.25	0.57
2:C:36:ARG:HA	2:C:39:GLN:NE2	2.20	0.57
1:B:80:PHE:HD1	1:B:166:ARG:HB2	1.69	0.57
1:B:105:VAL:CG1	1:B:108:ASN:HA	2.35	0.57
1:B:232:SER:O	1:B:236:ALA:HB2	2.03	0.57
1:B:369:GLY:O	1:B:373:LEU:HG	2.05	0.57
1:E:305:ILE:CG2	1:E:307:LEU:HD11	2.34	0.57
1:E:561:THR:CA	1:E:564:LEU:HD12	2.34	0.57
1:E:597:ASP:OD1	1:E:597:ASP:N	2.34	0.57
1:A:267:ILE:CD1	1:A:277:LEU:CD2	2.82	0.57
1:A:492:PRO:C	1:A:495:ILE:HG13	2.22	0.57
2:C:309:TYR:CE1	2:C:313:GLN:NE2	2.73	0.57
2:D:69:ASP:HA	2:D:77:VAL:HG21	0.85	0.57
2:D:498:PRO:CG	1:B:602:ILE:HG23	2.34	0.57
1:B:387:PHE:CE1	1:B:401:THR:HG21	2.38	0.57
1:B:504:ILE:HD12	1:B:575:ILE:HG22	1.72	0.57
1:B:590:SER:O	1:B:594:ILE:O	2.22	0.57
1:E:91:LEU:HB3	1:E:95:PHE:CE1	2.39	0.57
1:E:98:GLN:CB	1:E:117:ILE:HG22	2.35	0.57
2:F:51:TYR:CD2	2:F:51:TYR:N	2.73	0.57
2:F:58:SER:OG	2:F:95:PHE:HB2	2.04	0.57
2:F:201:LYS:O	2:F:205:LEU:HG	2.05	0.57
2:F:349:PHE:CE1	2:F:375:MET:CE	2.87	0.57
2:F:349:PHE:CD1	2:F:375:MET:CE	2.87	0.57
2:F:389:TRP:CD1	2:F:390:ARG:CD	2.88	0.57
1:A:399:GLU:OE2	1:A:399:GLU:N	2.38	0.57
2:D:96:VAL:CG1	2:D:100:LEU:CB	2.83	0.57
2:D:494:TRP:CH2	2:D:497:LYS:CG	2.88	0.57
1:B:289:TYR:CD2	1:B:289:TYR:N	2.73	0.57
1:A:278:VAL:O	1:A:278:VAL:HG23	2.04	0.57
2:C:108:PHE:CD1	2:C:108:PHE:N	2.73	0.57
2:C:312:GLN:OE1	2:C:323:LYS:CE	2.52	0.57
2:D:199:LEU:HD11	2:D:281:ASN:HB2	1.87	0.57
1:B:469:ILE:O	1:B:552:MET:N	2.38	0.57
1:E:392:ASN:N	1:E:393:SER:HA	2.20	0.57
1:E:509:TYR:CD1	1:E:510:SER:N	2.73	0.57
1:A:239:ASP:CB	1:A:355:GLY:H	2.17	0.57
1:A:374:ASN:ND2	1:A:400:LEU:O	2.38	0.57
2:D:351:ASN:OD1	2:D:351:ASN:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ASP:O	1:B:169:ASN:HB2	2.05	0.57
1:E:106:TYR:HD2	1:E:120:PHE:HE2	1.52	0.57
1:E:417:GLU:OE1	1:E:417:GLU:HA	2.04	0.57
2:F:272:ASN:O	2:F:276:GLU:HG3	2.05	0.57
1:A:194:PRO:O	1:A:211:ASP:OD1	2.22	0.56
1:A:359:LEU:HD12	1:A:360:ASN:CA	2.31	0.56
1:A:467:LEU:CD2	1:A:556:VAL:CG2	2.81	0.56
2:C:53:PRO:CD	2:C:56:VAL:HG21	2.35	0.56
2:C:125:PHE:O	2:C:128:LEU:CG	2.49	0.56
1:B:347:HIS:CD2	1:B:351:GLN:CG	2.88	0.56
1:B:348:LEU:CD1	1:B:353:PHE:CB	2.75	0.56
1:B:366:LYS:CD	1:B:395:ARG:NH1	2.68	0.56
1:A:486:GLU:O	1:A:487:PHE:HB2	2.04	0.56
2:C:125:PHE:CA	2:C:128:LEU:CD2	2.81	0.56
2:D:108:PHE:CD2	2:D:108:PHE:N	2.73	0.56
2:D:122:PRO:HD3	2:D:154:TRP:NE1	2.20	0.56
2:D:125:PHE:HA	2:D:128:LEU:HB2	1.87	0.56
2:D:349:PHE:CE2	2:D:356:TRP:NE1	2.72	0.56
1:B:80:PHE:CE1	1:B:166:ARG:HB2	2.40	0.56
1:B:92:SER:OG	1:B:189:TRP:O	2.23	0.56
1:B:405:SER:O	1:B:407:SER:O	2.22	0.56
1:B:485:MET:SD	1:B:485:MET:N	2.78	0.56
1:E:133:PHE:CD2	1:E:134:SER:N	2.73	0.56
1:E:245:ILE:HD13	1:E:373:LEU:CD1	2.19	0.56
1:E:333:GLU:OE1	1:E:336:SER:N	2.28	0.56
1:E:531:SER:O	1:E:534:LYS:HG3	2.06	0.56
2:F:369:LEU:HD12	2:F:415:LEU:HB3	1.86	0.56
1:A:128:ILE:O	1:A:215:SER:CB	2.53	0.56
1:A:236:ALA:O	1:A:237:ALA:HB3	2.05	0.56
2:C:97:ASN:HD21	2:C:129:ARG:HD2	1.70	0.56
2:C:145:ARG:NH2	3:C:602:HOH:O	2.39	0.56
2:D:154:TRP:HE3	2:D:155:LEU:HD23	1.60	0.56
1:B:313:GLN:HB3	1:B:456:TYR:OH	2.04	0.56
1:B:588:LEU:O	1:B:588:LEU:HD13	2.05	0.56
1:E:106:TYR:CE2	1:E:120:PHE:HD2	2.18	0.56
1:E:118:LEU:CB	1:E:305:ILE:CG2	2.84	0.56
1:E:359:LEU:HD12	1:E:360:ASN:CA	2.35	0.56
1:E:451:ILE:C	1:E:452:THR:HG23	2.25	0.56
2:F:139:PRO:CG	2:F:144:LEU:HD11	2.18	0.56
2:F:280:ASN:O	2:F:325:LYS:HE3	2.06	0.56
2:D:69:ASP:HB3	2:D:84:ILE:CD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:ILE:O	2:D:88:TYR:HD2	1.89	0.56
1:B:127:SER:HB3	1:B:214:GLN:HG3	1.87	0.56
1:E:100:VAL:CG1	1:E:101:LYS:HE2	2.35	0.56
1:E:353:PHE:CE1	1:E:355:GLY:HA3	2.41	0.56
1:E:493:GLN:HE22	2:F:36:ARG:NH2	2.02	0.56
1:E:546:ASP:CG	1:E:549:GLN:HE22	2.09	0.56
1:A:71:TYR:CD2	1:A:72:GLU:N	2.73	0.56
1:A:96:ARG:O	1:A:168:PHE:HD1	1.80	0.56
1:A:174:GLY:C	1:A:177:GLU:OE1	2.44	0.56
1:A:187:TYR:CZ	1:A:192:LYS:CB	2.88	0.56
1:A:223:SER:O	1:A:227:GLU:HB3	2.06	0.56
1:B:105:VAL:O	1:B:105:VAL:HG12	2.05	0.56
2:D:122:PRO:HG2	2:D:125:PHE:HE2	1.69	0.56
2:D:188:LEU:CD1	2:D:192:MET:HG2	2.36	0.56
1:B:388:LEU:CA	1:B:421:VAL:O	2.48	0.56
1:B:573:TRP:CD1	1:B:573:TRP:N	2.73	0.56
1:E:106:TYR:CE2	1:E:120:PHE:CE2	2.93	0.56
1:E:610:ARG:CD	2:F:167:ASP:CB	2.78	0.56
1:A:213:ILE:HD12	1:A:213:ILE:C	2.26	0.56
1:A:365:ILE:HD13	1:A:366:LYS:HD3	1.88	0.56
2:D:122:PRO:HD2	2:D:125:PHE:CD2	2.41	0.56
2:D:194:SER:HA	2:D:197:LYS:HB2	1.85	0.56
1:B:124:LEU:HB2	1:B:188:LEU:O	2.05	0.56
2:F:110:ILE:HG21	2:F:114:THR:HG22	1.87	0.56
1:A:218:VAL:O	1:A:218:VAL:HG13	2.05	0.56
1:A:365:ILE:CD1	1:A:366:LYS:H	2.14	0.56
1:A:518:LYS:O	1:A:525:ILE:N	2.33	0.56
2:C:133:THR:HG22	2:D:97:ASN:HD22	1.68	0.56
2:D:336:LEU:CD1	2:D:340:ILE:HD11	2.29	0.56
1:B:221:TYR:CD2	1:B:221:TYR:N	2.73	0.56
1:B:391:ALA:C	1:B:393:SER:HA	2.26	0.56
1:B:569:GLU:HG3	1:B:570:ASP:N	2.20	0.56
1:E:360:ASN:HD22	1:E:360:ASN:H	1.53	0.56
1:E:561:THR:CG2	1:E:562:GLN:HA	2.36	0.56
2:F:21:TRP:HE3	2:F:37:ALA:HA	1.71	0.56
2:F:98:GLY:O	2:F:102:PRO:HG3	2.04	0.56
2:F:152:LEU:N	2:F:155:LEU:HD11	2.20	0.56
1:A:96:ARG:HD3	1:A:170:SER:HA	1.87	0.56
1:A:248:LYS:O	1:A:249:ASN:HB3	2.05	0.56
1:A:284:PRO:C	1:A:287:PRO:HD3	2.27	0.56
2:C:54:HIS:HD2	2:C:98:GLY:C	2.07	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:388:SER:N	2:C:391:ASN:HD21	2.03	0.56
2:D:82:ILE:HG22	2:D:83:PRO:CD	2.32	0.56
1:B:331:GLN:HG3	1:B:364:TRP:CZ2	2.41	0.56
1:B:389:GLU:HA	1:B:389:GLU:OE2	2.04	0.56
1:E:83:LEU:HD22	1:E:166:ARG:HE	1.71	0.56
1:E:111:TYR:N	1:E:111:TYR:CD1	2.73	0.56
1:E:610:ARG:HD2	2:F:167:ASP:CG	2.26	0.56
1:A:81:VAL:HG12	1:A:82:GLY:N	2.21	0.56
1:A:282:LEU:CD1	1:A:359:LEU:HD21	2.35	0.56
1:A:617:TRP:CD1	1:A:618:LYS:N	2.73	0.56
2:C:53:PRO:CB	2:C:56:VAL:HG23	2.35	0.56
2:D:46:LEU:HD22	1:B:577:ARG:CD	2.35	0.56
2:D:133:THR:C	2:D:134:HIS:HD2	2.09	0.56
2:D:134:HIS:CD2	2:D:134:HIS:N	2.73	0.56
1:E:74:ASP:OD2	1:E:75:GLU:N	2.34	0.56
1:E:123:PRO:HB3	1:E:311:LEU:CD2	2.35	0.56
2:F:122:PRO:HB2	2:F:124:TRP:HD1	1.69	0.56
1:A:471:TYR:CE1	1:A:545:ILE:CG2	2.88	0.55
1:A:562:GLN:HB2	1:A:565:ASP:HB2	1.89	0.55
2:C:224:ILE:CG2	2:C:229:PHE:CZ	2.89	0.55
2:D:4:PRO:CB	1:B:607:PHE:CZ	2.51	0.55
2:D:5:ARG:CZ	1:B:610:ARG:CG	2.80	0.55
2:D:96:VAL:HG13	2:D:100:LEU:CB	2.36	0.55
2:D:102:PRO:O	2:D:104:GLN:N	2.34	0.55
1:B:211:ASP:HA	1:B:212:ARG:NH2	2.21	0.55
1:E:195:TYR:HD1	1:E:210:SER:HG	1.53	0.55
1:E:245:ILE:HD11	1:E:373:LEU:HD21	1.87	0.55
1:E:384:HIS:CD2	1:E:384:HIS:N	2.73	0.55
1:E:389:GLU:HB3	1:E:394:LYS:HB3	1.87	0.55
2:F:272:ASN:C	2:F:275:LEU:HD12	2.23	0.55
1:A:311:LEU:HD22	1:A:311:LEU:N	2.21	0.55
1:A:460:PRO:CB	1:A:594:ILE:HD11	2.33	0.55
1:A:518:LYS:CB	1:A:527:GLN:HG2	2.36	0.55
2:C:32:ASP:OD1	2:C:34:ARG:HG2	2.06	0.55
2:C:112:LEU:HD23	2:C:112:LEU:H	1.71	0.55
2:C:209:PHE:HD2	2:C:254:ILE:HD13	1.71	0.55
2:C:353:TRP:CE3	2:C:404:ILE:CG2	2.89	0.55
2:D:329:TRP:CB	2:D:424:ILE:HG23	2.36	0.55
1:B:230:TYR:CD1	1:B:263:PHE:CD1	2.93	0.55
1:B:236:ALA:O	1:B:237:ALA:HB3	2.06	0.55
1:B:570:ASP:N	1:B:570:ASP:OD2	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:PHE:CE2	1:E:120:PHE:CG	2.95	0.55
1:E:111:TYR:HD1	1:E:111:TYR:N	2.03	0.55
1:E:205:HIS:O	1:E:207:LEU:HD23	2.06	0.55
1:E:241:ARG:NH1	1:E:381:LYS:HD2	2.21	0.55
1:A:69:ILE:HG21	1:A:80:PHE:CB	2.34	0.55
1:A:84:LYS:H	1:A:139:TRP:CB	2.19	0.55
1:A:106:TYR:HE2	1:A:120:PHE:CD2	2.25	0.55
2:C:78:HIS:ND1	2:C:78:HIS:O	2.39	0.55
2:C:119:ILE:HG12	2:C:121:LEU:H	1.71	0.55
1:B:77:GLU:O	1:B:204:TYR:OH	2.23	0.55
1:B:99:VAL:HG22	1:B:166:ARG:HE	1.68	0.55
1:B:387:PHE:HE2	1:B:397:LEU:CD1	2.19	0.55
1:B:523:PHE:HB2	1:B:525:ILE:HD11	1.88	0.55
1:E:105:VAL:O	1:E:105:VAL:HG12	2.06	0.55
1:E:389:GLU:HG3	1:E:394:LYS:HA	1.80	0.55
1:A:168:PHE:HD1	1:A:168:PHE:H	1.55	0.55
1:A:361:LEU:HD11	1:A:376:ILE:CD1	2.35	0.55
1:A:373:LEU:HD23	1:A:373:LEU:H	1.69	0.55
1:B:589:PRO:HG2	1:B:596:TRP:CZ2	2.38	0.55
1:E:289:TYR:C	1:E:317:PHE:HE2	2.10	0.55
2:F:51:TYR:N	2:F:51:TYR:HD2	2.05	0.55
1:A:502:THR:CG2	1:A:577:ARG:HH22	2.19	0.55
1:A:562:GLN:O	1:A:565:ASP:HB2	2.07	0.55
2:D:341:ILE:HD13	2:D:374:SER:HB3	1.88	0.55
1:E:395:ARG:HH21	1:E:395:ARG:CG	2.15	0.55
1:E:504:ILE:HG13	1:E:540:GLY:O	2.05	0.55
1:E:518:LYS:O	1:E:525:ILE:N	2.26	0.55
2:F:17:GLU:HG2	2:F:21:TRP:CZ2	2.41	0.55
1:A:255:PHE:CE2	1:A:259:LEU:CD2	2.89	0.55
1:A:370:MET:O	1:A:374:ASN:CG	2.45	0.55
2:D:492:GLN:C	2:D:493:ASN:HD22	2.10	0.55
1:E:179:GLY:HA2	1:E:185:VAL:CG1	2.36	0.55
1:A:74:ASP:OD1	1:A:75:GLU:CA	2.55	0.55
1:A:241:ARG:O	1:A:383:THR:OG1	2.21	0.55
1:A:480:GLY:HA2	1:A:524:PRO:HG2	1.88	0.55
2:D:209:PHE:CZ	2:D:254:ILE:HG22	2.39	0.55
1:B:482:GLN:OE1	1:B:526:LEU:CD2	2.55	0.55
1:E:546:ASP:HB3	1:E:551:ILE:HG12	1.89	0.55
2:F:191:TYR:OH	2:F:264:LEU:O	2.21	0.55
2:F:276:GLU:O	2:F:280:ASN:ND2	2.40	0.55
2:F:335:ARG:HG3	2:F:335:ARG:NH1	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PHE:HE1	1:A:355:GLY:N	2.05	0.55
1:A:374:ASN:HD21	1:A:400:LEU:C	2.10	0.55
1:A:518:LYS:O	1:A:525:ILE:CG1	2.55	0.55
2:C:55:VAL:HG23	2:C:155:LEU:HD21	1.89	0.55
2:C:283:ASP:HB3	2:C:286:LEU:HB2	1.89	0.55
2:D:108:PHE:O	2:D:109:ALA:HB3	2.07	0.55
2:D:312:GLN:NE2	2:D:323:LYS:CD	2.68	0.55
2:D:329:TRP:CG	2:D:424:ILE:HG23	2.41	0.55
1:B:90:HIS:HE1	1:B:213:ILE:CD1	2.13	0.55
2:F:147:ALA:O	2:F:151:ALA:N	2.34	0.55
1:A:561:THR:HG23	1:A:562:GLN:HA	1.89	0.55
2:C:52:LEU:CD1	2:C:53:PRO:N	2.53	0.55
2:C:235:VAL:HG12	2:C:236:ASN:N	2.22	0.55
2:D:193:GLU:O	2:D:197:LYS:HG3	2.07	0.55
2:D:218:ASN:ND2	2:D:221:ASP:HB2	2.21	0.55
2:D:358:LYS:CB	2:D:490:ARG:NE	2.66	0.55
1:B:65:LEU:HD12	1:B:65:LEU:O	2.07	0.55
1:E:214:GLN:OE1	1:E:427:ASN:CA	2.54	0.55
2:F:111:PRO:O	2:F:114:THR:HB	2.06	0.55
1:A:562:GLN:O	1:A:565:ASP:N	2.40	0.55
2:C:329:TRP:CG	2:C:424:ILE:HG23	2.41	0.55
2:D:90:MET:O	2:D:94:ARG:HG3	2.06	0.55
1:B:93:GLY:H	1:B:122:HIS:HB3	1.71	0.55
1:E:454:PHE:CD2	1:E:454:PHE:N	2.73	0.55
2:F:410:GLU:O	2:F:414:ASN:CB	2.55	0.55
2:C:332:LEU:HD23	2:C:337:LEU:HB2	1.89	0.54
2:D:21:TRP:HB3	2:D:37:ALA:HB2	1.89	0.54
2:D:154:TRP:CE3	2:D:155:LEU:HA	2.42	0.54
2:D:188:LEU:CD1	2:D:192:MET:CG	2.86	0.54
1:B:397:LEU:CD1	1:B:400:LEU:CG	2.86	0.54
2:F:131:TRP:CD1	2:F:139:PRO:HD3	2.42	0.54
1:A:359:LEU:HD12	1:A:360:ASN:C	2.27	0.54
1:A:606:THR:HG23	2:C:5:ARG:NH1	2.22	0.54
2:C:83:PRO:HB3	2:D:68:LEU:HD22	1.88	0.54
2:C:359:LEU:O	2:C:359:LEU:HD23	2.07	0.54
2:D:96:VAL:C	2:D:100:LEU:CB	2.69	0.54
1:B:180:HIS:HB3	1:B:592:ARG:NH1	2.15	0.54
1:B:589:PRO:N	1:B:596:TRP:HH2	2.03	0.54
1:E:385:LEU:O	1:E:419:VAL:HG23	2.07	0.54
1:E:471:TYR:CZ	1:E:523:PHE:HE1	2.25	0.54
2:F:22:PHE:CD1	2:F:37:ALA:CB	2.91	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:110:ILE:CG2	2:F:114:THR:CG2	2.86	0.54
2:F:391:ASN:N	2:F:391:ASN:OD1	2.38	0.54
2:C:125:PHE:O	2:C:127:ASP:N	2.41	0.54
2:D:499:PHE:CD1	1:B:543:HIS:HA	2.41	0.54
1:A:101:LYS:HA	1:A:113:ALA:HB3	1.90	0.54
1:A:503:VAL:HG22	1:A:582:THR:HB	1.89	0.54
1:A:589:PRO:CB	1:A:594:ILE:CD1	2.85	0.54
2:C:83:PRO:O	2:C:86:LEU:HB2	2.06	0.54
2:C:350:LYS:HG2	2:C:404:ILE:CD1	2.37	0.54
1:B:395:ARG:HE	1:B:396:HIS:CB	2.20	0.54
1:B:544:SER:OG	1:B:553:ASN:CB	2.56	0.54
1:E:83:LEU:H	1:E:83:LEU:CD2	2.01	0.54
1:E:333:GLU:CD	1:E:336:SER:HB2	2.28	0.54
1:E:474:GLY:N	1:E:475:LYS:HA	2.21	0.54
1:E:480:GLY:H	1:E:524:PRO:HB2	1.72	0.54
1:E:562:GLN:HA	1:E:565:ASP:HB2	1.88	0.54
1:A:90:HIS:HE2	1:A:213:ILE:HD11	1.73	0.54
1:A:255:PHE:HE2	1:A:259:LEU:CD2	2.21	0.54
2:C:61:GLN:HE22	2:C:94:ARG:HE	1.55	0.54
2:C:101:ASP:OD1	2:C:101:ASP:N	2.38	0.54
2:D:122:PRO:CB	2:D:125:PHE:CD2	2.86	0.54
2:D:344:LEU:O	2:D:378:LYS:NZ	2.38	0.54
1:B:364:TRP:CE3	1:B:364:TRP:CA	2.90	0.54
1:B:467:LEU:HD23	1:B:554:ILE:O	2.07	0.54
1:A:91:LEU:HD23	1:A:95:PHE:CE2	2.42	0.54
1:A:95:PHE:CE2	1:A:120:PHE:HB2	2.43	0.54
1:A:282:LEU:HD13	1:A:359:LEU:HD21	1.89	0.54
1:A:369:GLY:O	1:A:373:LEU:HG	2.07	0.54
2:C:53:PRO:CD	2:C:56:VAL:CG2	2.86	0.54
2:C:97:ASN:CG	2:C:129:ARG:HE	2.09	0.54
2:C:323:LYS:HA	2:C:326:PHE:O	2.07	0.54
2:D:146:TRP:CH2	2:D:150:GLU:CD	2.73	0.54
1:B:484:PRO:HG2	1:B:487:PHE:HD1	1.71	0.54
1:E:487:PHE:CE2	2:F:46:LEU:CA	2.82	0.54
2:F:68:LEU:HD22	2:F:84:ILE:CG1	2.31	0.54
2:F:305:VAL:HG21	2:F:336:LEU:CD2	2.36	0.54
1:A:449:HIS:HB3	1:A:457:ASP:O	2.07	0.54
1:B:361:LEU:HD22	1:B:376:ILE:HD11	1.84	0.54
1:B:435:HIS:HB2	1:B:438:GLN:HB3	1.88	0.54
1:B:595:THR:O	1:B:595:THR:HG22	2.06	0.54
1:E:85:GLU:C	1:E:133:PHE:HD1	2.11	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:31:GLU:HG2	2:C:31:GLU:O	2.07	0.54
2:C:82:ILE:CG2	2:C:83:PRO:HD3	2.37	0.54
2:C:138:LEU:CD2	2:D:94:ARG:HH11	2.18	0.54
2:C:138:LEU:HD23	2:D:94:ARG:CZ	2.30	0.54
2:D:79:GLN:HA	2:D:79:GLN:HE21	1.73	0.54
1:B:261:GLU:CA	1:B:264:THR:HG1	2.17	0.54
1:E:199:ASN:CB	1:E:202:THR:CG2	2.85	0.54
1:E:471:TYR:CE2	1:E:523:PHE:HD1	2.26	0.54
1:E:549:GLN:HE21	1:E:549:GLN:N	2.06	0.54
2:F:62:ILE:HD12	2:F:155:LEU:HD21	1.89	0.54
2:F:312:GLN:NE2	2:F:323:LYS:NZ	2.55	0.54
1:A:97:LEU:O	1:A:118:LEU:N	2.31	0.54
1:A:226:LEU:CD1	1:A:230:TYR:HE1	2.14	0.54
2:D:350:LYS:HZ1	2:D:401:THR:HG22	1.72	0.54
2:D:494:TRP:CH2	2:D:497:LYS:HG3	2.42	0.54
1:B:590:SER:CB	1:B:593:THR:OG1	2.55	0.54
1:E:489:ASP:C	1:E:490:LEU:HD12	2.28	0.54
1:A:120:PHE:HA	1:A:307:LEU:O	2.08	0.54
1:A:234:LYS:HE2	1:A:270:SER:OG	2.08	0.54
1:A:503:VAL:CG2	1:A:582:THR:HB	2.38	0.54
2:C:54:HIS:O	2:C:54:HIS:ND1	2.42	0.54
2:D:96:VAL:HG13	2:D:100:LEU:HB2	1.89	0.54
2:D:279:PHE:HD1	2:D:304:TRP:CH2	2.24	0.54
1:B:254:THR:O	1:B:258:LEU:HG	2.08	0.54
1:E:77:GLU:CD	1:E:169:ASN:HD22	2.09	0.54
1:E:210:SER:O	1:E:212:ARG:HG3	2.08	0.54
1:E:384:HIS:HA	1:E:417:GLU:HB3	1.87	0.54
1:E:451:ILE:HB	1:E:455:ASP:OD1	2.07	0.54
2:F:125:PHE:HD1	2:F:128:LEU:HD23	1.73	0.54
1:A:183:ARG:HH21	1:A:183:ARG:HG2	1.73	0.53
1:A:388:LEU:O	1:A:423:ALA:N	2.42	0.53
2:C:110:ILE:N	2:C:110:ILE:HD12	2.23	0.53
2:C:312:GLN:CD	2:C:323:LYS:HD2	2.27	0.53
2:D:154:TRP:CZ3	2:D:155:LEU:CD2	2.86	0.53
1:B:310:HIS:C	1:B:311:LEU:HD22	2.27	0.53
1:B:545:ILE:HG12	1:B:552:MET:HG3	1.90	0.53
1:E:175:LEU:HD21	1:E:189:TRP:HE1	1.70	0.53
1:A:91:LEU:HD12	1:A:205:HIS:O	2.09	0.53
2:D:82:ILE:CG2	2:D:83:PRO:CD	2.86	0.53
2:D:331:GLU:O	2:D:335:ARG:HB2	2.06	0.53
1:B:99:VAL:HG13	1:B:166:ARG:HH21	1.70	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LYS:HD3	1:B:395:ARG:CZ	2.38	0.53
1:B:490:LEU:CD1	1:B:491:ASN:H	2.21	0.53
1:E:188:LEU:HD11	1:E:434:PHE:CD1	2.43	0.53
1:E:610:ARG:NE	2:F:167:ASP:CG	2.62	0.53
1:A:128:ILE:O	1:A:215:SER:HB2	2.09	0.53
1:A:269:ASP:OD2	1:A:269:ASP:N	2.41	0.53
1:A:325:ALA:C	1:A:578:ASN:ND2	2.61	0.53
1:B:110:HIS:HD2	1:B:111:TYR:N	2.06	0.53
1:B:324:TYR:CB	1:B:536:PHE:CE2	2.85	0.53
1:B:578:ASN:CG	1:B:579:LYS:N	2.62	0.53
1:E:289:TYR:CB	1:E:317:PHE:CD2	2.81	0.53
1:E:385:LEU:O	1:E:419:VAL:HG22	2.07	0.53
1:E:471:TYR:O	1:E:550:GLN:CB	2.56	0.53
2:C:68:LEU:HD12	2:C:68:LEU:C	2.29	0.53
2:D:21:TRP:N	2:D:21:TRP:CD1	2.73	0.53
1:B:387:PHE:CE2	1:B:397:LEU:HD11	2.42	0.53
1:B:397:LEU:CD1	1:B:400:LEU:HG	2.39	0.53
1:E:471:TYR:CD1	1:E:550:GLN:C	2.82	0.53
1:E:473:LYS:HD2	1:E:473:LYS:H	1.71	0.53
1:E:501:GLY:HA3	2:F:499:PHE:HD1	1.74	0.53
1:E:554:ILE:HG21	2:F:488:TRP:CZ3	2.44	0.53
1:A:124:LEU:H	1:A:188:LEU:CD2	2.22	0.53
1:A:267:ILE:CD1	1:A:277:LEU:HD21	2.39	0.53
1:A:518:LYS:O	1:A:525:ILE:HG13	2.09	0.53
1:A:527:GLN:HE21	1:A:527:GLN:C	2.10	0.53
2:D:336:LEU:CD1	2:D:340:ILE:CD1	2.86	0.53
2:D:350:LYS:HZ1	2:D:401:THR:CG2	2.21	0.53
1:B:122:HIS:ND1	1:B:128:ILE:HB	2.14	0.53
1:B:175:LEU:O	1:B:458:PHE:HZ	1.88	0.53
1:B:208:HIS:CE1	1:B:209:GLU:HG2	2.42	0.53
1:E:241:ARG:HB2	1:E:383:THR:N	2.23	0.53
1:E:486:GLU:O	2:F:42:GLN:OE1	2.27	0.53
1:E:562:GLN:CB	1:E:565:ASP:HB2	2.39	0.53
1:E:562:GLN:HB2	1:E:565:ASP:HB3	1.90	0.53
1:A:504:ILE:HD11	1:A:575:ILE:HG23	1.81	0.53
2:C:160:TRP:HA	2:C:160:TRP:CE3	2.43	0.53
1:E:295:ILE:HD11	1:E:337:TYR:CE2	2.43	0.53
2:F:312:GLN:HE22	2:F:323:LYS:NZ	2.07	0.53
1:A:245:ILE:HD12	1:A:245:ILE:C	2.27	0.53
1:A:260:LEU:HD23	1:A:277:LEU:CD1	2.39	0.53
1:A:617:TRP:CH2	2:D:133:THR:O	2.61	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:207:ASN:CA	2:C:210:LEU:CD1	2.87	0.53
1:B:589:PRO:CD	1:B:596:TRP:CZ2	2.84	0.53
1:E:324:TYR:CB	1:E:536:PHE:CE2	2.76	0.53
1:E:444:ILE:HD12	1:E:581:GLU:OE1	2.09	0.53
1:E:612:LYS:CD	2:F:164:GLU:CG	2.87	0.53
2:F:108:PHE:N	2:F:108:PHE:CD2	2.77	0.53
2:F:298:ASP:OD2	2:F:356:TRP:HZ2	1.91	0.53
2:F:492:GLN:H	2:F:492:GLN:CD	2.11	0.53
2:C:497:LYS:CE	2:C:502:LEU:O	2.57	0.53
2:D:69:ASP:CB	2:D:77:VAL:HG11	2.38	0.53
1:B:92:SER:HB2	1:B:207:LEU:CD1	2.33	0.53
1:B:264:THR:O	1:B:267:ILE:HG12	2.09	0.53
1:B:381:LYS:HD3	1:B:410:LEU:HA	1.90	0.53
1:E:559:CYS:SG	1:E:560:HIS:N	2.81	0.53
1:A:97:LEU:O	1:A:117:ILE:HA	2.09	0.53
1:A:617:TRP:C	1:A:618:LYS:HG3	2.28	0.53
2:D:199:LEU:HD13	2:D:281:ASN:OD1	2.08	0.53
2:D:283:ASP:OD1	2:D:285:LEU:N	2.40	0.53
2:D:333:GLN:O	2:D:338:ASP:N	2.37	0.53
1:E:182:TYR:HD1	1:E:184:ASP:H	1.55	0.53
1:E:222:TRP:HD1	1:E:422:PRO:HB2	1.69	0.53
2:F:365:SER:C	2:F:419:PHE:CD1	2.82	0.53
1:A:84:LYS:H	1:A:139:TRP:HB3	1.74	0.53
1:A:305:ILE:HG22	1:A:307:LEU:CD1	2.35	0.53
1:A:478:ILE:HD13	1:A:573:TRP:HB2	1.91	0.53
2:C:74:CYS:HA	2:C:75:LEU:C	2.30	0.53
2:C:86:LEU:CD2	2:C:138:LEU:HD12	2.29	0.53
2:C:110:ILE:HG23	2:C:111:PRO:HD2	1.90	0.53
2:C:332:LEU:CD2	2:C:337:LEU:HB2	2.39	0.53
2:C:349:PHE:HZ	2:C:353:TRP:CZ3	2.24	0.53
1:B:286:GLN:HG3	1:B:286:GLN:O	2.09	0.53
1:B:454:PHE:C	1:B:455:ASP:OD1	2.48	0.53
1:E:114:SER:O	1:E:115:ARG:HB3	2.07	0.53
1:E:175:LEU:CD2	1:E:189:TRP:NE1	2.50	0.53
1:E:471:TYR:CZ	1:E:523:PHE:CD1	2.97	0.53
1:E:488:GLN:HB3	1:E:489:ASP:OD1	2.09	0.53
1:A:115:ARG:HG2	1:A:115:ARG:O	2.09	0.52
1:A:198:LEU:CD2	1:A:205:HIS:NE2	2.73	0.52
2:C:78:HIS:CB	2:D:35:GLN:NE2	2.55	0.52
2:D:4:PRO:HD3	1:B:607:PHE:CE1	2.43	0.52
2:D:262:GLN:O	2:D:266:LYS:HG3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:LEU:HD13	1:B:89:LEU:C	2.30	0.52
1:B:175:LEU:CA	1:B:458:PHE:CZ	2.91	0.52
1:A:257:ARG:HA	1:A:260:LEU:HB2	1.91	0.52
2:C:207:ASN:O	2:C:210:LEU:HD13	2.08	0.52
2:D:291:MET:CE	2:D:340:ILE:HG23	2.39	0.52
2:D:349:PHE:CD2	2:D:356:TRP:NE1	2.77	0.52
1:B:321:LEU:HD21	1:B:344:LEU:HD13	1.81	0.52
1:B:562:GLN:HB2	1:B:565:ASP:HB2	1.91	0.52
1:E:96:ARG:HG2	1:E:168:PHE:O	2.09	0.52
2:F:155:LEU:CD1	2:F:155:LEU:H	2.10	0.52
2:F:394:ARG:O	2:F:398:ILE:HG13	2.10	0.52
1:A:446:ALA:O	1:A:450:LYS:HB2	2.09	0.52
1:A:472:GLY:N	1:A:475:LYS:CB	2.72	0.52
1:A:603:PRO:HG2	2:C:500:GLY:HA3	1.91	0.52
2:D:358:LYS:O	2:D:362:GLU:CA	2.56	0.52
1:B:503:VAL:HG12	1:B:539:LEU:HD22	1.91	0.52
1:E:120:PHE:HA	1:E:307:LEU:O	2.08	0.52
1:E:388:LEU:HD12	1:E:388:LEU:N	2.24	0.52
1:A:83:LEU:HD12	1:A:138:GLY:HA3	1.90	0.52
1:A:106:TYR:HE2	1:A:120:PHE:HD2	1.55	0.52
1:A:488:GLN:HE21	1:A:527:GLN:HE22	0.52	0.52
2:C:119:ILE:CG1	2:C:121:LEU:HB2	2.38	0.52
2:C:394:ARG:HH11	2:C:394:ARG:HG2	1.74	0.52
1:E:587:PHE:O	1:E:587:PHE:HD2	1.92	0.52
1:A:311:LEU:N	1:A:311:LEU:CD2	2.73	0.52
1:A:366:LYS:CE	1:A:395:ARG:CZ	2.79	0.52
1:A:480:GLY:N	1:A:524:PRO:CG	2.70	0.52
2:D:5:ARG:NE	1:B:610:ARG:HG3	2.24	0.52
2:D:77:VAL:HG13	2:D:84:ILE:CG1	2.30	0.52
2:D:113:HIS:HA	2:D:116:ALA:CB	2.39	0.52
2:D:302:ILE:HD12	2:D:356:TRP:HZ3	1.74	0.52
1:B:242:ILE:N	1:B:242:ILE:CD1	2.73	0.52
1:E:81:VAL:HG12	1:E:82:GLY:N	2.25	0.52
1:E:112:ASN:OD1	1:E:112:ASN:N	2.43	0.52
1:E:196:PHE:CD2	1:E:197:PRO:HD2	2.44	0.52
1:E:264:THR:O	1:E:268:ARG:NH1	2.43	0.52
1:E:493:GLN:HE22	2:F:36:ARG:HH21	1.58	0.52
1:E:518:LYS:HB3	1:E:525:ILE:O	2.09	0.52
2:C:223:LEU:N	2:C:223:LEU:CD2	2.73	0.52
1:B:395:ARG:NE	1:B:396:HIS:CA	2.73	0.52
1:E:184:ASP:OD1	1:E:184:ASP:N	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:HIS:CB	1:E:263:PHE:HE2	2.23	0.52
1:A:74:ASP:CG	1:A:75:GLU:N	2.49	0.52
1:A:270:SER:HB3	1:A:273:SER:OG	2.09	0.52
1:A:338:LEU:HD21	1:A:372:ILE:CG1	2.22	0.52
2:C:101:ASP:O	2:C:104:GLN:OE1	2.28	0.52
2:C:129:ARG:HG2	2:C:129:ARG:HH11	1.72	0.52
2:C:191:TYR:HE2	2:C:264:LEU:HD22	1.74	0.52
2:C:312:GLN:NE2	2:C:323:LYS:HB2	2.23	0.52
2:C:314:ASP:CB	2:C:495:LYS:HZ1	2.23	0.52
2:D:341:ILE:HG23	2:D:375:MET:SD	2.50	0.52
1:B:318:GLN:HG3	1:B:318:GLN:O	2.09	0.52
1:E:106:TYR:CD2	1:E:120:PHE:CE2	2.97	0.52
1:E:588:LEU:HD11	2:F:6:ILE:HD11	1.92	0.52
1:E:610:ARG:HE	2:F:167:ASP:CG	2.13	0.52
1:A:330:PRO:HG2	1:A:362:PRO:HG3	1.91	0.52
1:A:431:SER:O	1:A:434:PHE:N	2.36	0.52
2:D:84:ILE:HD12	2:D:88:TYR:HD2	1.74	0.52
2:D:329:TRP:CZ3	2:D:424:ILE:HD13	2.38	0.52
1:B:268:ARG:CZ	1:B:305:ILE:HD12	2.39	0.52
1:B:549:GLN:HB2	1:B:551:ILE:HG23	1.91	0.52
1:E:182:TYR:CE1	1:E:184:ASP:OD1	2.33	0.52
1:E:280:LEU:HD11	1:E:345:ILE:HG12	1.92	0.52
1:E:365:ILE:CD1	1:E:366:LYS:N	2.73	0.52
2:F:108:PHE:N	2:F:108:PHE:HD2	2.06	0.52
1:A:491:ASN:HD22	2:C:36:ARG:CD	2.23	0.52
1:A:617:TRP:HA	2:C:102:PRO:HB3	1.92	0.52
2:C:404:ILE:O	2:C:408:LEU:HD12	2.10	0.52
2:D:96:VAL:CG1	2:D:100:LEU:HB2	2.40	0.52
2:D:250:SER:O	2:D:254:ILE:HG13	2.10	0.52
1:B:97:LEU:HB2	1:B:120:PHE:CE1	2.44	0.52
1:B:287:PRO:HG3	1:B:292:PRO:HA	1.92	0.52
1:B:471:TYR:CD1	1:B:471:TYR:N	2.76	0.52
1:B:478:ILE:HD13	1:B:478:ILE:H	1.72	0.52
1:B:482:GLN:HB2	1:B:526:LEU:HD22	1.92	0.52
2:F:129:ARG:NH2	2:F:129:ARG:CB	2.73	0.52
2:F:299:TRP:O	2:F:303:GLU:N	2.37	0.52
1:A:74:ASP:OD1	1:A:75:GLU:O	2.28	0.52
1:A:469:ILE:CD1	2:C:488:TRP:CE2	2.87	0.52
2:C:207:ASN:C	2:C:210:LEU:HD13	2.30	0.52
1:B:68:ASN:CB	1:B:81:VAL:HA	2.40	0.52
1:B:490:LEU:CD1	1:B:491:ASN:N	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:538:THR:CG2	1:B:539:LEU:N	2.73	0.52
1:E:268:ARG:CG	1:E:268:ARG:NH1	2.73	0.52
1:E:305:ILE:HG22	1:E:307:LEU:HD11	1.91	0.52
1:E:358:LEU:N	1:E:358:LEU:CD2	2.73	0.52
1:E:449:HIS:HD2	1:E:458:PHE:HA	1.75	0.52
1:A:385:LEU:HD23	1:A:386:LEU:N	2.25	0.51
2:C:356:TRP:CE3	2:C:359:LEU:HD13	2.45	0.51
2:D:113:HIS:O	2:D:117:ALA:N	2.42	0.51
2:D:232:ASP:OD1	2:D:232:ASP:N	2.37	0.51
1:B:175:LEU:HA	1:B:458:PHE:CE2	2.45	0.51
1:B:289:TYR:HD2	1:B:289:TYR:N	2.08	0.51
1:B:311:LEU:N	1:B:311:LEU:CD2	2.73	0.51
1:B:450:LYS:NZ	1:B:450:LYS:CB	2.73	0.51
1:B:589:PRO:CG	1:B:596:TRP:CZ2	2.93	0.51
1:E:289:TYR:HD1	1:E:317:PHE:HD2	1.45	0.51
1:E:469:ILE:CB	1:E:478:ILE:HD11	2.33	0.51
1:E:524:PRO:O	1:E:525:ILE:CD1	2.46	0.51
1:E:560:HIS:O	1:E:563:ILE:HB	2.09	0.51
2:F:68:LEU:HD22	2:F:84:ILE:HD11	1.72	0.51
2:F:154:TRP:CE2	2:F:158:HIS:ND1	2.76	0.51
1:A:176:LEU:CD2	1:A:176:LEU:N	2.73	0.51
1:A:418:VAL:O	1:A:419:VAL:HG13	2.10	0.51
2:C:40:ARG:HD3	2:C:44:TYR:CZ	2.44	0.51
2:D:312:GLN:OE1	2:D:430:ILE:CD1	2.58	0.51
1:B:213:ILE:O	1:B:213:ILE:HG13	2.09	0.51
1:B:289:TYR:HA	1:B:317:PHE:CE1	2.45	0.51
1:E:75:GLU:OE1	1:E:76:ASP:HB2	2.09	0.51
1:E:88:LYS:HB3	1:E:130:THR:CG2	2.40	0.51
1:E:182:TYR:HD1	1:E:182:TYR:C	2.14	0.51
1:E:562:GLN:O	1:E:566:LYS:N	2.44	0.51
2:F:315:ASP:OD2	3:F:601:HOH:O	2.19	0.51
1:A:77:GLU:CG	1:A:201:ARG:O	2.58	0.51
1:A:104:ILE:CD1	1:A:104:ILE:N	2.73	0.51
1:A:124:LEU:CB	1:A:188:LEU:O	2.54	0.51
1:A:196:PHE:CE2	1:A:197:PRO:HD2	2.46	0.51
1:A:299:LYS:C	1:A:300:ILE:CD1	2.79	0.51
1:A:365:ILE:C	1:A:396:HIS:CE1	2.77	0.51
2:C:358:LYS:O	2:C:362:GLU:HB2	2.10	0.51
2:D:95:PHE:CZ	2:D:155:LEU:HD21	2.42	0.51
2:D:212:TYR:CE2	2:D:250:SER:HB3	2.46	0.51
2:D:218:ASN:ND2	2:D:221:ASP:CB	2.73	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:TRP:N	2:D:428:ASP:OD1	2.43	0.51
1:B:400:LEU:CD2	1:B:400:LEU:N	2.73	0.51
1:E:104:ILE:N	1:E:104:ILE:CD1	2.73	0.51
1:E:468:GLN:O	2:F:488:TRP:HA	2.10	0.51
1:E:490:LEU:HD12	1:E:490:LEU:N	2.25	0.51
2:F:36:ARG:HH12	2:F:40:ARG:HH21	1.56	0.51
1:A:183:ARG:CG	1:A:183:ARG:NH2	2.73	0.51
1:A:498:ALA:O	1:A:502:THR:CG2	2.59	0.51
2:C:110:ILE:N	2:C:110:ILE:CD1	2.73	0.51
2:C:128:LEU:HD12	2:C:129:ARG:N	2.25	0.51
1:B:114:SER:O	1:B:115:ARG:NE	2.43	0.51
1:B:473:LYS:CE	1:B:474:GLY:N	2.73	0.51
1:E:97:LEU:CB	1:E:167:VAL:H	2.23	0.51
1:E:394:LYS:HD2	1:E:394:LYS:C	2.29	0.51
1:E:612:LYS:HD3	2:F:164:GLU:CG	2.40	0.51
1:A:508:THR:OG1	1:A:537:ILE:HD11	2.10	0.51
2:C:209:PHE:CE2	2:C:254:ILE:CG1	2.92	0.51
2:C:209:PHE:HE2	2:C:254:ILE:HG12	1.67	0.51
1:B:99:VAL:CG1	1:B:166:ARG:NH2	2.68	0.51
1:E:233:HIS:CB	1:E:263:PHE:CE2	2.94	0.51
1:E:289:TYR:CD1	1:E:317:PHE:HD2	2.21	0.51
2:F:52:LEU:HD23	2:F:57:ASP:HB2	1.89	0.51
2:F:280:ASN:C	2:F:325:LYS:HE3	2.30	0.51
1:A:107:ASN:HD22	1:A:258:LEU:HD21	1.72	0.51
1:B:69:ILE:N	1:B:69:ILE:CD1	2.73	0.51
1:B:85:GLU:O	1:B:133:PHE:CD1	2.64	0.51
1:B:310:HIS:CD2	1:B:314:GLY:CA	2.79	0.51
1:B:503:VAL:HG12	1:B:539:LEU:CD2	2.40	0.51
1:E:469:ILE:CG2	1:E:470:SER:N	2.73	0.51
1:E:491:ASN:HD22	2:F:36:ARG:HE	1.53	0.51
1:A:169:ASN:CB	1:A:203:THR:HG23	2.41	0.51
1:A:176:LEU:N	1:A:176:LEU:HD22	2.26	0.51
1:A:291:LEU:CD1	1:A:291:LEU:N	2.73	0.51
1:A:477:GLY:C	1:A:478:ILE:HD13	2.30	0.51
1:A:524:PRO:O	1:A:524:PRO:HG2	2.10	0.51
2:C:119:ILE:CG1	2:C:121:LEU:N	2.74	0.51
2:C:160:TRP:HA	2:C:160:TRP:HE3	1.76	0.51
2:D:209:PHE:CE1	2:D:254:ILE:HG21	2.43	0.51
1:B:467:LEU:CD2	1:B:554:ILE:O	2.59	0.51
1:E:95:PHE:CE2	1:E:120:PHE:HB2	2.45	0.51
1:E:389:GLU:HB3	1:E:394:LYS:CB	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:ARG:NH2	1:E:593:THR:N	2.57	0.51
1:E:599:ASN:OD1	1:E:600:ILE:HG12	2.10	0.51
1:A:371:GLN:NE2	1:A:371:GLN:CA	2.73	0.51
2:C:359:LEU:HD23	2:C:359:LEU:C	2.31	0.51
2:C:405:GLU:HA	2:C:408:LEU:HD12	1.93	0.51
1:E:387:PHE:CZ	1:E:401:THR:CG2	2.94	0.51
1:A:177:GLU:HG2	2:C:267:LEU:HD23	1.91	0.51
1:A:226:LEU:CG	1:A:230:TYR:OH	2.58	0.51
1:A:300:ILE:CD1	1:A:300:ILE:N	2.73	0.51
1:A:365:ILE:CG2	1:A:397:LEU:HD21	2.34	0.51
1:A:603:PRO:O	2:C:10:ARG:HA	2.10	0.51
2:C:96:VAL:HG11	2:C:128:LEU:CD1	2.35	0.51
2:C:122:PRO:HB2	2:C:124:TRP:CD1	2.46	0.51
2:C:127:ASP:O	2:C:131:TRP:HB2	2.10	0.51
2:D:88:TYR:HB3	2:D:144:LEU:HD13	1.92	0.51
1:E:265:GLN:O	1:E:269:ASP:OD2	2.29	0.51
1:E:280:LEU:O	1:E:359:LEU:HB2	2.10	0.51
2:F:45:ARG:O	2:F:48:GLY:O	2.28	0.51
1:A:395:ARG:NH2	1:A:395:ARG:CG	2.73	0.51
2:D:182:TYR:O	2:D:186:ASP:N	2.42	0.51
2:D:356:TRP:C	2:D:360:ILE:HG13	2.29	0.51
1:B:175:LEU:CA	1:B:458:PHE:CE2	2.94	0.51
1:E:245:ILE:CG2	1:E:387:PHE:CE2	2.94	0.51
1:E:588:LEU:HD21	2:F:6:ILE:CD1	2.40	0.51
1:E:601:GLN:NE2	1:E:601:GLN:CA	2.73	0.51
2:F:12:PHE:O	2:F:12:PHE:HD1	1.94	0.51
2:F:53:PRO:HD2	2:F:56:VAL:HG21	1.93	0.51
2:F:359:LEU:HD23	2:F:360:ILE:CA	2.40	0.51
2:C:129:ARG:NH1	2:C:129:ARG:CG	2.73	0.50
2:C:212:TYR:N	2:C:212:TYR:CD2	2.79	0.50
2:C:224:ILE:CB	2:C:229:PHE:CE2	2.86	0.50
2:D:102:PRO:HG3	1:B:615:HIS:NE2	2.26	0.50
2:D:329:TRP:HB2	2:D:424:ILE:HG23	1.93	0.50
1:B:245:ILE:O	1:B:388:LEU:CD1	2.59	0.50
1:B:536:PHE:HD1	1:B:537:ILE:N	2.09	0.50
1:E:74:ASP:CG	1:E:75:GLU:H	2.07	0.50
1:A:198:LEU:HD23	1:A:205:HIS:HE2	1.76	0.50
1:A:527:GLN:NE2	1:A:527:GLN:CA	2.73	0.50
1:B:98:GLN:HB3	1:B:165:LEU:HD13	1.92	0.50
1:B:311:LEU:O	1:B:312:CYS:HB2	2.12	0.50
1:E:364:TRP:CE3	3:E:705:HOH:O	2.64	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:538:THR:CG2	1:E:539:LEU:N	2.73	0.50
1:E:546:ASP:HB3	1:E:551:ILE:CG1	2.40	0.50
1:A:71:TYR:CE2	1:A:73:GLY:N	2.73	0.50
1:A:79:MET:CE	1:A:81:VAL:CG2	2.90	0.50
1:A:105:VAL:HG12	1:A:105:VAL:O	2.10	0.50
1:A:481:ILE:HG23	1:A:575:ILE:CG1	2.41	0.50
2:D:154:TRP:HZ3	2:D:155:LEU:HD23	1.71	0.50
2:D:193:GLU:O	2:D:197:LYS:CG	2.60	0.50
1:B:358:LEU:N	1:B:358:LEU:CD2	2.73	0.50
1:B:590:SER:C	1:B:593:THR:HG1	2.10	0.50
1:E:491:ASN:HD21	2:F:39:GLN:CB	2.23	0.50
2:F:349:PHE:CD1	2:F:375:MET:HE2	2.45	0.50
1:A:106:TYR:CD2	1:A:120:PHE:CE2	2.98	0.50
1:A:165:LEU:N	1:A:165:LEU:CD1	2.73	0.50
1:A:469:ILE:CG2	2:C:488:TRP:CD2	2.94	0.50
2:D:133:THR:HB	2:D:134:HIS:HD2	1.76	0.50
2:D:336:LEU:CD1	2:D:340:ILE:CG1	2.90	0.50
1:B:92:SER:HA	1:B:122:HIS:HB3	1.93	0.50
1:B:121:TRP:CB	1:B:309:GLN:O	2.59	0.50
1:B:175:LEU:HD22	1:B:456:TYR:HE2	1.76	0.50
1:B:448:PHE:CB	1:B:461:LEU:HD21	2.41	0.50
1:E:98:GLN:CB	1:E:117:ILE:CG2	2.89	0.50
1:E:118:LEU:N	1:E:118:LEU:CD2	2.73	0.50
1:E:399:GLU:OE2	1:E:400:LEU:CA	2.60	0.50
2:F:66:VAL:HA	2:F:88:TYR:CZ	2.45	0.50
1:A:97:LEU:HA	1:A:166:ARG:O	2.11	0.50
1:A:204:TYR:CD1	1:A:204:TYR:N	2.79	0.50
1:A:224:THR:HB	1:A:225:PRO:HD3	1.94	0.50
1:A:589:PRO:HG2	1:A:596:TRP:CZ3	2.46	0.50
2:C:96:VAL:CG2	2:C:128:LEU:HD11	2.42	0.50
2:D:69:ASP:CB	2:D:77:VAL:HG21	2.27	0.50
2:D:330:LYS:O	2:D:334:LYS:HG2	2.11	0.50
1:B:103:GLY:O	1:B:134:SER:CB	2.56	0.50
1:B:211:ASP:CA	1:B:212:ARG:NH2	2.75	0.50
1:B:488:GLN:HA	1:B:488:GLN:HE21	1.77	0.50
1:E:97:LEU:HB2	1:E:167:VAL:H	1.76	0.50
1:E:98:GLN:HB2	1:E:117:ILE:CG2	2.42	0.50
1:E:213:ILE:HD12	1:E:215:SER:N	2.26	0.50
1:E:267:ILE:CD1	1:E:302:SER:HB3	2.38	0.50
1:E:584:PHE:CE1	1:E:588:LEU:CD1	2.95	0.50
2:F:398:ILE:HA	2:F:401:THR:HG23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:O	1:A:133:PHE:CD2	2.64	0.50
1:A:174:GLY:HA3	1:A:456:TYR:O	2.11	0.50
1:A:471:TYR:O	1:A:550:GLN:O	2.30	0.50
2:D:199:LEU:HD12	2:D:281:ASN:OD1	2.11	0.50
1:B:184:ASP:HB3	1:B:438:GLN:OE1	2.12	0.50
1:B:536:PHE:CD1	1:B:536:PHE:C	2.85	0.50
1:E:84:LYS:HA	1:E:133:PHE:CZ	2.45	0.50
1:E:110:HIS:CD2	1:E:111:TYR:N	2.80	0.50
1:E:257:ARG:HE	1:E:308:GLY:C	2.14	0.50
1:E:331:GLN:HG3	1:E:364:TRP:CH2	2.19	0.50
1:A:241:ARG:NE	1:A:380:TYR:O	2.43	0.50
1:A:265:GLN:HA	1:A:268:ARG:NH1	2.26	0.50
1:A:347:HIS:C	1:A:347:HIS:CD2	2.85	0.50
1:A:484:PRO:HG2	1:A:487:PHE:CD1	2.47	0.50
2:C:309:TYR:CD1	2:C:309:TYR:C	2.85	0.50
2:D:112:LEU:N	2:D:112:LEU:CD2	2.73	0.50
2:D:156:TYR:C	2:D:156:TYR:CD1	2.85	0.50
2:D:184:ARG:CG	1:B:592:ARG:CD	2.90	0.50
2:D:210:LEU:HG	2:D:285:LEU:HD11	1.93	0.50
1:B:167:VAL:O	1:B:204:TYR:CZ	2.65	0.50
1:B:334:PRO:O	1:B:338:LEU:HD12	2.11	0.50
1:B:482:GLN:HB3	1:B:576:VAL:HG22	1.92	0.50
1:B:541:LEU:O	1:B:555:TYR:N	2.45	0.50
1:E:353:PHE:HE1	1:E:355:GLY:HA3	1.77	0.50
2:F:154:TRP:CE3	2:F:154:TRP:C	2.85	0.50
2:F:359:LEU:HD21	2:F:368:ILE:CD1	2.37	0.50
1:A:267:ILE:CD1	1:A:277:LEU:HD23	2.42	0.50
1:A:353:PHE:CD1	1:A:353:PHE:C	2.85	0.50
1:A:491:ASN:ND2	2:C:36:ARG:CD	2.74	0.50
2:D:154:TRP:CE3	2:D:154:TRP:C	2.85	0.50
1:E:182:TYR:CE1	1:E:184:ASP:HB2	2.42	0.50
1:E:182:TYR:C	1:E:182:TYR:CD1	2.85	0.50
1:E:549:GLN:NE2	1:E:549:GLN:N	2.60	0.50
2:F:110:ILE:CG2	2:F:114:THR:HG22	2.42	0.50
2:F:298:ASP:CG	2:F:356:TRP:CZ2	2.85	0.50
2:F:350:LYS:HZ3	2:F:401:THR:CG2	1.98	0.50
1:A:307:LEU:N	1:A:307:LEU:CD1	2.73	0.50
1:A:371:GLN:NE2	1:A:371:GLN:HA	2.25	0.50
1:A:457:ASP:OD2	2:C:268:SER:HB2	2.12	0.50
2:C:357:GLU:HG2	2:C:361:ASP:OD1	2.12	0.50
1:B:450:LYS:HB3	1:B:450:LYS:HZ3	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:ARG:HH11	1:E:268:ARG:HG3	1.74	0.50
1:E:474:GLY:N	1:E:475:LYS:CA	2.74	0.50
1:E:587:PHE:C	1:E:587:PHE:CD2	2.85	0.50
1:E:589:PRO:CG	1:E:596:TRP:CH2	2.95	0.50
2:F:53:PRO:HD2	2:F:56:VAL:CG2	2.41	0.50
1:A:353:PHE:CE1	1:A:354:PHE:C	2.86	0.49
1:A:589:PRO:HG3	1:A:596:TRP:CH2	2.46	0.49
1:A:617:TRP:HD1	1:A:618:LYS:H	1.60	0.49
2:C:307:ARG:NH1	2:C:307:ARG:CG	2.73	0.49
1:B:389:GLU:HB3	1:B:394:LYS:CA	2.42	0.49
1:B:390:THR:CG2	1:B:391:ALA:H	2.02	0.49
1:B:587:PHE:C	1:B:587:PHE:CD2	2.85	0.49
1:E:214:GLN:HG3	1:E:214:GLN:O	2.12	0.49
1:E:445:LEU:HD13	1:E:583:PRO:HG3	1.93	0.49
1:E:473:LYS:HD2	1:E:474:GLY:N	2.27	0.49
1:E:473:LYS:CD	1:E:474:GLY:H	2.25	0.49
1:E:549:GLN:NE2	1:E:549:GLN:H	2.10	0.49
2:C:23:TYR:HD2	2:C:156:TYR:CE2	2.29	0.49
2:C:292:LEU:N	2:C:292:LEU:HD23	2.26	0.49
2:C:314:ASP:HB3	2:C:495:LYS:HZ1	1.76	0.49
2:D:282:TYR:CD1	2:D:282:TYR:C	2.86	0.49
1:B:167:VAL:HG23	1:B:167:VAL:O	2.11	0.49
1:E:71:TYR:CZ	1:E:73:GLY:HA3	2.47	0.49
1:E:279:TYR:HB2	1:E:300:ILE:HD11	1.93	0.49
1:E:523:PHE:CB	1:E:525:ILE:HD11	2.42	0.49
2:F:319:THR:HG21	2:F:433:GLU:N	2.23	0.49
2:C:260:GLN:O	2:C:264:LEU:HG	2.11	0.49
2:C:325:LYS:C	2:C:326:PHE:CD1	2.85	0.49
1:B:172:HIS:CD2	1:B:454:PHE:C	2.81	0.49
1:E:195:TYR:CD1	1:E:208:HIS:HB3	2.47	0.49
1:E:208:HIS:ND1	1:E:209:GLU:N	2.60	0.49
2:F:131:TRP:CD1	2:F:131:TRP:C	2.85	0.49
2:F:146:TRP:C	2:F:146:TRP:CD1	2.85	0.49
1:A:107:ASN:O	1:A:109:VAL:HG13	2.12	0.49
1:A:169:ASN:HB3	1:A:203:THR:CG2	2.42	0.49
1:A:245:ILE:HD11	1:A:363:GLY:C	2.33	0.49
1:A:317:PHE:C	1:A:317:PHE:CD2	2.86	0.49
1:A:470:SER:HB2	1:A:550:GLN:O	2.12	0.49
1:A:592:ARG:HH21	2:C:184:ARG:HE	1.58	0.49
2:D:69:ASP:HB2	2:D:77:VAL:HG11	1.93	0.49
2:D:82:ILE:HG23	2:D:83:PRO:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:TYR:O	1:B:196:PHE:HD1	1.96	0.49
1:B:490:LEU:HD12	1:B:491:ASN:H	1.74	0.49
1:E:110:HIS:C	1:E:110:HIS:CD2	2.85	0.49
1:E:389:GLU:HB2	1:E:397:LEU:HD11	1.94	0.49
2:F:188:LEU:O	2:F:192:MET:HG2	2.12	0.49
2:F:270:TYR:C	2:F:274:VAL:HG23	2.31	0.49
1:A:169:ASN:ND2	1:A:203:THR:HG23	2.26	0.49
1:A:541:LEU:HD11	2:C:499:PHE:HE1	1.77	0.49
1:A:614:GLU:HB2	2:C:53:PRO:HB3	1.94	0.49
2:C:209:PHE:HD2	2:C:254:ILE:CD1	2.25	0.49
2:D:278:PHE:CE1	2:D:279:PHE:HE2	2.30	0.49
1:B:94:VAL:HG12	1:B:95:PHE:N	2.28	0.49
1:E:182:TYR:CD1	1:E:184:ASP:N	2.79	0.49
1:E:236:ALA:O	1:E:237:ALA:HB3	2.13	0.49
1:E:245:ILE:HG21	1:E:387:PHE:HE2	1.77	0.49
1:E:365:ILE:HG21	1:E:389:GLU:OE2	2.13	0.49
1:E:390:THR:O	1:E:394:LYS:CG	2.61	0.49
1:E:536:PHE:HD1	1:E:536:PHE:C	2.15	0.49
2:F:282:TYR:CD1	2:F:282:TYR:C	2.86	0.49
1:A:552:MET:O	1:A:554:ILE:HG22	2.11	0.49
1:A:592:ARG:NH2	2:C:184:ARG:NE	2.53	0.49
1:A:603:PRO:HD3	2:C:498:PRO:HG2	1.94	0.49
2:D:154:TRP:HZ3	2:D:155:LEU:CD2	2.25	0.49
2:D:487:ASN:ND2	2:D:488:TRP:CD1	2.75	0.49
1:B:450:LYS:CD	1:B:456:TYR:HH	2.05	0.49
1:B:544:SER:OG	1:B:553:ASN:CG	2.50	0.49
2:F:54:HIS:ND1	2:F:54:HIS:O	2.43	0.49
2:F:80:ASP:OD1	2:F:80:ASP:N	2.35	0.49
1:A:105:VAL:C	1:A:132:ASP:HB2	2.33	0.49
1:A:169:ASN:HB3	1:A:203:THR:HG21	1.94	0.49
1:A:472:GLY:CA	1:A:475:LYS:CB	2.91	0.49
2:C:128:LEU:O	2:C:131:TRP:HB3	2.12	0.49
2:C:218:ASN:OD1	2:C:218:ASN:N	2.45	0.49
2:D:191:TYR:CD1	2:D:191:TYR:C	2.86	0.49
1:B:93:GLY:O	1:B:95:PHE:CE1	2.65	0.49
1:B:245:ILE:HD12	1:B:246:GLY:H	1.77	0.49
1:B:277:LEU:HA	1:B:356:THR:O	2.12	0.49
1:B:364:TRP:HE3	1:B:364:TRP:H	1.60	0.49
1:E:316:ASN:O	1:E:316:ASN:ND2	2.44	0.49
1:E:536:PHE:C	1:E:536:PHE:CD1	2.86	0.49
2:F:98:GLY:O	2:F:102:PRO:CB	2.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:372:CYS:HB3	2:F:412:ILE:HD11	1.93	0.49
1:A:129:PRO:HB3	1:A:217:SER:HA	1.93	0.49
1:A:205:HIS:ND1	1:A:206:LEU:N	2.60	0.49
1:A:243:MET:SD	1:A:361:LEU:CD2	3.01	0.49
1:A:280:LEU:HD11	1:A:297:LEU:CD1	2.39	0.49
1:A:383:THR:HB	1:A:384:HIS:CE1	2.47	0.49
2:C:353:TRP:CH2	2:C:408:LEU:CD2	2.82	0.49
1:B:65:LEU:HD12	1:B:66:ILE:O	2.13	0.49
1:B:122:HIS:HE1	1:B:128:ILE:HD13	1.78	0.49
1:B:337:TYR:C	1:B:337:TYR:CD2	2.85	0.49
1:B:590:SER:N	1:B:593:THR:HG1	2.08	0.49
1:E:103:GLY:O	1:E:104:ILE:HD12	2.13	0.49
1:E:133:PHE:CD2	1:E:133:PHE:C	2.86	0.49
1:E:181:LEU:HD13	1:E:181:LEU:C	2.32	0.49
1:E:233:HIS:CD2	1:E:356:THR:HG21	2.48	0.49
1:E:424:HIS:C	1:E:424:HIS:CD2	2.85	0.49
1:E:431:SER:OG	1:E:435:HIS:N	2.45	0.49
1:E:538:THR:HG21	1:E:557:PRO:HD2	1.94	0.49
2:F:154:TRP:HE3	2:F:155:LEU:N	2.11	0.49
1:A:168:PHE:CD1	1:A:168:PHE:N	2.81	0.49
1:A:364:TRP:CD1	1:A:369:GLY:HA3	2.43	0.49
1:A:471:TYR:C	1:A:471:TYR:CD2	2.85	0.49
2:C:125:PHE:CD1	2:C:128:LEU:HD23	2.48	0.49
2:C:202:TRP:HH2	2:C:289:VAL:HG21	1.77	0.49
2:C:497:LYS:CD	2:C:502:LEU:C	2.54	0.49
2:D:389:TRP:CD1	2:D:389:TRP:C	2.86	0.49
2:D:423:GLU:O	2:D:426:LEU:HB2	2.13	0.49
1:B:247:GLY:HA3	1:B:365:ILE:CG2	2.43	0.49
1:B:288:GLU:C	1:B:289:TYR:CD2	2.85	0.49
1:B:305:ILE:HG22	1:B:307:LEU:HD21	1.95	0.49
1:B:471:TYR:CZ	1:B:550:GLN:HA	2.39	0.49
2:F:271:HIS:C	2:F:274:VAL:HG23	2.33	0.49
1:A:280:LEU:CG	1:A:297:LEU:HD12	2.42	0.49
1:A:337:TYR:CD1	1:A:337:TYR:C	2.86	0.49
1:A:357:SER:OG	1:A:380:TYR:OH	1.95	0.49
1:A:517:VAL:HG13	1:A:517:VAL:O	2.13	0.49
1:A:615:HIS:ND1	1:A:615:HIS:N	2.60	0.49
2:C:312:GLN:OE1	2:C:323:LYS:NZ	2.45	0.49
2:D:419:PHE:CD2	2:D:419:PHE:N	2.81	0.49
1:B:400:LEU:CD2	1:B:401:THR:H	2.21	0.49
1:B:509:TYR:CZ	1:B:513:ASP:HB2	2.44	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:MET:SD	1:E:377:ILE:HG12	2.52	0.49
1:E:317:PHE:HD1	1:E:317:PHE:H	1.59	0.49
1:E:501:GLY:CA	2:F:499:PHE:HD1	2.26	0.49
1:A:388:LEU:HG	1:A:421:VAL:HG21	1.95	0.48
2:C:62:ILE:HG12	2:C:91:ALA:HB1	1.94	0.48
2:C:75:LEU:HD23	2:C:76:GLY:C	2.34	0.48
2:C:202:TRP:CH2	2:C:289:VAL:HG21	2.48	0.48
2:D:493:ASN:N	2:D:493:ASN:ND2	2.60	0.48
1:B:469:ILE:HB	1:B:478:ILE:HD11	1.94	0.48
2:F:125:PHE:HD1	2:F:128:LEU:CD2	2.25	0.48
1:A:171:ASN:O	1:A:454:PHE:HB2	2.12	0.48
1:A:261:GLU:CG	1:A:307:LEU:HD23	2.43	0.48
1:A:373:LEU:CD2	1:A:373:LEU:N	2.73	0.48
1:A:487:PHE:HD2	2:C:42:GLN:OE1	1.96	0.48
2:D:5:ARG:CD	1:B:610:ARG:CG	2.91	0.48
2:D:54:HIS:HE1	2:D:58:SER:OG	1.96	0.48
1:B:371:GLN:HA	1:B:371:GLN:NE2	2.27	0.48
1:B:534:LYS:N	1:B:534:LYS:HD2	2.28	0.48
1:E:168:PHE:CD2	1:E:168:PHE:C	2.85	0.48
1:E:214:GLN:OE1	1:E:427:ASN:CB	2.60	0.48
1:E:390:THR:OG1	1:E:422:PRO:HA	2.13	0.48
1:E:473:LYS:H	1:E:473:LYS:CD	2.25	0.48
2:F:337:LEU:CD1	2:F:338:ASP:N	2.73	0.48
1:A:75:GLU:CA	2:C:259:ARG:NH2	2.63	0.48
1:A:256:LEU:CD1	1:A:360:ASN:HB3	2.40	0.48
1:A:282:LEU:CD1	1:A:359:LEU:CD1	2.85	0.48
1:A:330:PRO:HB3	1:A:337:TYR:CD2	2.48	0.48
1:A:472:GLY:HA2	1:A:550:GLN:NE2	2.28	0.48
1:A:611:LYS:HA	2:C:164:GLU:O	2.14	0.48
2:C:23:TYR:HE2	2:C:160:TRP:HD1	1.57	0.48
2:C:197:LYS:O	2:C:201:LYS:HG3	2.12	0.48
2:D:71:LYS:HB3	2:D:71:LYS:HZ2	1.77	0.48
2:D:278:PHE:CD1	2:D:278:PHE:C	2.86	0.48
2:D:329:TRP:CG	2:D:424:ILE:CD1	2.65	0.48
1:B:127:SER:CB	1:B:214:GLN:HG3	2.43	0.48
1:B:507:TYR:HD1	1:B:535:ASN:O	1.96	0.48
2:F:67:LEU:O	2:F:67:LEU:HD23	2.14	0.48
2:F:418:ARG:C	2:F:419:PHE:CD2	2.85	0.48
1:A:71:TYR:CD2	1:A:73:GLY:N	2.79	0.48
1:A:98:GLN:HG2	1:A:115:ARG:HA	1.85	0.48
1:A:253:SER:O	1:A:257:ARG:HG3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:PRO:HB3	1:A:521:ASN:HB2	1.95	0.48
2:C:182:TYR:HE1	2:F:183:ARG:HG3	1.69	0.48
2:C:202:TRP:CE2	2:C:286:LEU:CD1	2.97	0.48
2:C:325:LYS:O	2:C:326:PHE:HD1	1.95	0.48
2:C:353:TRP:CE3	2:C:404:ILE:HG23	2.48	0.48
2:D:312:GLN:CD	2:D:427:TYR:CE2	2.87	0.48
1:B:599:ASN:ND2	1:B:600:ILE:N	2.60	0.48
1:E:584:PHE:C	1:E:584:PHE:CD1	2.86	0.48
1:A:313:GLN:NE2	1:A:313:GLN:N	2.60	0.48
2:C:125:PHE:CB	2:C:128:LEU:CD2	2.91	0.48
2:C:148:ALA:O	2:C:152:LEU:HG	2.14	0.48
2:C:278:PHE:HE2	2:C:286:LEU:HD23	0.51	0.48
2:C:291:MET:HE3	2:C:340:ILE:HG22	1.78	0.48
2:D:110:ILE:HG22	2:D:111:PRO:O	2.14	0.48
1:B:73:GLY:HA2	1:B:74:ASP:C	2.33	0.48
1:B:395:ARG:NE	1:B:396:HIS:HA	2.28	0.48
1:E:195:TYR:HD1	1:E:210:SER:OG	1.97	0.48
1:E:254:THR:HA	1:E:257:ARG:NH1	2.28	0.48
1:A:196:PHE:CG	1:A:197:PRO:CD	2.94	0.48
1:A:481:ILE:HG23	1:A:575:ILE:CB	2.41	0.48
2:C:130:HIS:CB	2:C:134:HIS:ND1	2.73	0.48
2:C:310:ARG:HH11	2:C:310:ARG:HG3	1.77	0.48
2:D:215:VAL:HG13	2:D:255:ARG:NH2	2.28	0.48
1:A:81:VAL:HG12	1:A:82:GLY:H	1.79	0.48
1:A:541:LEU:C	1:A:554:ILE:HG13	2.34	0.48
2:C:96:VAL:HG21	2:C:128:LEU:HD11	1.96	0.48
2:C:278:PHE:CE1	2:C:287:LEU:CD1	2.97	0.48
1:B:76:ASP:HB3	1:B:169:ASN:HB2	1.95	0.48
1:E:480:GLY:N	1:E:524:PRO:HB2	2.28	0.48
1:A:244:VAL:HB	1:A:256:LEU:HD21	1.96	0.48
1:A:401:THR:HA	1:A:404:GLN:CB	2.43	0.48
1:A:543:HIS:HE1	2:C:502:LEU:HA	1.77	0.48
1:A:617:TRP:HH2	2:D:133:THR:O	1.96	0.48
2:C:15:LEU:O	2:C:15:LEU:HD23	2.14	0.48
2:D:21:TRP:HB3	2:D:33:LYS:O	2.14	0.48
2:D:278:PHE:HE1	2:D:279:PHE:CD2	2.27	0.48
2:D:320:THR:OG1	2:D:323:LYS:HB2	2.13	0.48
2:D:423:GLU:O	2:D:426:LEU:N	2.46	0.48
1:B:263:PHE:HD1	1:B:263:PHE:H	1.61	0.48
1:B:347:HIS:HA	1:B:350:GLU:HB2	1.96	0.48
1:B:488:GLN:NE2	1:B:488:GLN:CA	2.73	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:ILE:HD13	1:B:552:MET:HE2	1.95	0.48
1:E:295:ILE:HG22	1:E:344:LEU:HD21	1.94	0.48
1:E:297:LEU:HB3	1:E:321:LEU:HD23	1.96	0.48
1:A:100:VAL:O	1:A:101:LYS:HD2	2.14	0.48
1:A:124:LEU:H	1:A:188:LEU:HD23	1.79	0.48
2:D:69:ASP:CB	2:D:84:ILE:HG12	2.44	0.48
2:D:334:LYS:HA	2:D:338:ASP:HB2	1.96	0.48
2:D:492:GLN:H	2:D:492:GLN:HG2	1.46	0.48
1:B:263:PHE:CD1	1:B:263:PHE:N	2.82	0.48
1:E:223:SER:O	1:E:227:GLU:N	2.47	0.48
1:E:282:LEU:HD23	1:E:295:ILE:HG23	1.94	0.48
1:E:394:LYS:HD2	1:E:395:ARG:N	2.28	0.48
1:E:452:THR:HB	1:E:454:PHE:HE2	1.79	0.48
1:E:531:SER:O	1:E:531:SER:OG	2.30	0.48
1:A:472:GLY:H	1:A:475:LYS:CB	2.27	0.48
2:C:88:TYR:O	2:C:92:LEU:HG	2.13	0.48
2:C:141:LEU:HD23	2:C:145:ARG:HH22	1.79	0.48
2:D:54:HIS:NE2	2:D:99:LEU:CD1	2.75	0.48
2:D:84:ILE:HD12	2:D:84:ILE:C	2.34	0.48
1:E:83:LEU:O	1:E:133:PHE:CD1	2.66	0.48
1:E:96:ARG:O	1:E:168:PHE:N	2.47	0.48
1:E:233:HIS:CG	1:E:263:PHE:HE2	2.30	0.48
2:F:337:LEU:CD1	2:F:341:ILE:HD11	2.44	0.48
2:C:291:MET:HE3	2:C:340:ILE:CG2	2.38	0.47
2:D:59:THR:OG1	2:D:155:LEU:CD1	2.62	0.47
2:D:133:THR:C	2:D:134:HIS:CD2	2.87	0.47
1:B:611:LYS:O	1:B:614:GLU:HG3	2.14	0.47
1:E:211:ASP:C	1:E:212:ARG:HG3	2.33	0.47
1:E:263:PHE:O	1:E:267:ILE:HG23	2.14	0.47
1:E:389:GLU:CB	1:E:394:LYS:HA	2.42	0.47
1:E:480:GLY:H	1:E:524:PRO:HG3	1.79	0.47
2:F:193:GLU:HG2	2:F:197:LYS:HD2	1.96	0.47
2:F:285:LEU:O	2:F:289:VAL:HG23	2.14	0.47
1:A:288:GLU:OE2	1:A:289:TYR:HE2	1.96	0.47
1:A:465:ALA:CA	2:C:494:TRP:CE3	2.88	0.47
1:A:584:PHE:CD1	1:A:584:PHE:C	2.86	0.47
1:A:590:SER:HG	2:C:184:ARG:NE	2.09	0.47
1:A:616:VAL:HG23	1:A:618:LYS:NZ	2.28	0.47
2:C:182:TYR:OH	2:F:183:ARG:HG2	2.14	0.47
2:D:55:VAL:HG21	2:D:159:TYR:CG	2.49	0.47
2:D:279:PHE:CE1	2:D:304:TRP:CE3	2.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:ARG:HB3	1:B:380:TYR:CE2	2.49	0.47
1:E:100:VAL:HG12	1:E:101:LYS:CE	2.43	0.47
1:E:182:TYR:HD1	1:E:183:ARG:N	2.12	0.47
1:E:444:ILE:CD1	1:E:581:GLU:OE1	2.63	0.47
1:E:471:TYR:CE2	1:E:523:PHE:CD1	3.01	0.47
1:E:495:ILE:HG21	1:E:523:PHE:HD2	1.78	0.47
2:F:333:GLN:HG3	2:F:370:TYR:CZ	2.49	0.47
1:A:114:SER:O	1:A:114:SER:OG	2.29	0.47
1:A:348:LEU:HD12	1:A:348:LEU:O	2.14	0.47
1:A:359:LEU:CD1	1:A:360:ASN:C	2.82	0.47
1:A:464:SER:C	2:C:494:TRP:CZ3	2.81	0.47
2:C:394:ARG:CG	2:C:394:ARG:NH1	2.73	0.47
2:D:86:LEU:HD12	2:D:138:LEU:HD22	1.89	0.47
1:B:583:PRO:HG2	1:B:586:ASP:HB3	1.97	0.47
1:E:289:TYR:CG	1:E:317:PHE:CD2	2.99	0.47
1:E:481:ILE:HG13	1:E:524:PRO:O	2.14	0.47
1:E:537:ILE:C	1:E:538:THR:HG1	2.17	0.47
2:F:324:ARG:HB3	2:F:324:ARG:HH11	1.78	0.47
1:A:367:GLY:O	2:D:124:TRP:HB3	2.14	0.47
2:C:209:PHE:HE2	2:C:254:ILE:CG1	2.25	0.47
2:C:387:ASN:CA	2:C:391:ASN:HD21	2.28	0.47
2:D:112:LEU:HD23	2:D:112:LEU:H	1.73	0.47
2:D:209:PHE:CE1	2:D:254:ILE:HG22	2.45	0.47
2:D:329:TRP:CZ3	2:D:424:ILE:CD1	2.97	0.47
1:E:361:LEU:CD2	1:E:376:ILE:HD11	2.44	0.47
1:E:383:THR:C	1:E:384:HIS:CD2	2.88	0.47
1:A:97:LEU:O	1:A:118:LEU:CD2	2.63	0.47
1:A:184:ASP:N	1:A:184:ASP:OD1	2.48	0.47
1:A:330:PRO:HG3	1:A:337:TYR:CE2	2.49	0.47
2:C:54:HIS:HD2	2:C:98:GLY:O	1.98	0.47
2:C:232:ASP:OD1	2:C:232:ASP:N	2.47	0.47
2:C:333:GLN:HG2	2:C:338:ASP:OD2	2.14	0.47
1:B:230:TYR:HE1	1:B:263:PHE:CD1	2.20	0.47
1:E:71:TYR:CD1	1:E:80:PHE:HE2	2.26	0.47
1:E:109:VAL:HG21	1:E:111:TYR:OH	2.12	0.47
1:E:199:ASN:HB3	1:E:202:THR:CG2	2.28	0.47
1:E:491:ASN:HB2	1:E:494:ASP:OD1	2.15	0.47
1:A:462:LEU:HD11	2:C:499:PHE:CD2	2.49	0.47
2:C:85:ARG:HE	2:C:138:LEU:HD12	1.79	0.47
2:C:133:THR:HG21	2:D:93:ILE:HG21	1.93	0.47
2:C:163:GLU:O	2:C:165:LEU:HD13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:79:GLN:NE2	2:D:79:GLN:CA	2.73	0.47
2:D:163:GLU:O	2:D:165:LEU:HD22	2.14	0.47
2:D:358:LYS:C	2:D:361:ASP:OD2	2.51	0.47
1:B:408:THR:CB	1:B:415:ALA:H	2.26	0.47
1:E:387:PHE:CE1	1:E:401:THR:HG23	2.48	0.47
1:E:587:PHE:HD2	1:E:587:PHE:C	2.18	0.47
2:F:278:PHE:C	2:F:278:PHE:CD2	2.86	0.47
1:A:83:LEU:O	1:A:133:PHE:CG	2.68	0.47
1:A:271:THR:HA	1:A:272:THR:HA	1.45	0.47
1:A:390:THR:OG1	1:A:422:PRO:CA	2.62	0.47
1:A:531:SER:O	1:A:534:LYS:HG3	2.14	0.47
1:A:543:HIS:CE1	2:C:502:LEU:HA	2.50	0.47
1:A:562:GLN:O	1:A:566:LYS:N	2.48	0.47
2:C:14:GLU:O	2:C:17:GLU:HB3	2.14	0.47
2:C:85:ARG:NH1	1:B:486:GLU:OE1	2.48	0.47
2:C:136:ARG:HA	1:B:617:TRP:CG	2.48	0.47
2:C:271:HIS:ND1	2:C:300:LYS:HE3	2.30	0.47
2:C:337:LEU:HD23	2:C:337:LEU:C	2.35	0.47
1:B:167:VAL:O	1:B:204:TYR:OH	2.33	0.47
1:B:207:LEU:CD1	1:B:213:ILE:HD13	2.38	0.47
1:B:288:GLU:O	1:B:289:TYR:HB2	2.14	0.47
1:B:331:GLN:HG3	1:B:364:TRP:HZ2	1.80	0.47
1:B:358:LEU:HD22	1:B:358:LEU:H	1.77	0.47
1:B:590:SER:H	1:B:593:THR:HG1	1.59	0.47
1:E:206:LEU:O	1:E:207:LEU:HD23	2.14	0.47
1:E:301:LEU:CD1	1:E:301:LEU:N	2.73	0.47
1:E:502:THR:O	1:E:541:LEU:HD12	2.14	0.47
2:F:8:PRO:CD	2:F:51:TYR:O	2.63	0.47
2:F:34:ARG:O	2:F:35:GLN:C	2.50	0.47
2:F:96:VAL:HG11	2:F:129:ARG:HD2	1.95	0.47
1:A:73:GLY:CA	1:A:78:THR:HG23	2.40	0.47
1:A:462:LEU:HD11	2:C:499:PHE:CE2	2.50	0.47
1:A:470:SER:HB3	2:C:485:VAL:CG2	2.44	0.47
1:A:589:PRO:HD3	1:A:596:TRP:CH2	2.29	0.47
2:C:34:ARG:HA	2:C:37:ALA:HB3	1.97	0.47
2:D:113:HIS:ND1	2:D:113:HIS:N	2.62	0.47
2:D:278:PHE:HZ	2:D:287:LEU:HD13	1.78	0.47
1:B:469:ILE:HG12	1:B:552:MET:HB3	1.95	0.47
1:E:235:ASN:N	1:E:235:ASN:ND2	2.60	0.47
1:E:324:TYR:CB	1:E:536:PHE:HE2	2.25	0.47
1:E:471:TYR:O	1:E:550:GLN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:ILE:HD11	1:E:554:ILE:HD11	1.97	0.47
2:F:110:ILE:HG23	2:F:111:PRO:HD2	1.97	0.47
2:F:207:ASN:O	2:F:211:GLU:HG3	2.14	0.47
1:A:77:GLU:HG3	1:A:201:ARG:C	2.35	0.47
1:A:99:VAL:HB	1:A:113:ALA:CB	2.45	0.47
1:A:242:ILE:HB	1:A:358:LEU:HD23	1.96	0.47
2:C:310:ARG:CG	2:C:310:ARG:NH1	2.73	0.47
2:D:47:LYS:HG2	1:B:502:THR:HG21	1.97	0.47
2:D:111:PRO:HG2	2:D:114:THR:CB	2.45	0.47
2:D:184:ARG:CG	1:B:592:ARG:HD3	2.44	0.47
2:D:346:ASN:HD22	2:D:382:GLU:CD	2.17	0.47
1:B:395:ARG:CD	1:B:396:HIS:N	2.78	0.47
1:B:531:SER:O	1:B:531:SER:OG	2.30	0.47
1:A:466:PRO:HD3	2:C:494:TRP:CZ2	2.50	0.47
1:A:490:LEU:HD11	2:C:43:SER:CB	2.44	0.47
1:E:175:LEU:HD23	1:E:175:LEU:C	2.35	0.47
1:E:178:ALA:O	1:E:458:PHE:CD1	2.68	0.47
1:E:224:THR:HB	1:E:225:PRO:HD3	1.96	0.47
1:E:295:ILE:HD11	1:E:337:TYR:HD2	1.78	0.47
1:E:361:LEU:HD21	1:E:376:ILE:CD1	2.45	0.47
1:E:592:ARG:NH2	1:E:592:ARG:CG	2.73	0.47
1:A:69:ILE:CG2	1:A:80:PHE:CB	2.92	0.46
1:A:198:LEU:CD2	1:A:205:HIS:HE2	2.28	0.46
1:A:226:LEU:CD1	1:A:230:TYR:HH	1.92	0.46
1:A:366:LYS:CG	1:A:396:HIS:HB3	2.34	0.46
1:A:469:ILE:HG23	2:C:488:TRP:CE3	2.49	0.46
2:C:128:LEU:HA	2:C:131:TRP:CB	2.45	0.46
2:C:332:LEU:HD23	2:C:332:LEU:O	2.14	0.46
2:D:494:TRP:CH2	2:D:497:LYS:CB	2.98	0.46
1:E:171:ASN:ND2	1:E:454:PHE:CD1	2.83	0.46
1:E:460:PRO:HG2	1:E:593:THR:HG22	1.98	0.46
2:F:158:HIS:O	2:F:162:ASP:CG	2.54	0.46
1:A:94:VAL:HG12	1:A:170:SER:CB	2.45	0.46
1:A:501:GLY:O	1:A:582:THR:HG21	2.14	0.46
2:C:92:LEU:N	2:C:92:LEU:CD2	2.73	0.46
2:D:11:ASP:OD1	2:D:13:ALA:HB3	2.15	0.46
2:D:139:PRO:CG	2:D:144:LEU:HD21	2.42	0.46
1:B:450:LYS:HA	1:B:456:TYR:HD1	1.80	0.46
1:E:398:ASP:OD2	1:E:398:ASP:N	2.40	0.46
1:E:431:SER:HG	1:E:434:PHE:N	2.02	0.46
1:A:214:GLN:HE21	1:A:214:GLN:HB3	1.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ILE:HD12	1:A:277:LEU:HD21	1.97	0.46
2:D:397:GLN:O	2:D:401:THR:HG23	2.15	0.46
1:B:79:MET:C	1:B:79:MET:SD	2.94	0.46
1:B:342:ASP:HA	1:B:345:ILE:HD12	1.98	0.46
1:B:364:TRP:CD1	1:B:372:ILE:CG2	2.86	0.46
1:B:524:PRO:O	1:B:524:PRO:HG2	2.15	0.46
2:F:84:ILE:HD12	2:F:84:ILE:HA	1.77	0.46
2:F:154:TRP:HE3	2:F:155:LEU:CA	2.28	0.46
1:A:71:TYR:CD2	1:A:71:TYR:C	2.89	0.46
1:A:79:MET:SD	1:A:79:MET:C	2.94	0.46
1:A:392:ASN:N	1:A:393:SER:CA	2.78	0.46
1:A:588:LEU:HD11	2:C:6:ILE:CD1	2.46	0.46
2:C:61:GLN:O	2:C:64:CYS:HB2	2.15	0.46
1:E:71:TYR:C	1:E:71:TYR:CD2	2.89	0.46
1:E:360:ASN:ND2	1:E:360:ASN:H	2.13	0.46
1:E:360:ASN:N	1:E:360:ASN:HD22	2.12	0.46
2:F:32:ASP:OD2	2:F:34:ARG:HG3	2.15	0.46
2:F:337:LEU:HD12	2:F:338:ASP:CA	2.45	0.46
1:A:364:TRP:HB3	1:A:369:GLY:HA3	1.97	0.46
1:A:554:ILE:HG12	1:A:555:TYR:N	2.31	0.46
1:A:587:PHE:HD2	1:A:587:PHE:O	1.97	0.46
1:A:603:PRO:O	2:C:10:ARG:C	2.53	0.46
2:C:130:HIS:CG	2:C:134:HIS:ND1	2.83	0.46
2:D:96:VAL:HG12	2:D:100:LEU:CB	2.46	0.46
2:D:222:SER:O	2:D:222:SER:OG	2.28	0.46
1:B:90:HIS:CE1	1:B:128:ILE:HG12	2.43	0.46
1:B:175:LEU:C	1:B:458:PHE:CZ	2.89	0.46
1:B:347:HIS:NE2	1:B:351:GLN:OE1	2.48	0.46
1:E:228:LYS:HB2	1:E:228:LYS:HE2	1.58	0.46
1:E:387:PHE:HE1	1:E:401:THR:HG21	1.75	0.46
1:E:528:SER:C	1:E:529:CYS:SG	2.94	0.46
2:F:335:ARG:HH11	2:F:335:ARG:HG3	1.78	0.46
1:A:229:LEU:HD11	1:A:386:LEU:HD11	1.96	0.46
2:C:360:ILE:HD13	2:C:372:CYS:SG	2.56	0.46
2:D:167:ASP:HA	1:B:612:LYS:HG2	1.96	0.46
1:B:389:GLU:CG	1:B:394:LYS:HA	2.45	0.46
1:E:280:LEU:HB3	1:E:359:LEU:HB2	1.97	0.46
1:E:487:PHE:CZ	2:F:46:LEU:HA	2.51	0.46
2:F:100:LEU:N	2:F:100:LEU:CD2	2.73	0.46
1:A:607:PHE:HE1	2:C:4:PRO:CG	1.83	0.46
2:C:125:PHE:HD1	2:C:128:LEU:HD23	1.75	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:LEU:O	2:D:46:LEU:HD23	2.16	0.46
2:D:55:VAL:HG13	2:D:159:TYR:CE2	2.50	0.46
1:B:114:SER:O	1:B:114:SER:OG	2.30	0.46
1:B:216:LEU:HD23	1:B:217:SER:H	1.75	0.46
1:E:501:GLY:CA	2:F:499:PHE:CD1	2.99	0.46
2:F:278:PHE:CE2	2:F:282:TYR:CB	2.99	0.46
1:A:83:LEU:N	1:A:83:LEU:CD2	2.73	0.46
1:A:84:LYS:CB	1:A:139:TRP:C	2.84	0.46
1:A:118:LEU:HD12	1:A:120:PHE:CZ	2.50	0.46
2:C:125:PHE:CB	2:C:128:LEU:HD21	2.44	0.46
2:D:14:GLU:O	2:D:17:GLU:HG2	2.16	0.46
2:D:278:PHE:CZ	2:D:287:LEU:HD13	2.51	0.46
2:D:358:LYS:N	2:D:361:ASP:OD2	2.48	0.46
1:B:330:PRO:HD2	1:B:364:TRP:HZ2	1.70	0.46
1:B:347:HIS:CD2	1:B:347:HIS:C	2.87	0.46
1:B:353:PHE:CG	1:B:354:PHE:N	2.84	0.46
1:B:388:LEU:N	1:B:388:LEU:CD1	2.73	0.46
1:B:431:SER:HB2	1:B:434:PHE:O	2.16	0.46
1:E:369:GLY:O	1:E:372:ILE:HG22	2.16	0.46
1:E:376:ILE:HA	1:E:379:LYS:HB3	1.97	0.46
1:E:491:ASN:HD22	2:F:36:ARG:NE	2.00	0.46
1:E:562:GLN:HB2	1:E:565:ASP:CB	2.45	0.46
2:F:280:ASN:OD1	2:F:321:ILE:CG2	2.63	0.46
2:C:291:MET:SD	2:C:340:ILE:HG23	2.56	0.46
2:C:387:ASN:C	2:C:391:ASN:HD21	2.19	0.46
2:D:184:ARG:CD	1:B:592:ARG:HD3	2.44	0.46
2:D:283:ASP:OD1	2:D:285:LEU:HB2	2.16	0.46
1:B:177:GLU:OE2	1:B:456:TYR:O	2.34	0.46
1:B:297:LEU:HB3	1:B:321:LEU:HD22	1.95	0.46
1:B:467:LEU:HD23	1:B:467:LEU:C	2.36	0.46
1:E:169:ASN:HD21	1:E:203:THR:HG23	1.79	0.46
1:E:245:ILE:CG2	1:E:387:PHE:HE2	2.28	0.46
1:E:291:LEU:O	1:E:294:SER:HB3	2.14	0.46
1:E:536:PHE:HZ	1:E:539:LEU:HD23	1.81	0.46
1:E:543:HIS:CE1	2:F:494:TRP:HZ2	2.34	0.46
2:F:79:GLN:O	2:F:79:GLN:HG2	2.16	0.46
2:F:322:LEU:HD21	2:F:332:LEU:CD1	2.45	0.46
1:A:81:VAL:H	1:A:166:ARG:CG	2.28	0.46
1:A:169:ASN:CB	1:A:203:THR:CG2	2.93	0.46
1:A:196:PHE:CE1	1:A:197:PRO:HD2	2.51	0.46
1:A:366:LYS:HG2	1:A:395:ARG:CZ	2.37	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:MET:O	1:A:374:ASN:CB	2.64	0.46
2:C:9:TRP:HA	2:C:14:GLU:OE2	2.15	0.46
2:C:116:ALA:HB2	2:C:126:VAL:HG21	1.98	0.46
2:C:327:ASN:OD1	2:C:331:GLU:OE2	2.34	0.46
2:D:371:PHE:CZ	2:D:375:MET:HG3	2.51	0.46
1:B:271:THR:HA	1:B:272:THR:HA	1.58	0.46
1:B:541:LEU:O	1:B:554:ILE:HG13	2.15	0.46
1:E:96:ARG:HB3	1:E:119:THR:HG22	1.97	0.46
1:E:241:ARG:HH11	1:E:381:LYS:HD2	1.80	0.46
2:F:362:GLU:O	2:F:363:ASN:ND2	2.39	0.46
1:A:264:THR:HG22	1:A:268:ARG:HD3	1.97	0.45
1:A:498:ALA:O	1:A:502:THR:HG23	2.16	0.45
1:A:534:LYS:HG3	1:A:534:LYS:H	1.50	0.45
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.31	0.45
2:C:21:TRP:CZ3	2:C:36:ARG:HG3	2.51	0.45
2:D:346:ASN:N	2:D:346:ASN:OD1	2.49	0.45
2:D:377:ALA:O	2:D:381:THR:HG23	2.15	0.45
2:D:488:TRP:HE3	1:B:467:LEU:HG	1.81	0.45
1:B:507:TYR:CD1	1:B:535:ASN:O	2.69	0.45
1:E:98:GLN:HB2	1:E:117:ILE:HG22	1.95	0.45
1:E:105:VAL:CG1	1:E:108:ASN:HA	2.45	0.45
1:E:289:TYR:CD1	1:E:317:PHE:CE2	3.03	0.45
2:F:83:PRO:O	2:F:86:LEU:HB2	2.15	0.45
1:A:246:GLY:O	1:A:363:GLY:HA2	2.09	0.45
1:A:299:LYS:HB2	1:A:320:LEU:HD11	1.98	0.45
1:B:93:GLY:N	1:B:122:HIS:HB3	2.31	0.45
1:B:110:HIS:CD2	1:B:111:TYR:N	2.84	0.45
1:B:321:LEU:CD1	1:B:347:HIS:HD1	2.20	0.45
1:E:208:HIS:ND1	1:E:210:SER:N	2.60	0.45
1:E:432:SER:O	1:E:432:SER:OG	2.31	0.45
1:E:504:ILE:HD13	1:E:575:ILE:HD13	1.98	0.45
2:F:122:PRO:HB2	2:F:124:TRP:CD1	2.49	0.45
2:F:372:CYS:CB	2:F:412:ILE:HD11	2.46	0.45
2:F:376:LEU:O	2:F:380:GLU:N	2.50	0.45
1:A:123:PRO:HG3	1:A:311:LEU:HD21	1.98	0.45
1:A:173:THR:O	1:A:177:GLU:OE2	2.35	0.45
1:A:289:TYR:HD1	1:A:298:ASN:HD21	1.63	0.45
1:A:326:GLY:N	1:A:578:ASN:ND2	2.59	0.45
1:A:588:LEU:HD21	1:A:605:ALA:CB	2.47	0.45
2:D:113:HIS:O	2:D:116:ALA:HB3	2.14	0.45
2:D:154:TRP:HE3	2:D:155:LEU:N	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:288:LYS:CG	2:D:343:ASN:ND2	2.74	0.45
2:D:312:GLN:HE22	2:D:323:LYS:HG3	0.43	0.45
1:B:174:GLY:C	1:B:458:PHE:CE2	2.67	0.45
1:E:109:VAL:HG21	1:E:111:TYR:CZ	2.50	0.45
1:E:375:HIS:O	1:E:378:ARG:HB3	2.17	0.45
1:A:194:PRO:HG3	1:A:198:LEU:CD2	2.46	0.45
1:A:540:GLY:HA3	1:A:554:ILE:HD11	1.99	0.45
2:C:110:ILE:HG22	2:C:111:PRO:O	2.15	0.45
1:B:451:ILE:N	1:B:451:ILE:CD1	2.73	0.45
1:B:506:ILE:CD1	1:B:540:GLY:HA3	2.45	0.45
1:B:536:PHE:HD1	1:B:536:PHE:C	2.19	0.45
1:E:389:GLU:CG	1:E:393:SER:O	2.64	0.45
1:E:399:GLU:OE2	1:E:400:LEU:HA	2.15	0.45
1:E:454:PHE:HD2	1:E:454:PHE:H	1.62	0.45
1:E:592:ARG:HD2	1:E:592:ARG:O	2.16	0.45
2:F:146:TRP:NE1	2:F:150:GLU:OE1	2.46	0.45
1:A:116:GLU:O	1:A:118:LEU:HD23	2.17	0.45
1:A:187:TYR:CD2	1:A:192:LYS:CB	2.98	0.45
1:A:190:LYS:NZ	1:A:202:THR:O	2.43	0.45
1:A:313:GLN:CG	1:A:456:TYR:OH	2.61	0.45
2:C:36:ARG:HA	2:C:39:GLN:HE21	1.82	0.45
1:B:392:ASN:N	1:B:393:SER:CA	2.77	0.45
1:E:481:ILE:HA	1:E:575:ILE:O	2.17	0.45
2:F:45:ARG:NH2	2:F:61:GLN:HE21	2.14	0.45
1:A:88:LYS:H	1:A:88:LYS:HG3	1.59	0.45
2:D:220:ASN:O	2:D:220:ASN:ND2	2.50	0.45
2:D:502:LEU:CB	1:B:546:ASP:OD1	2.65	0.45
1:B:90:HIS:CG	1:B:207:LEU:HB2	2.51	0.45
1:E:76:ASP:C	1:E:77:GLU:HG2	2.37	0.45
1:E:537:ILE:O	1:E:538:THR:OG1	2.32	0.45
2:F:89:VAL:HG21	2:F:138:LEU:HD23	1.98	0.45
1:A:294:SER:OG	1:A:295:ILE:N	2.50	0.45
1:A:348:LEU:CD1	1:A:353:PHE:CB	2.86	0.45
2:C:53:PRO:CG	2:C:56:VAL:CG2	2.94	0.45
1:B:467:LEU:CD2	1:B:467:LEU:N	2.80	0.45
1:A:223:SER:O	1:A:227:GLU:CB	2.65	0.45
1:A:255:PHE:CE2	1:A:259:LEU:HD22	2.51	0.45
1:A:607:PHE:CE2	2:C:4:PRO:HB3	2.37	0.45
2:C:359:LEU:C	2:C:359:LEU:CD2	2.85	0.45
2:D:426:LEU:O	2:D:430:ILE:CD1	2.65	0.45
1:E:241:ARG:HB2	1:E:383:THR:OG1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:365:ILE:HD13	1:E:366:LYS:N	2.29	0.45
1:E:562:GLN:CB	1:E:565:ASP:CB	2.95	0.45
2:F:156:TYR:CZ	2:F:161:ASN:ND2	2.82	0.45
2:F:389:TRP:NE1	2:F:390:ARG:CD	2.73	0.45
1:A:83:LEU:HD23	1:A:166:ARG:CZ	2.47	0.45
1:A:123:PRO:HD3	1:A:309:GLN:O	2.17	0.45
1:A:326:GLY:N	1:A:578:ASN:HD22	2.13	0.45
1:A:392:ASN:CB	1:A:393:SER:C	2.85	0.45
2:C:34:ARG:HH21	2:C:67:LEU:HG	1.81	0.45
2:C:82:ILE:HG23	2:C:83:PRO:HD3	1.98	0.45
2:C:128:LEU:HA	2:C:131:TRP:HB2	1.99	0.45
2:C:235:VAL:CG1	2:C:236:ASN:N	2.79	0.45
2:C:314:ASP:CB	2:C:495:LYS:HZ3	2.30	0.45
1:B:317:PHE:CD2	1:B:317:PHE:O	2.70	0.45
1:E:95:PHE:CD2	1:E:95:PHE:O	2.70	0.45
1:E:194:PRO:CB	1:E:205:HIS:CE1	2.91	0.45
1:E:425:SER:OG	1:E:426:LEU:HA	2.16	0.45
1:E:452:THR:OG1	1:E:454:PHE:CD2	2.70	0.45
1:E:473:LYS:CD	1:E:474:GLY:N	2.80	0.45
1:E:523:PHE:HB3	1:E:525:ILE:HD11	1.98	0.45
2:F:108:PHE:CG	2:F:108:PHE:O	2.70	0.45
2:F:332:LEU:C	2:F:332:LEU:CD2	2.85	0.45
1:A:396:HIS:O	1:A:396:HIS:CD2	2.70	0.45
1:A:613:LEU:O	1:A:615:HIS:CE1	2.70	0.45
2:C:50:GLN:OE1	2:C:51:TYR:CE2	2.70	0.45
2:C:107:GLN:OE1	2:C:108:PHE:CD2	2.70	0.45
2:D:17:GLU:O	2:D:21:TRP:CD1	2.70	0.45
1:B:473:LYS:CG	1:B:474:GLY:N	2.80	0.45
1:B:599:ASN:ND2	1:B:600:ILE:CD1	2.73	0.45
1:E:331:GLN:HG3	1:E:364:TRP:HZ2	0.30	0.45
1:E:460:PRO:HG2	1:E:593:THR:CG2	2.47	0.45
2:F:12:PHE:O	2:F:12:PHE:CD1	2.70	0.45
2:F:52:LEU:HD21	2:F:57:ASP:CA	2.46	0.45
1:A:606:THR:HG23	2:C:5:ARG:HH11	1.80	0.44
2:C:84:ILE:O	2:C:88:TYR:CD2	2.70	0.44
2:C:130:HIS:CB	2:C:134:HIS:CE1	3.01	0.44
2:C:364:ALA:H	2:C:493:ASN:ND2	2.14	0.44
2:D:82:ILE:CG2	2:D:83:PRO:N	2.80	0.44
2:D:133:THR:OG1	2:D:134:HIS:CD2	2.70	0.44
2:D:237:TYR:CD1	2:D:237:TYR:O	2.71	0.44
2:D:323:LYS:HD2	2:D:430:ILE:HG13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:LEU:CB	1:B:456:TYR:CD2	2.67	0.44
1:E:76:ASP:C	1:E:77:GLU:CG	2.85	0.44
1:E:181:LEU:C	1:E:181:LEU:CD1	2.86	0.44
1:E:241:ARG:CB	1:E:383:THR:OG1	2.65	0.44
1:E:306:SER:C	1:E:307:LEU:CD1	2.85	0.44
2:F:275:LEU:HB3	2:F:279:PHE:HE2	1.82	0.44
2:F:349:PHE:CD2	2:F:349:PHE:O	2.70	0.44
1:A:168:PHE:HD1	1:A:168:PHE:N	2.15	0.44
1:A:288:GLU:OE2	1:A:289:TYR:CE2	2.70	0.44
1:A:339:ASN:O	1:A:343:LYS:CG	2.64	0.44
2:D:99:LEU:C	2:D:102:PRO:CD	2.86	0.44
1:B:294:SER:OG	1:B:323:PHE:O	2.29	0.44
1:E:208:HIS:CG	1:E:209:GLU:N	2.85	0.44
1:E:257:ARG:NE	1:E:308:GLY:O	2.50	0.44
1:A:168:PHE:CD1	1:A:168:PHE:O	2.70	0.44
1:A:195:TYR:O	1:A:195:TYR:CD1	2.70	0.44
1:A:617:TRP:C	1:A:618:LYS:CG	2.85	0.44
2:C:51:TYR:N	2:C:51:TYR:CD2	2.84	0.44
2:C:62:ILE:O	2:C:65:ALA:N	2.50	0.44
2:C:122:PRO:HD2	2:C:125:PHE:CD2	2.52	0.44
2:C:224:ILE:HG21	2:C:229:PHE:CZ	2.40	0.44
2:D:298:ASP:OD1	2:D:299:TRP:N	2.50	0.44
2:D:488:TRP:CH2	1:B:469:ILE:HG21	2.52	0.44
1:B:260:LEU:HD23	1:B:277:LEU:HD12	1.99	0.44
2:F:156:TYR:HA	2:F:160:TRP:HB2	2.00	0.44
1:A:128:ILE:O	1:A:215:SER:HA	2.18	0.44
1:A:188:LEU:O	1:A:188:LEU:HD23	2.17	0.44
1:A:388:LEU:HG	1:A:421:VAL:CG2	2.47	0.44
1:A:445:LEU:HD13	1:A:583:PRO:HG3	2.00	0.44
1:A:469:ILE:HD12	2:C:488:TRP:CZ2	2.41	0.44
1:A:471:TYR:CE2	1:A:522:THR:O	2.71	0.44
1:A:589:PRO:HB2	1:A:594:ILE:HG13	1.98	0.44
2:D:4:PRO:N	1:B:607:PHE:HE1	2.15	0.44
2:D:291:MET:HE1	2:D:340:ILE:HG23	1.98	0.44
2:D:349:PHE:CE1	2:D:375:MET:HE2	2.52	0.44
1:B:243:MET:HE2	1:B:243:MET:HB2	1.85	0.44
1:B:347:HIS:CD2	1:B:347:HIS:O	2.70	0.44
1:E:261:GLU:HG2	1:E:307:LEU:HD23	1.98	0.44
1:E:394:LYS:C	1:E:394:LYS:CD	2.86	0.44
1:E:477:GLY:C	1:E:478:ILE:HG13	2.37	0.44
2:F:278:PHE:O	2:F:278:PHE:CD2	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:CA	1:A:168:PHE:HE1	2.31	0.44
2:C:310:ARG:HH21	2:C:314:ASP:CG	2.12	0.44
2:C:364:ALA:H	2:C:493:ASN:HD21	1.65	0.44
2:D:146:TRP:C	2:D:146:TRP:CD2	2.90	0.44
1:B:471:TYR:CD1	1:B:471:TYR:O	2.71	0.44
1:E:271:THR:HA	1:E:272:THR:HA	1.64	0.44
1:E:342:ASP:OD2	1:E:375:HIS:NE2	2.38	0.44
1:E:389:GLU:CD	1:E:392:ASN:CB	2.86	0.44
1:E:495:ILE:HG21	1:E:523:PHE:CD2	2.52	0.44
1:E:501:GLY:HA2	2:F:499:PHE:CE1	2.53	0.44
1:E:588:LEU:HD21	2:F:6:ILE:HD13	1.98	0.44
2:F:411:ASN:O	2:F:414:ASN:HB3	2.18	0.44
1:A:260:LEU:CD2	1:A:277:LEU:HD12	2.48	0.44
1:A:317:PHE:CD2	1:A:317:PHE:O	2.70	0.44
1:A:347:HIS:CE1	1:A:351:GLN:OE1	2.70	0.44
2:D:128:LEU:C	2:D:128:LEU:CD2	2.86	0.44
2:D:403:GLU:O	2:D:407:LYS:HG3	2.18	0.44
1:B:172:HIS:CB	1:B:454:PHE:O	2.66	0.44
1:E:313:GLN:OE1	1:E:450:LYS:NZ	2.50	0.44
2:F:499:PHE:N	2:F:499:PHE:CD2	2.84	0.44
1:A:491:ASN:HD22	2:C:36:ARG:HD3	1.81	0.44
1:A:603:PRO:HB2	1:A:604:PHE:CD2	2.51	0.44
2:C:107:GLN:OE1	2:C:108:PHE:CZ	2.71	0.44
2:C:337:LEU:C	2:C:337:LEU:CD2	2.86	0.44
1:B:463:LYS:HE2	1:B:594:ILE:HG12	1.98	0.44
2:F:159:TYR:C	2:F:159:TYR:CD2	2.91	0.44
2:F:278:PHE:CD2	2:F:282:TYR:HA	2.53	0.44
1:A:195:TYR:O	1:A:195:TYR:CG	2.70	0.44
1:A:280:LEU:HG	1:A:297:LEU:HD12	1.98	0.44
1:A:306:SER:C	1:A:307:LEU:HD12	2.37	0.44
1:A:353:PHE:CD1	1:A:354:PHE:N	2.86	0.44
1:A:365:ILE:CD1	1:A:366:LYS:N	2.77	0.44
1:A:613:LEU:O	1:A:615:HIS:ND1	2.51	0.44
1:A:614:GLU:O	1:A:614:GLU:HG3	2.17	0.44
2:C:84:ILE:O	2:C:88:TYR:HD2	2.00	0.44
2:C:202:TRP:CZ2	2:C:286:LEU:HD12	2.53	0.44
1:B:103:GLY:O	1:B:134:SER:CA	2.65	0.44
1:E:311:LEU:O	1:E:312:CYS:HB2	2.17	0.44
1:E:385:LEU:HD22	1:E:387:PHE:CE2	2.52	0.44
1:E:389:GLU:HG2	1:E:397:LEU:HD11	2.00	0.44
1:E:462:LEU:O	2:F:494:TRP:HZ3	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:496:LYS:HG2	1:E:500:GLU:OE2	2.17	0.44
1:E:562:GLN:H	1:E:562:GLN:CD	2.20	0.44
2:F:108:PHE:CD2	2:F:108:PHE:O	2.70	0.44
2:F:278:PHE:CE2	2:F:282:TYR:CA	3.00	0.44
1:A:485:MET:H	1:A:485:MET:HG2	1.58	0.44
1:A:515:LEU:H	1:A:515:LEU:HG	1.57	0.44
1:A:543:HIS:CE1	2:C:502:LEU:C	2.89	0.44
2:D:102:PRO:O	2:D:104:GLN:NE2	2.51	0.44
1:B:89:LEU:HD13	1:B:90:HIS:CA	2.47	0.44
1:B:265:GLN:HA	1:B:265:GLN:OE1	2.17	0.44
1:B:273:SER:HB3	1:B:275:GLU:HG2	1.99	0.44
1:E:103:GLY:C	1:E:104:ILE:CD1	2.85	0.44
1:E:317:PHE:O	1:E:317:PHE:CD1	2.70	0.44
1:E:482:GLN:HE21	1:E:576:VAL:CG1	2.31	0.44
2:F:309:TYR:OH	2:F:423:GLU:OE2	2.36	0.44
1:A:105:VAL:CG1	1:A:132:ASP:OD2	2.62	0.43
1:A:166:ARG:HB3	1:A:167:VAL:H	1.60	0.43
1:A:248:LYS:H	1:A:248:LYS:HG2	1.56	0.43
1:A:473:LYS:H	1:A:473:LYS:HG2	1.45	0.43
2:C:54:HIS:HE1	2:C:58:SER:OG	2.00	0.43
2:C:107:GLN:OE1	2:C:108:PHE:CD1	2.71	0.43
2:C:107:GLN:OE1	2:C:108:PHE:CG	2.71	0.43
2:C:278:PHE:CZ	2:C:287:LEU:HD12	2.52	0.43
2:C:285:LEU:O	2:C:285:LEU:HD22	2.18	0.43
2:D:188:LEU:CD1	2:D:192:MET:HG3	2.48	0.43
2:D:356:TRP:O	2:D:360:ILE:CB	2.66	0.43
1:B:108:ASN:ND2	1:B:108:ASN:O	2.51	0.43
1:B:122:HIS:HE1	1:B:128:ILE:CD1	2.31	0.43
1:B:421:VAL:O	1:B:421:VAL:HG23	2.18	0.43
1:E:494:ASP:OD1	1:E:494:ASP:N	2.47	0.43
1:E:587:PHE:O	1:E:587:PHE:CD2	2.71	0.43
2:F:17:GLU:CG	2:F:21:TRP:CE2	3.01	0.43
1:A:255:PHE:HE2	1:A:259:LEU:HD21	1.83	0.43
2:C:332:LEU:C	2:C:332:LEU:CD2	2.85	0.43
2:D:389:TRP:CD1	2:D:389:TRP:O	2.70	0.43
1:B:405:SER:O	1:B:406:PHE:C	2.55	0.43
1:E:348:LEU:HB3	1:E:349:GLU:OE1	2.19	0.43
1:E:469:ILE:CG2	1:E:470:SER:H	2.22	0.43
2:F:101:ASP:N	2:F:102:PRO:CD	2.82	0.43
2:F:352:LYS:HE3	2:F:352:LYS:HB2	1.94	0.43
1:A:368:PHE:CD2	1:A:368:PHE:O	2.70	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:PHE:CD1	2:C:128:LEU:HD21	2.51	0.43
2:C:329:TRP:CD1	2:C:424:ILE:CG2	3.02	0.43
1:B:90:HIS:CE1	1:B:128:ILE:HD13	2.30	0.43
1:B:97:LEU:HD13	1:B:120:PHE:CE1	2.53	0.43
1:B:368:PHE:O	1:B:372:ILE:N	2.48	0.43
1:B:591:PRO:O	1:B:592:ARG:CB	2.49	0.43
1:E:133:PHE:HD2	1:E:134:SER:N	2.15	0.43
1:E:424:HIS:CD2	1:E:424:HIS:O	2.70	0.43
1:E:424:HIS:O	1:E:424:HIS:CG	2.70	0.43
1:E:509:TYR:HE1	1:E:533:SER:HB3	1.83	0.43
1:E:541:LEU:HD12	1:E:542:ILE:H	1.83	0.43
2:F:81:SER:O	2:F:84:ILE:HG22	2.17	0.43
2:F:98:GLY:O	2:F:102:PRO:HB3	2.18	0.43
2:F:99:LEU:C	2:F:102:PRO:CD	2.86	0.43
2:F:426:LEU:HD23	2:F:426:LEU:HA	1.89	0.43
1:A:98:GLN:CG	1:A:115:ARG:C	2.82	0.43
1:A:105:VAL:HG12	1:A:132:ASP:HB2	1.96	0.43
1:A:389:GLU:HB3	1:A:394:LYS:HB3	1.98	0.43
1:A:420:ARG:HH21	1:A:420:ARG:CG	2.23	0.43
1:A:502:THR:HG22	1:A:577:ARG:HH22	1.84	0.43
1:A:505:GLY:HA2	1:A:539:LEU:HA	1.99	0.43
1:A:541:LEU:C	1:A:541:LEU:CD1	2.85	0.43
1:A:561:THR:CG2	1:A:562:GLN:HA	2.48	0.43
2:C:90:MET:CB	2:D:86:LEU:HG	2.45	0.43
2:C:107:GLN:OE1	2:C:108:PHE:CE1	2.70	0.43
2:C:209:PHE:CD2	2:C:254:ILE:HG12	2.53	0.43
2:D:358:LYS:HG2	2:D:358:LYS:H	1.58	0.43
2:D:365:SER:O	2:D:368:ILE:N	2.51	0.43
2:D:427:TYR:CD2	2:D:427:TYR:O	2.70	0.43
1:B:175:LEU:HD12	1:B:458:PHE:HZ	1.84	0.43
1:B:194:PRO:CG	1:B:205:HIS:NE2	2.81	0.43
1:B:317:PHE:O	1:B:317:PHE:HD2	2.01	0.43
1:B:366:LYS:HD3	1:B:395:ARG:NH1	2.33	0.43
1:E:277:LEU:HD23	1:E:277:LEU:H	1.83	0.43
1:E:518:LYS:O	1:E:525:ILE:O	2.36	0.43
2:F:337:LEU:C	2:F:337:LEU:CD1	2.86	0.43
1:A:170:SER:OG	1:A:172:HIS:CE1	2.70	0.43
1:A:341:ALA:O	1:A:344:LEU:N	2.50	0.43
1:A:451:ILE:C	1:A:452:THR:CG2	2.86	0.43
2:C:209:PHE:CD2	2:C:254:ILE:HD13	2.51	0.43
2:C:333:GLN:HA	2:C:337:LEU:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:389:TRP:CE3	2:C:389:TRP:HA	2.52	0.43
2:D:212:TYR:OH	2:D:250:SER:OG	2.36	0.43
2:D:488:TRP:CZ3	1:B:469:ILE:CG2	3.01	0.43
1:B:208:HIS:O	1:B:210:SER:N	2.41	0.43
1:B:395:ARG:C	1:B:395:ARG:CD	2.86	0.43
1:B:453:GLN:H	1:B:453:GLN:HG2	1.49	0.43
1:E:189:TRP:HA	1:E:189:TRP:CE3	2.54	0.43
1:E:234:LYS:HA	1:E:234:LYS:HD2	1.74	0.43
1:E:252:LYS:HE3	1:E:361:LEU:O	2.19	0.43
1:E:617:TRP:O	1:E:617:TRP:CD1	2.70	0.43
2:F:17:GLU:HG2	2:F:21:TRP:CE2	2.53	0.43
2:F:333:GLN:CB	2:F:337:LEU:HD21	2.46	0.43
1:A:177:GLU:HG2	2:C:267:LEU:HD22	1.99	0.43
1:A:549:GLN:HB3	1:A:551:ILE:HG23	2.01	0.43
2:C:107:GLN:OE1	2:C:108:PHE:CE2	2.70	0.43
2:C:340:ILE:H	2:C:340:ILE:HG13	1.56	0.43
2:D:188:LEU:HD12	2:D:192:MET:HG2	2.00	0.43
2:D:330:LYS:O	2:D:334:LYS:CG	2.66	0.43
1:B:94:VAL:C	1:B:95:PHE:CD1	2.92	0.43
1:B:111:TYR:CE1	1:B:265:GLN:HB2	2.54	0.43
1:B:178:ALA:HA	1:B:458:PHE:CB	2.25	0.43
1:B:337:TYR:OH	1:B:362:PRO:CD	2.66	0.43
1:E:74:ASP:CG	1:E:75:GLU:N	2.70	0.43
1:E:389:GLU:HG3	1:E:393:SER:O	2.17	0.43
2:F:99:LEU:HD23	2:F:99:LEU:HA	1.82	0.43
1:A:282:LEU:O	1:A:337:TYR:CZ	2.72	0.43
1:A:417:GLU:HG3	1:A:418:VAL:N	2.34	0.43
1:A:450:LYS:HB2	1:A:456:TYR:CE1	2.54	0.43
1:A:484:PRO:HG2	1:A:487:PHE:HD1	1.84	0.43
2:D:71:LYS:NZ	2:D:71:LYS:CB	2.73	0.43
1:B:73:GLY:CA	1:B:74:ASP:C	2.86	0.43
1:B:241:ARG:NE	1:B:380:TYR:O	2.51	0.43
1:B:310:HIS:N	1:B:310:HIS:ND1	2.60	0.43
1:B:365:ILE:O	1:B:396:HIS:CG	2.70	0.43
1:B:467:LEU:HD22	1:B:467:LEU:H	1.84	0.43
1:B:545:ILE:CD1	1:B:552:MET:HE2	2.49	0.43
1:A:396:HIS:CD2	1:A:396:HIS:C	2.92	0.43
2:C:82:ILE:HG22	2:C:83:PRO:HD3	2.01	0.43
2:C:116:ALA:O	2:C:119:ILE:HG12	2.19	0.43
2:C:206:ARG:C	2:C:210:LEU:CD1	2.69	0.43
2:D:88:TYR:CD1	2:D:144:LEU:HB3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LEU:N	2:D:152:LEU:HD23	2.33	0.43
2:D:352:LYS:O	2:D:355:ASN:CB	2.62	0.43
2:D:497:LYS:HD2	2:D:501:VAL:HG23	1.99	0.43
1:B:344:LEU:O	1:B:347:HIS:HB3	2.19	0.43
1:B:372:ILE:HG23	1:B:373:LEU:N	2.33	0.43
1:B:471:TYR:HD1	1:B:471:TYR:O	2.01	0.43
1:B:471:TYR:O	1:B:550:GLN:NE2	2.46	0.43
1:E:361:LEU:HD21	1:E:376:ILE:HD11	2.01	0.43
2:F:319:THR:CG2	2:F:432:ALA:HA	2.48	0.43
1:A:208:HIS:O	1:A:209:GLU:HB2	2.18	0.43
1:A:291:LEU:N	1:A:291:LEU:HD13	2.32	0.43
1:A:615:HIS:N	1:A:615:HIS:HD1	2.17	0.43
2:C:112:LEU:N	2:C:112:LEU:CD2	2.73	0.43
2:C:257:ASN:O	2:C:261:TRP:HD1	2.00	0.43
1:B:338:LEU:HD11	1:B:372:ILE:HD13	2.00	0.43
1:B:364:TRP:HA	1:B:364:TRP:HE3	1.81	0.43
1:B:397:LEU:HD12	1:B:400:LEU:HG	1.98	0.43
1:B:522:THR:HG23	1:B:522:THR:O	2.18	0.43
1:E:81:VAL:CG1	1:E:82:GLY:N	2.81	0.43
1:E:309:GLN:CD	1:E:311:LEU:HD13	2.37	0.43
2:F:312:GLN:OE1	2:F:323:LYS:HD3	2.09	0.43
2:F:353:TRP:CE2	2:F:357:GLU:OE2	2.70	0.43
1:A:612:LYS:HA	1:A:613:LEU:HA	1.45	0.43
2:C:116:ALA:HB2	2:C:126:VAL:CG2	2.48	0.43
2:C:209:PHE:HE2	2:C:254:ILE:CB	2.32	0.43
2:D:312:GLN:CD	2:D:430:ILE:HG13	2.33	0.43
2:D:489:SER:O	1:B:468:GLN:N	2.52	0.43
1:B:611:LYS:N	1:B:614:GLU:OE1	2.51	0.43
1:E:491:ASN:HD21	2:F:39:GLN:HB2	1.83	0.43
1:E:508:THR:N	1:E:535:ASN:O	2.36	0.43
1:E:529:CYS:C	1:E:530:THR:OG1	2.54	0.43
2:F:48:GLY:HA2	2:F:50:GLN:N	2.34	0.43
2:F:126:VAL:HA	2:F:129:ARG:HD3	1.99	0.43
1:A:283:ASP:OD1	1:A:285:GLY:N	2.35	0.42
1:A:502:THR:O	1:A:504:ILE:HG23	2.19	0.42
2:C:122:PRO:HD2	2:C:125:PHE:CE2	2.54	0.42
2:C:128:LEU:HD12	2:C:129:ARG:HA	2.00	0.42
2:C:411:ASN:O	2:C:415:LEU:HG	2.18	0.42
2:C:490:ARG:HE	2:C:490:ARG:HB2	1.54	0.42
2:D:195:LEU:HD22	2:D:274:VAL:HG22	2.00	0.42
1:B:245:ILE:O	1:B:388:LEU:HD11	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:TYR:CD1	1:B:550:GLN:HB3	2.54	0.42
1:E:331:GLN:NE2	1:E:368:PHE:CB	2.82	0.42
1:E:385:LEU:HB2	1:E:417:GLU:O	2.19	0.42
1:E:389:GLU:HG3	1:E:392:ASN:CB	2.49	0.42
2:F:68:LEU:HD23	2:F:68:LEU:O	2.19	0.42
2:F:340:ILE:HG22	2:F:344:LEU:HD11	1.99	0.42
2:C:357:GLU:O	2:C:361:ASP:CB	2.65	0.42
1:B:69:ILE:HD13	1:B:69:ILE:N	2.34	0.42
1:B:115:ARG:HH21	1:B:115:ARG:CB	2.30	0.42
1:B:347:HIS:NE2	1:B:351:GLN:CG	2.82	0.42
1:E:431:SER:HB2	1:E:435:HIS:HA	2.01	0.42
1:E:504:ILE:N	1:E:540:GLY:O	2.34	0.42
1:A:181:LEU:CD1	1:A:181:LEU:C	2.85	0.42
2:D:104:GLN:HG2	2:D:105:GLN:OE1	2.19	0.42
1:B:110:HIS:CD2	1:B:110:HIS:C	2.92	0.42
1:B:395:ARG:HE	1:B:396:HIS:CA	2.32	0.42
1:B:461:LEU:O	1:B:555:TYR:CZ	2.73	0.42
1:B:530:THR:HB	1:B:531:SER:H	1.63	0.42
1:B:545:ILE:HD11	1:B:552:MET:CE	2.48	0.42
2:F:497:LYS:HG2	2:F:501:VAL:HB	2.01	0.42
1:A:68:ASN:HB3	1:A:69:ILE:HG13	2.01	0.42
1:A:265:GLN:O	1:A:268:ARG:HG2	2.20	0.42
1:A:371:GLN:NE2	1:A:371:GLN:C	2.73	0.42
1:A:466:PRO:HD3	2:C:494:TRP:CH2	2.54	0.42
1:A:604:PHE:HE1	2:C:47:LYS:HD2	1.85	0.42
2:C:96:VAL:CG2	2:C:128:LEU:HD21	2.22	0.42
2:C:353:TRP:CZ3	2:C:404:ILE:CG2	3.02	0.42
2:D:115:LEU:O	2:D:115:LEU:HD23	2.20	0.42
2:D:296:ASN:HB3	2:D:299:TRP:CZ2	2.54	0.42
1:B:100:VAL:HG23	1:B:101:LYS:N	2.34	0.42
1:B:105:VAL:O	1:B:132:ASP:OD2	2.38	0.42
1:B:211:ASP:C	1:B:212:ARG:NH2	2.73	0.42
1:B:543:HIS:C	1:B:543:HIS:ND1	2.73	0.42
1:E:123:PRO:CB	1:E:311:LEU:HD21	2.49	0.42
1:E:169:ASN:OD1	1:E:203:THR:OG1	2.31	0.42
1:E:239:ASP:HA	1:E:355:GLY:O	2.20	0.42
1:E:364:TRP:CD1	1:E:368:PHE:C	2.89	0.42
2:F:97:ASN:OD1	2:F:129:ARG:CZ	2.56	0.42
1:A:79:MET:SD	1:A:80:PHE:C	2.98	0.42
2:C:54:HIS:CE1	2:C:58:SER:OG	2.72	0.42
2:C:135:GLU:O	2:C:136:ARG:C	2.56	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:VAL:HB	2:D:9:TRP:CE2	2.55	0.42
2:D:81:SER:OG	2:D:141:LEU:HD22	2.19	0.42
1:B:130:THR:HG23	1:B:215:SER:HB2	2.02	0.42
1:B:169:ASN:HD21	1:B:202:THR:HA	1.85	0.42
1:B:534:LYS:HD2	1:B:534:LYS:H	1.84	0.42
1:E:280:LEU:HB3	1:E:359:LEU:CB	2.50	0.42
2:F:48:GLY:HA2	2:F:49:SER:C	2.39	0.42
2:F:54:HIS:CD2	2:F:98:GLY:CA	3.00	0.42
1:A:181:LEU:HD22	1:A:181:LEU:HA	1.84	0.42
1:A:399:GLU:N	1:A:399:GLU:CD	2.73	0.42
1:A:606:THR:HG21	2:C:5:ARG:NH1	2.31	0.42
2:C:272:ASN:O	2:C:276:GLU:HG3	2.19	0.42
2:C:323:LYS:HE2	2:C:430:ILE:HB	2.01	0.42
2:D:61:GLN:OE1	2:D:94:ARG:NE	2.53	0.42
2:D:279:PHE:HE1	2:D:304:TRP:CZ3	2.01	0.42
1:B:65:LEU:HD12	1:B:66:ILE:C	2.40	0.42
1:B:263:PHE:HD1	1:B:263:PHE:N	2.17	0.42
1:B:372:ILE:HD12	1:B:372:ILE:O	2.19	0.42
1:B:509:TYR:OH	1:B:513:ASP:HB3	2.18	0.42
1:E:240:THR:HG1	1:E:356:THR:HG22	1.82	0.42
1:E:295:ILE:HG22	1:E:344:LEU:CD2	2.50	0.42
1:E:467:LEU:HB2	2:F:489:SER:C	2.40	0.42
1:E:469:ILE:HD12	1:E:478:ILE:CD1	2.45	0.42
1:E:562:GLN:CD	1:E:562:GLN:N	2.73	0.42
2:F:21:TRP:HB3	2:F:37:ALA:HB2	2.00	0.42
1:A:289:TYR:HD1	1:A:298:ASN:ND2	2.18	0.42
1:A:301:LEU:HD12	1:A:301:LEU:H	1.85	0.42
1:A:369:GLY:C	1:A:372:ILE:HG22	2.40	0.42
1:A:383:THR:C	1:A:384:HIS:ND1	2.73	0.42
2:C:359:LEU:HD23	2:C:363:ASN:HD21	1.85	0.42
2:C:484:PRO:N	2:C:485:VAL:C	2.73	0.42
2:D:492:GLN:C	2:D:493:ASN:ND2	2.73	0.42
1:E:100:VAL:O	1:E:101:LYS:HD3	2.20	0.42
1:E:186:ASN:C	1:E:186:ASN:ND2	2.73	0.42
1:E:462:LEU:O	2:F:494:TRP:CZ3	2.72	0.42
2:F:50:GLN:C	2:F:51:TYR:CD2	2.93	0.42
2:F:139:PRO:HG2	2:F:144:LEU:HD12	1.91	0.42
2:F:154:TRP:CE3	2:F:155:LEU:CA	3.01	0.42
2:F:500:GLY:O	2:F:501:VAL:HG23	2.19	0.42
1:A:471:TYR:HB3	1:A:552:MET:SD	2.59	0.42
1:A:474:GLY:N	1:A:475:LYS:HA	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:PHE:C	2:C:12:PHE:CD1	2.93	0.42
2:C:52:LEU:CD1	2:C:52:LEU:C	2.86	0.42
2:C:78:HIS:ND1	2:C:78:HIS:C	2.73	0.42
2:C:128:LEU:HD12	2:C:129:ARG:CA	2.49	0.42
2:D:69:ASP:HB3	2:D:88:TYR:HE2	1.84	0.42
2:D:498:PRO:HG2	1:B:602:ILE:HG23	2.01	0.42
1:B:94:VAL:C	1:B:95:PHE:HD1	2.23	0.42
1:B:175:LEU:C	1:B:458:PHE:CE2	2.93	0.42
1:B:231:LEU:O	1:B:235:ASN:CG	2.58	0.42
1:B:313:GLN:CD	1:B:313:GLN:N	2.73	0.42
1:B:491:ASN:HD22	1:B:491:ASN:HA	1.62	0.42
1:E:254:THR:HA	1:E:257:ARG:HH11	1.85	0.42
1:E:301:LEU:HD11	1:E:316:ASN:HA	2.00	0.42
1:A:175:LEU:HD23	1:A:175:LEU:O	2.20	0.42
1:A:311:LEU:C	1:A:312:CYS:SG	2.99	0.42
2:C:46:LEU:HD22	2:C:46:LEU:C	2.38	0.42
2:D:20:LEU:HD23	2:D:20:LEU:HA	1.87	0.42
2:D:102:PRO:O	2:D:104:GLN:CD	2.58	0.42
1:B:474:GLY:N	1:B:475:LYS:CA	2.79	0.42
1:B:482:GLN:CG	1:B:526:LEU:HD23	2.50	0.42
1:B:503:VAL:HG11	1:B:539:LEU:HD22	2.00	0.42
1:B:575:ILE:N	1:B:575:ILE:CD1	2.73	0.42
1:E:95:PHE:CD2	1:E:95:PHE:C	2.92	0.42
1:E:464:SER:O	2:F:494:TRP:CZ3	2.72	0.42
1:E:501:GLY:HA2	2:F:499:PHE:CD1	2.55	0.42
3:E:701:HOH:O	2:F:502:LEU:HD21	2.13	0.42
2:F:275:LEU:O	2:F:279:PHE:CD2	2.70	0.42
2:F:501:VAL:C	2:F:502:LEU:CG	2.86	0.42
1:A:188:LEU:CD2	1:A:188:LEU:C	2.88	0.42
1:A:588:LEU:HD21	1:A:605:ALA:HB2	2.00	0.42
2:C:6:ILE:HG21	2:C:51:TYR:CD1	2.54	0.42
2:C:55:VAL:HG23	2:C:155:LEU:HD23	2.00	0.42
2:C:82:ILE:HG23	2:C:83:PRO:CD	2.50	0.42
2:C:125:PHE:HB3	2:C:128:LEU:CD2	2.49	0.42
2:D:195:LEU:HD21	2:D:277:LYS:HB3	2.02	0.42
1:B:89:LEU:HD13	1:B:90:HIS:C	2.40	0.42
1:B:175:LEU:HD22	1:B:456:TYR:CE2	2.55	0.42
1:B:216:LEU:HD23	1:B:216:LEU:C	2.41	0.42
1:B:364:TRP:CA	1:B:364:TRP:HE3	2.33	0.42
1:B:366:LYS:HD2	1:B:395:ARG:NH1	2.34	0.42
1:B:397:LEU:CG	1:B:400:LEU:HD11	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ASN:ND2	1:B:599:ASN:C	2.73	0.42
1:B:615:HIS:ND1	1:B:615:HIS:C	2.73	0.42
1:E:96:ARG:NE	1:E:168:PHE:CE2	2.87	0.42
1:E:493:GLN:HE21	1:E:493:GLN:HB2	1.68	0.42
1:E:548:SER:H	1:E:548:SER:HG	1.52	0.42
1:E:573:TRP:NE1	2:F:487:ASN:OD1	2.53	0.42
2:F:10:ARG:HE	2:F:10:ARG:HB3	1.65	0.42
2:F:50:GLN:O	2:F:51:TYR:HB2	2.19	0.42
2:F:154:TRP:HE3	2:F:155:LEU:HA	1.81	0.42
2:F:499:PHE:N	2:F:499:PHE:HD2	2.18	0.42
1:A:368:PHE:O	1:A:368:PHE:CG	2.72	0.41
1:A:386:LEU:CD2	1:A:419:VAL:HG21	2.50	0.41
1:A:498:ALA:O	1:A:502:THR:HG21	2.20	0.41
1:A:610:ARG:HD2	2:C:167:ASP:OD2	2.20	0.41
2:C:53:PRO:HD2	2:C:56:VAL:HG23	1.98	0.41
1:B:96:ARG:HG2	1:B:119:THR:OG1	2.20	0.41
1:B:431:SER:O	1:B:434:PHE:HB2	2.20	0.41
1:E:123:PRO:CB	1:E:311:LEU:CD2	2.98	0.41
1:E:171:ASN:ND2	1:E:454:PHE:HD1	2.18	0.41
1:E:244:VAL:HG13	1:E:388:LEU:HD11	2.02	0.41
1:E:491:ASN:CG	2:F:36:ARG:HD2	2.25	0.41
1:E:546:ASP:CG	1:E:549:GLN:NE2	2.73	0.41
2:F:31:GLU:O	2:F:33:LYS:N	2.52	0.41
1:A:480:GLY:H	1:A:524:PRO:HG3	1.82	0.41
2:C:228:ASN:OD1	2:C:228:ASN:N	2.31	0.41
2:D:42:GLN:NE2	1:B:487:PHE:CE2	2.88	0.41
2:D:349:PHE:CD2	2:D:356:TRP:CE2	3.07	0.41
1:B:359:LEU:CD1	1:B:360:ASN:C	2.86	0.41
1:B:472:GLY:HA3	1:B:476:SER:H	1.84	0.41
1:E:96:ARG:O	1:E:168:PHE:CD2	2.73	0.41
1:E:469:ILE:CG1	1:E:478:ILE:HD11	2.50	0.41
2:F:48:GLY:CA	2:F:49:SER:C	2.88	0.41
2:F:112:LEU:H	2:F:112:LEU:HG	1.58	0.41
1:A:291:LEU:HD13	1:A:291:LEU:H	1.85	0.41
2:C:314:ASP:OD2	2:C:495:LYS:CE	2.68	0.41
2:C:356:TRP:O	2:C:360:ILE:N	2.31	0.41
2:C:413:ASP:O	2:C:417:LEU:HG	2.20	0.41
2:D:85:ARG:NH2	2:D:138:LEU:O	2.53	0.41
2:D:92:LEU:O	2:D:95:PHE:HB3	2.20	0.41
2:D:234:LEU:HD13	2:D:236:ASN:HB2	2.02	0.41
1:B:390:THR:CG2	1:B:391:ALA:N	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:LEU:N	1:B:588:LEU:CD1	2.73	0.41
1:E:100:VAL:C	1:E:101:LYS:CG	2.86	0.41
1:E:316:ASN:C	1:E:316:ASN:ND2	2.73	0.41
2:F:272:ASN:O	2:F:275:LEU:CD1	2.65	0.41
1:A:79:MET:SD	1:A:80:PHE:O	2.79	0.41
1:A:135:HIS:HA	1:A:136:PHE:HA	1.83	0.41
1:A:226:LEU:HD13	1:A:259:LEU:HD13	2.03	0.41
1:A:395:ARG:HH21	1:A:395:ARG:HG2	1.84	0.41
1:A:527:GLN:NE2	1:A:527:GLN:HA	2.35	0.41
1:A:617:TRP:HZ2	2:D:134:HIS:HA	1.84	0.41
2:C:336:LEU:O	2:C:340:ILE:HG13	2.20	0.41
2:D:49:SER:O	2:D:49:SER:OG	2.34	0.41
2:D:159:TYR:HE1	1:B:614:GLU:CD	2.17	0.41
2:D:220:ASN:ND2	2:D:220:ASN:C	2.73	0.41
1:B:293:ASP:OD2	1:B:580:THR:HG23	2.21	0.41
1:B:317:PHE:CD2	1:B:317:PHE:C	2.93	0.41
1:B:338:LEU:HD11	1:B:372:ILE:CD1	2.50	0.41
1:B:385:LEU:O	1:B:386:LEU:HG	2.19	0.41
1:E:96:ARG:O	1:E:168:PHE:HD2	2.03	0.41
1:E:239:ASP:CB	1:E:355:GLY:O	2.68	0.41
1:E:289:TYR:CG	1:E:317:PHE:CE2	3.07	0.41
1:E:581:GLU:H	1:E:581:GLU:HG3	1.63	0.41
2:F:36:ARG:HD2	2:F:36:ARG:HA	1.63	0.41
2:F:54:HIS:ND1	2:F:54:HIS:C	2.73	0.41
1:A:221:TYR:CD1	1:A:221:TYR:N	2.88	0.41
1:A:592:ARG:HD3	2:C:184:ARG:HE	1.77	0.41
2:C:312:GLN:HE21	2:C:320:THR:HG23	1.85	0.41
2:D:268:SER:HA	2:D:271:HIS:CD2	2.55	0.41
2:D:329:TRP:CH2	2:D:424:ILE:CD1	2.99	0.41
1:B:96:ARG:HH22	1:B:171:ASN:ND2	1.97	0.41
1:B:349:GLU:C	1:B:352:ALA:H	2.23	0.41
1:B:485:MET:HE3	1:B:485:MET:H	1.85	0.41
1:B:506:ILE:HD11	1:B:540:GLY:CA	2.47	0.41
1:B:519:SER:O	1:B:520:LEU:HD23	2.21	0.41
1:E:554:ILE:HG21	2:F:488:TRP:HZ3	1.83	0.41
1:E:568:PRO:HG2	1:E:571:ALA:HB2	2.01	0.41
1:A:173:THR:O	1:A:177:GLU:OE1	2.39	0.41
1:A:492:PRO:HA	1:A:495:ILE:CG1	2.49	0.41
1:A:492:PRO:HB3	1:A:520:LEU:HB3	2.02	0.41
2:C:12:PHE:HD1	2:C:12:PHE:C	2.23	0.41
2:C:96:VAL:HA	2:C:99:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:ARG:HA	1:B:617:TRP:CE3	2.54	0.41
2:D:81:SER:HA	2:D:84:ILE:HG22	2.03	0.41
2:D:359:LEU:HD23	2:D:360:ILE:N	2.36	0.41
2:D:489:SER:C	1:B:467:LEU:HB2	2.29	0.41
1:B:233:HIS:HD1	1:B:233:HIS:C	2.21	0.41
1:E:487:PHE:O	1:E:490:LEU:HD12	2.04	0.41
1:E:600:ILE:HG12	1:E:600:ILE:H	1.63	0.41
2:F:41:VAL:O	2:F:44:TYR:N	2.48	0.41
2:F:349:PHE:CE1	2:F:375:MET:HE3	2.55	0.41
1:A:97:LEU:HG	1:A:166:ARG:O	2.21	0.41
1:A:225:PRO:HG2	1:A:421:VAL:HG12	2.02	0.41
1:A:446:ALA:O	1:A:450:LYS:CB	2.69	0.41
1:A:488:GLN:NE2	1:A:527:GLN:OE1	2.52	0.41
2:C:143:MET:O	2:C:143:MET:SD	2.79	0.41
2:C:146:TRP:CD1	2:C:146:TRP:C	2.94	0.41
2:D:271:HIS:O	2:D:275:LEU:HG	2.21	0.41
2:D:325:LYS:HD3	2:D:325:LYS:HA	1.62	0.41
1:B:521:ASN:O	1:B:523:PHE:CD2	2.74	0.41
1:B:542:ILE:CD1	1:B:552:MET:HE2	2.50	0.41
1:E:387:PHE:HE1	1:E:401:THR:HG23	1.82	0.41
1:E:389:GLU:CB	1:E:397:LEU:HD11	2.50	0.41
1:E:449:HIS:CD2	1:E:458:PHE:HA	2.54	0.41
2:F:68:LEU:O	2:F:71:LYS:HB2	2.20	0.41
2:F:191:TYR:CE2	2:F:264:LEU:HD22	2.56	0.41
2:F:492:GLN:CD	2:F:492:GLN:N	2.73	0.41
1:A:180:HIS:HB2	2:C:269:ILE:CD1	2.47	0.41
1:A:347:HIS:CD2	1:A:347:HIS:O	2.74	0.41
2:C:415:LEU:O	2:C:418:ARG:N	2.48	0.41
2:D:36:ARG:HH11	1:B:494:ASP:CG	2.24	0.41
2:D:302:ILE:HD12	2:D:356:TRP:CZ3	2.55	0.41
1:B:107:ASN:HA	1:B:218:VAL:HG12	2.03	0.41
1:B:337:TYR:CZ	1:B:362:PRO:HG2	2.55	0.41
1:B:480:GLY:CA	1:B:524:PRO:O	2.66	0.41
1:A:98:GLN:HB3	1:A:165:LEU:N	2.35	0.41
1:A:395:ARG:NH2	1:A:395:ARG:HG3	2.35	0.41
1:A:492:PRO:HG3	1:A:520:LEU:HB3	2.03	0.41
2:C:54:HIS:ND1	2:C:54:HIS:C	2.73	0.41
2:C:90:MET:HE1	2:D:89:VAL:HG12	2.02	0.41
2:D:489:SER:OG	1:B:468:GLN:HG2	2.21	0.41
1:B:93:GLY:O	1:B:95:PHE:CD1	2.74	0.41
1:B:175:LEU:N	1:B:456:TYR:HB2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:HG3	1:B:458:PHE:CD2	2.43	0.41
1:B:261:GLU:HA	1:B:264:THR:HG1	1.77	0.41
1:B:295:ILE:O	1:B:323:PHE:N	2.34	0.41
1:B:364:TRP:CG	1:B:369:GLY:HA3	2.55	0.41
1:E:76:ASP:OD1	1:E:169:ASN:HB3	2.20	0.41
1:E:310:HIS:CG	1:E:314:GLY:CA	3.02	0.41
1:E:421:VAL:HB	1:E:422:PRO:HD2	2.03	0.41
1:E:471:TYR:HA	1:E:478:ILE:HB	2.02	0.41
1:E:509:TYR:HD1	1:E:510:SER:H	1.69	0.41
2:F:349:PHE:CD2	2:F:349:PHE:C	2.93	0.41
1:A:106:TYR:CE2	1:A:120:PHE:CD2	3.06	0.41
1:A:249:ASN:ND2	1:A:249:ASN:C	2.73	0.41
1:A:461:LEU:HD22	1:A:555:TYR:CD2	2.56	0.41
1:A:469:ILE:CG2	2:C:488:TRP:CA	2.98	0.41
2:C:388:SER:N	2:C:391:ASN:ND2	2.69	0.41
2:D:374:SER:O	2:D:377:ALA:N	2.53	0.41
2:D:398:ILE:O	2:D:402:VAL:HG23	2.21	0.41
1:B:366:LYS:CG	1:B:395:ARG:HH11	2.34	0.41
1:B:387:PHE:CE2	1:B:397:LEU:CD1	3.01	0.41
1:B:526:LEU:HD12	1:B:526:LEU:HA	1.77	0.41
1:B:545:ILE:CD1	1:B:552:MET:CE	2.99	0.41
1:E:440:ARG:O	1:E:444:ILE:HG13	2.21	0.41
1:E:546:ASP:OD1	1:E:548:SER:OG	2.38	0.41
2:F:18:LEU:CD1	2:F:44:TYR:HE2	2.34	0.41
2:F:100:LEU:HD23	2:F:100:LEU:H	1.83	0.41
2:F:154:TRP:CE3	2:F:155:LEU:N	2.89	0.41
1:A:480:GLY:CA	1:A:524:PRO:O	2.45	0.40
1:A:502:THR:CG2	1:A:577:ARG:HH21	2.25	0.40
2:C:96:VAL:HA	2:C:99:LEU:CD2	2.51	0.40
2:C:136:ARG:NE	2:D:49:SER:O	2.54	0.40
2:D:418:ARG:CB	2:D:419:PHE:CE2	2.92	0.40
2:D:427:TYR:HD2	2:D:430:ILE:HD11	1.87	0.40
2:D:487:ASN:O	1:B:468:GLN:O	2.39	0.40
1:B:96:ARG:HA	1:B:119:THR:HA	2.02	0.40
1:B:96:ARG:O	1:B:168:PHE:CB	2.69	0.40
1:E:89:LEU:N	1:E:131:ILE:O	2.46	0.40
1:E:127:SER:O	1:E:129:PRO:HD3	2.20	0.40
1:E:176:LEU:N	1:E:176:LEU:HD13	2.36	0.40
1:E:268:ARG:HD3	1:E:302:SER:HB2	2.01	0.40
1:E:471:TYR:OH	1:E:522:THR:O	2.38	0.40
2:F:68:LEU:CD2	2:F:68:LEU:C	2.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:333:GLN:CA	2:F:337:LEU:CD2	2.98	0.40
1:A:249:ASN:C	1:A:249:ASN:HD22	2.25	0.40
1:A:268:ARG:HG2	1:A:268:ARG:H	1.59	0.40
2:C:38:VAL:O	2:C:42:GLN:HB2	2.20	0.40
2:C:74:CYS:HB2	2:C:75:LEU:HA	2.03	0.40
2:C:325:LYS:O	2:C:326:PHE:CD1	2.73	0.40
2:D:5:ARG:CD	1:B:610:ARG:HG3	2.52	0.40
2:D:41:VAL:O	2:D:45:ARG:HG3	2.21	0.40
2:D:237:TYR:O	2:D:237:TYR:HD1	2.04	0.40
2:D:341:ILE:CD1	2:D:374:SER:HB3	2.52	0.40
2:D:492:GLN:HE21	2:D:492:GLN:HB3	1.61	0.40
1:B:436:ALA:O	1:B:440:ARG:HB2	2.21	0.40
1:E:97:LEU:HA	1:E:167:VAL:H	1.87	0.40
1:E:168:PHE:HD2	1:E:168:PHE:O	2.05	0.40
1:E:306:SER:C	1:E:307:LEU:CG	2.89	0.40
1:E:362:PRO:CB	3:E:705:HOH:O	2.60	0.40
1:E:507:TYR:HD1	1:E:535:ASN:O	2.03	0.40
2:F:18:LEU:HD11	2:F:44:TYR:HE2	1.86	0.40
2:F:126:VAL:HA	2:F:129:ARG:CD	2.50	0.40
2:F:372:CYS:HB2	2:F:412:ILE:HG12	2.03	0.40
2:F:411:ASN:CA	2:F:414:ASN:HB3	2.51	0.40
1:A:110:HIS:C	1:A:111:TYR:CD1	2.95	0.40
2:C:207:ASN:C	2:C:210:LEU:CD1	2.89	0.40
2:C:358:LYS:CB	2:C:490:ARG:HH12	2.29	0.40
1:B:521:ASN:O	1:B:523:PHE:HD2	2.03	0.40
1:B:600:ILE:CG2	3:B:703:HOH:O	2.70	0.40
1:E:474:GLY:N	1:E:475:LYS:CB	2.85	0.40
2:F:34:ARG:HA	2:F:37:ALA:HB3	2.04	0.40
2:F:298:ASP:HB2	2:F:356:TRP:HH2	1.86	0.40
1:A:100:VAL:C	1:A:101:LYS:HG2	2.42	0.40
1:A:324:TYR:OH	1:A:580:THR:OG1	2.04	0.40
1:A:398:ASP:CG	1:A:399:GLU:N	2.73	0.40
2:C:195:LEU:O	2:C:198:THR:N	2.52	0.40
2:C:237:TYR:HD1	2:C:237:TYR:HA	1.82	0.40
2:C:256:GLU:O	2:C:260:GLN:HG3	2.22	0.40
2:C:287:LEU:HD12	2:C:287:LEU:HA	1.85	0.40
1:B:472:GLY:O	1:B:475:LYS:CB	2.69	0.40
1:E:121:TRP:O	1:E:123:PRO:HD3	2.21	0.40
1:E:373:LEU:O	1:E:377:ILE:HG13	2.22	0.40
2:F:156:TYR:OH	2:F:161:ASN:ND2	2.54	0.40
1:A:197:PRO:HG2	1:A:197:PRO:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:SER:OG	1:A:545:ILE:N	2.54	0.40
1:A:562:GLN:H	1:A:562:GLN:HG2	1.57	0.40
2:C:291:MET:SD	2:C:340:ILE:CG2	3.10	0.40
1:B:289:TYR:CD1	1:B:317:PHE:HD1	2.39	0.40
1:E:175:LEU:HD22	1:E:189:TRP:CD1	2.53	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:331:GLN:O	2:F:143:MET:CE[2_555]	1.76	0.44
2:F:49:SER:C	2:F:136:ARG:NH2[2_555]	1.94	0.26
2:F:49:SER:O	2:F:136:ARG:NH2[2_555]	1.99	0.21
1:E:486:GLU:O	2:F:81:SER:OG[2_555]	2.08	0.12
2:F:94:ARG:NH2	2:F:136:ARG:O[2_555]	2.08	0.12
1:E:371:GLN:NE2	2:F:150:GLU:OE1[2_555]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	525/632 (83%)	494 (94%)	29 (6%)	2 (0%)	34	69
1	B	522/632 (83%)	488 (94%)	31 (6%)	3 (1%)	25	62
1	E	521/632 (82%)	492 (94%)	28 (5%)	1 (0%)	47	78
2	C	422/502 (84%)	404 (96%)	18 (4%)	0	100	100
2	D	421/502 (84%)	399 (95%)	20 (5%)	2 (0%)	29	66
2	F	385/502 (77%)	372 (97%)	11 (3%)	2 (0%)	29	66
All	All	2796/3402 (82%)	2649 (95%)	137 (5%)	10 (0%)	34	69

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	PRO
2	D	131	TRP
1	B	416	PRO
1	E	416	PRO
2	F	501	VAL
1	B	422	PRO
1	A	194	PRO
1	B	466	PRO
2	D	101	ASP
2	F	101	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	441/579 (76%)	303 (69%)	138 (31%)	0 1
1	B	430/579 (74%)	319 (74%)	111 (26%)	0 4
1	E	433/579 (75%)	313 (72%)	120 (28%)	0 2
2	C	392/461 (85%)	311 (79%)	81 (21%)	1 7
2	D	391/461 (85%)	320 (82%)	71 (18%)	1 11
2	F	364/461 (79%)	297 (82%)	67 (18%)	1 10
All	All	2451/3120 (79%)	1863 (76%)	588 (24%)	0 5

All (588) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	67	ASP
1	A	68	ASN
1	A	71	TYR
1	A	74	ASP
1	A	75	GLU
1	A	76	ASP
1	A	78	THR
1	A	80	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	83	LEU
1	A	88	LYS
1	A	96	ARG
1	A	106	TYR
1	A	108	ASN
1	A	115	ARG
1	A	118	LEU
1	A	119	THR
1	A	124	LEU
1	A	135	HIS
1	A	166	ARG
1	A	168	PHE
1	A	170	SER
1	A	175	LEU
1	A	180	HIS
1	A	183	ARG
1	A	184	ASP
1	A	186	ASN
1	A	188	LEU
1	A	190	LYS
1	A	193	GLU
1	A	198	LEU
1	A	203	THR
1	A	206	LEU
1	A	207	LEU
1	A	208	HIS
1	A	209	GLU
1	A	210	SER
1	A	214	GLN
1	A	216	LEU
1	A	217	SER
1	A	221	TYR
1	A	226	LEU
1	A	245	ILE
1	A	248	LYS
1	A	249	ASN
1	A	259	LEU
1	A	260	LEU
1	A	261	GLU
1	A	268	ARG
1	A	269	ASP
1	A	271	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	THR
1	A	275	GLU
1	A	276	GLU
1	A	277	LEU
1	A	280	LEU
1	A	282	LEU
1	A	290	SER
1	A	291	LEU
1	A	294	SER
1	A	298	ASN
1	A	300	ILE
1	A	301	LEU
1	A	303	SER
1	A	305	ILE
1	A	306	SER
1	A	307	LEU
1	A	309	GLN
1	A	313	GLN
1	A	328	SER
1	A	329	SER
1	A	337	TYR
1	A	342	ASP
1	A	344	LEU
1	A	345	ILE
1	A	356	THR
1	A	359	LEU
1	A	361	LEU
1	A	364	TRP
1	A	371	GLN
1	A	373	LEU
1	A	383	THR
1	A	394	LYS
1	A	395	ARG
1	A	397	LEU
1	A	399	GLU
1	A	406	PHE
1	A	420	ARG
1	A	425	SER
1	A	432	SER
1	A	450	LYS
1	A	454	PHE
1	A	455	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	457	ASP
1	A	473	LYS
1	A	476	SER
1	A	481	ILE
1	A	485	MET
1	A	490	LEU
1	A	493	GLN
1	A	497	SER
1	A	499	LEU
1	A	507	TYR
1	A	509	TYR
1	A	515	LEU
1	A	521	ASN
1	A	522	THR
1	A	525	ILE
1	A	526	LEU
1	A	527	GLN
1	A	528	SER
1	A	530	THR
1	A	534	LYS
1	A	539	LEU
1	A	541	LEU
1	A	544	SER
1	A	550	GLN
1	A	554	ILE
1	A	559	CYS
1	A	560	HIS
1	A	562	GLN
1	A	566	LYS
1	A	575	ILE
1	A	577	ARG
1	A	579	LYS
1	A	584	PHE
1	A	585	CYS
1	A	587	PHE
1	A	592	ARG
1	A	593	THR
1	A	596	TRP
1	A	597	ASP
1	A	601	GLN
1	A	609	ARG
1	A	610	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	611	LYS
1	A	613	LEU
1	A	616	VAL
2	C	11	ASP
2	C	12	PHE
2	C	15	LEU
2	C	18	LEU
2	C	29	THR
2	C	30	ILE
2	C	33	LYS
2	C	42	GLN
2	C	43	SER
2	C	46	LEU
2	C	49	SER
2	C	50	GLN
2	C	52	LEU
2	C	54	HIS
2	C	68	LEU
2	C	69	ASP
2	C	71	LYS
2	C	78	HIS
2	C	79	GLN
2	C	80	ASP
2	C	87	SER
2	C	92	LEU
2	C	97	ASN
2	C	99	LEU
2	C	100	LEU
2	C	101	ASP
2	C	105	GLN
2	C	107	GLN
2	C	108	PHE
2	C	112	LEU
2	C	115	LEU
2	C	129	ARG
2	C	142	GLU
2	C	143	MET
2	C	146	TRP
2	C	155	LEU
2	C	160	TRP
2	C	161	ASN
2	C	182	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	184	ARG
2	C	210	LEU
2	C	213	LYS
2	C	216	TRP
2	C	217	GLU
2	C	218	ASN
2	C	221	ASP
2	C	223	LEU
2	C	224	ILE
2	C	228	ASN
2	C	232	ASP
2	C	236	ASN
2	C	248	SER
2	C	249	SER
2	C	250	SER
2	C	285	LEU
2	C	287	LEU
2	C	288	LYS
2	C	307	ARG
2	C	309	TYR
2	C	310	ARG
2	C	311	THR
2	C	312	GLN
2	C	317	ASN
2	C	325	LYS
2	C	327	ASN
2	C	330	LYS
2	C	340	ILE
2	C	345	ASN
2	C	348	ASN
2	C	354	GLN
2	C	359	LEU
2	C	361	ASP
2	C	363	ASN
2	C	385	THR
2	C	387	ASN
2	C	389	TRP
2	C	394	ARG
2	C	395	ARG
2	C	487	ASN
2	C	490	ARG
2	C	492	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	12	PHE
2	D	18	LEU
2	D	20	LEU
2	D	32	ASP
2	D	43	SER
2	D	46	LEU
2	D	54	HIS
2	D	71	LYS
2	D	72	GLU
2	D	75	LEU
2	D	77	VAL
2	D	79	GLN
2	D	84	ILE
2	D	86	LEU
2	D	99	LEU
2	D	100	LEU
2	D	103	THR
2	D	104	GLN
2	D	105	GLN
2	D	106	SER
2	D	107	GLN
2	D	108	PHE
2	D	112	LEU
2	D	113	HIS
2	D	115	LEU
2	D	121	LEU
2	D	127	ASP
2	D	129	ARG
2	D	131	TRP
2	D	137	ASP
2	D	146	TRP
2	D	162	ASP
2	D	163	GLU
2	D	182	TYR
2	D	188	LEU
2	D	189	GLU
2	D	199	LEU
2	D	205	LEU
2	D	210	LEU
2	D	222	SER
2	D	225	THR
2	D	228	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	232	ASP
2	D	234	LEU
2	D	236	ASN
2	D	250	SER
2	D	255	ARG
2	D	278	PHE
2	D	282	TYR
2	D	310	ARG
2	D	323	LYS
2	D	325	LYS
2	D	332	LEU
2	D	334	LYS
2	D	336	LEU
2	D	344	LEU
2	D	346	ASN
2	D	347	LYS
2	D	350	LYS
2	D	351	ASN
2	D	352	LYS
2	D	358	LYS
2	D	361	ASP
2	D	365	SER
2	D	388	SER
2	D	390	ARG
2	D	421	GLU
2	D	425	LYS
2	D	430	ILE
2	D	492	GLN
2	D	493	ASN
1	B	65	LEU
1	B	67	ASP
1	B	69	ILE
1	B	74	ASP
1	B	77	GLU
1	B	78	THR
1	B	79	MET
1	B	90	HIS
1	B	108	ASN
1	B	115	ARG
1	B	117	ILE
1	B	118	LEU
1	B	122	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	124	LEU
1	B	135	HIS
1	B	139	TRP
1	B	165	LEU
1	B	166	ARG
1	B	173	THR
1	B	176	LEU
1	B	181	LEU
1	B	182	TYR
1	B	190	LYS
1	B	195	TYR
1	B	196	PHE
1	B	209	GLU
1	B	210	SER
1	B	212	ARG
1	B	217	SER
1	B	221	TYR
1	B	230	TYR
1	B	233	HIS
1	B	243	MET
1	B	250	SER
1	B	252	LYS
1	B	253	SER
1	B	263	PHE
1	B	264	THR
1	B	268	ARG
1	B	273	SER
1	B	277	LEU
1	B	286	GLN
1	B	289	TYR
1	B	307	LEU
1	B	310	HIS
1	B	313	GLN
1	B	317	PHE
1	B	318	GLN
1	B	321	LEU
1	B	332	ASP
1	B	333	GLU
1	B	337	TYR
1	B	345	ILE
1	B	349	GLU
1	B	350	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	353	PHE
1	B	356	THR
1	B	358	LEU
1	B	359	LEU
1	B	364	TRP
1	B	371	GLN
1	B	372	ILE
1	B	379	LYS
1	B	388	LEU
1	B	389	GLU
1	B	394	LYS
1	B	395	ARG
1	B	397	LEU
1	B	398	ASP
1	B	399	GLU
1	B	400	LEU
1	B	401	THR
1	B	425	SER
1	B	429	THR
1	B	450	LYS
1	B	453	GLN
1	B	455	ASP
1	B	461	LEU
1	B	462	LEU
1	B	467	LEU
1	B	471	TYR
1	B	473	LYS
1	B	476	SER
1	B	478	ILE
1	B	481	ILE
1	B	485	MET
1	B	488	GLN
1	B	490	LEU
1	B	491	ASN
1	B	515	LEU
1	B	520	LEU
1	B	522	THR
1	B	524	PRO
1	B	525	ILE
1	B	530	THR
1	B	531	SER
1	B	534	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	536	PHE
1	B	549	GLN
1	B	569	GLU
1	B	570	ASP
1	B	577	ARG
1	B	585	CYS
1	B	588	LEU
1	B	592	ARG
1	B	596	TRP
1	B	599	ASN
1	B	612	LYS
1	B	613	LEU
1	B	615	HIS
1	B	616	VAL
1	E	69	ILE
1	E	71	TYR
1	E	72	GLU
1	E	75	GLU
1	E	79	MET
1	E	83	LEU
1	E	90	HIS
1	E	98	GLN
1	E	104	ILE
1	E	106	TYR
1	E	111	TYR
1	E	112	ASN
1	E	114	SER
1	E	117	ILE
1	E	118	LEU
1	E	130	THR
1	E	166	ARG
1	E	168	PHE
1	E	170	SER
1	E	176	LEU
1	E	177	GLU
1	E	180	HIS
1	E	181	LEU
1	E	182	TYR
1	E	184	ASP
1	E	186	ASN
1	E	196	PHE
1	E	206	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	207	LEU
1	E	209	GLU
1	E	212	ARG
1	E	216	LEU
1	E	222	TRP
1	E	230	TYR
1	E	234	LYS
1	E	235	ASN
1	E	245	ILE
1	E	248	LYS
1	E	268	ARG
1	E	269	ASP
1	E	273	SER
1	E	277	LEU
1	E	279	TYR
1	E	286	GLN
1	E	290	SER
1	E	291	LEU
1	E	293	ASP
1	E	301	LEU
1	E	307	LEU
1	E	309	GLN
1	E	310	HIS
1	E	311	LEU
1	E	316	ASN
1	E	317	PHE
1	E	327	SER
1	E	332	ASP
1	E	333	GLU
1	E	336	SER
1	E	356	THR
1	E	358	LEU
1	E	359	LEU
1	E	360	ASN
1	E	365	ILE
1	E	378	ARG
1	E	381	LYS
1	E	383	THR
1	E	384	HIS
1	E	385	LEU
1	E	388	LEU
1	E	393	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	394	LYS
1	E	395	ARG
1	E	397	LEU
1	E	399	GLU
1	E	400	LEU
1	E	417	GLU
1	E	449	HIS
1	E	450	LYS
1	E	454	PHE
1	E	461	LEU
1	E	467	LEU
1	E	471	TYR
1	E	473	LYS
1	E	489	ASP
1	E	493	GLN
1	E	499	LEU
1	E	502	THR
1	E	517	VAL
1	E	526	LEU
1	E	529	CYS
1	E	534	LYS
1	E	536	PHE
1	E	539	LEU
1	E	544	SER
1	E	547	THR
1	E	548	SER
1	E	549	GLN
1	E	560	HIS
1	E	562	GLN
1	E	564	LEU
1	E	565	ASP
1	E	566	LYS
1	E	567	GLN
1	E	581	GLU
1	E	582	THR
1	E	586	ASP
1	E	587	PHE
1	E	588	LEU
1	E	592	ARG
1	E	594	ILE
1	E	595	THR
1	E	596	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	597	ASP
1	E	598	ASP
1	E	601	GLN
1	E	608	GLU
1	E	609	ARG
1	E	610	ARG
1	E	614	GLU
1	E	615	HIS
2	F	10	ARG
2	F	12	PHE
2	F	18	LEU
2	F	25	LYS
2	F	26	SER
2	F	29	THR
2	F	32	ASP
2	F	34	ARG
2	F	36	ARG
2	F	46	LEU
2	F	47	LYS
2	F	50	GLN
2	F	51	TYR
2	F	52	LEU
2	F	54	HIS
2	F	62	ILE
2	F	77	VAL
2	F	80	ASP
2	F	81	SER
2	F	100	LEU
2	F	101	ASP
2	F	108	PHE
2	F	110	ILE
2	F	112	LEU
2	F	118	LYS
2	F	125	PHE
2	F	127	ASP
2	F	128	LEU
2	F	129	ARG
2	F	131	TRP
2	F	133	THR
2	F	136	ARG
2	F	138	LEU
2	F	144	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	146	TRP
2	F	152	LEU
2	F	155	LEU
2	F	162	ASP
2	F	182	TYR
2	F	259	ARG
2	F	274	VAL
2	F	275	LEU
2	F	278	PHE
2	F	282	TYR
2	F	283	ASP
2	F	321	ILE
2	F	323	LYS
2	F	324	ARG
2	F	335	ARG
2	F	336	LEU
2	F	349	PHE
2	F	350	LYS
2	F	352	LYS
2	F	359	LEU
2	F	363	ASN
2	F	365	SER
2	F	367	LEU
2	F	388	SER
2	F	390	ARG
2	F	391	ASN
2	F	417	LEU
2	F	423	GLU
2	F	489	SER
2	F	490	ARG
2	F	494	TRP
2	F	497	LYS
2	F	502	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	98	GLN
1	A	108	ASN
1	A	126	GLN
1	A	169	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	214	GLN
1	A	249	ASN
1	A	313	GLN
1	A	318	GLN
1	A	331	GLN
1	A	371	GLN
1	A	488	GLN
1	A	491	ASN
1	A	493	GLN
1	A	543	HIS
1	A	560	HIS
1	A	567	GLN
1	A	572	GLN
1	A	615	HIS
2	C	39	GLN
2	C	54	HIS
2	C	79	GLN
2	C	97	ASN
2	C	105	GLN
2	C	130	HIS
2	C	161	ASN
2	C	293	ASN
2	C	313	GLN
2	C	355	ASN
2	C	363	ASN
2	C	391	ASN
2	C	493	ASN
2	D	79	GLN
2	D	104	GLN
2	D	107	GLN
2	D	134	HIS
2	D	161	ASN
2	D	218	ASN
2	D	220	ASN
2	D	312	GLN
2	D	327	ASN
2	D	343	ASN
2	D	492	GLN
2	D	493	ASN
1	B	90	HIS
1	B	108	ASN
1	B	171	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	172	HIS
1	B	233	HIS
1	B	371	GLN
1	B	396	HIS
1	B	435	HIS
1	B	438	GLN
1	B	488	GLN
1	B	549	GLN
1	B	599	ASN
1	E	110	HIS
1	E	186	ASN
1	E	205	HIS
1	E	235	ASN
1	E	316	ASN
1	E	360	ASN
1	E	384	HIS
1	E	424	HIS
1	E	482	GLN
1	E	491	ASN
1	E	493	GLN
1	E	549	GLN
1	E	560	HIS
1	E	567	GLN
1	E	601	GLN
2	F	42	GLN
2	F	105	GLN
2	F	161	ASN
2	F	333	GLN
2	F	345	ASN
2	F	492	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	529/632 (83%)	-0.20	13 (2%) 57 45	30, 74, 134, 150	0
1	B	528/632 (83%)	0.17	27 (5%) 28 21	28, 109, 157, 177	0
1	E	527/632 (83%)	-0.01	10 (1%) 66 55	49, 89, 133, 163	0
2	C	430/502 (85%)	0.11	39 (9%) 9 7	29, 72, 158, 200	0
2	D	429/502 (85%)	0.16	36 (8%) 11 8	45, 93, 152, 198	0
2	F	397/502 (79%)	0.61	59 (14%) 2 2	45, 133, 176, 198	0
All	All	2840/3402 (83%)	0.12	184 (6%) 18 12	28, 91, 158, 200	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	387	ASN	13.3
1	E	137	ALA	11.3
2	C	433	GLU	8.3
2	C	233	ASN	7.3
2	F	386	GLY	6.6
2	C	399	ASP	6.6
1	E	138	GLY	6.5
1	B	397	LEU	6.4
2	C	434	LYS	6.3
2	F	396	LYS	6.2
2	C	432	ALA	6.0
2	F	394	ARG	6.0
2	C	106	SER	5.9
2	C	235	VAL	5.8
2	C	237	TYR	5.5
2	D	233	ASN	5.3
1	B	401	THR	5.2
1	E	401	THR	5.0
2	D	225	THR	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	382	GLU	4.8
2	C	232	ASP	4.6
2	F	78	HIS	4.5
2	C	225	THR	4.3
2	C	76	GLY	4.3
2	D	388	SER	4.2
2	C	236	ASN	4.1
2	F	180	TYR	4.1
2	C	231	GLY	4.1
2	C	234	LEU	4.0
1	A	427	ASN	3.9
2	D	232	ASP	3.9
2	F	399	ASP	3.9
2	F	314	ASP	3.9
2	C	230	SER	3.9
1	B	390	THR	3.8
2	D	2	ILE	3.8
2	F	191	TYR	3.8
2	F	318	ILE	3.8
1	B	111	TYR	3.7
1	B	427	ASN	3.7
1	B	112	ASN	3.7
2	D	391	ASN	3.7
1	E	139	TRP	3.6
2	C	107	GLN	3.6
2	C	26	SER	3.5
2	C	429	PHE	3.5
2	D	433	GLU	3.5
1	E	165	LEU	3.5
2	C	226	SER	3.5
1	B	365	ILE	3.5
2	F	393	LYS	3.4
2	D	184	ARG	3.4
2	D	183	ARG	3.4
2	F	76	GLY	3.3
2	C	228	ASN	3.3
2	D	226	SER	3.3
2	F	397	GLN	3.3
2	D	167	ASP	3.3
2	F	428	ASP	3.3
1	B	394	LYS	3.2
2	F	348	ASN	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	100	VAL	3.2
1	A	390	THR	3.2
2	C	388	SER	3.2
2	C	390	ARG	3.1
1	B	196	PHE	3.1
1	B	110	HIS	3.1
2	D	185	ASN	3.1
2	F	403	GLU	3.1
2	F	395	ARG	3.1
2	D	392	LYS	3.0
2	C	223	LEU	3.0
1	A	137	ALA	3.0
2	F	186	ASP	3.0
2	F	308	ASN	3.0
2	C	395	ARG	3.0
1	A	424	HIS	3.0
1	A	409	SER	3.0
2	F	298	ASP	3.0
1	B	135	HIS	3.0
2	F	350	LYS	3.0
2	D	228	ASN	2.9
2	F	410	GLU	2.9
2	C	391	ASN	2.9
2	D	3	PRO	2.9
2	D	319	THR	2.9
2	D	108	PHE	2.9
2	C	227	SER	2.9
2	C	387	ASN	2.9
2	F	307	ARG	2.9
2	F	383	LYS	2.8
2	F	184	ARG	2.8
2	F	351	ASN	2.8
2	F	427	TYR	2.8
2	D	110	ILE	2.8
2	C	78	HIS	2.8
2	D	235	VAL	2.8
2	C	389	TRP	2.7
2	D	109	ALA	2.7
2	D	399	ASP	2.7
2	D	230	SER	2.7
2	D	222	SER	2.7
2	F	79	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	237	TYR	2.7
2	F	319	THR	2.7
1	A	401	THR	2.6
1	A	112	ASN	2.6
2	D	389	TRP	2.6
2	C	219	ALA	2.6
2	D	432	ALA	2.6
2	D	236	ASN	2.6
2	F	377	ALA	2.6
1	E	427	ASN	2.6
2	F	392	LYS	2.6
2	F	388	SER	2.6
1	B	137	ALA	2.6
1	A	425	SER	2.6
1	B	138	GLY	2.6
2	F	289	VAL	2.5
1	B	301	LEU	2.5
2	F	357	GLU	2.5
2	D	395	ARG	2.5
1	A	391	ALA	2.5
2	C	158	HIS	2.5
2	C	317	ASN	2.5
1	B	230	TYR	2.5
2	D	396	LYS	2.5
2	F	306	ALA	2.5
1	B	391	ALA	2.5
1	E	237	ALA	2.5
2	D	231	GLY	2.4
2	F	346	ASN	2.4
2	F	255	ARG	2.4
2	F	409	LYS	2.4
1	B	100	VAL	2.4
2	F	391	ASN	2.4
2	F	420	ASN	2.4
2	F	315	ASP	2.4
2	F	385	THR	2.4
2	F	384	ILE	2.3
2	C	385	THR	2.3
2	D	429	PHE	2.3
1	B	206	LEU	2.3
2	F	75	LEU	2.3
2	F	356	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	222	SER	2.3
2	D	234	LEU	2.3
2	D	434	LYS	2.3
1	B	114	SER	2.3
2	F	194	SER	2.3
1	B	422	PRO	2.3
2	F	432	ALA	2.3
1	B	116	GLU	2.3
2	C	398	ILE	2.3
2	D	387	ASN	2.3
1	A	402	ILE	2.2
2	C	221	ASP	2.2
1	A	420	ARG	2.2
2	F	265	TRP	2.2
2	F	400	SER	2.2
1	E	391	ALA	2.2
1	B	165	LEU	2.2
1	B	409	SER	2.2
2	D	112	LEU	2.2
2	F	376	LEU	2.2
1	B	420	ARG	2.2
2	F	292	LEU	2.2
1	B	218	VAL	2.2
1	E	403	PRO	2.2
2	F	484	PRO	2.2
2	F	264	LEU	2.1
1	B	431	SER	2.1
2	C	218	ASN	2.1
1	B	569	GLU	2.1
2	F	77	VAL	2.1
2	C	25	LYS	2.1
2	F	485	VAL	2.1
1	E	167	VAL	2.1
1	A	398	ASP	2.1
2	F	103	THR	2.1
2	F	317	ASN	2.1
2	D	383	LYS	2.0
2	C	75	LEU	2.0
2	F	123	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.