Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 08:58 PM EDT

PDB ID	:	2HPC
Title	:	Crystal structure of fragment D from Human Fibrinogen Complexed with Gly-Pro-Arg-Pro-amide.
Authors	:	Doolittle, R.F.; Kollman, J.M.; Chen, A.; Pandi, L.
Deposited on	:	2006-07-17
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

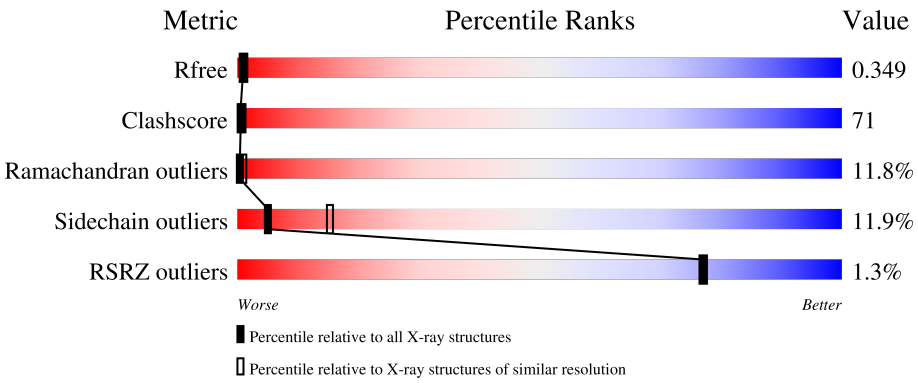
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	87	2%, 8%, 56%, 20%, •, 15%
1	D	87	23%, 47%, 10%, •, 18%
1	G	87	2%, 10%, 51%, 22%, •, 15%
1	J	87	23%, 54%, 14%, 9%
2	B	328	%, 17%, 61%, 12%, •, 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	328	29% 51% 12% • 7%
2	H	328	% 18% 60% 12% • 6%
2	K	328	30% 53% 10% • 7%
3	C	323	4% 18% 54% 22% • 6%
3	F	323	25% 58% 8% • 7%
3	I	323	4% 16% 55% 22% • 6%
3	L	323	24% 58% 10% • 7%
4	M	5	20% 80% 20%
4	N	5	100%
4	O	5	60% 40%
4	P	5	40% 40% 20%
4	Q	5	60% 40%
4	R	5	20% 60% 20%
4	S	5	40% 60%
4	T	5	60% 20% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	470	X	-	-	-
5	NAG	E	470	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22270 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 Fibrinogen alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	74	608	377	115	113	3	0	0	0
1	D	71	584	361	112	108	3	0	0	0
1	G	74	608	377	115	113	3	0	0	0
1	J	79	652	402	126	121	3	0	0	0

- Molecule 2 is a protein called Fibrinogen beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	307	2462	1535	433	472	22	0	0	0
2	E	304	2434	1514	430	468	22	0	0	0
2	H	307	2462	1535	433	472	22	0	0	0
2	K	305	2442	1520	431	469	22	0	0	0

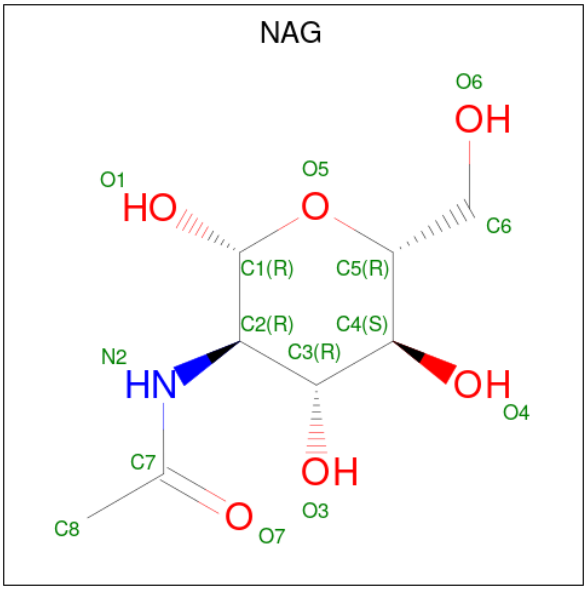
- Molecule 3 is a protein called Fibrinogen, gamma polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	305	2446	1552	410	472	12	0	0	0
3	F	300	2410	1529	405	464	12	0	0	0
3	I	305	2446	1552	410	472	12	0	0	0
3	L	300	2410	1529	405	464	12	0	0	0

- Molecule 4 is a protein called Gly-Pro-Arg-Pro-amide peptide ligand.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	M	5	30	18	8	4	0	0	1
4	N	5	30	18	8	4	0	0	1
4	O	5	30	18	8	4	0	0	1
4	P	5	30	18	8	4	0	0	1
4	Q	5	30	18	8	4	0	0	1
4	R	5	30	18	8	4	0	0	1
4	S	5	30	18	8	4	0	0	1
4	T	5	30	18	8	4	0	0	1

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
5	E	1	14	8	1	5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	H	1	14	8	1	5	0	0
			Total	C	N	O		
5	K	1	14	8	1	5	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

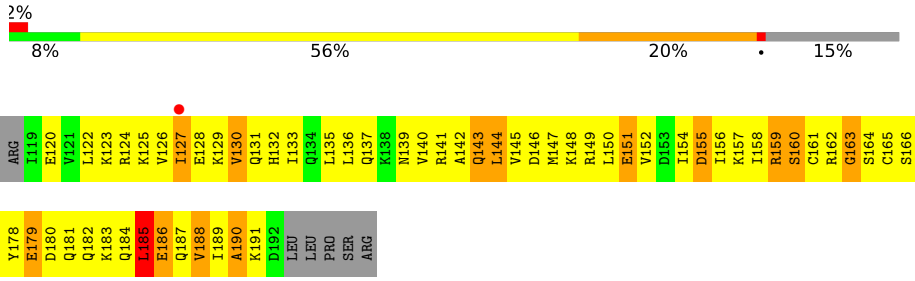
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	B	1	1	1	0	0
			Total	Ca		
6	C	1	1	1	0	0
			Total	Ca		
6	E	2	2	2	0	0
			Total	Ca		
6	F	1	1	1	0	0
			Total	Ca		
6	H	1	1	1	0	0
			Total	Ca		
6	I	1	1	1	0	0
			Total	Ca		
6	K	2	2	2	0	0
			Total	Ca		
6	L	1	1	1	0	0

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.

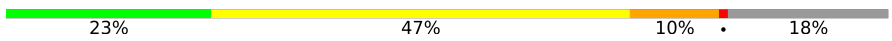
• Molecule 1: Fibrinogen alpha chain

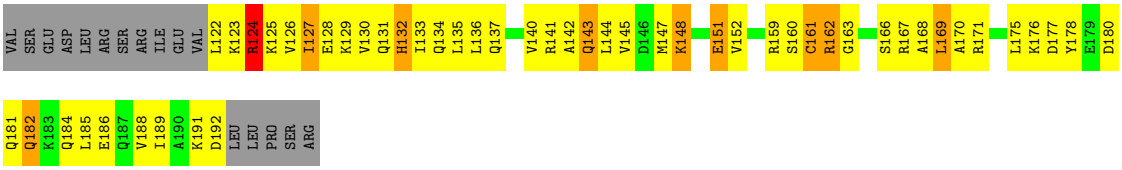
Chain A:



• Molecule 1: Fibrinogen alpha chain

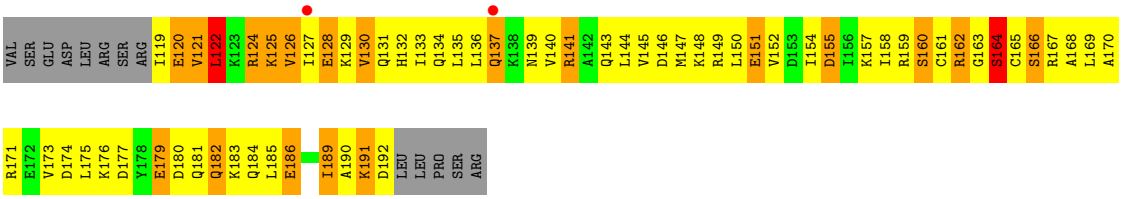
Chain D:





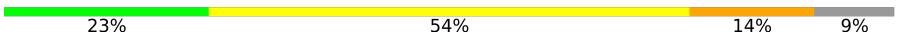
• Molecule 1: Fibrinogen alpha chain

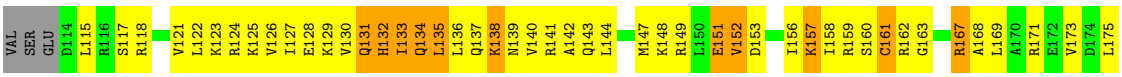
Chain G:



• Molecule 1: Fibrinogen alpha chain

Chain J:





K176 D177 Y178 E179 D180 Q181 Q182 K183 Q184 L185 E186 Q187 V188 I189 A190 K191 D192 LEU LEU PRO SER ARG

• Molecule 2: Fibrinogen beta chain

Chain B: % 17% 61% 12% • 6%

ASP ASN GLU ASN VAL VAL ASN GLU TYR SER SER GLU LEU GLU LYS HIS GLN L151 Y152 I153 D154 E155 T156 V157 N158 S159 N160 I161 P162 T163 N164 L165 R166 V167 L168 R169 S170 I171 L172 E173 N174 L175 R176 S177 K178 I179 Q180 K181 L182 E183 S184 D185 V186 S187 A188 Q189 M190 E191 Y192 C193

R194 C197 T198 V199 S200 C201 N202 I203 P204 V205 V206 S207 G208 K209 E210 C211 E212 E213 I214 I215 R216 K217 G218 G219 S222 E223 M224 Y225 L226 I227 Q228 P229 D230 S231 S232 V233 K234 P235 Y236 R237 V238 Y239 C240 D241 M242 N246 G247 G248 W249 T250 V251 I252 Q253 N254 R255 Q256 D257

G258 S259 V260 D261 F262 G263 R264 K265 W266 D267 P268 Y269 K270 Q271 G272 F273 V276 A277 T278 N279 T280 D281 N284 Y285 C286 G287 L288 P289 G290 E291 Y292 W293 L294 G295 N296 D297 K298 I299 S300 Q301 L302 T303 R304 E309 L310 L311 I312 E315 D316 W317 D320 K321 V322 K323 A324

H325 Y326 G327 G328 F329 T330 V331 Q332 N333 E334 A335 N336 K337 Y338 Q339 I340 S341 V342 N343 K344 Y345 R346 G347 T348 A349 G350 N351 A352 L353 M354 D355 G356 A357 S358 Q359 L360 M361 G362 E363 N364 R365 T366 M367 T368 I369 H370 N371 G372 M373 F374 F375 S376 R380 G384 W385 L386 T387 S388

D389 P390 Q393 C394 S395 K396 E397 D398 G399 G400 G401 W402 W403 Y404 N405 R406 C407 H408 A409 A410 N411 P412 N413 G414 R415 Y416 Y417 W418 Q421 Y422 T423 W424 D425 M426 A427 K428 H429 D432 D433 G434 V435 V436 W437 M438 N439 W440 K441 G442 S443 W444 Y445 S446 M447 R448 K449 N450 S451

M452 K453 I454 R455 P456 F457 PHE PRO GLN GLN

• Molecule 2: Fibrinogen beta chain

Chain E: 29% 51% 12% • 7%

ASP ASN GLU ASN VAL VAL ASN GLU TYR SER SER GLU LEU GLU LYS HIS GLN LEU TYR ILE D154 E155 T156 V157 N158 S159 N160 I161 P162 T163 N164 L165 R166 V167 L168 R169 S170 I171 L172 E173 N174 L175 R176 S177 K178 I179 Q180 K181 L182 E183 S184 D185 V186 Q189 M190 E191 Y192 C193 R194

T195 T198 V199 S200 C201 N202 I203 P204 V205 V206 K209 E210 C211 E212 E213 I214 I215 R216 K217 G218 G219 E220 T221 S222 E223 M224 Y225 L226 I227 Q228 P229 D230 S231 S232 V233 K234 P235 Y236 R237 V238 Y239 C240 D241 M242 N243 T244 E245 N246 G247 G248 W249 T250 V251 I252 Q253 N254 R255 Q256

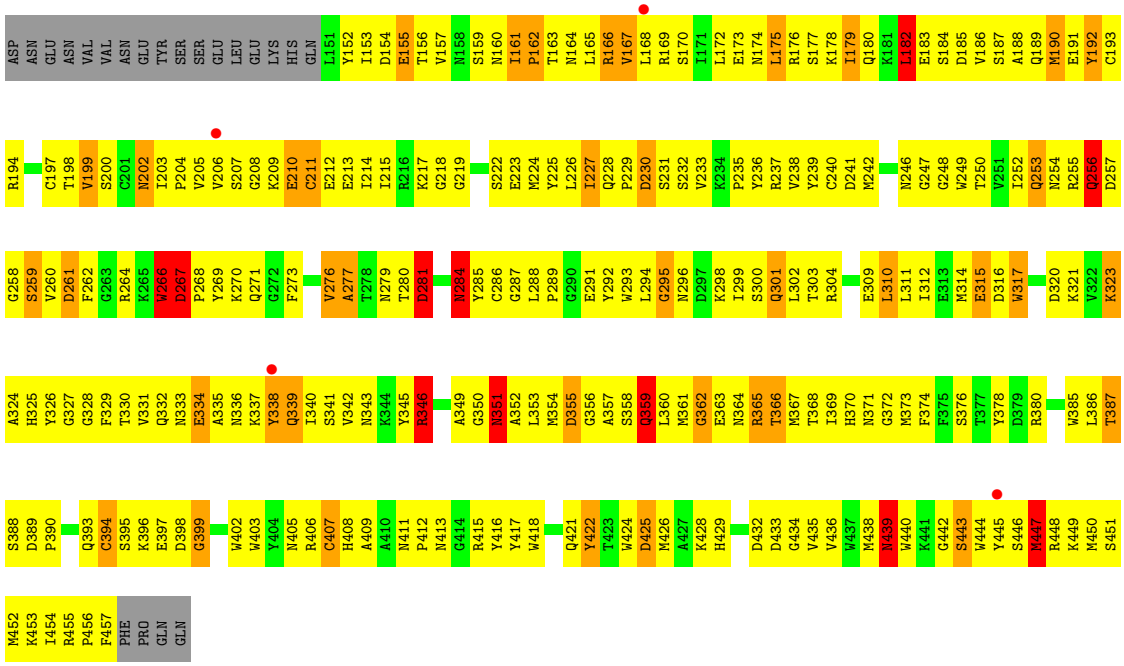
D257 G258 S259 R264 K265 W266 D267 P268 Y269 K270 Q271 G272 F273 V276 A277 T278 N279 T280 D281 C286 G287 L288 P289 G290 E291 Y292 W293 L294 G295 N296 D297 K298 Q301 L302 T303 R304 M305 G306 P307 T308 E309 L310 L311 I312 E313 M314 E315 K318 K321 V322 K323 A324 H325 Y326

G327 G328 Q332 N333 N336 K337 Y338 Q339 I340 S341 V342 N343 K344 Y345 R346 G347 T348 N351 A352 L353 M354 D355 S358 Q359 N364 R365 T366 M367 T368 I369 H370 M373 F374 F375 S376 T377 Y378 D379 R380 D381 N382 D383 G384 W385 L386 T387 S388 D389 P390 R391 K392 Q393 C394 S395

K396 E397 D398 G399 W402 W403 Y404 N405 R406 C407 H408 A409 A410 N411 P412 N413 G414 R415 D425 M426 H429 G430 T431 D432 D433 G434 V435 V436 W437 M438 N439 W440 K441 W444 Y445 S446 M447 R448 M452 K453 I454 R455 P456 F457 PHE PRO GLN GLN

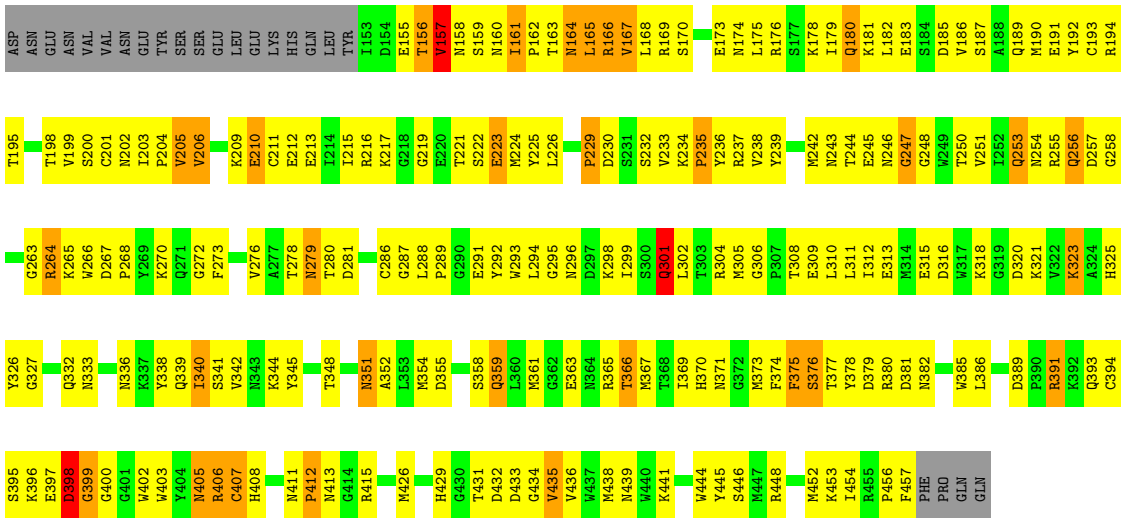
• Molecule 2: Fibrinogen beta chain

Chain H: % 18% 60% 12% • 6%



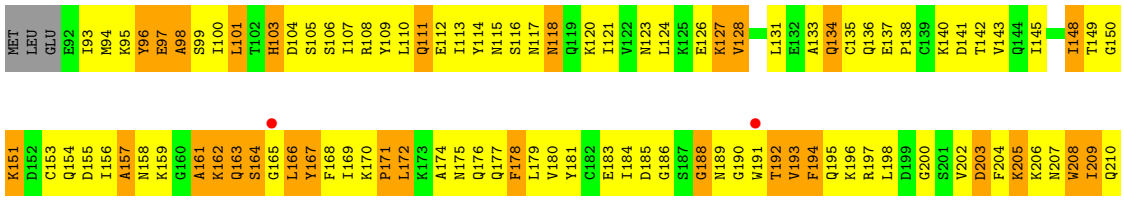
• Molecule 2: Fibrinogen beta chain

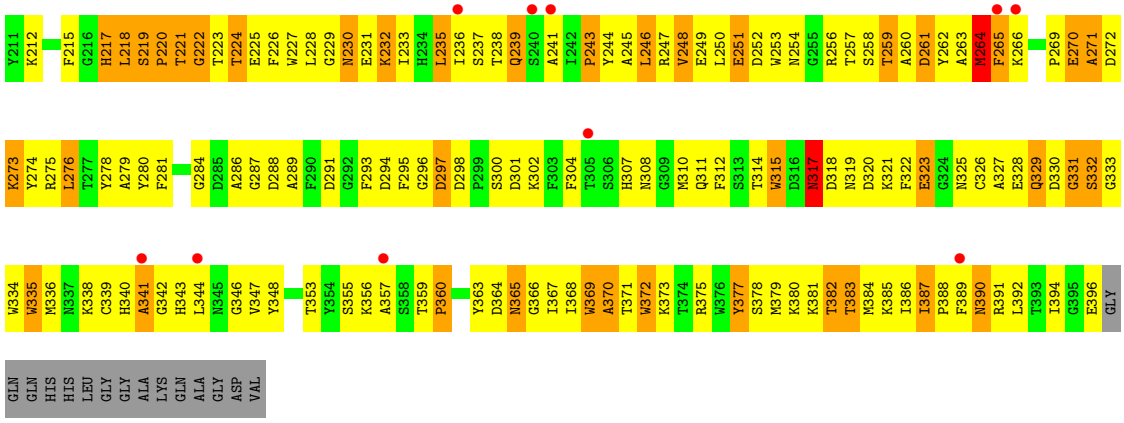
Chain K: 30% 53% 10% • 7%



• Molecule 3: Fibrinogen, gamma polypeptide

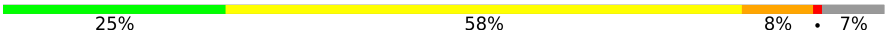
Chain C: 4% 18% 54% 22% • 6%

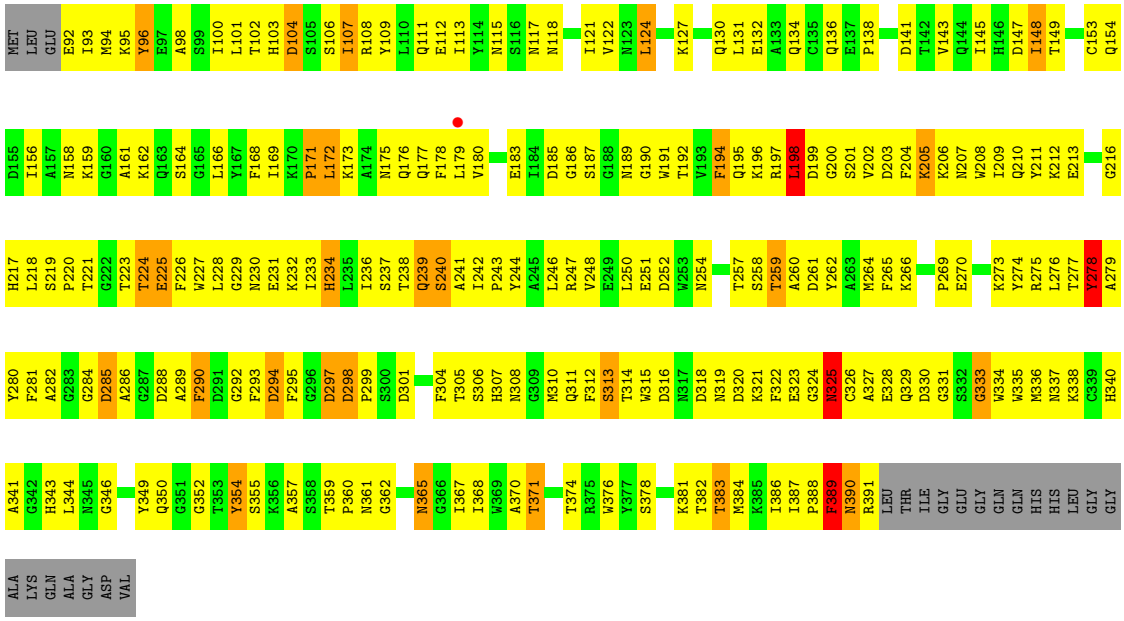




- Molecule 3: Fibrinogen, gamma polypeptide

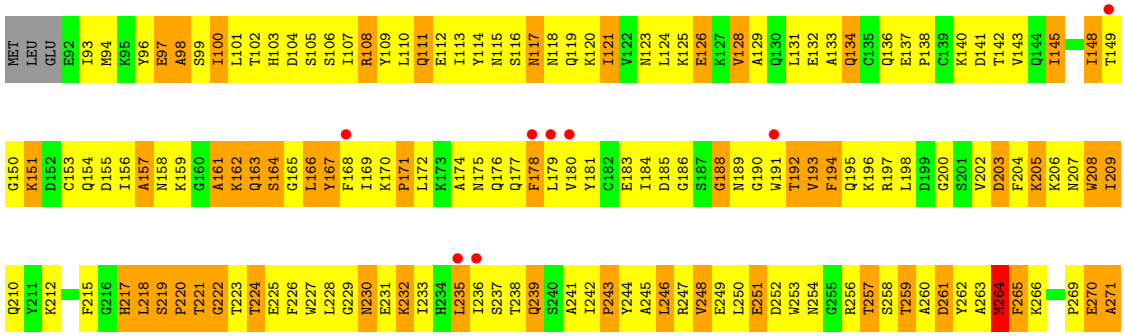
Chain F:





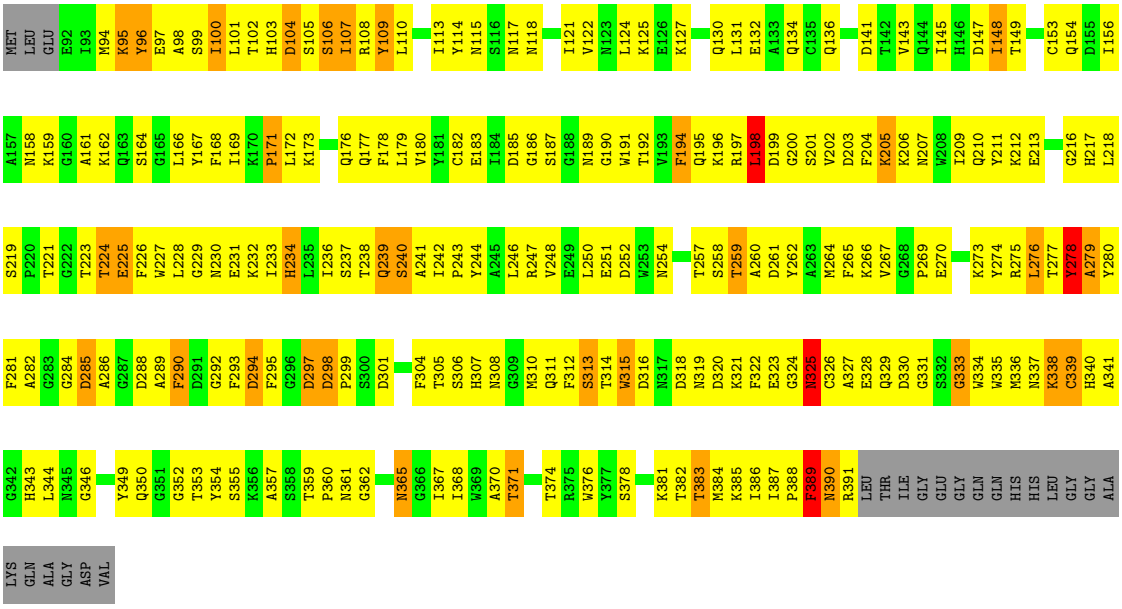
- Molecule 3: Fibrinogen, gamma polypeptide

Chain I:



• Molecule 3: Fibrinogen, gamma polypeptide

Chain L: 24% 58% 10% • 7%



• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain M: 20% 80% 20%

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain N: 100%

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain O: 60% 40%

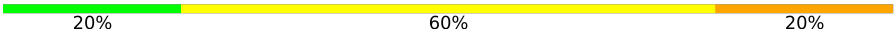
• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain P:

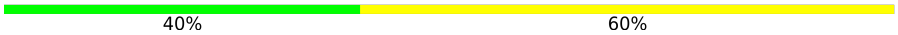
• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain Q:

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain R: 

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain S: 

• Molecule 4: Gly-Pro-Arg-Pro-amide peptide ligand

Chain T:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	81.68Å 46.07Å 429.90Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 49.09 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-2.90) 86.5 (49.09-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.54Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.360 0.266 , 0.349	Depositor DCC
R_{free} test set	3644 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 28.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22270	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CA, NH2

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	0.38	0/609	0.75	0/811
1	D	0.44	0/585	0.77	0/778
1	G	0.42	0/609	0.78	0/811
1	J	0.42	0/653	0.74	0/869
2	B	0.40	0/2523	0.76	2/3409 (0.1%)
2	E	0.50	0/2494	0.78	1/3369 (0.0%)
2	H	0.41	0/2523	0.76	1/3409 (0.0%)
2	K	0.50	0/2502	0.79	3/3380 (0.1%)
3	C	0.40	0/2512	0.68	0/3396
3	F	0.44	0/2476	0.72	1/3347 (0.0%)
3	I	0.40	0/2512	0.70	1/3396 (0.0%)
3	L	0.43	0/2476	0.73	2/3347 (0.1%)
4	M	0.45	0/30	0.66	0/40
4	N	0.65	0/30	0.72	0/40
4	O	0.51	0/30	0.71	0/40
4	P	0.48	0/30	0.80	0/40
4	Q	0.52	0/30	0.73	0/40
4	R	0.56	0/30	0.66	0/40
4	S	0.49	0/30	0.59	0/40
4	T	0.53	0/30	0.79	0/40
All	All	0.43	0/22714	0.74	11/30642 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	406	ARG	C-N-CA	5.83	136.28	121.70
2	K	412	PRO	N-CA-C	-5.72	97.22	112.10
2	E	412	PRO	N-CA-C	-5.71	97.26	112.10
2	K	406	ARG	CA-C-N	-5.70	104.66	117.20
2	H	346	ARG	N-CA-C	-5.53	96.08	111.00
3	I	338	LYS	C-N-CA	5.25	134.83	121.70
2	B	346	ARG	N-CA-C	-5.25	96.84	111.00
3	L	338	LYS	C-N-CA	5.21	134.71	121.70
3	L	333	GLY	N-CA-C	-5.13	100.28	113.10
3	F	333	GLY	N-CA-C	-5.06	100.45	113.10
2	B	175	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	378	TYR	Sidechain

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	608	0	649	142	0
1	D	584	0	623	80	0
1	G	608	0	649	118	0
1	J	652	0	695	97	0
2	B	2462	0	2327	497	0
2	E	2434	0	2295	236	0
2	H	2462	0	2326	430	0
2	K	2442	0	2307	234	0
3	C	2446	0	2294	450	0
3	F	2410	0	2256	293	0
3	I	2446	0	2294	443	0
3	L	2410	0	2256	303	0
4	M	30	0	32	2	0
4	N	30	0	32	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	30	0	32	3	0
4	P	30	0	32	4	0
4	Q	30	0	32	2	0
4	R	30	0	32	8	0
4	S	30	0	32	7	0
4	T	30	0	32	3	0
5	B	14	0	13	1	0
5	E	14	0	13	0	0
5	H	14	0	13	4	0
5	K	14	0	13	3	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	E	2	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	K	2	0	0	0	0
6	L	1	0	0	0	0
All	All	22270	0	21279	3110	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

All (3110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:LEU:H	2:B:166:ARG:NH2	1.45	1.15
3:C:197:ARG:HA	3:C:225:GLU:HG2	1.27	1.14
3:I:197:ARG:HA	3:I:225:GLU:HG2	1.30	1.12
3:I:171:PRO:HB2	3:I:174:ALA:HB2	1.33	1.06
3:C:171:PRO:HB2	3:C:174:ALA:HB2	1.33	1.05
2:B:165:LEU:N	2:B:166:ARG:HH21	1.56	1.03
3:C:154:GLN:HE22	3:C:189:ASN:HA	1.25	1.01
3:C:212:LYS:HG2	3:C:231:GLU:HB2	1.42	1.01
3:I:169:ILE:HD12	3:I:171:PRO:HD3	1.41	1.01
3:I:212:LYS:HG2	3:I:231:GLU:HB2	1.43	1.01
1:D:147:MET:HG3	2:E:175:LEU:HD22	1.41	1.00
3:F:148:ILE:HD12	3:F:148:ILE:H	1.24	1.00
2:B:176:ARG:HA	2:B:179:ILE:HD12	1.40	0.99
3:C:169:ILE:HD12	3:C:171:PRO:HD3	1.43	0.99
2:B:249:TRP:HH2	2:B:325:HIS:HE2	1.11	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:249:TRP:HH2	2:H:325:HIS:HE2	1.12	0.98
3:I:154:GLN:HE22	3:I:189:ASN:HA	1.29	0.98
3:L:96:TYR:H	3:L:96:TYR:HD2	1.09	0.97
2:K:367:MET:HB2	2:K:406:ARG:HB3	1.48	0.96
3:I:189:ASN:ND2	3:I:391:ARG:HB3	1.79	0.96
2:B:193:CYS:HB3	3:C:134:GLN:HE22	1.32	0.95
2:K:367:MET:SD	2:K:406:ARG:HG2	2.07	0.95
2:H:210:GLU:HA	2:H:227:ILE:HB	1.49	0.94
3:C:193:VAL:HG12	3:C:194:PHE:N	1.83	0.94
2:E:212:GLU:O	2:E:215:ILE:HG22	1.70	0.92
2:K:212:GLU:O	2:K:215:ILE:HG22	1.70	0.92
2:B:204:PRO:HA	3:C:217:HIS:HA	1.52	0.92
3:I:154:GLN:HE21	3:I:158:ASN:ND2	1.68	0.92
3:C:209:ILE:H	3:C:209:ILE:HD12	1.35	0.92
3:I:193:VAL:HG12	3:I:194:PHE:N	1.85	0.91
2:H:357:ALA:HA	2:H:439:ASN:HD21	1.34	0.91
3:C:193:VAL:HG12	3:C:194:PHE:H	1.32	0.91
2:H:204:PRO:HA	3:I:217:HIS:HA	1.53	0.91
2:H:359:GLN:O	2:H:360:LEU:HD23	1.70	0.91
3:I:209:ILE:H	3:I:209:ILE:HD12	1.35	0.91
3:C:189:ASN:ND2	3:C:391:ARG:HB3	1.85	0.90
3:C:154:GLN:HE21	3:C:158:ASN:ND2	1.69	0.90
2:B:210:GLU:HA	2:B:227:ILE:HB	1.53	0.90
3:I:193:VAL:HG12	3:I:194:PHE:H	1.34	0.90
3:C:249:GLU:HB3	3:C:383:THR:HG23	1.54	0.90
3:I:249:GLU:HB3	3:I:383:THR:HG23	1.54	0.90
3:L:148:ILE:H	3:L:148:ILE:HD12	1.33	0.90
2:B:180:GLN:O	2:B:183:GLU:HB3	1.71	0.89
3:I:103:HIS:O	3:I:107:ILE:HG12	1.73	0.89
1:A:143:GLN:HA	1:A:143:GLN:HE21	1.35	0.89
3:F:227:TRP:HZ2	3:F:230:ASN:HD21	1.20	0.89
3:L:230:ASN:HA	3:L:233:ILE:HD12	1.54	0.89
1:A:167:ARG:HH12	1:A:169:LEU:HD23	1.35	0.89
3:L:258:SER:HB2	3:L:286:ALA:HB2	1.55	0.89
3:C:287:GLY:HA3	3:C:371:THR:O	1.72	0.88
1:A:148:LYS:NZ	2:B:425:ASP:HB2	1.89	0.88
2:B:357:ALA:HA	2:B:439:ASN:HD21	1.39	0.88
2:E:373:MET:HG3	2:E:405:ASN:HB2	1.56	0.88
2:H:373:MET:SD	2:H:405:ASN:HB2	2.13	0.88
3:C:196:LYS:HG2	3:C:198:LEU:HD11	1.56	0.88
2:B:310:LEU:HD11	2:B:312:ILE:HG13	1.56	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:227:TRP:HZ2	3:L:230:ASN:HD21	1.17	0.88
3:I:107:ILE:HG13	3:I:108:ARG:H	1.38	0.88
2:B:256:GLN:HE21	2:B:449:LYS:HE2	1.36	0.87
3:I:196:LYS:HG2	3:I:198:LEU:HD11	1.57	0.87
2:H:310:LEU:HD11	2:H:312:ILE:HG13	1.56	0.87
1:J:167:ARG:HA	1:J:167:ARG:CZ	2.03	0.87
2:B:165:LEU:HD23	2:B:166:ARG:NH2	1.90	0.87
3:F:258:SER:HB2	3:F:286:ALA:HB2	1.57	0.87
1:G:148:LYS:HD3	1:G:182:GLN:HE22	1.38	0.87
3:F:172:LEU:HD13	3:F:240:SER:HB3	1.56	0.87
2:K:373:MET:HG3	2:K:405:ASN:HB2	1.55	0.87
1:A:144:LEU:HD21	1:A:182:GLN:HG2	1.54	0.87
3:I:196:LYS:HE3	3:I:198:LEU:HD21	1.56	0.87
2:H:357:ALA:HA	2:H:439:ASN:ND2	1.90	0.86
3:F:251:GLU:HB3	3:F:381:LYS:HB2	1.54	0.86
2:K:412:PRO:O	2:K:413:ASN:HB2	1.76	0.86
2:B:256:GLN:HB3	2:B:449:LYS:HE2	1.57	0.86
3:C:196:LYS:HE3	3:C:198:LEU:HD21	1.57	0.86
3:I:109:TYR:O	3:I:112:GLU:HB3	1.76	0.85
3:L:172:LEU:HD13	3:L:240:SER:HB3	1.58	0.85
2:H:292:TYR:HE2	2:H:294:LEU:HB2	1.42	0.85
2:H:237:ARG:HH11	2:H:237:ARG:HG3	1.41	0.85
2:B:193:CYS:HB3	3:C:134:GLN:NE2	1.91	0.85
2:B:215:ILE:HB	2:B:242:MET:HE1	1.59	0.85
2:B:398:ASP:HA	2:B:433:ASP:CB	2.07	0.85
1:D:143:GLN:HE22	3:F:117:ASN:HB2	1.39	0.85
1:A:128:GLU:O	1:A:131:GLN:HG2	1.76	0.84
3:C:118:ASN:HD22	3:C:118:ASN:H	1.20	0.84
1:G:147:MET:HE2	2:H:179:ILE:HG12	1.57	0.84
3:I:154:GLN:HE21	3:I:158:ASN:HD21	1.23	0.84
1:A:169:LEU:HD13	1:A:170:ALA:N	1.91	0.84
3:C:340:HIS:O	4:O:1:GLY:HA2	1.77	0.84
2:K:175:LEU:O	2:K:179:ILE:HG13	1.78	0.84
2:H:256:GLN:HE21	2:H:449:LYS:HE2	1.43	0.84
3:C:230:ASN:HD22	3:C:230:ASN:N	1.72	0.84
2:H:168:LEU:HD23	3:I:110:LEU:HD12	1.60	0.84
1:G:160:SER:OG	2:H:261:ASP:HB3	1.78	0.84
3:C:154:GLN:HE21	3:C:158:ASN:HD21	1.22	0.84
2:H:166:ARG:HH12	2:H:169:ARG:HD2	1.41	0.84
2:H:238:VAL:HG21	2:H:250:THR:HG23	1.59	0.84
2:H:215:ILE:HB	2:H:242:MET:HE1	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:ALA:HA	2:B:439:ASN:ND2	1.94	0.83
2:B:237:ARG:HG3	2:B:237:ARG:HH11	1.42	0.83
3:I:287:GLY:HA3	3:I:371:THR:O	1.77	0.83
3:C:193:VAL:CG1	3:C:194:PHE:H	1.91	0.83
3:C:230:ASN:HD22	3:C:230:ASN:H	1.23	0.83
3:I:250:LEU:HD12	3:I:382:THR:HA	1.61	0.83
2:H:215:ILE:HD12	2:H:219:GLY:O	1.79	0.83
3:F:230:ASN:HA	3:F:233:ILE:HD12	1.60	0.82
2:B:237:ARG:HH21	3:C:143:VAL:HG23	1.43	0.82
3:I:325:ASN:HD21	3:I:327:ALA:HB3	1.42	0.82
3:L:194:PHE:HD1	3:L:233:ILE:HG12	1.41	0.82
2:H:161:ILE:HG21	3:I:103:HIS:CE1	2.13	0.82
2:H:309:GLU:HB3	2:H:325:HIS:HE1	1.42	0.82
3:F:149:THR:O	3:F:156:ILE:HG12	1.78	0.82
1:J:129:LYS:O	1:J:133:ILE:HG22	1.79	0.82
3:F:166:LEU:HB3	3:F:179:LEU:HD11	1.60	0.82
2:H:256:GLN:HB3	2:H:449:LYS:HE2	1.60	0.82
3:I:227:TRP:HZ2	3:I:230:ASN:HD21	1.25	0.82
3:F:278:TYR:CZ	3:F:308:ASN:HB2	2.14	0.82
2:H:398:ASP:HA	2:H:433:ASP:CB	2.10	0.82
3:I:107:ILE:HG13	3:I:108:ARG:N	1.94	0.82
2:B:238:VAL:HG21	2:B:250:THR:HG23	1.61	0.81
3:C:163:GLN:HA	3:C:163:GLN:HE21	1.44	0.81
3:C:230:ASN:H	3:C:230:ASN:ND2	1.76	0.81
3:I:230:ASN:HD22	3:I:230:ASN:N	1.76	0.81
3:L:251:GLU:HB3	3:L:381:LYS:HB2	1.60	0.81
2:H:215:ILE:HD13	2:H:242:MET:HB3	1.62	0.81
2:B:164:ASN:H	2:B:166:ARG:NE	1.77	0.81
2:B:309:GLU:HB3	2:B:325:HIS:HE1	1.44	0.81
3:I:246:LEU:HD12	3:I:247:ARG:N	1.96	0.81
2:B:359:GLN:O	2:B:360:LEU:HD23	1.80	0.81
2:H:237:ARG:HH21	3:I:143:VAL:HG23	1.44	0.81
1:A:160:SER:OG	2:B:261:ASP:HB3	1.80	0.81
2:B:166:ARG:NE	2:B:166:ARG:H	1.78	0.81
2:E:175:LEU:O	2:E:179:ILE:HG13	1.80	0.80
3:C:246:LEU:HD12	3:C:247:ARG:N	1.96	0.80
3:C:250:LEU:HD12	3:C:382:THR:HA	1.62	0.80
3:F:194:PHE:HD1	3:F:233:ILE:HG12	1.44	0.80
2:B:267:ASP:HB2	2:B:268:PRO:HD3	1.62	0.80
3:C:143:VAL:HG12	3:C:220:PRO:HD3	1.63	0.80
2:E:265:LYS:O	2:E:268:PRO:HD2	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:179:ILE:O	2:K:183:GLU:HG3	1.81	0.80
3:I:273:LYS:HE3	3:I:319:ASN:ND2	1.96	0.80
1:D:132:HIS:HB3	3:F:107:ILE:HD11	1.63	0.80
3:I:230:ASN:HD22	3:I:230:ASN:H	1.29	0.80
2:B:398:ASP:HA	2:B:433:ASP:HB3	1.63	0.80
1:D:132:HIS:HB3	3:F:107:ILE:CD1	2.12	0.79
3:F:117:ASN:O	3:F:121:ILE:HG13	1.80	0.79
3:I:193:VAL:CG1	3:I:194:PHE:H	1.95	0.79
2:B:373:MET:SD	2:B:405:ASN:HB2	2.22	0.79
3:L:149:THR:O	3:L:156:ILE:HG12	1.82	0.79
3:L:338:LYS:HG3	4:T:3:ARG:HB2	1.63	0.79
3:C:278:TYR:OH	3:C:308:ASN:HB2	1.82	0.79
2:K:393:GLN:HB2	2:K:396:LYS:HG2	1.62	0.79
1:A:128:GLU:HG2	1:A:129:LYS:HD2	1.64	0.79
2:E:412:PRO:O	2:E:413:ASN:HB2	1.83	0.79
1:G:181:GLN:O	1:G:184:GLN:HG3	1.82	0.79
3:I:367:ILE:HG22	3:I:379:MET:HG2	1.64	0.79
3:L:278:TYR:CZ	3:L:308:ASN:HB2	2.17	0.79
2:B:176:ARG:HA	2:B:179:ILE:CD1	2.13	0.78
2:B:399:GLY:HA3	2:B:415:ARG:HD3	1.63	0.78
3:C:325:ASN:HD21	3:C:327:ALA:HB3	1.46	0.78
1:G:169:LEU:HD22	1:G:170:ALA:H	1.47	0.78
3:I:330:ASP:HB3	3:I:365:ASN:HB3	1.64	0.78
3:I:163:GLN:HA	3:I:163:GLN:HE21	1.47	0.78
2:B:292:TYR:HE2	2:B:294:LEU:HB2	1.48	0.78
3:C:273:LYS:HE3	3:C:319:ASN:ND2	1.98	0.78
3:I:340:HIS:O	4:S:1:GLY:HA2	1.84	0.78
3:L:322:PHE:HB2	3:L:338:LYS:HD2	1.66	0.78
2:B:215:ILE:HD13	2:B:242:MET:HB3	1.66	0.78
2:B:455:ARG:HG3	2:B:456:PRO:HD2	1.66	0.78
3:C:110:LEU:C	3:C:112:GLU:H	1.85	0.78
2:E:205:VAL:HG12	2:E:206:VAL:N	1.97	0.78
1:A:155:ASP:HA	1:A:171:ARG:NH2	1.99	0.78
1:D:185:LEU:HB2	2:E:171:ILE:CD1	2.13	0.77
2:H:267:ASP:HB2	2:H:268:PRO:HD3	1.64	0.77
2:H:270:LYS:HA	2:H:296:ASN:HB2	1.66	0.77
3:I:230:ASN:H	3:I:230:ASN:ND2	1.80	0.77
3:L:195:GLN:HG3	3:L:227:TRP:CE3	2.18	0.77
2:H:223:GLU:HB2	2:H:287:GLY:HA2	1.66	0.77
3:I:256:ARG:HG3	3:I:256:ARG:HH11	1.46	0.77
3:C:367:ILE:HG22	3:C:379:MET:HG2	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:193:VAL:HG12	3:I:195:GLN:H	1.48	0.77
3:L:262:TYR:OH	3:L:290:PHE:HB2	1.84	0.77
1:A:122:LEU:HD23	1:A:122:LEU:H	1.49	0.77
3:C:228:LEU:HD12	3:C:228:LEU:O	1.84	0.77
2:B:162:PRO:C	2:B:166:ARG:HD2	2.05	0.77
3:C:256:ARG:HH11	3:C:256:ARG:HG3	1.47	0.77
2:H:186:VAL:HG11	3:I:128:VAL:HG22	1.67	0.77
2:K:351:ASN:HD21	2:K:354:MET:H	1.32	0.77
3:L:166:LEU:HB3	3:L:179:LEU:HD11	1.66	0.77
2:B:284:ASN:H	2:B:284:ASN:HD22	1.30	0.77
3:C:154:GLN:NE2	3:C:189:ASN:HA	1.99	0.77
3:L:117:ASN:O	3:L:121:ILE:HG13	1.85	0.77
2:B:187:SER:HA	2:B:190:MET:HB3	1.66	0.77
3:F:195:GLN:HG3	3:F:227:TRP:CE3	2.20	0.77
2:H:411:ASN:HB3	2:H:436:VAL:HG22	1.66	0.77
2:B:223:GLU:HB2	2:B:287:GLY:HA2	1.66	0.76
4:R:3:ARG:HB3	4:R:4:PRO:CD	2.15	0.76
2:B:165:LEU:N	2:B:166:ARG:NH2	2.23	0.76
2:B:165:LEU:HD11	3:C:107:ILE:HA	1.67	0.76
2:B:177:SER:HA	2:B:180:GLN:CG	2.16	0.76
2:K:352:ALA:HB2	2:K:439:ASN:ND2	1.99	0.76
3:F:183:GLU:HB3	3:F:191:TRP:HB2	1.67	0.76
3:C:330:ASP:HB3	3:C:365:ASN:HB3	1.65	0.76
3:I:170:LYS:HE3	3:I:177:GLN:HB3	1.67	0.76
1:G:144:LEU:HD21	1:G:182:GLN:HG3	1.67	0.76
1:G:186:GLU:HA	1:G:189:ILE:HG22	1.68	0.76
3:I:278:TYR:OH	3:I:308:ASN:HB2	1.86	0.76
2:K:205:VAL:HG12	2:K:206:VAL:N	2.00	0.76
3:L:281:PHE:HB2	3:L:288:ASP:OD2	1.85	0.76
2:B:161:ILE:HG21	3:C:103:HIS:CD2	2.20	0.76
2:H:399:GLY:HA3	2:H:415:ARG:HD3	1.67	0.76
2:B:411:ASN:HB3	2:B:436:VAL:HG22	1.68	0.76
3:F:212:LYS:HG3	3:F:231:GLU:HB2	1.67	0.76
2:K:216:ARG:HB2	2:K:216:ARG:NH1	2.00	0.76
3:F:262:TYR:OH	3:F:290:PHE:HB2	1.84	0.75
2:H:455:ARG:HG3	2:H:456:PRO:HD2	1.68	0.75
2:K:216:ARG:CB	2:K:216:ARG:HH11	1.99	0.75
1:A:143:GLN:HE22	3:C:118:ASN:ND2	1.85	0.75
2:H:309:GLU:HB3	2:H:325:HIS:CE1	2.22	0.75
2:H:346:ARG:HH11	2:H:346:ARG:HB2	1.50	0.75
2:H:333:ASN:OD1	2:H:335:ALA:HB3	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:315:GLU:HB2	2:H:321:LYS:HB3	1.68	0.75
1:J:143:GLN:HE22	3:L:117:ASN:HB2	1.50	0.75
3:C:154:GLN:NE2	3:C:158:ASN:HD21	1.84	0.75
3:F:94:MET:HB3	3:F:96:TYR:CE1	2.21	0.75
1:D:124:ARG:HD3	1:D:124:ARG:H	1.50	0.75
3:C:342:GLY:H	3:C:368:ILE:HG13	1.52	0.75
3:F:251:GLU:HA	3:F:257:THR:HG22	1.68	0.75
2:H:187:SER:O	2:H:191:GLU:HB2	1.86	0.75
3:I:304:PHE:HB3	3:I:338:LYS:HB3	1.69	0.75
1:J:158:ILE:HG23	2:K:189:GLN:HE21	1.51	0.75
2:H:398:ASP:HA	2:H:433:ASP:HB3	1.69	0.74
2:B:270:LYS:HA	2:B:296:ASN:HB2	1.68	0.74
2:B:309:GLU:HB3	2:B:325:HIS:CE1	2.23	0.74
3:C:193:VAL:HG12	3:C:195:GLN:H	1.51	0.74
2:E:352:ALA:HB2	2:E:439:ASN:ND2	2.02	0.74
2:E:393:GLN:HB2	2:E:396:LYS:HG2	1.68	0.74
3:I:143:VAL:HG12	3:I:220:PRO:HD3	1.68	0.74
3:F:281:PHE:HB2	3:F:288:ASP:OD2	1.86	0.74
2:H:369:ILE:H	2:H:405:ASN:HD22	1.36	0.74
3:I:154:GLN:NE2	3:I:158:ASN:HD21	1.84	0.74
3:F:229:GLY:O	3:F:233:ILE:HG13	1.88	0.74
3:I:203:ASP:O	3:I:206:LYS:HE3	1.87	0.74
3:I:264:MET:N	3:I:264:MET:SD	2.60	0.74
3:C:170:LYS:HE3	3:C:177:GLN:HB3	1.69	0.74
2:E:216:ARG:CB	2:E:216:ARG:HH11	2.00	0.74
3:F:297:ASP:O	3:F:298:ASP:HB3	1.88	0.74
3:C:172:LEU:HB2	3:C:239:GLN:HB3	1.70	0.74
3:L:292:GLY:N	3:L:306:SER:HA	2.02	0.74
3:C:227:TRP:HZ2	3:C:230:ASN:HD21	1.34	0.74
2:H:199:VAL:O	3:I:142:THR:HG23	1.88	0.74
3:I:250:LEU:O	3:I:257:THR:HB	1.87	0.74
3:L:212:LYS:HG3	3:L:231:GLU:HB2	1.69	0.74
2:H:284:ASN:HD22	2:H:284:ASN:H	1.34	0.74
3:F:96:TYR:H	3:F:96:TYR:HD1	1.35	0.73
3:I:154:GLN:NE2	3:I:189:ASN:HA	2.02	0.73
2:K:312:ILE:HG12	2:K:452:MET:HG2	1.68	0.73
3:C:172:LEU:HD13	3:C:239:GLN:CB	2.19	0.73
3:C:382:THR:HG22	3:C:382:THR:O	1.88	0.73
1:D:136:LEU:HD23	2:E:168:LEU:HD13	1.70	0.73
2:H:385:TRP:HB2	2:H:406:ARG:HA	1.71	0.73
1:J:144:LEU:HD23	2:K:175:LEU:HD21	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:TRP:CZ3	2:B:448:ARG:HD3	2.23	0.73
3:F:278:TYR:OH	3:F:308:ASN:HB2	1.87	0.73
2:B:185:ASP:HA	2:B:188:ALA:HB3	1.68	0.73
2:E:180:GLN:HG3	2:E:181:LYS:N	2.03	0.73
2:E:216:ARG:NH1	2:E:216:ARG:HB2	2.03	0.73
2:B:215:ILE:HD12	2:B:219:GLY:O	1.88	0.73
2:B:310:LEU:HD11	2:B:312:ILE:CG1	2.18	0.73
3:C:281:PHE:CE2	3:C:288:ASP:HB2	2.23	0.73
3:I:117:ASN:N	3:I:117:ASN:HD22	1.86	0.73
3:L:229:GLY:O	3:L:233:ILE:HG13	1.89	0.73
2:H:176:ARG:HA	2:H:179:ILE:CD1	2.18	0.73
3:L:183:GLU:HB3	3:L:191:TRP:HB2	1.70	0.73
1:G:169:LEU:HD13	1:G:171:ARG:N	2.04	0.73
3:I:218:LEU:O	3:I:219:SER:HB3	1.87	0.73
1:A:133:ILE:O	1:A:137:GLN:HB2	1.88	0.73
1:A:156:ILE:HD11	2:B:416:TYR:N	2.04	0.73
2:E:229:PRO:HG3	2:E:301:GLN:HE22	1.52	0.73
2:H:310:LEU:HD11	2:H:312:ILE:CG1	2.19	0.73
1:A:123:LYS:H	1:A:124:ARG:HH11	1.36	0.72
2:B:169:ARG:O	2:B:173:GLU:HB2	1.89	0.72
2:H:161:ILE:HG22	2:H:162:PRO:HD3	1.70	0.72
3:I:172:LEU:HB2	3:I:239:GLN:HB3	1.71	0.72
3:C:222:GLY:O	3:C:224:THR:HG22	1.89	0.72
3:F:240:SER:O	3:F:242:ILE:HG13	1.89	0.72
3:L:251:GLU:HA	3:L:257:THR:HG22	1.71	0.72
3:C:172:LEU:H	3:C:172:LEU:HD12	1.54	0.72
3:L:297:ASP:O	3:L:298:ASP:HB3	1.89	0.72
2:B:315:GLU:HB2	2:B:321:LYS:HB3	1.70	0.72
3:C:203:ASP:O	3:C:206:LYS:HE3	1.90	0.72
3:F:238:THR:HG22	3:F:266:LYS:HE2	1.70	0.72
2:H:176:ARG:HA	2:H:179:ILE:HD12	1.69	0.72
1:J:161:CYS:C	1:J:163:GLY:H	1.91	0.72
2:B:300:SER:O	2:B:304:ARG:HG2	1.89	0.72
1:D:140:VAL:HG13	1:D:141:ARG:N	2.04	0.72
2:E:155:GLU:HG3	2:E:156:THR:N	2.05	0.72
2:E:230:ASP:OD2	2:E:232:SER:HB2	1.89	0.72
3:I:222:GLY:O	3:I:224:THR:HG22	1.90	0.72
3:C:218:LEU:O	3:C:219:SER:HB3	1.88	0.72
2:H:223:GLU:CB	2:H:287:GLY:HA2	2.19	0.72
3:I:342:GLY:H	3:I:368:ILE:HG13	1.54	0.72
3:I:364:ASP:OD2	3:I:368:ILE:HD13	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:ASP:OD2	2:B:443:SER:OG	2.07	0.72
3:I:228:LEU:HD12	3:I:228:LEU:O	1.89	0.72
2:H:241:ASP:HB3	2:H:249:TRP:HB2	1.71	0.72
1:A:144:LEU:HD23	1:A:145:VAL:HG23	1.72	0.71
1:A:133:ILE:HG21	2:B:164:ASN:ND2	2.05	0.71
3:I:120:LYS:HA	3:I:123:ASN:HD22	1.55	0.71
2:B:199:VAL:O	3:C:142:THR:HG23	1.90	0.71
1:G:164:SER:HB3	3:I:137:GLU:O	1.89	0.71
2:H:346:ARG:HH11	2:H:346:ARG:CB	2.03	0.71
3:L:325:ASN:HD21	3:L:327:ALA:HB3	1.55	0.71
1:A:158:ILE:HD11	2:B:189:GLN:HB3	1.72	0.71
3:F:246:LEU:HD22	3:F:265:PHE:CD1	2.25	0.71
3:I:103:HIS:HA	3:I:106:SER:HB3	1.72	0.71
3:I:110:LEU:C	3:I:112:GLU:H	1.92	0.71
2:B:346:ARG:HB2	2:B:346:ARG:HH11	1.55	0.71
1:G:159:ARG:HB3	2:H:258:GLY:HA3	1.72	0.71
2:H:159:SER:C	2:H:162:PRO:HD2	2.10	0.71
2:H:292:TYR:CE2	2:H:294:LEU:HB2	2.25	0.71
2:H:300:SER:O	2:H:304:ARG:HG2	1.90	0.71
3:I:171:PRO:CB	3:I:174:ALA:HB2	2.18	0.71
3:I:189:ASN:HD21	3:I:391:ARG:HB3	1.54	0.71
3:I:337:ASN:C	3:I:339:CYS:H	1.93	0.71
3:L:204:PHE:C	3:L:206:LYS:H	1.94	0.71
2:B:256:GLN:HA	2:B:449:LYS:HG2	1.72	0.71
2:B:346:ARG:HH11	2:B:346:ARG:CB	2.04	0.71
2:B:369:ILE:H	2:B:405:ASN:HD22	1.38	0.71
2:E:179:ILE:O	2:E:183:GLU:HG3	1.89	0.71
2:H:172:LEU:HD23	2:H:172:LEU:O	1.90	0.71
3:C:197:ARG:C	3:C:198:LEU:HD12	2.11	0.71
3:L:105:SER:HA	3:L:108:ARG:HG2	1.71	0.71
3:L:145:ILE:HG21	3:L:168:PHE:CE2	2.26	0.71
2:B:165:LEU:HD23	2:B:166:ARG:HH22	1.56	0.70
2:B:241:ASP:HB3	2:B:249:TRP:HB2	1.72	0.70
3:C:171:PRO:CB	3:C:174:ALA:HB2	2.19	0.70
2:B:333:ASN:OD1	2:B:335:ALA:HB3	1.91	0.70
3:I:325:ASN:ND2	3:I:327:ALA:HB3	2.06	0.70
2:H:242:MET:SD	2:H:248:GLY:HA2	2.31	0.70
2:H:317:TRP:CZ3	2:H:448:ARG:HD3	2.26	0.70
1:J:151:GLU:HG3	1:J:178:TYR:CE2	2.25	0.70
3:L:320:ASP:HB2	3:L:337:ASN:O	1.91	0.70
3:L:337:ASN:C	3:L:339:CYS:H	1.93	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:GLU:OE2	2:B:212:GLU:HB3	1.91	0.70
3:C:250:LEU:O	3:C:257:THR:HB	1.91	0.70
3:F:270:GLU:HB2	3:F:274:TYR:OH	1.92	0.70
1:G:157:LYS:O	1:G:160:SER:HB3	1.91	0.70
3:I:382:THR:HG22	3:I:382:THR:O	1.90	0.70
2:B:157:VAL:O	2:B:158:ASN:HB2	1.90	0.70
2:B:178:LYS:C	2:B:180:GLN:H	1.95	0.70
2:E:200:SER:H	2:E:279:ASN:ND2	1.89	0.70
3:F:101:LEU:O	3:F:104:ASP:HB3	1.91	0.70
3:F:251:GLU:CB	3:F:381:LYS:HB2	2.21	0.70
1:G:147:MET:CE	2:H:179:ILE:HG12	2.20	0.70
1:A:176:LYS:O	1:A:180:ASP:HB2	1.92	0.70
3:C:118:ASN:HD22	3:C:118:ASN:N	1.90	0.70
3:C:264:MET:N	3:C:264:MET:SD	2.64	0.70
2:H:256:GLN:HA	2:H:449:LYS:HG2	1.73	0.70
2:B:183:GLU:O	2:B:186:VAL:HG12	1.91	0.70
2:B:223:GLU:CB	2:B:287:GLY:HA2	2.21	0.70
3:L:194:PHE:CD1	3:L:233:ILE:HG12	2.25	0.70
2:B:242:MET:SD	2:B:248:GLY:HA2	2.32	0.70
2:B:253:GLN:HB2	2:B:293:TRP:CE3	2.26	0.70
2:B:439:ASN:HD22	2:B:439:ASN:H	1.40	0.70
3:C:365:ASN:HD22	3:C:365:ASN:H	1.38	0.70
1:A:184:GLN:HE21	1:A:185:LEU:HB2	1.57	0.70
3:F:292:GLY:N	3:F:306:SER:HA	2.06	0.70
3:I:263:ALA:HB3	3:I:279:ALA:HB3	1.73	0.70
3:I:365:ASN:HD22	3:I:365:ASN:H	1.38	0.70
3:L:278:TYR:HD1	3:L:279:ALA:N	1.88	0.70
3:F:204:PHE:C	3:F:206:LYS:H	1.95	0.69
3:F:243:PRO:O	3:F:389:PHE:N	2.25	0.69
3:C:170:LYS:HG3	3:C:175:ASN:O	1.92	0.69
1:D:185:LEU:HB2	2:E:171:ILE:HD13	1.74	0.69
2:E:215:ILE:HA	2:E:219:GLY:O	1.92	0.69
2:E:406:ARG:HH21	4:N:5:NH2:N	1.90	0.69
3:I:97:GLU:C	3:I:99:SER:H	1.93	0.69
3:I:367:ILE:HB	3:I:379:MET:H	1.56	0.69
2:B:345:TYR:CE2	2:B:351:ASN:HB2	2.28	0.69
3:F:391:ARG:NH1	3:F:391:ARG:HB2	2.07	0.69
3:I:197:ARG:C	3:I:198:LEU:HD12	2.12	0.69
2:B:164:ASN:C	2:B:166:ARG:HE	1.96	0.69
2:E:235:PRO:HG2	3:F:168:PHE:HE1	1.56	0.69
3:F:278:TYR:HD1	3:F:279:ALA:N	1.89	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:365:ASN:HD22	3:F:365:ASN:H	1.36	0.69
3:I:318:ASP:HB2	3:I:320:ASP:OD1	1.92	0.69
2:K:373:MET:SD	2:K:405:ASN:ND2	2.65	0.69
3:L:243:PRO:O	3:L:389:PHE:N	2.26	0.69
3:L:246:LEU:HD22	3:L:265:PHE:CD1	2.27	0.69
3:L:391:ARG:NH1	3:L:391:ARG:HB2	2.07	0.69
3:C:221:THR:OG1	3:C:222:GLY:N	2.23	0.69
2:H:434:GLY:O	2:H:436:VAL:N	2.26	0.69
3:I:343:HIS:O	3:I:367:ILE:HA	1.91	0.69
1:D:143:GLN:NE2	3:F:117:ASN:HB2	2.08	0.69
3:C:322:PHE:HD1	3:C:338:LYS:HG3	1.56	0.69
3:F:320:ASP:HB2	3:F:337:ASN:O	1.93	0.69
2:H:316:ASP:HB2	2:H:445:TYR:HE2	1.57	0.69
2:H:351:ASN:ND2	2:H:354:MET:H	1.90	0.69
3:I:325:ASN:HD21	3:I:327:ALA:CB	2.06	0.69
2:K:406:ARG:HE	4:R:3:ARG:HB2	1.58	0.69
3:C:364:ASP:OD2	3:C:368:ILE:HD13	1.93	0.69
2:E:351:ASN:HD21	2:E:354:MET:H	1.40	0.69
2:E:373:MET:SD	2:E:405:ASN:ND2	2.66	0.69
3:F:325:ASN:C	3:F:325:ASN:HD22	1.96	0.69
2:H:301:GLN:HE21	2:H:301:GLN:C	1.95	0.69
2:H:310:LEU:HA	2:H:454:ILE:HG22	1.74	0.69
3:I:172:LEU:H	3:I:172:LEU:HD12	1.57	0.69
1:J:126:VAL:HG13	1:J:127:ILE:N	2.06	0.69
3:L:238:THR:HG22	3:L:266:LYS:HE2	1.75	0.69
2:B:193:CYS:CB	3:C:134:GLN:HE22	2.06	0.69
3:C:343:HIS:O	3:C:367:ILE:HA	1.92	0.69
2:B:173:GLU:HA	2:B:176:ARG:HB2	1.75	0.68
3:C:227:TRP:CD1	3:C:229:GLY:HA2	2.28	0.68
2:E:406:ARG:NH2	4:N:5:NH2:N	2.41	0.68
3:F:96:TYR:C	3:F:98:ALA:H	1.95	0.68
3:L:240:SER:O	3:L:242:ILE:HG13	1.93	0.68
3:F:289:ALA:HB2	3:F:371:THR:OG1	1.93	0.68
4:N:3:ARG:HB3	4:N:4:PRO:HD2	1.76	0.68
2:H:345:TYR:CE2	2:H:351:ASN:HB2	2.29	0.68
1:A:184:GLN:C	1:A:186:GLU:H	1.95	0.68
3:I:227:TRP:CD1	3:I:229:GLY:HA2	2.29	0.68
3:I:278:TYR:CZ	3:I:308:ASN:HB2	2.29	0.68
2:K:351:ASN:ND2	2:K:354:MET:H	1.91	0.68
3:C:151:LYS:HB2	3:C:155:ASP:HB2	1.74	0.68
2:H:172:LEU:HD21	3:I:113:ILE:HG22	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:172:LEU:HD13	3:I:239:GLN:CB	2.24	0.68
2:K:229:PRO:HG3	2:K:301:GLN:HE22	1.58	0.68
2:K:265:LYS:O	2:K:268:PRO:HD2	1.93	0.68
3:L:270:GLU:HB2	3:L:274:TYR:OH	1.94	0.68
3:C:179:LEU:HD23	3:C:218:LEU:HD12	1.74	0.68
3:C:278:TYR:CZ	3:C:308:ASN:HB2	2.29	0.68
3:F:94:MET:HB3	3:F:96:TYR:HE1	1.57	0.68
3:I:120:LYS:HA	3:I:123:ASN:ND2	2.08	0.68
3:L:325:ASN:C	3:L:325:ASN:HD22	1.97	0.68
3:L:365:ASN:HD22	3:L:365:ASN:H	1.39	0.68
2:H:412:PRO:HA	2:H:450:MET:HE1	1.76	0.68
2:K:352:ALA:HB2	2:K:439:ASN:HD22	1.56	0.68
3:I:197:ARG:NH2	3:I:346:GLY:O	2.27	0.68
2:B:161:ILE:HG21	3:C:103:HIS:HD2	1.59	0.68
2:B:301:GLN:NE2	2:B:302:LEU:HD23	2.09	0.68
2:B:370:HIS:O	2:B:373:MET:HB2	1.94	0.68
3:C:251:GLU:HB3	3:C:381:LYS:HB2	1.76	0.68
3:C:273:LYS:HE3	3:C:319:ASN:HD21	1.58	0.68
2:H:402:TRP:CH2	2:H:412:PRO:HG2	2.29	0.68
2:E:312:ILE:HG12	2:E:452:MET:HG2	1.76	0.67
1:J:133:ILE:CD1	2:K:161:ILE:HG23	2.24	0.67
3:I:110:LEU:HD23	3:I:110:LEU:N	2.08	0.67
2:K:180:GLN:HG3	2:K:181:LYS:N	2.08	0.67
2:B:402:TRP:CH2	2:B:412:PRO:HG2	2.29	0.67
2:H:210:GLU:OE2	2:H:212:GLU:HB3	1.94	0.67
3:I:365:ASN:HD22	3:I:365:ASN:N	1.89	0.67
2:B:316:ASP:HB2	2:B:445:TYR:HE2	1.58	0.67
2:B:434:GLY:O	2:B:436:VAL:N	2.28	0.67
3:C:263:ALA:HB3	3:C:279:ALA:HB3	1.75	0.67
2:H:193:CYS:HB3	3:I:134:GLN:NE2	2.10	0.67
3:I:111:GLN:HG2	3:I:111:GLN:O	1.93	0.67
3:I:221:THR:OG1	3:I:222:GLY:N	2.21	0.67
3:I:281:PHE:CE2	3:I:288:ASP:HB2	2.29	0.67
2:H:299:ILE:O	2:H:303:THR:HG23	1.94	0.67
1:J:117:SER:O	1:J:121:VAL:HG23	1.95	0.67
3:L:278:TYR:OH	3:L:308:ASN:HB2	1.94	0.67
2:E:239:TYR:CZ	2:E:289:PRO:HD3	2.30	0.67
2:E:352:ALA:HB2	2:E:439:ASN:HD22	1.59	0.67
3:F:195:GLN:HG3	3:F:227:TRP:CZ3	2.28	0.67
2:H:304:ARG:NH2	2:H:333:ASN:N	2.43	0.67
3:C:365:ASN:HD22	3:C:365:ASN:N	1.89	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:194:PHE:CD1	3:F:233:ILE:HG12	2.29	0.67
2:H:287:GLY:O	2:H:288:LEU:HD23	1.95	0.67
2:B:238:VAL:HG22	2:B:239:TYR:N	2.09	0.67
2:E:393:GLN:HB2	2:E:396:LYS:CG	2.25	0.67
2:H:364:ASN:ND2	5:H:470:NAG:H62	2.10	0.67
3:I:251:GLU:HB3	3:I:381:LYS:HB2	1.77	0.67
1:A:179:GLU:HG3	1:A:182:GLN:OE1	1.94	0.67
1:D:160:SER:HA	2:E:258:GLY:O	1.95	0.67
3:F:100:ILE:HG22	3:F:103:HIS:HB2	1.76	0.67
3:F:305:THR:HB	3:F:341:ALA:HB2	1.77	0.67
2:B:202:ASN:ND2	2:B:284:ASN:HB2	2.10	0.66
2:B:204:PRO:HA	3:C:217:HIS:CA	2.22	0.66
3:C:197:ARG:NH2	3:C:346:GLY:O	2.29	0.66
2:E:203:ILE:HD12	2:E:203:ILE:N	2.10	0.66
3:C:230:ASN:N	3:C:230:ASN:ND2	2.39	0.66
3:F:237:SER:HB3	3:F:266:LYS:HA	1.76	0.66
3:I:170:LYS:HG3	3:I:175:ASN:O	1.95	0.66
2:K:230:ASP:OD2	2:K:232:SER:HB2	1.94	0.66
2:K:391:ARG:HG2	2:K:391:ARG:HH11	1.59	0.66
3:C:367:ILE:HB	3:C:379:MET:H	1.59	0.66
1:G:132:HIS:C	1:G:133:ILE:HD12	2.16	0.66
1:G:139:ASN:HB3	3:I:114:TYR:CZ	2.30	0.66
2:H:162:PRO:C	2:H:164:ASN:H	1.96	0.66
2:H:301:GLN:HE21	2:H:302:LEU:N	1.93	0.66
2:H:439:ASN:HD22	2:H:439:ASN:H	1.42	0.66
3:I:133:ALA:HA	3:I:136:GLN:HG2	1.76	0.66
3:I:151:LYS:HB2	3:I:155:ASP:HB2	1.75	0.66
3:I:250:LEU:HD23	3:I:372:TRP:CZ3	2.30	0.66
2:B:165:LEU:N	2:B:166:ARG:HE	1.92	0.66
2:B:236:TYR:OH	2:B:302:LEU:HD21	1.96	0.66
3:F:145:ILE:HD13	3:F:168:PHE:HE2	1.59	0.66
1:G:124:ARG:H	1:G:124:ARG:HD2	1.60	0.66
2:H:270:LYS:HE3	2:H:334:GLU:OE1	1.95	0.66
2:H:432:ASP:OD2	2:H:443:SER:OG	2.14	0.66
1:J:133:ILE:O	1:J:133:ILE:HG12	1.94	0.66
2:K:203:ILE:HD12	2:K:203:ILE:N	2.10	0.66
1:A:167:ARG:HG3	2:B:192:TYR:HB3	1.78	0.66
2:B:191:GLU:C	2:B:193:CYS:H	1.99	0.66
2:B:241:ASP:O	2:B:248:GLY:N	2.28	0.66
2:H:301:GLN:NE2	2:H:302:LEU:HD23	2.11	0.66
1:J:138:LYS:HB2	1:J:138:LYS:NZ	2.09	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:305:THR:HB	3:L:341:ALA:HB2	1.76	0.66
2:B:213:GLU:HG2	2:B:217:LYS:HE3	1.78	0.66
3:C:97:GLU:C	3:C:99:SER:H	1.96	0.66
2:H:203:ILE:HG21	2:H:226:LEU:HD22	1.77	0.66
2:H:204:PRO:HA	3:I:217:HIS:CA	2.23	0.66
2:K:393:GLN:HB2	2:K:396:LYS:CG	2.26	0.66
3:C:325:ASN:ND2	3:C:327:ALA:HB3	2.11	0.66
3:F:325:ASN:HD21	3:F:327:ALA:HB3	1.61	0.66
2:H:213:GLU:HG2	2:H:217:LYS:HE3	1.78	0.66
3:I:273:LYS:HE3	3:I:319:ASN:HD21	1.58	0.66
2:B:266:TRP:HA	2:B:266:TRP:CE3	2.29	0.66
2:B:351:ASN:ND2	2:B:354:MET:H	1.92	0.66
3:C:227:TRP:CZ2	3:C:230:ASN:ND2	2.64	0.66
2:H:237:ARG:HG3	2:H:237:ARG:NH1	2.06	0.66
2:H:241:ASP:O	2:H:248:GLY:N	2.28	0.66
3:I:163:GLN:HE21	3:I:163:GLN:CA	2.08	0.66
3:L:227:TRP:CZ2	3:L:230:ASN:ND2	2.61	0.66
2:B:162:PRO:HA	2:B:166:ARG:HD2	1.78	0.66
2:B:412:PRO:HG3	2:B:450:MET:HE1	1.76	0.66
3:C:167:TYR:CD1	3:C:167:TYR:N	2.64	0.66
3:C:251:GLU:HA	3:C:257:THR:HA	1.75	0.66
3:F:234:HIS:NE2	3:F:269:PRO:HB3	2.11	0.66
2:H:370:HIS:O	2:H:373:MET:HB2	1.96	0.66
2:K:215:ILE:HA	2:K:219:GLY:O	1.95	0.66
2:K:267:ASP:HB3	2:K:268:PRO:HD3	1.78	0.66
3:L:141:ASP:OD1	3:L:143:VAL:HG22	1.96	0.66
2:B:165:LEU:HD13	3:C:110:LEU:HD22	1.78	0.66
2:B:345:TYR:CD2	2:B:351:ASN:HB2	2.31	0.66
3:C:178:PHE:CE1	3:C:232:LYS:HG2	2.31	0.66
3:F:145:ILE:HG21	3:F:168:PHE:CE2	2.31	0.66
1:G:121:VAL:HG12	1:G:124:ARG:HE	1.60	0.66
3:I:330:ASP:HB3	3:I:365:ASN:CB	2.26	0.66
2:K:406:ARG:NH2	4:R:5:NH2:N	2.43	0.66
3:L:96:TYR:CD2	3:L:96:TYR:N	2.63	0.66
3:L:292:GLY:HA2	3:L:305:THR:C	2.17	0.66
4:R:3:ARG:HB3	4:R:4:PRO:HD2	1.77	0.66
1:D:161:CYS:C	1:D:163:GLY:H	1.98	0.65
2:E:391:ARG:HG2	2:E:391:ARG:HH11	1.59	0.65
2:H:214:ILE:HD13	2:H:225:TYR:HD2	1.61	0.65
3:I:230:ASN:N	3:I:230:ASN:ND2	2.42	0.65
3:L:251:GLU:CB	3:L:381:LYS:HB2	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:PRO:HA	2:B:450:MET:HE1	1.77	0.65
3:C:141:ASP:OD2	3:C:143:VAL:HG22	1.96	0.65
1:G:132:HIS:O	1:G:133:ILE:HD12	1.97	0.65
2:K:161:ILE:HB	2:K:162:PRO:HD3	1.77	0.65
2:K:167:VAL:HG12	2:K:168:LEU:HD22	1.77	0.65
2:B:294:LEU:O	2:B:295:GLY:O	2.14	0.65
3:C:189:ASN:HD21	3:C:391:ARG:HB3	1.59	0.65
2:E:302:LEU:HD13	2:E:454:ILE:HD11	1.77	0.65
3:F:162:LYS:HE3	3:F:186:GLY:HA2	1.78	0.65
1:A:124:ARG:N	1:A:124:ARG:HD2	2.12	0.65
1:A:167:ARG:HD2	1:A:168:ALA:N	2.12	0.65
2:B:203:ILE:HG21	2:B:226:LEU:HD22	1.78	0.65
3:C:103:HIS:HA	3:C:106:SER:HB2	1.78	0.65
3:I:178:PHE:CE1	3:I:232:LYS:HG2	2.32	0.65
2:B:292:TYR:CE2	2:B:294:LEU:HB2	2.31	0.65
3:C:197:ARG:HA	3:C:225:GLU:CG	2.16	0.65
3:C:330:ASP:HB3	3:C:365:ASN:CB	2.27	0.65
3:F:246:LEU:HD13	3:F:265:PHE:CE2	2.30	0.65
3:I:227:TRP:HZ2	3:I:230:ASN:ND2	1.94	0.65
2:B:177:SER:HA	2:B:180:GLN:HG3	1.79	0.65
2:E:166:ARG:O	2:E:169:ARG:HB3	1.97	0.65
2:E:251:VAL:HG22	2:E:453:LYS:HG2	1.78	0.65
2:E:256:GLN:N	2:E:291:GLU:OE2	2.29	0.65
2:E:267:ASP:HB3	2:E:268:PRO:HD3	1.79	0.65
2:H:294:LEU:O	2:H:295:GLY:O	2.15	0.65
1:A:148:LYS:HE3	2:B:425:ASP:O	1.97	0.65
2:B:270:LYS:HE3	2:B:334:GLU:OE1	1.97	0.65
2:B:328:GLY:O	2:B:342:VAL:HA	1.96	0.65
3:C:193:VAL:CG1	3:C:195:GLN:H	2.10	0.65
2:E:199:VAL:HG23	3:F:141:ASP:HA	1.79	0.65
2:E:359:GLN:OE1	2:E:438:MET:HB3	1.96	0.65
2:H:202:ASN:ND2	2:H:284:ASN:HB2	2.11	0.65
2:K:239:TYR:CZ	2:K:289:PRO:HD3	2.32	0.65
2:K:302:LEU:HD13	2:K:454:ILE:HD11	1.76	0.65
3:L:166:LEU:HD22	3:L:218:LEU:HB3	1.79	0.65
2:B:252:ILE:HD11	2:B:454:ILE:HG12	1.79	0.65
2:H:255:ARG:NH1	2:H:413:ASN:HA	2.12	0.65
2:H:304:ARG:NH2	2:H:333:ASN:H	1.95	0.65
3:I:249:GLU:HB3	3:I:383:THR:CG2	2.24	0.65
2:B:238:VAL:CG2	2:B:239:TYR:N	2.59	0.65
2:B:369:ILE:H	2:B:405:ASN:ND2	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ARG:NH2	2:B:333:ASN:N	2.45	0.64
3:C:343:HIS:HB3	3:C:366:GLY:O	1.97	0.64
3:C:367:ILE:O	3:C:378:SER:HA	1.98	0.64
2:H:253:GLN:HB2	2:H:293:TRP:CE3	2.32	0.64
2:H:345:TYR:CD2	2:H:351:ASN:HB2	2.32	0.64
3:I:97:GLU:O	3:I:99:SER:N	2.29	0.64
3:L:145:ILE:HG21	3:L:168:PHE:HE2	1.62	0.64
2:B:158:ASN:HA	2:B:162:PRO:HG2	1.79	0.64
3:C:235:LEU:H	3:C:235:LEU:HD12	1.63	0.64
3:C:318:ASP:HB2	3:C:320:ASP:OD1	1.97	0.64
2:E:351:ASN:C	2:E:351:ASN:HD22	1.98	0.64
1:G:168:ALA:HA	2:H:189:GLN:NE2	2.12	0.64
3:I:141:ASP:OD2	3:I:143:VAL:HG22	1.97	0.64
3:L:97:GLU:HA	3:L:100:ILE:HG13	1.79	0.64
2:B:159:SER:N	2:B:162:PRO:HD2	2.13	0.64
2:B:162:PRO:HA	2:B:166:ARG:HH11	1.62	0.64
2:B:299:ILE:O	2:B:303:THR:HG23	1.97	0.64
3:I:347:VAL:HG23	3:I:365:ASN:O	1.98	0.64
2:E:189:GLN:O	2:E:193:CYS:SG	2.54	0.64
2:H:328:GLY:O	2:H:342:VAL:HA	1.97	0.64
2:K:327:GLY:HA3	2:K:344:LYS:HB2	1.77	0.64
1:A:140:VAL:O	1:A:143:GLN:N	2.30	0.64
2:B:237:ARG:HG3	2:B:237:ARG:NH1	2.07	0.64
3:C:100:ILE:O	3:C:100:ILE:HG22	1.98	0.64
3:C:389:PHE:HE1	3:C:392:LEU:HD22	1.61	0.64
2:E:200:SER:H	2:E:279:ASN:HD21	1.44	0.64
2:H:190:MET:O	2:H:193:CYS:HB2	1.97	0.64
2:K:200:SER:H	2:K:279:ASN:ND2	1.95	0.64
4:N:3:ARG:HB3	4:N:4:PRO:CD	2.27	0.64
3:C:325:ASN:HD21	3:C:327:ALA:CB	2.11	0.64
2:H:266:TRP:HA	2:H:266:TRP:CE3	2.31	0.64
2:H:369:ILE:H	2:H:405:ASN:ND2	1.94	0.64
2:K:189:GLN:O	2:K:193:CYS:SG	2.54	0.64
2:E:272:GLY:HA2	2:E:293:TRP:O	1.98	0.64
3:I:251:GLU:HA	3:I:257:THR:HA	1.77	0.64
2:K:315:GLU:HG3	2:K:321:LYS:HG2	1.78	0.64
1:A:128:GLU:HG2	1:A:129:LYS:CD	2.28	0.64
2:B:287:GLY:O	2:B:288:LEU:HD23	1.98	0.64
2:B:310:LEU:HA	2:B:454:ILE:HG22	1.80	0.64
3:F:166:LEU:HD22	3:F:218:LEU:HB3	1.80	0.64
3:F:227:TRP:CZ2	3:F:230:ASN:ND2	2.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:193:VAL:CG1	3:I:195:GLN:H	2.11	0.64
3:L:237:SER:HB3	3:L:266:LYS:HA	1.78	0.64
2:B:240:CYS:HB3	2:B:242:MET:SD	2.37	0.64
2:E:237:ARG:HH11	2:E:237:ARG:HG3	1.63	0.64
3:I:244:TYR:CD2	3:I:386:ILE:HD12	2.32	0.64
3:I:343:HIS:HB3	3:I:366:GLY:O	1.98	0.64
2:K:270:LYS:HA	2:K:296:ASN:HB2	1.79	0.64
3:L:162:LYS:HE3	3:L:186:GLY:HA2	1.80	0.64
3:L:246:LEU:HD13	3:L:265:PHE:CE2	2.33	0.64
3:I:339:CYS:SG	4:S:3:ARG:CZ	2.86	0.64
2:B:412:PRO:CA	2:B:450:MET:HE1	2.28	0.63
2:K:406:ARG:HH21	4:R:5:NH2:N	1.96	0.63
3:L:228:LEU:HD23	3:L:232:LYS:HD2	1.80	0.63
3:C:249:GLU:HB3	3:C:383:THR:CG2	2.26	0.63
3:C:339:CYS:SG	4:O:3:ARG:NH1	2.71	0.63
3:F:194:PHE:CD2	3:F:384:MET:O	2.51	0.63
1:J:171:ARG:HD2	2:K:185:ASP:OD1	1.98	0.63
2:K:406:ARG:NE	4:R:3:ARG:HB2	2.13	0.63
2:B:340:ILE:HG22	2:B:373:MET:O	1.98	0.63
3:C:193:VAL:CG1	3:C:194:PHE:N	2.50	0.63
1:D:191:LYS:HG3	1:D:192:ASP:H	1.61	0.63
3:F:228:LEU:HD23	3:F:232:LYS:HD2	1.81	0.63
3:F:312:PHE:HA	3:F:335:TRP:HA	1.81	0.63
3:I:161:ALA:O	3:I:162:LYS:HB2	1.97	0.63
2:B:165:LEU:HB2	2:B:166:ARG:CZ	2.27	0.63
2:B:165:LEU:HD12	3:C:106:SER:O	1.99	0.63
3:C:250:LEU:HD23	3:C:372:TRP:CZ3	2.32	0.63
2:E:367:MET:SD	2:E:406:ARG:HG2	2.38	0.63
3:L:289:ALA:HB2	3:L:371:THR:OG1	1.98	0.63
2:B:301:GLN:HE21	2:B:302:LEU:N	1.97	0.63
2:B:408:HIS:CD2	2:B:411:ASN:HB2	2.33	0.63
3:C:244:TYR:CD2	3:C:386:ILE:HD12	2.33	0.63
2:H:296:ASN:HB3	2:H:338:TYR:CE1	2.33	0.63
2:K:351:ASN:C	2:K:351:ASN:HD22	2.00	0.63
2:B:163:THR:N	2:B:166:ARG:HD2	2.14	0.63
3:C:293:PHE:N	3:C:302:LYS:HG3	2.13	0.63
3:F:292:GLY:HA2	3:F:305:THR:C	2.19	0.63
2:B:255:ARG:NH1	2:B:413:ASN:HA	2.13	0.63
3:C:126:GLU:C	3:C:128:VAL:H	2.01	0.63
2:E:160:ASN:H	2:E:162:PRO:HD2	1.64	0.63
1:G:121:VAL:O	1:G:122:LEU:HD22	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:389:ASP:OD1	2:K:391:ARG:HB2	1.98	0.63
3:C:166:LEU:HD21	3:C:219:SER:O	1.98	0.63
1:D:128:GLU:HA	1:D:131:GLN:HG2	1.81	0.63
2:H:238:VAL:HG22	2:H:239:TYR:N	2.13	0.63
2:B:214:ILE:HD13	2:B:225:TYR:HD2	1.63	0.63
3:C:161:ALA:O	3:C:162:LYS:HB2	1.98	0.63
3:C:163:GLN:O	3:C:167:TYR:OH	2.17	0.63
2:E:389:ASP:OD1	2:E:391:ARG:HB2	1.97	0.63
2:K:359:GLN:OE1	2:K:438:MET:HB3	1.99	0.63
3:L:194:PHE:CD2	3:L:384:MET:O	2.52	0.63
2:B:296:ASN:HB3	2:B:338:TYR:CE1	2.34	0.62
3:C:178:PHE:CD1	3:C:232:LYS:HG2	2.33	0.62
1:G:148:LYS:NZ	2:H:425:ASP:HB2	2.14	0.62
2:H:173:GLU:C	2:H:175:LEU:H	2.01	0.62
2:H:408:HIS:CD2	2:H:411:ASN:HB2	2.34	0.62
1:J:133:ILE:HD12	2:K:161:ILE:HG23	1.81	0.62
3:L:216:GLY:O	3:L:217:HIS:HD2	1.82	0.62
3:I:208:TRP:HA	3:I:314:THR:HG21	1.80	0.62
3:L:96:TYR:O	3:L:100:ILE:HG13	1.99	0.62
3:L:234:HIS:NE2	3:L:269:PRO:HB3	2.15	0.62
3:C:208:TRP:HA	3:C:314:THR:HG21	1.80	0.62
3:C:338:LYS:O	3:C:338:LYS:HG2	1.98	0.62
2:E:210:GLU:OE1	2:E:456:PRO:HG3	1.98	0.62
1:G:144:LEU:HD23	1:G:182:GLN:HE21	1.64	0.62
2:H:252:ILE:HD11	2:H:454:ILE:HG12	1.82	0.62
1:J:185:LEU:O	1:J:185:LEU:HD13	1.99	0.62
3:L:224:THR:O	3:L:226:PHE:HD1	1.80	0.62
1:A:143:GLN:NE2	3:C:118:ASN:ND2	2.48	0.62
3:I:110:LEU:HD23	3:I:110:LEU:H	1.65	0.62
3:I:178:PHE:CE2	3:I:228:LEU:HD11	2.34	0.62
3:I:235:LEU:HD12	3:I:235:LEU:H	1.65	0.62
2:E:308:THR:HA	2:E:456:PRO:HA	1.80	0.62
2:E:355:ASP:HA	2:E:369:ILE:HD13	1.82	0.62
3:F:143:VAL:O	3:F:143:VAL:HG23	2.00	0.62
2:H:169:ARG:O	2:H:173:GLU:HG2	1.98	0.62
3:I:197:ARG:HA	3:I:225:GLU:CG	2.19	0.62
1:J:160:SER:HA	2:K:258:GLY:O	1.98	0.62
1:J:167:ARG:HA	1:J:167:ARG:NE	2.14	0.62
1:J:191:LYS:HB2	1:J:191:LYS:NZ	2.14	0.62
2:K:199:VAL:HG23	3:L:141:ASP:HA	1.82	0.62
2:B:175:LEU:O	2:B:178:LYS:HB2	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:ILE:HG21	2:B:225:TYR:CE2	2.34	0.62
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.07	0.62
2:K:165:LEU:HA	2:K:168:LEU:HD23	1.82	0.62
2:B:255:ARG:HA	2:B:291:GLU:OE2	2.00	0.62
3:C:124:LEU:HD12	3:C:127:LYS:HB3	1.80	0.62
3:C:246:LEU:HD12	3:C:247:ARG:H	1.63	0.62
2:H:417:TYR:HE1	2:H:433:ASP:O	1.82	0.62
3:I:208:TRP:HZ2	3:I:270:GLU:HG3	1.64	0.62
1:A:144:LEU:CD2	1:A:182:GLN:HG2	2.27	0.62
2:B:177:SER:HA	2:B:180:GLN:HG2	1.81	0.62
3:C:154:GLN:CD	3:C:190:GLY:H	2.02	0.62
3:C:227:TRP:HZ2	3:C:230:ASN:ND2	1.96	0.62
3:F:198:LEU:HB3	3:F:381:LYS:HE2	1.81	0.62
1:G:148:LYS:CD	1:G:182:GLN:HE22	2.11	0.62
2:H:255:ARG:HA	2:H:291:GLU:OE2	2.00	0.62
3:I:167:TYR:N	3:I:167:TYR:CD1	2.68	0.62
3:I:227:TRP:CZ2	3:I:230:ASN:ND2	2.64	0.62
3:L:236:ILE:CG2	3:L:386:ILE:HD11	2.29	0.62
1:A:150:LEU:O	1:A:154:ILE:HB	2.00	0.62
2:B:369:ILE:N	2:B:405:ASN:HD22	1.97	0.62
3:C:344:LEU:HD12	3:C:384:MET:SD	2.40	0.62
2:E:315:GLU:HG3	2:E:321:LYS:HG2	1.81	0.62
3:I:154:GLN:CD	3:I:190:GLY:H	2.02	0.62
2:K:256:GLN:N	2:K:291:GLU:OE2	2.31	0.62
1:A:143:GLN:NE2	3:C:118:ASN:HD21	1.98	0.62
2:B:161:ILE:O	2:B:163:THR:N	2.28	0.62
2:E:198:THR:O	2:E:199:VAL:HG13	1.99	0.62
3:F:153:CYS:SG	3:F:192:THR:HA	2.39	0.62
2:H:214:ILE:HG21	2:H:225:TYR:CE2	2.35	0.62
3:I:297:ASP:HB2	3:I:301:ASP:OD2	2.00	0.62
3:I:367:ILE:O	3:I:378:SER:HA	2.00	0.62
2:B:373:MET:CG	2:B:405:ASN:HB2	2.29	0.61
1:J:140:VAL:HG13	1:J:141:ARG:N	2.14	0.61
3:L:320:ASP:HA	3:L:336:MET:O	1.99	0.61
2:E:366:THR:HA	2:E:369:ILE:HG13	1.82	0.61
2:H:176:ARG:HA	2:H:179:ILE:CG1	2.30	0.61
2:K:352:ALA:CB	2:K:439:ASN:ND2	2.63	0.61
2:B:271:GLN:O	2:B:295:GLY:HA3	1.99	0.61
3:C:232:LYS:O	3:C:236:ILE:HG12	2.00	0.61
3:C:389:PHE:C	3:C:391:ARG:H	2.03	0.61
2:H:416:TYR:OH	2:H:448:ARG:HD2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:178:PHE:CD1	3:I:232:LYS:HG2	2.35	0.61
3:L:312:PHE:HA	3:L:335:TRP:HA	1.83	0.61
2:E:351:ASN:ND2	2:E:354:MET:H	1.98	0.61
3:F:203:ASP:O	3:F:206:LYS:HG2	1.99	0.61
2:B:301:GLN:HE21	2:B:301:GLN:C	2.03	0.61
3:L:195:GLN:HG3	3:L:227:TRP:CZ3	2.34	0.61
1:G:129:LYS:O	1:G:130:VAL:HG23	2.01	0.61
2:H:236:TYR:OH	2:H:302:LEU:HD21	2.01	0.61
2:H:238:VAL:CG2	2:H:239:TYR:N	2.63	0.61
3:I:166:LEU:HD21	3:I:219:SER:O	2.00	0.61
3:I:260:ALA:HB2	3:I:286:ALA:HB3	1.82	0.61
3:L:118:ASN:O	3:L:122:VAL:HG23	2.00	0.61
2:B:184:SER:O	2:B:187:SER:N	2.33	0.61
3:C:196:LYS:HG2	3:C:198:LEU:CD1	2.30	0.61
2:E:429:HIS:O	2:E:431:THR:HG23	2.00	0.61
1:G:144:LEU:CD2	1:G:182:GLN:HG3	2.29	0.61
3:I:193:VAL:HG12	3:I:195:GLN:N	2.14	0.61
3:I:220:PRO:HG2	3:I:221:THR:H	1.65	0.61
3:I:272:ASP:O	3:I:273:LYS:HB2	1.99	0.61
2:K:159:SER:C	2:K:160:ASN:HD22	2.03	0.61
2:K:198:THR:O	2:K:199:VAL:HG13	2.00	0.61
2:K:235:PRO:HG2	3:L:168:PHE:HE1	1.64	0.61
2:K:361:MET:O	5:K:470:NAG:H82	2.00	0.61
2:K:415:ARG:O	2:K:434:GLY:HA2	2.00	0.61
3:C:368:ILE:HG21	3:C:375:ARG:HA	1.83	0.61
2:E:264:ARG:HG2	3:F:136:GLN:HE22	1.64	0.61
2:H:369:ILE:N	2:H:405:ASN:HD22	1.98	0.61
3:I:237:SER:OG	3:I:266:LYS:HA	2.01	0.61
3:I:256:ARG:HG3	3:I:256:ARG:NH1	2.15	0.61
1:J:127:ILE:O	1:J:130:VAL:HB	2.00	0.61
2:K:169:ARG:O	2:K:173:GLU:HG3	2.01	0.61
2:B:304:ARG:NH2	2:B:333:ASN:H	1.99	0.61
3:C:272:ASP:O	3:C:273:LYS:HB2	2.00	0.61
3:F:92:GLU:HG2	3:F:93:ILE:N	2.15	0.61
3:F:154:GLN:C	3:F:156:ILE:H	2.04	0.61
2:H:298:LYS:O	2:H:302:LEU:HG	2.00	0.61
3:I:103:HIS:C	3:I:105:SER:H	2.04	0.61
3:I:383:THR:OG1	3:I:384:MET:N	2.33	0.61
3:L:194:PHE:CE2	3:L:384:MET:HB2	2.36	0.61
2:B:416:TYR:OH	2:B:448:ARG:HD2	2.01	0.61
3:F:246:LEU:HB2	3:F:265:PHE:CG	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:161:CYS:HB3	1:G:165:CYS:SG	2.40	0.61
2:H:161:ILE:HG22	2:H:162:PRO:CD	2.31	0.61
3:I:196:LYS:HG2	3:I:198:LEU:CD1	2.30	0.61
3:I:389:PHE:C	3:I:391:ARG:H	2.04	0.61
2:K:332:GLN:HB3	2:K:336:ASN:HB2	1.83	0.61
3:L:153:CYS:SG	3:L:192:THR:HA	2.40	0.61
3:I:179:LEU:HD23	3:I:218:LEU:HD12	1.82	0.60
1:J:157:LYS:HA	1:J:157:LYS:HE3	1.83	0.60
2:K:255:ARG:HA	2:K:291:GLU:OE2	2.01	0.60
2:B:156:THR:HA	2:B:160:ASN:HB2	1.82	0.60
1:D:131:GLN:HG3	1:D:132:HIS:N	2.15	0.60
3:F:194:PHE:CE2	3:F:384:MET:HB2	2.36	0.60
3:F:276:LEU:HD11	3:F:290:PHE:CE2	2.36	0.60
1:J:181:GLN:NE2	2:K:174:ASN:ND2	2.49	0.60
3:L:278:TYR:CD1	3:L:279:ALA:N	2.69	0.60
3:C:260:ALA:HB2	3:C:286:ALA:HB3	1.82	0.60
3:F:141:ASP:OD1	3:F:143:VAL:HG22	2.00	0.60
3:C:256:ARG:HG3	3:C:256:ARG:NH1	2.16	0.60
3:F:108:ARG:O	3:F:112:GLU:HG3	2.01	0.60
2:H:359:GLN:HE21	2:H:359:GLN:H	1.48	0.60
2:K:251:VAL:HG22	2:K:453:LYS:HG2	1.82	0.60
2:K:366:THR:HA	2:K:369:ILE:HG13	1.83	0.60
1:A:136:LEU:HD11	3:C:111:GLN:HB2	1.84	0.60
3:C:365:ASN:N	3:C:365:ASN:ND2	2.46	0.60
3:F:278:TYR:CD1	3:F:279:ALA:N	2.69	0.60
3:F:389:PHE:O	3:F:391:ARG:N	2.33	0.60
2:H:271:GLN:O	2:H:295:GLY:HA3	2.01	0.60
3:I:204:PHE:HE1	3:I:225:GLU:HB3	1.67	0.60
3:I:342:GLY:HA2	3:I:368:ILE:O	2.01	0.60
1:G:140:VAL:O	1:G:143:GLN:N	2.29	0.60
3:I:380:LYS:HD2	3:I:381:LYS:HG2	1.83	0.60
3:L:154:GLN:C	3:L:156:ILE:H	2.05	0.60
3:L:178:PHE:CZ	3:L:232:LYS:HG2	2.37	0.60
3:C:172:LEU:HD13	3:C:239:GLN:HB3	1.84	0.60
3:C:193:VAL:HG12	3:C:195:GLN:N	2.16	0.60
3:C:204:PHE:HE1	3:C:225:GLU:HB3	1.67	0.60
3:I:232:LYS:O	3:I:236:ILE:HG12	2.01	0.60
3:I:322:PHE:HD1	3:I:338:LYS:HG3	1.66	0.60
2:K:210:GLU:OE1	2:K:456:PRO:HG3	2.01	0.60
2:B:266:TRP:HA	2:B:266:TRP:HE3	1.67	0.60
3:C:178:PHE:CE2	3:C:228:LEU:HD11	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:VAL:HG21	2:E:426:MET:O	2.01	0.60
1:G:151:GLU:OE2	1:G:173:VAL:HG11	2.00	0.60
3:I:246:LEU:HD12	3:I:247:ARG:H	1.66	0.60
3:I:360:PRO:HD2	3:I:365:ASN:OD1	2.02	0.60
3:I:365:ASN:N	3:I:365:ASN:ND2	2.47	0.60
2:K:358:SER:HA	2:K:365:ARG:NH1	2.16	0.60
3:L:389:PHE:O	3:L:391:ARG:N	2.34	0.60
3:F:194:PHE:HA	3:F:228:LEU:HB2	1.84	0.60
2:H:215:ILE:HB	2:H:242:MET:CE	2.30	0.60
2:H:340:ILE:HG22	2:H:373:MET:O	2.01	0.60
3:L:143:VAL:HG23	3:L:143:VAL:O	2.02	0.60
2:B:166:ARG:H	2:B:166:ARG:CD	2.14	0.60
3:C:252:ASP:OD2	3:C:254:ASN:HB2	2.02	0.60
2:H:373:MET:CG	2:H:405:ASN:HB2	2.31	0.60
3:I:310:MET:O	3:I:335:TRP:HD1	1.85	0.60
3:L:242:ILE:CG2	3:L:243:PRO:HD2	2.32	0.60
3:C:163:GLN:O	3:C:165:GLY:N	2.35	0.59
1:D:123:LYS:C	1:D:125:LYS:H	2.04	0.59
2:E:255:ARG:HA	2:E:291:GLU:OE2	2.02	0.59
2:E:352:ALA:CB	2:E:439:ASN:ND2	2.64	0.59
3:F:191:TRP:CZ3	3:F:387:ILE:HB	2.37	0.59
2:H:257:ASP:OD2	2:H:291:GLU:HG3	2.01	0.59
3:I:193:VAL:CG1	3:I:194:PHE:N	2.53	0.59
2:B:215:ILE:HB	2:B:242:MET:CE	2.29	0.59
3:C:172:LEU:H	3:C:172:LEU:CD1	2.14	0.59
3:C:383:THR:OG1	3:C:384:MET:N	2.34	0.59
3:C:389:PHE:CE1	3:C:392:LEU:HD22	2.37	0.59
2:E:264:ARG:HG2	2:E:264:ARG:HH11	1.67	0.59
2:H:394:CYS:SG	2:H:407:CYS:N	2.75	0.59
2:K:215:ILE:HD12	2:K:248:GLY:N	2.17	0.59
3:L:194:PHE:HA	3:L:228:LEU:HB2	1.84	0.59
1:A:181:GLN:O	1:A:184:GLN:HG3	2.02	0.59
2:B:153:ILE:C	2:B:155:GLU:H	2.05	0.59
2:E:270:LYS:HA	2:E:296:ASN:HB2	1.83	0.59
3:F:216:GLY:O	3:F:217:HIS:HD2	1.85	0.59
1:G:135:LEU:HD12	1:G:136:LEU:HD22	1.83	0.59
3:I:339:CYS:SG	4:S:3:ARG:NH1	2.76	0.59
3:I:367:ILE:HB	3:I:378:SER:OG	2.02	0.59
3:I:368:ILE:HG21	3:I:375:ARG:HA	1.84	0.59
2:K:308:THR:HA	2:K:456:PRO:HA	1.82	0.59
3:I:163:GLN:O	3:I:165:GLY:N	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:266:TRP:HE1	2:B:380:ARG:CZ	2.16	0.59
2:B:402:TRP:CE2	2:B:412:PRO:HD2	2.36	0.59
3:C:191:TRP:CE3	3:C:385:LYS:HE2	2.37	0.59
3:C:304:PHE:CD1	3:C:338:LYS:HD3	2.38	0.59
3:C:360:PRO:HD2	3:C:365:ASN:OD1	2.03	0.59
1:G:124:ARG:O	1:G:126:VAL:N	2.35	0.59
2:H:191:GLU:C	2:H:193:CYS:H	2.05	0.59
2:H:239:TYR:CZ	2:H:289:PRO:HD3	2.37	0.59
2:H:412:PRO:CA	2:H:450:MET:HE1	2.32	0.59
2:H:175:LEU:O	2:H:179:ILE:HG13	2.02	0.59
3:I:194:PHE:CZ	3:I:384:MET:HB3	2.37	0.59
3:F:236:ILE:CG2	3:F:386:ILE:HD11	2.32	0.59
1:G:137:GLN:OE1	1:G:189:ILE:HD12	2.02	0.59
1:G:143:GLN:C	1:G:145:VAL:H	2.05	0.59
2:H:162:PRO:O	2:H:164:ASN:N	2.35	0.59
3:I:246:LEU:HD21	3:I:248:VAL:HG23	1.85	0.59
2:K:405:ASN:C	2:K:407:CYS:N	2.53	0.59
1:A:189:ILE:O	1:A:190:ALA:CB	2.51	0.59
2:B:165:LEU:H	2:B:166:ARG:HH21	0.71	0.59
2:E:216:ARG:HH11	2:E:216:ARG:HB2	1.60	0.59
2:E:332:GLN:HB3	2:E:336:ASN:HB2	1.85	0.59
3:F:207:ASN:OD1	3:F:210:GLN:HG3	2.02	0.59
2:H:212:GLU:O	2:H:215:ILE:HG22	2.02	0.59
2:H:351:ASN:HD21	2:H:354:MET:H	1.51	0.59
3:L:198:LEU:HB3	3:L:381:LYS:HE2	1.84	0.59
3:L:203:ASP:O	3:L:206:LYS:HG2	2.02	0.59
3:C:208:TRP:HZ2	3:C:270:GLU:HG3	1.67	0.59
2:E:223:GLU:HB2	2:E:286:CYS:O	2.03	0.59
2:E:310:LEU:HD21	2:E:312:ILE:HD11	1.85	0.59
3:I:116:SER:O	3:I:119:GLN:HB3	2.03	0.59
2:K:272:GLY:HA2	2:K:293:TRP:O	2.02	0.59
2:B:178:LYS:C	2:B:180:GLN:N	2.56	0.59
3:C:96:TYR:CD1	3:C:96:TYR:C	2.76	0.59
3:F:196:LYS:O	3:F:197:ARG:HD2	2.02	0.59
3:I:200:GLY:N	3:I:225:GLU:OE2	2.20	0.59
3:I:209:ILE:H	3:I:209:ILE:CD1	2.10	0.59
1:J:191:LYS:HB2	1:J:191:LYS:HZ3	1.66	0.59
3:C:209:ILE:H	3:C:209:ILE:CD1	2.10	0.58
3:C:220:PRO:HG2	3:C:221:THR:H	1.67	0.58
3:F:224:THR:O	3:F:226:PHE:HD1	1.85	0.58
3:F:242:ILE:CG2	3:F:243:PRO:HD2	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:276:LEU:HD23	3:F:277:THR:N	2.18	0.58
2:H:345:TYR:HB3	2:H:354:MET:HE2	1.84	0.58
2:H:439:ASN:HD22	2:H:439:ASN:N	2.01	0.58
1:A:136:LEU:HD23	1:A:139:ASN:HD22	1.67	0.58
2:B:202:ASN:HD22	2:B:284:ASN:HB2	1.67	0.58
2:B:359:GLN:HE21	2:B:359:GLN:H	1.50	0.58
3:I:117:ASN:O	3:I:119:GLN:N	2.36	0.58
3:I:293:PHE:N	3:I:302:LYS:HG3	2.17	0.58
3:I:393:THR:HG22	3:I:393:THR:O	2.02	0.58
1:J:124:ARG:O	1:J:124:ARG:HD3	2.01	0.58
2:B:214:ILE:HG21	2:B:225:TYR:CD2	2.38	0.58
3:C:109:TYR:C	3:C:110:LEU:HD12	2.24	0.58
2:H:240:CYS:HB3	2:H:242:MET:SD	2.42	0.58
1:J:152:VAL:HG21	2:K:426:MET:O	2.03	0.58
2:K:355:ASP:HA	2:K:369:ILE:HD13	1.86	0.58
2:B:212:GLU:O	2:B:215:ILE:HG22	2.03	0.58
3:C:327:ALA:O	3:C:331:GLY:N	2.36	0.58
2:E:215:ILE:HD12	2:E:248:GLY:N	2.18	0.58
1:G:148:LYS:CE	2:H:425:ASP:HB2	2.33	0.58
2:H:434:GLY:O	2:H:436:VAL:HG13	2.03	0.58
3:I:124:LEU:HD12	3:I:124:LEU:N	2.19	0.58
3:I:389:PHE:O	3:I:391:ARG:N	2.34	0.58
1:A:149:ARG:HG2	2:B:426:MET:O	2.02	0.58
3:C:172:LEU:HD13	3:C:239:GLN:HB2	1.85	0.58
3:C:297:ASP:HB2	3:C:301:ASP:OD2	2.02	0.58
3:C:342:GLY:HA2	3:C:368:ILE:O	2.03	0.58
3:C:380:LYS:HD2	3:C:381:LYS:HG2	1.85	0.58
1:D:185:LEU:O	1:D:185:LEU:HD13	2.04	0.58
2:H:254:ASN:OD1	2:H:451:SER:HB3	2.03	0.58
3:L:189:ASN:ND2	3:L:391:ARG:HD3	2.18	0.58
3:L:246:LEU:HB2	3:L:265:PHE:CG	2.38	0.58
2:B:417:TYR:HB2	2:B:446:SER:HB3	1.85	0.58
3:C:322:PHE:CD1	3:C:338:LYS:HG3	2.38	0.58
2:E:381:ASP:OD2	2:E:393:GLN:HG2	2.04	0.58
1:A:161:CYS:O	1:A:163:GLY:N	2.31	0.58
3:C:237:SER:OG	3:C:266:LYS:HA	2.04	0.58
2:E:397:GLU:O	2:E:399:GLY:N	2.37	0.58
3:F:168:PHE:HD1	3:F:177:GLN:HG3	1.68	0.58
2:H:186:VAL:O	2:H:186:VAL:HG12	2.03	0.58
3:L:276:LEU:HD11	3:L:290:PHE:CE2	2.39	0.58
3:C:286:ALA:O	3:C:372:TRP:HB2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:H	1:D:144:LEU:HD12	1.69	0.58
2:E:183:GLU:HA	3:F:124:LEU:HD21	1.86	0.58
3:F:178:PHE:CZ	3:F:232:LYS:HG2	2.38	0.58
2:K:160:ASN:O	2:K:161:ILE:C	2.42	0.58
3:L:196:LYS:O	3:L:197:ARG:HD2	2.04	0.58
2:B:172:LEU:O	2:B:172:LEU:HD13	2.03	0.58
2:B:190:MET:O	2:B:193:CYS:HB2	2.03	0.58
2:B:258:GLY:O	2:B:260:VAL:N	2.36	0.58
3:C:367:ILE:HB	3:C:378:SER:OG	2.04	0.58
1:G:162:ARG:HG2	1:G:168:ALA:HB2	1.85	0.58
2:H:214:ILE:HG21	2:H:225:TYR:CD2	2.39	0.58
1:A:143:GLN:CD	3:C:118:ASN:HD21	2.07	0.58
2:B:165:LEU:N	2:B:166:ARG:NE	2.51	0.58
2:B:239:TYR:CZ	2:B:289:PRO:HD3	2.39	0.58
2:B:328:GLY:O	2:B:343:ASN:N	2.37	0.58
1:D:140:VAL:CG1	1:D:141:ARG:N	2.67	0.58
2:H:184:SER:O	2:H:187:SER:N	2.35	0.58
3:I:344:LEU:HD12	3:I:384:MET:SD	2.44	0.58
1:J:152:VAL:HG23	1:J:153:ASP:H	1.68	0.58
3:L:304:PHE:CD1	3:L:338:LYS:HB2	2.38	0.58
2:B:298:LYS:O	2:B:302:LEU:HG	2.03	0.57
3:C:200:GLY:N	3:C:225:GLU:OE2	2.22	0.57
3:C:347:VAL:HG23	3:C:365:ASN:O	2.04	0.57
1:G:154:ILE:HG22	1:G:171:ARG:HH12	1.68	0.57
3:I:131:LEU:HD23	3:I:131:LEU:C	2.24	0.57
3:I:194:PHE:CE2	3:I:384:MET:HB3	2.39	0.57
3:I:383:THR:O	3:I:384:MET:HG3	2.04	0.57
2:K:216:ARG:NH1	2:K:216:ARG:CB	2.64	0.57
3:C:155:ASP:O	3:C:159:LYS:HG3	2.04	0.57
3:F:118:ASN:O	3:F:122:VAL:HG23	2.04	0.57
1:G:176:LYS:O	1:G:176:LYS:HG2	2.03	0.57
2:H:333:ASN:C	2:H:335:ALA:H	2.07	0.57
1:J:156:ILE:HG22	1:J:157:LYS:NZ	2.19	0.57
3:L:172:LEU:HD13	3:L:240:SER:CB	2.32	0.57
1:A:147:MET:HG3	2:B:175:LEU:HD21	1.85	0.57
1:A:159:ARG:HB3	2:B:258:GLY:HA3	1.84	0.57
2:B:412:PRO:HA	2:B:450:MET:CE	2.34	0.57
3:C:137:GLU:HB3	3:C:138:PRO:HD2	1.86	0.57
2:H:266:TRP:HA	2:H:266:TRP:HE3	1.69	0.57
3:L:259:THR:O	3:L:286:ALA:HB3	2.04	0.57
1:A:143:GLN:OE1	3:C:118:ASN:ND2	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:TYR:CE2	2:B:298:LYS:HD3	2.40	0.57
2:B:284:ASN:H	2:B:284:ASN:ND2	2.02	0.57
3:C:118:ASN:H	3:C:118:ASN:ND2	1.99	0.57
3:C:310:MET:O	3:C:335:TRP:HD1	1.87	0.57
2:E:183:GLU:HG2	3:F:124:LEU:HG	1.84	0.57
2:E:209:LYS:HG3	2:E:213:GLU:OE1	2.04	0.57
3:F:153:CYS:O	3:F:156:ILE:HB	2.04	0.57
3:F:196:LYS:HA	3:F:382:THR:O	2.04	0.57
1:G:168:ALA:HA	2:H:189:GLN:HE22	1.69	0.57
2:H:166:ARG:O	2:H:167:VAL:HG23	2.04	0.57
2:H:402:TRP:CE2	2:H:412:PRO:HD2	2.39	0.57
3:L:154:GLN:OE1	3:L:189:ASN:HA	2.04	0.57
3:L:198:LEU:HA	3:L:381:LYS:HG2	1.87	0.57
1:A:144:LEU:HD11	1:A:182:GLN:HG2	1.85	0.57
1:A:149:ARG:HG2	2:B:426:MET:C	2.25	0.57
1:A:159:ARG:NH2	2:B:418:TRP:CE3	2.73	0.57
3:F:320:ASP:HA	3:F:336:MET:O	2.03	0.57
3:L:273:LYS:HE3	3:L:319:ASN:HD21	1.69	0.57
3:L:322:PHE:CB	3:L:338:LYS:HD2	2.33	0.57
1:A:124:ARG:C	1:A:126:VAL:H	2.06	0.57
2:B:224:MET:SD	2:B:237:ARG:HB3	2.45	0.57
2:B:367:MET:O	2:B:405:ASN:O	2.23	0.57
2:E:398:ASP:O	2:E:399:GLY:O	2.23	0.57
3:F:280:TYR:O	3:F:281:PHE:C	2.42	0.57
2:H:176:ARG:HA	2:H:179:ILE:HG13	1.85	0.57
2:H:367:MET:HB2	2:H:406:ARG:HB3	1.85	0.57
3:I:198:LEU:HD22	3:I:223:THR:HA	1.86	0.57
3:L:153:CYS:O	3:L:156:ILE:HB	2.04	0.57
3:L:196:LYS:HA	3:L:382:THR:O	2.05	0.57
3:C:171:PRO:HB3	3:C:239:GLN:HG2	1.87	0.57
3:C:246:LEU:HD21	3:C:248:VAL:HG23	1.86	0.57
3:C:295:PHE:HB2	3:C:301:ASP:OD2	2.04	0.57
3:C:339:CYS:SG	4:O:3:ARG:CZ	2.93	0.57
2:H:166:ARG:NH1	2:H:169:ARG:HD2	2.14	0.57
2:H:180:GLN:O	2:H:183:GLU:N	2.38	0.57
1:J:131:GLN:NE2	1:J:132:HIS:N	2.53	0.57
1:J:175:LEU:HD21	2:K:426:MET:CE	2.35	0.57
1:A:148:LYS:HZ2	2:B:425:ASP:HB2	1.66	0.57
3:F:131:LEU:O	3:F:134:GLN:N	2.28	0.57
3:F:172:LEU:HB2	3:F:239:GLN:HB2	1.87	0.57
2:H:276:VAL:O	2:H:277:ALA:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:345:TYR:CB	2:H:354:MET:HE2	2.34	0.57
3:I:355:SER:O	3:I:359:THR:HG23	2.05	0.57
1:J:135:LEU:O	1:J:135:LEU:HD22	2.05	0.57
3:L:276:LEU:HD23	3:L:277:THR:N	2.20	0.57
2:B:175:LEU:HA	2:B:178:LYS:HG3	1.86	0.57
2:B:198:THR:HA	3:C:140:LYS:O	2.05	0.57
2:B:224:MET:SD	2:B:237:ARG:HD3	2.44	0.57
1:J:161:CYS:C	1:J:163:GLY:N	2.59	0.57
2:K:264:ARG:HG2	3:L:136:GLN:HE22	1.70	0.57
2:K:315:GLU:OE2	2:K:448:ARG:NH2	2.38	0.57
3:L:180:VAL:HB	3:L:228:LEU:HD11	1.87	0.57
1:A:151:GLU:HG3	1:A:152:VAL:N	2.20	0.56
3:C:133:ALA:HA	3:C:136:GLN:HG2	1.87	0.56
3:C:336:MET:HE1	3:C:340:HIS:HD2	1.69	0.56
1:D:126:VAL:O	1:D:127:ILE:C	2.43	0.56
2:E:154:ASP:OD2	2:E:154:ASP:N	2.38	0.56
3:F:145:ILE:HG21	3:F:168:PHE:HE2	1.69	0.56
2:H:230:ASP:O	2:H:232:SER:N	2.34	0.56
2:B:165:LEU:HB2	2:B:166:ARG:NH2	2.20	0.56
3:F:251:GLU:OE1	3:F:381:LYS:HD2	2.05	0.56
3:I:117:ASN:N	3:I:117:ASN:ND2	2.53	0.56
3:I:246:LEU:HB3	3:I:265:PHE:CD1	2.40	0.56
3:I:327:ALA:O	3:I:331:GLY:N	2.38	0.56
1:J:126:VAL:CG1	1:J:127:ILE:N	2.68	0.56
2:K:367:MET:HB2	2:K:406:ARG:CB	2.31	0.56
2:K:398:ASP:O	2:K:399:GLY:O	2.23	0.56
3:L:168:PHE:HD1	3:L:177:GLN:HG3	1.69	0.56
3:L:207:ASN:OD1	3:L:210:GLN:HG3	2.05	0.56
1:A:159:ARG:O	2:B:259:SER:N	2.37	0.56
1:A:184:GLN:OE1	2:B:167:VAL:HB	2.06	0.56
2:B:164:ASN:N	2:B:166:ARG:NE	2.51	0.56
2:B:304:ARG:HH22	2:B:333:ASN:HB3	1.69	0.56
2:B:345:TYR:CB	2:B:354:MET:HE2	2.35	0.56
3:C:232:LYS:HA	3:C:235:LEU:CD1	2.36	0.56
2:H:412:PRO:HA	2:H:450:MET:CE	2.36	0.56
3:I:117:ASN:C	3:I:119:GLN:H	2.09	0.56
3:I:155:ASP:O	3:I:159:LYS:HG3	2.05	0.56
3:I:181:TYR:CG	3:I:181:TYR:O	2.56	0.56
2:K:264:ARG:HD3	2:K:273:PHE:CD2	2.40	0.56
2:B:333:ASN:C	2:B:335:ALA:H	2.08	0.56
1:D:169:LEU:H	2:E:189:GLN:HE22	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:343:HIS:O	3:F:367:ILE:HA	2.04	0.56
2:H:417:TYR:HB2	2:H:446:SER:HB3	1.86	0.56
2:H:455:ARG:CG	2:H:456:PRO:HD2	2.34	0.56
2:K:361:MET:HB2	5:K:470:NAG:H81	1.86	0.56
1:A:128:GLU:HA	1:A:131:GLN:HG2	1.86	0.56
1:A:151:GLU:OE2	1:A:173:VAL:HG12	2.06	0.56
2:B:385:TRP:N	2:B:406:ARG:HB2	2.20	0.56
2:B:393:GLN:HB2	2:B:396:LYS:HG3	1.86	0.56
3:C:355:SER:O	3:C:359:THR:HG23	2.06	0.56
1:D:162:ARG:O	1:D:162:ARG:HG2	2.06	0.56
3:I:172:LEU:H	3:I:172:LEU:CD1	2.18	0.56
3:I:193:VAL:HA	3:I:385:LYS:HB3	1.87	0.56
3:I:219:SER:OG	3:I:224:THR:HG21	2.06	0.56
3:I:330:ASP:CB	3:I:365:ASN:HB3	2.35	0.56
2:B:179:ILE:O	2:B:183:GLU:HB2	2.05	0.56
2:B:237:ARG:HH21	3:C:143:VAL:CG2	2.17	0.56
2:B:310:LEU:HD12	2:B:311:LEU:N	2.20	0.56
2:B:385:TRP:CD1	2:B:387:THR:HG22	2.41	0.56
2:B:439:ASN:HD22	2:B:439:ASN:N	2.04	0.56
1:D:159:ARG:O	1:D:159:ARG:HG2	2.06	0.56
2:E:169:ARG:O	2:E:173:GLU:HG3	2.05	0.56
2:E:216:ARG:CB	2:E:216:ARG:NH1	2.66	0.56
2:E:406:ARG:O	2:E:406:ARG:CG	2.54	0.56
3:F:259:THR:O	3:F:286:ALA:HB3	2.06	0.56
3:F:293:PHE:CD1	3:F:294:ASP:N	2.74	0.56
1:G:126:VAL:C	1:G:128:GLU:N	2.59	0.56
1:G:176:LYS:O	1:G:180:ASP:HB2	2.05	0.56
2:H:202:ASN:HD22	2:H:284:ASN:HB2	1.68	0.56
3:I:124:LEU:C	3:I:126:GLU:H	2.08	0.56
1:J:143:GLN:NE2	3:L:117:ASN:HB2	2.20	0.56
2:K:373:MET:HA	2:K:373:MET:HE3	1.88	0.56
2:K:397:GLU:O	2:K:399:GLY:N	2.38	0.56
3:L:104:ASP:O	3:L:107:ILE:HG22	2.06	0.56
2:B:417:TYR:HE1	2:B:433:ASP:O	1.88	0.56
2:E:327:GLY:HA3	2:E:344:LYS:HB2	1.86	0.56
3:F:185:ASP:OD2	3:F:187:SER:HB3	2.06	0.56
2:H:176:ARG:HH11	2:H:176:ARG:HG2	1.70	0.56
2:H:385:TRP:CD1	2:H:387:THR:HG22	2.41	0.56
3:I:171:PRO:HB3	3:I:239:GLN:HG2	1.88	0.56
3:I:171:PRO:HG2	3:I:236:ILE:HG22	1.88	0.56
1:A:148:LYS:HZ1	2:B:425:ASP:HB2	1.67	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ASP:OD2	2:B:291:GLU:HG3	2.04	0.56
1:G:186:GLU:HA	1:G:189:ILE:CG2	2.34	0.56
2:H:224:MET:SD	2:H:237:ARG:HB3	2.46	0.56
3:I:286:ALA:O	3:I:372:TRP:HB2	2.05	0.56
2:B:161:ILE:HG22	2:B:166:ARG:HH12	1.70	0.56
2:B:398:ASP:CA	2:B:433:ASP:HB3	2.33	0.56
1:G:147:MET:HE1	1:G:150:LEU:HD23	1.87	0.56
2:H:226:LEU:O	2:H:227:ILE:O	2.24	0.56
3:I:315:TRP:HA	3:I:325:ASN:OD1	2.06	0.56
1:J:148:LYS:O	1:J:152:VAL:HG22	2.06	0.56
2:K:342:VAL:HG23	2:K:354:MET:HG3	1.86	0.56
3:L:195:GLN:HG3	3:L:227:TRP:HE3	1.64	0.56
2:B:254:ASN:OD1	2:B:451:SER:HB3	2.06	0.56
2:B:390:PRO:O	2:B:396:LYS:HE2	2.06	0.56
3:C:194:PHE:CZ	3:C:384:MET:HB3	2.40	0.56
2:E:415:ARG:O	2:E:434:GLY:HA2	2.06	0.56
2:H:365:ARG:O	2:H:367:MET:N	2.39	0.56
3:I:245:ALA:O	3:I:386:ILE:HA	2.06	0.56
3:L:251:GLU:OE1	3:L:381:LYS:HD2	2.06	0.56
2:B:249:TRP:CH2	2:B:325:HIS:NE2	2.71	0.55
3:C:194:PHE:CE2	3:C:384:MET:HB3	2.41	0.55
3:F:180:VAL:HB	3:F:228:LEU:HD11	1.87	0.55
3:I:252:ASP:OD2	3:I:254:ASN:HB2	2.06	0.55
1:J:152:VAL:HG23	1:J:153:ASP:N	2.22	0.55
3:L:194:PHE:HD1	3:L:233:ILE:CG1	2.16	0.55
3:L:344:LEU:HD22	3:L:382:THR:HG21	1.87	0.55
1:A:156:ILE:HD11	2:B:416:TYR:H	1.71	0.55
2:B:164:ASN:HB2	2:B:166:ARG:NH2	2.20	0.55
2:B:168:LEU:HD23	3:C:110:LEU:CD2	2.36	0.55
1:D:161:CYS:O	1:D:163:GLY:N	2.39	0.55
3:F:346:GLY:O	3:F:367:ILE:HG12	2.06	0.55
2:H:230:ASP:C	2:H:232:SER:H	2.09	0.55
2:H:310:LEU:HB2	2:H:329:PHE:CD2	2.41	0.55
3:I:195:GLN:HA	3:I:226:PHE:O	2.06	0.55
3:L:343:HIS:O	3:L:367:ILE:HA	2.06	0.55
2:B:165:LEU:N	2:B:166:ARG:CZ	2.69	0.55
2:B:181:LYS:C	2:B:183:GLU:H	2.10	0.55
2:B:202:ASN:ND2	2:B:284:ASN:O	2.40	0.55
1:D:144:LEU:HD12	1:D:144:LEU:N	2.21	0.55
3:F:172:LEU:HD13	3:F:240:SER:CB	2.31	0.55
3:F:322:PHE:HB2	3:F:338:LYS:HD2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:293:TRP:HE1	2:H:296:ASN:ND2	2.04	0.55
3:I:295:PHE:HB2	3:I:301:ASP:OD2	2.05	0.55
3:C:198:LEU:HD22	3:C:223:THR:HA	1.88	0.55
3:C:205:LYS:O	3:C:205:LYS:HG2	2.06	0.55
3:C:389:PHE:O	3:C:391:ARG:N	2.36	0.55
3:F:154:GLN:OE1	3:F:189:ASN:HA	2.06	0.55
1:G:159:ARG:C	1:G:161:CYS:H	2.09	0.55
3:I:96:TYR:O	3:I:98:ALA:N	2.40	0.55
2:B:152:TYR:O	2:B:154:ASP:N	2.39	0.55
2:B:162:PRO:HA	2:B:166:ARG:NH1	2.21	0.55
3:C:197:ARG:HH21	3:C:367:ILE:HD11	1.69	0.55
1:D:185:LEU:O	1:D:189:ILE:HG13	2.06	0.55
3:F:148:ILE:H	3:F:148:ILE:CD1	2.00	0.55
3:F:217:HIS:HB2	3:F:224:THR:OG1	2.06	0.55
2:H:178:LYS:C	2:H:180:GLN:H	2.10	0.55
2:H:393:GLN:HB2	2:H:396:LYS:HG3	1.87	0.55
3:I:209:ILE:HD12	3:I:209:ILE:N	2.14	0.55
3:I:367:ILE:HG22	3:I:379:MET:CG	2.36	0.55
2:K:429:HIS:O	2:K:431:THR:HG23	2.06	0.55
3:C:219:SER:HB3	3:C:224:THR:HG21	1.89	0.55
3:F:191:TRP:CE3	3:F:387:ILE:HB	2.42	0.55
3:F:246:LEU:HD22	3:F:265:PHE:CE1	2.41	0.55
3:F:293:PHE:CD2	3:F:370:ALA:HB1	2.42	0.55
3:I:117:ASN:ND2	3:I:117:ASN:H	2.05	0.55
3:I:172:LEU:HD13	3:I:239:GLN:HB3	1.89	0.55
3:I:329:GLN:HE22	3:I:363:TYR:HE2	1.55	0.55
1:J:115:LEU:C	1:J:117:SER:H	2.09	0.55
1:J:124:ARG:HG2	1:J:124:ARG:HH11	1.71	0.55
2:K:378:TYR:HB2	2:K:396:LYS:HD3	1.88	0.55
3:L:293:PHE:CD2	3:L:370:ALA:HB1	2.42	0.55
1:A:155:ASP:O	1:A:158:ILE:HG22	2.06	0.55
2:B:359:GLN:O	2:B:359:GLN:HG2	2.07	0.55
3:C:315:TRP:HA	3:C:325:ASN:OD1	2.07	0.55
3:I:334:TRP:CH2	3:I:344:LEU:HB2	2.42	0.55
3:I:344:LEU:C	3:I:346:GLY:H	2.10	0.55
1:J:122:LEU:HD21	3:L:98:ALA:CB	2.36	0.55
3:L:191:TRP:CZ3	3:L:387:ILE:HB	2.42	0.55
2:B:412:PRO:CG	2:B:450:MET:HE1	2.37	0.55
3:C:166:LEU:HD11	3:C:219:SER:O	2.07	0.55
3:C:279:ALA:HB2	3:F:308:ASN:ND2	2.22	0.55
2:H:175:LEU:O	2:H:178:LYS:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:304:ARG:HH22	2:H:333:ASN:HB3	1.71	0.55
2:B:227:ILE:HD13	2:B:238:VAL:HG11	1.88	0.55
2:B:360:LEU:O	2:B:361:MET:HG2	2.07	0.55
3:C:330:ASP:CB	3:C:365:ASN:HB3	2.36	0.55
1:D:186:GLU:OE1	1:D:186:GLU:HA	2.07	0.55
3:F:194:PHE:H	3:F:194:PHE:HD2	1.53	0.55
3:F:195:GLN:NE2	3:F:344:LEU:O	2.40	0.55
3:F:227:TRP:HE1	3:F:230:ASN:ND2	2.05	0.55
1:G:168:ALA:HA	2:H:189:GLN:OE1	2.07	0.55
1:G:169:LEU:HD13	1:G:170:ALA:N	2.22	0.55
2:H:153:ILE:O	2:H:153:ILE:HG12	2.06	0.55
2:H:249:TRP:CH2	2:H:325:HIS:NE2	2.71	0.55
2:H:351:ASN:OD1	2:H:354:MET:HB2	2.07	0.55
1:J:180:ASP:O	1:J:184:GLN:HG3	2.07	0.55
3:L:259:THR:OG1	3:L:260:ALA:N	2.39	0.55
3:L:293:PHE:CD1	3:L:294:ASP:N	2.75	0.55
1:A:139:ASN:HB3	3:C:114:TYR:CZ	2.42	0.55
1:A:164:SER:HB3	3:C:137:GLU:O	2.05	0.55
2:B:164:ASN:O	2:B:167:VAL:N	2.40	0.55
2:B:255:ARG:HB2	2:B:450:MET:H	1.72	0.55
2:B:345:TYR:HB3	2:B:354:MET:HE2	1.88	0.55
2:B:421:GLN:HG2	2:B:445:TYR:HD1	1.72	0.55
2:B:440:TRP:CE3	2:B:447:MET:HE1	2.43	0.55
3:C:344:LEU:C	3:C:346:GLY:H	2.10	0.55
2:E:358:SER:HA	2:E:365:ARG:NH1	2.21	0.55
3:F:199:ASP:OD1	3:F:201:SER:HB3	2.06	0.55
2:H:390:PRO:O	2:H:396:LYS:HE2	2.07	0.55
2:K:200:SER:H	2:K:279:ASN:HD21	1.55	0.55
2:K:223:GLU:HB2	2:K:286:CYS:O	2.07	0.55
2:K:310:LEU:HD21	2:K:312:ILE:HD11	1.88	0.55
2:K:394:CYS:SG	2:K:407:CYS:N	2.80	0.55
3:L:280:TYR:O	3:L:281:PHE:C	2.45	0.55
2:E:264:ARG:HG2	2:E:264:ARG:NH1	2.19	0.54
2:E:342:VAL:HG23	2:E:354:MET:HG3	1.88	0.54
3:F:104:ASP:O	3:F:107:ILE:HG23	2.08	0.54
3:F:194:PHE:CE2	3:F:384:MET:O	2.60	0.54
2:H:301:GLN:C	2:H:301:GLN:NE2	2.61	0.54
3:I:110:LEU:O	3:I:112:GLU:N	2.38	0.54
3:I:161:ALA:HB1	3:I:184:ILE:CD1	2.38	0.54
3:L:100:ILE:O	3:L:100:ILE:HG22	2.06	0.54
2:B:230:ASP:O	2:B:232:SER:N	2.35	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:172:LEU:HD13	3:I:239:GLN:HB2	1.88	0.54
2:K:310:LEU:HB3	2:K:326:TYR:HB2	1.89	0.54
2:B:198:THR:O	2:B:199:VAL:HG13	2.07	0.54
3:C:246:LEU:O	3:C:261:ASP:HA	2.07	0.54
3:C:304:PHE:CG	3:C:338:LYS:HD3	2.43	0.54
3:F:354:TYR:O	3:F:376:TRP:HB3	2.08	0.54
2:H:198:THR:HA	3:I:140:LYS:O	2.07	0.54
2:H:328:GLY:O	2:H:343:ASN:N	2.37	0.54
2:H:359:GLN:O	2:H:359:GLN:HG2	2.07	0.54
3:I:196:LYS:CG	3:I:198:LEU:HD11	2.33	0.54
3:I:343:HIS:H	3:I:368:ILE:HG13	1.73	0.54
3:I:344:LEU:HD22	3:I:382:THR:HG21	1.90	0.54
3:L:236:ILE:HG21	3:L:386:ILE:HD11	1.89	0.54
3:L:246:LEU:HD22	3:L:265:PHE:CE1	2.42	0.54
2:B:222:SER:OG	2:B:240:CYS:O	2.22	0.54
3:C:356:LYS:HG2	3:C:356:LYS:O	2.08	0.54
3:F:194:PHE:HD1	3:F:233:ILE:CG1	2.16	0.54
2:H:198:THR:O	2:H:199:VAL:HG13	2.08	0.54
2:H:421:GLN:HG2	2:H:445:TYR:HD1	1.72	0.54
3:I:191:TRP:CE3	3:I:385:LYS:HE2	2.42	0.54
3:I:202:VAL:O	3:I:202:VAL:HG12	2.06	0.54
1:J:144:LEU:HD13	1:J:182:GLN:CG	2.38	0.54
1:J:181:GLN:HE22	2:K:174:ASN:ND2	2.05	0.54
2:K:435:VAL:O	2:K:446:SER:HA	2.08	0.54
3:C:281:PHE:CD2	3:C:288:ASP:HB2	2.42	0.54
3:C:343:HIS:H	3:C:368:ILE:HG13	1.72	0.54
3:C:367:ILE:HG22	3:C:379:MET:CG	2.37	0.54
2:E:345:TYR:CD2	2:E:351:ASN:HB2	2.42	0.54
1:G:136:LEU:O	1:G:140:VAL:HG13	2.07	0.54
3:I:110:LEU:C	3:I:112:GLU:N	2.61	0.54
2:B:175:LEU:O	2:B:179:ILE:HG13	2.08	0.54
2:B:352:ALA:HB2	2:B:439:ASN:HB2	1.89	0.54
3:C:105:SER:C	3:C:107:ILE:H	2.09	0.54
2:E:397:GLU:C	2:E:399:GLY:H	2.10	0.54
3:F:198:LEU:HA	3:F:381:LYS:HG2	1.90	0.54
1:G:186:GLU:OE2	1:G:189:ILE:HG21	2.07	0.54
2:H:442:GLY:O	2:H:444:TRP:N	2.41	0.54
3:I:163:GLN:O	3:I:167:TYR:OH	2.20	0.54
3:I:232:LYS:HA	3:I:235:LEU:CD1	2.38	0.54
3:I:247:ARG:O	3:I:249:GLU:N	2.41	0.54
2:K:456:PRO:O	2:K:457:PHE:O	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:172:LEU:HB2	3:L:239:GLN:HB2	1.90	0.54
2:B:162:PRO:CA	2:B:166:ARG:HD2	2.37	0.54
2:B:200:SER:O	2:B:279:ASN:ND2	2.37	0.54
2:B:310:LEU:HB2	2:B:329:PHE:CD2	2.42	0.54
2:B:365:ARG:O	2:B:367:MET:N	2.41	0.54
3:C:373:LYS:HG3	3:C:379:MET:HE1	1.89	0.54
1:G:140:VAL:HG12	3:I:114:TYR:CD1	2.43	0.54
1:G:159:ARG:HH12	2:H:418:TRP:HB2	1.73	0.54
1:G:183:LYS:O	1:G:183:LYS:HD3	2.07	0.54
2:H:253:GLN:NE2	2:H:452:MET:HG3	2.23	0.54
2:H:258:GLY:O	2:H:260:VAL:N	2.40	0.54
2:H:300:SER:HA	2:H:331:VAL:O	2.07	0.54
2:H:351:ASN:ND2	2:H:354:MET:HB2	2.22	0.54
3:I:273:LYS:HE3	3:I:319:ASN:CG	2.28	0.54
3:L:217:HIS:HB2	3:L:224:THR:OG1	2.07	0.54
2:B:276:VAL:O	2:B:277:ALA:HB3	2.08	0.54
2:B:455:ARG:CG	2:B:456:PRO:HD2	2.37	0.54
3:C:246:LEU:HB3	3:C:265:PHE:CD1	2.42	0.54
1:D:177:ASP:O	1:D:181:GLN:HG3	2.07	0.54
2:H:237:ARG:HH21	3:I:143:VAL:CG2	2.20	0.54
2:H:352:ALA:HB2	2:H:439:ASN:HB2	1.90	0.54
3:I:205:LYS:HG2	3:I:205:LYS:O	2.08	0.54
2:B:238:VAL:HA	2:B:276:VAL:HG11	1.90	0.54
3:C:318:ASP:OD2	3:C:325:ASN:HB2	2.07	0.54
1:D:122:LEU:N	1:D:124:ARG:HE	2.06	0.54
2:E:378:TYR:HB2	2:E:396:LYS:HD3	1.90	0.54
2:E:406:ARG:NE	4:N:3:ARG:HB2	2.23	0.54
2:H:228:GLN:O	2:H:228:GLN:HG2	2.08	0.54
2:H:266:TRP:HE1	2:H:380:ARG:CZ	2.21	0.54
3:L:312:PHE:CE1	3:L:334:TRP:HA	2.43	0.54
3:L:328:GLU:C	3:L:330:ASP:H	2.11	0.54
2:B:230:ASP:C	2:B:232:SER:H	2.10	0.54
2:B:351:ASN:ND2	2:B:354:MET:HB2	2.22	0.54
2:H:359:GLN:H	2:H:359:GLN:NE2	2.03	0.54
3:I:246:LEU:O	3:I:261:ASP:HA	2.08	0.54
3:I:264:MET:HE3	3:L:279:ALA:HA	1.90	0.54
2:K:164:ASN:C	2:K:166:ARG:H	2.11	0.54
3:L:321:LYS:HA	3:L:321:LYS:HE2	1.90	0.54
3:C:196:LYS:CG	3:C:198:LEU:HD11	2.34	0.53
3:C:368:ILE:CG2	3:C:375:ARG:HA	2.38	0.53
2:E:270:LYS:O	2:E:270:LYS:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:120:GLU:CD	1:G:121:VAL:N	2.62	0.53
2:H:200:SER:O	2:H:279:ASN:ND2	2.37	0.53
2:H:215:ILE:CD1	2:H:242:MET:HB3	2.37	0.53
2:H:456:PRO:O	2:H:457:PHE:HB3	2.08	0.53
3:I:209:ILE:HG22	3:I:209:ILE:O	2.07	0.53
3:I:212:LYS:O	3:I:231:GLU:HB3	2.08	0.53
1:J:123:LYS:HA	1:J:126:VAL:HG12	1.89	0.53
3:L:224:THR:O	3:L:226:PHE:CD1	2.62	0.53
3:L:388:PRO:O	3:L:389:PHE:O	2.25	0.53
2:B:176:ARG:HD2	2:B:179:ILE:HD12	1.90	0.53
2:B:267:ASP:HB2	2:B:268:PRO:CD	2.37	0.53
3:C:156:ILE:C	3:C:158:ASN:H	2.11	0.53
2:E:170:SER:O	2:E:173:GLU:N	2.36	0.53
3:F:189:ASN:ND2	3:F:391:ARG:HD3	2.22	0.53
3:F:195:GLN:HG3	3:F:227:TRP:HE3	1.69	0.53
1:G:130:VAL:N	1:G:133:ILE:HD13	2.23	0.53
2:H:162:PRO:C	2:H:164:ASN:N	2.61	0.53
3:I:344:LEU:HD22	3:I:382:THR:CG2	2.38	0.53
3:L:94:MET:HB3	3:L:96:TYR:CE2	2.43	0.53
1:A:148:LYS:CE	2:B:425:ASP:HB2	2.38	0.53
2:B:226:LEU:O	2:B:227:ILE:O	2.26	0.53
2:B:310:LEU:HD12	2:B:310:LEU:C	2.29	0.53
3:C:329:GLN:HE22	3:C:363:TYR:HE2	1.57	0.53
1:D:175:LEU:HD21	2:E:426:MET:HE1	1.89	0.53
2:E:177:SER:HA	2:E:180:GLN:HG2	1.91	0.53
2:E:264:ARG:CG	3:F:136:GLN:HE22	2.21	0.53
3:F:227:TRP:HZ2	3:F:230:ASN:ND2	2.00	0.53
1:G:149:ARG:HG2	2:H:426:MET:C	2.29	0.53
2:H:222:SER:OG	2:H:240:CYS:O	2.23	0.53
2:H:386:LEU:O	2:H:386:LEU:HD13	2.08	0.53
2:K:270:LYS:O	2:K:270:LYS:HG2	2.08	0.53
1:A:184:GLN:O	1:A:186:GLU:N	2.41	0.53
2:B:158:ASN:CA	2:B:162:PRO:HG2	2.38	0.53
2:B:215:ILE:CD1	2:B:242:MET:HB3	2.37	0.53
2:B:310:LEU:H	2:B:325:HIS:CE1	2.26	0.53
3:C:149:THR:HB	3:C:168:PHE:O	2.08	0.53
1:A:122:LEU:HB2	1:A:124:ARG:HD3	1.89	0.53
3:C:317:ASN:HD22	3:C:317:ASN:C	2.12	0.53
3:F:96:TYR:HD1	3:F:96:TYR:N	2.02	0.53
3:F:295:PHE:HE2	3:F:305:THR:HG21	1.73	0.53
2:H:255:ARG:HB2	2:H:450:MET:H	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:266:TRP:CE3	2:K:380:ARG:HG2	2.44	0.53
3:L:101:LEU:O	3:L:104:ASP:HB3	2.07	0.53
1:A:183:LYS:O	1:A:183:LYS:HD3	2.09	0.53
2:B:351:ASN:HD21	2:B:354:MET:H	1.57	0.53
3:C:264:MET:CE	3:F:279:ALA:HA	2.38	0.53
2:E:237:ARG:HG3	2:E:237:ARG:NH1	2.23	0.53
3:I:157:ALA:HA	3:I:161:ALA:HB3	1.91	0.53
2:K:242:MET:HA	2:K:248:GLY:H	1.74	0.53
2:K:373:MET:HA	2:K:373:MET:CE	2.37	0.53
3:L:194:PHE:H	3:L:194:PHE:HD2	1.55	0.53
3:L:295:PHE:HE2	3:L:305:THR:HG21	1.74	0.53
3:C:103:HIS:O	3:C:107:ILE:HG22	2.09	0.53
3:C:167:TYR:N	3:C:167:TYR:HD1	2.06	0.53
3:C:171:PRO:HG2	3:C:236:ILE:HG22	1.91	0.53
1:G:140:VAL:HA	3:I:114:TYR:HE1	1.73	0.53
2:H:185:ASP:HA	2:H:188:ALA:HB3	1.90	0.53
2:H:325:HIS:O	2:H:345:TYR:HA	2.09	0.53
2:H:412:PRO:HG3	2:H:450:MET:HE1	1.91	0.53
3:I:149:THR:HB	3:I:168:PHE:O	2.09	0.53
3:I:304:PHE:CG	3:I:338:LYS:HD3	2.44	0.53
2:K:203:ILE:HD12	2:K:203:ILE:H	1.73	0.53
1:A:165:CYS:SG	3:C:135:CYS:SG	3.06	0.53
2:B:366:THR:O	2:B:369:ILE:HG13	2.09	0.53
3:C:191:TRP:HH2	3:C:247:ARG:HH11	1.57	0.53
2:H:242:MET:HA	2:H:247:GLY:CA	2.39	0.53
3:I:113:ILE:N	3:I:113:ILE:HD12	2.24	0.53
3:I:156:ILE:C	3:I:158:ASN:H	2.12	0.53
3:I:264:MET:O	3:I:265:PHE:C	2.47	0.53
2:K:216:ARG:HH11	2:K:216:ARG:HB3	1.72	0.53
2:K:333:ASN:HB3	2:K:336:ASN:HD22	1.73	0.53
3:L:97:GLU:O	3:L:100:ILE:N	2.39	0.53
2:B:300:SER:HA	2:B:331:VAL:O	2.08	0.53
3:C:227:TRP:HE1	3:C:230:ASN:ND2	2.06	0.53
2:E:333:ASN:HB3	2:E:336:ASN:HD22	1.73	0.53
3:F:251:GLU:CD	3:F:381:LYS:HD2	2.29	0.53
3:F:273:LYS:HE3	3:F:319:ASN:HD21	1.74	0.53
3:F:312:PHE:CE1	3:F:334:TRP:HA	2.44	0.53
3:F:328:GLU:C	3:F:330:ASP:H	2.12	0.53
3:I:149:THR:HA	3:I:156:ILE:CD1	2.38	0.53
3:I:196:LYS:HE3	3:I:198:LEU:HD11	1.91	0.53
3:I:197:ARG:HH21	3:I:367:ILE:HD11	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:123:LYS:O	1:J:127:ILE:HB	2.09	0.53
2:B:227:ILE:CD1	2:B:238:VAL:HG11	2.39	0.53
3:C:202:VAL:O	3:C:202:VAL:HG12	2.09	0.53
1:D:185:LEU:CD1	1:D:189:ILE:HD11	2.39	0.53
2:E:242:MET:HA	2:E:248:GLY:H	1.74	0.53
1:J:186:GLU:OE1	1:J:186:GLU:HA	2.08	0.53
3:L:191:TRP:CE3	3:L:387:ILE:HB	2.44	0.53
1:A:184:GLN:C	1:A:186:GLU:N	2.62	0.52
2:B:168:LEU:HD23	3:C:110:LEU:HD23	1.90	0.52
2:B:385:TRP:CZ3	4:M:3:ARG:NE	2.78	0.52
3:C:154:GLN:NE2	3:C:190:GLY:H	2.06	0.52
3:C:195:GLN:HA	3:C:226:PHE:O	2.09	0.52
3:C:212:LYS:O	3:C:231:GLU:HB3	2.08	0.52
2:E:276:VAL:HA	2:E:292:TYR:CD1	2.44	0.52
1:J:151:GLU:HG3	1:J:178:TYR:CZ	2.43	0.52
3:C:209:ILE:HD12	3:C:209:ILE:N	2.15	0.52
3:C:212:LYS:CG	3:C:231:GLU:HB2	2.28	0.52
2:E:315:GLU:OE2	2:E:448:ARG:NH2	2.42	0.52
2:H:169:ARG:NH2	3:I:109:TYR:HD2	2.07	0.52
2:H:224:MET:SD	2:H:237:ARG:HD3	2.48	0.52
3:I:227:TRP:NE1	3:I:229:GLY:HA2	2.25	0.52
3:I:274:TYR:HB2	3:I:312:PHE:HB3	1.90	0.52
3:I:373:LYS:HG3	3:I:379:MET:HE1	1.91	0.52
3:C:149:THR:HA	3:C:156:ILE:CD1	2.39	0.52
3:C:236:ILE:HG13	3:C:236:ILE:O	2.08	0.52
2:E:155:GLU:HG3	2:E:156:THR:H	1.73	0.52
2:E:236:TYR:CD2	2:E:298:LYS:HE2	2.43	0.52
3:F:194:PHE:HD2	3:F:384:MET:O	1.93	0.52
3:F:197:ARG:NE	3:F:204:PHE:CE1	2.77	0.52
3:F:304:PHE:CD1	3:F:338:LYS:HB3	2.45	0.52
2:H:238:VAL:HA	2:H:276:VAL:HG11	1.92	0.52
3:I:171:PRO:O	3:I:174:ALA:HB3	2.09	0.52
3:I:212:LYS:CG	3:I:231:GLU:HB2	2.29	0.52
3:I:274:TYR:HB2	3:I:312:PHE:CB	2.39	0.52
1:J:143:GLN:O	1:J:147:MET:HG2	2.09	0.52
2:K:180:GLN:HG3	2:K:181:LYS:H	1.70	0.52
2:K:211:CYS:SG	2:K:250:THR:HA	2.49	0.52
2:K:264:ARG:HG2	2:K:264:ARG:HH11	1.74	0.52
3:L:218:LEU:HD21	3:L:226:PHE:CE2	2.44	0.52
3:L:223:THR:O	3:L:224:THR:HB	2.10	0.52
1:A:133:ILE:CG2	2:B:164:ASN:ND2	2.72	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:TRP:HE1	2:B:296:ASN:ND2	2.08	0.52
3:C:202:VAL:O	3:C:203:ASP:C	2.47	0.52
3:C:394:ILE:C	3:C:396:GLU:H	2.12	0.52
1:D:140:VAL:HG22	1:D:144:LEU:HD11	1.90	0.52
3:I:117:ASN:C	3:I:119:GLN:N	2.63	0.52
3:I:312:PHE:CZ	3:I:333:GLY:O	2.63	0.52
2:K:381:ASP:OD2	2:K:393:GLN:HG2	2.10	0.52
3:L:194:PHE:CE2	3:L:384:MET:O	2.62	0.52
2:B:228:GLN:HG2	2:B:228:GLN:O	2.08	0.52
3:C:274:TYR:HB2	3:C:312:PHE:CB	2.39	0.52
2:H:187:SER:HA	2:H:190:MET:HB3	1.92	0.52
2:K:162:PRO:HG3	3:L:103:HIS:CE1	2.44	0.52
3:L:145:ILE:HD13	3:L:168:PHE:HE2	1.74	0.52
3:C:163:GLN:HA	3:C:163:GLN:NE2	2.18	0.52
3:C:394:ILE:O	3:C:396:GLU:N	2.39	0.52
3:F:322:PHE:CD2	4:P:3:ARG:HG3	2.45	0.52
2:H:328:GLY:HA3	2:H:343:ASN:OD1	2.10	0.52
3:L:194:PHE:HD2	3:L:384:MET:O	1.93	0.52
2:B:253:GLN:NE2	2:B:452:MET:HG3	2.25	0.52
2:B:351:ASN:OD1	2:B:354:MET:HB2	2.10	0.52
3:C:245:ALA:O	3:C:386:ILE:HA	2.10	0.52
3:C:274:TYR:HB2	3:C:312:PHE:HB3	1.91	0.52
3:F:388:PRO:O	3:F:389:PHE:O	2.27	0.52
2:H:202:ASN:ND2	2:H:284:ASN:O	2.43	0.52
2:H:227:ILE:HD13	2:H:238:VAL:HG11	1.91	0.52
2:H:367:MET:O	2:H:405:ASN:O	2.27	0.52
2:B:359:GLN:H	2:B:359:GLN:NE2	2.05	0.52
2:B:406:ARG:O	2:B:406:ARG:HG2	2.09	0.52
3:C:264:MET:O	3:C:265:PHE:C	2.48	0.52
2:E:164:ASN:O	2:E:164:ASN:ND2	2.33	0.52
2:E:266:TRP:CE3	2:E:380:ARG:HG2	2.45	0.52
1:G:128:GLU:CD	1:G:129:LYS:HZ2	2.13	0.52
1:G:161:CYS:C	1:G:163:GLY:H	2.13	0.52
3:I:169:ILE:HG12	3:I:180:VAL:HG11	1.91	0.52
3:I:261:ASP:O	3:I:262:TYR:CG	2.63	0.52
2:K:213:GLU:O	2:K:217:LYS:HG3	2.09	0.52
3:L:314:THR:O	3:L:316:ASP:N	2.43	0.52
1:A:127:ILE:O	1:A:130:VAL:HG12	2.10	0.52
3:C:96:TYR:C	3:C:96:TYR:HD1	2.11	0.52
3:C:247:ARG:O	3:C:249:GLU:N	2.43	0.52
3:C:287:GLY:HA3	3:C:371:THR:HB	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:167:VAL:HG23	2:E:168:LEU:N	2.24	0.52
1:G:169:LEU:HD22	1:G:170:ALA:N	2.21	0.52
2:H:387:THR:C	2:H:389:ASP:H	2.12	0.52
3:I:97:GLU:C	3:I:99:SER:N	2.63	0.52
3:I:107:ILE:CG1	3:I:108:ARG:H	2.17	0.52
1:A:133:ILE:CG2	2:B:164:ASN:HD22	2.22	0.52
1:A:143:GLN:HA	1:A:143:GLN:NE2	2.16	0.52
1:A:161:CYS:C	1:A:163:GLY:H	2.12	0.52
3:C:161:ALA:HB1	3:C:184:ILE:CD1	2.40	0.52
3:F:236:ILE:HG21	3:F:386:ILE:HD11	1.92	0.52
3:F:344:LEU:HD22	3:F:382:THR:HG21	1.91	0.52
2:H:267:ASP:HB2	2:H:268:PRO:CD	2.38	0.52
3:I:340:HIS:ND1	3:I:368:ILE:HD11	2.25	0.52
1:J:148:LYS:O	1:J:151:GLU:HB2	2.09	0.52
2:K:187:SER:HA	2:K:190:MET:CE	2.40	0.52
2:K:270:LYS:HG3	2:K:338:TYR:OH	2.09	0.52
2:K:345:TYR:CD2	2:K:351:ASN:HB2	2.45	0.52
2:B:456:PRO:O	2:B:457:PHE:HB3	2.10	0.51
3:C:94:MET:C	3:C:96:TYR:H	2.13	0.51
3:C:99:SER:C	3:C:101:LEU:H	2.13	0.51
3:C:149:THR:HA	3:C:156:ILE:HD13	1.92	0.51
3:C:219:SER:CB	3:C:224:THR:HG21	2.39	0.51
1:D:175:LEU:HD21	2:E:426:MET:CE	2.40	0.51
2:E:436:VAL:HG12	2:E:445:TYR:O	2.10	0.51
1:G:126:VAL:HG12	1:G:127:ILE:N	2.25	0.51
1:G:144:LEU:CD2	1:G:182:GLN:HE21	2.23	0.51
3:I:149:THR:HA	3:I:156:ILE:HD13	1.93	0.51
1:J:130:VAL:O	1:J:134:GLN:HB2	2.10	0.51
2:K:202:ASN:ND2	3:L:219:SER:HB3	2.25	0.51
2:K:234:LYS:HD3	2:K:234:LYS:C	2.30	0.51
2:K:355:ASP:O	2:K:365:ARG:HD3	2.10	0.51
3:L:227:TRP:HZ3	3:L:384:MET:HE2	1.75	0.51
2:B:164:ASN:HB2	2:B:166:ARG:HH21	1.76	0.51
2:B:256:GLN:CA	2:B:449:LYS:HG2	2.38	0.51
3:C:100:ILE:O	3:C:100:ILE:CG2	2.57	0.51
3:C:110:LEU:C	3:C:112:GLU:N	2.54	0.51
3:F:320:ASP:HB3	3:F:336:MET:HB2	1.92	0.51
3:I:356:LYS:O	3:I:356:LYS:HG2	2.10	0.51
3:L:195:GLN:NE2	3:L:344:LEU:O	2.43	0.51
2:B:373:MET:HG3	2:B:405:ASN:HB2	1.92	0.51
3:F:96:TYR:C	3:F:98:ALA:N	2.64	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:259:THR:OG1	3:F:260:ALA:N	2.41	0.51
2:H:408:HIS:NE2	2:H:436:VAL:HG21	2.25	0.51
1:J:175:LEU:HD21	2:K:426:MET:HE1	1.91	0.51
2:K:164:ASN:O	2:K:167:VAL:HG12	2.10	0.51
2:K:209:LYS:HG3	2:K:213:GLU:OE1	2.10	0.51
2:B:210:GLU:OE1	2:B:212:GLU:N	2.32	0.51
2:E:406:ARG:HG2	2:E:406:ARG:O	2.10	0.51
2:H:210:GLU:HA	2:H:227:ILE:CB	2.32	0.51
3:I:368:ILE:CG2	3:I:375:ARG:HA	2.40	0.51
1:J:153:ASP:O	1:J:156:ILE:HB	2.10	0.51
3:C:227:TRP:NE1	3:C:229:GLY:HA2	2.26	0.51
3:F:321:LYS:HE2	3:F:321:LYS:HA	1.92	0.51
1:G:168:ALA:HA	2:H:189:GLN:CD	2.30	0.51
2:H:361:MET:HB2	5:H:470:NAG:O7	2.10	0.51
1:J:126:VAL:O	1:J:127:ILE:C	2.48	0.51
1:J:161:CYS:O	1:J:163:GLY:N	2.42	0.51
3:L:346:GLY:O	3:L:367:ILE:HG12	2.10	0.51
1:A:136:LEU:HD11	3:C:111:GLN:CB	2.40	0.51
2:B:165:LEU:CD2	2:B:166:ARG:NH2	2.70	0.51
2:B:299:ILE:C	2:B:301:GLN:N	2.63	0.51
3:C:169:ILE:HG12	3:C:180:VAL:HG11	1.92	0.51
3:C:275:ARG:HB2	3:C:311:GLN:HG2	1.93	0.51
3:C:312:PHE:CZ	3:C:333:GLY:O	2.64	0.51
2:E:264:ARG:HD3	2:E:273:PHE:CD2	2.46	0.51
2:E:355:ASP:HA	2:E:369:ILE:CD1	2.41	0.51
2:E:373:MET:HA	2:E:373:MET:HE3	1.93	0.51
3:F:365:ASN:HD22	3:F:365:ASN:N	2.01	0.51
1:G:143:GLN:C	1:G:145:VAL:N	2.63	0.51
3:I:171:PRO:CG	3:I:236:ILE:HG22	2.40	0.51
3:I:219:SER:CB	3:I:224:THR:HG21	2.40	0.51
3:I:304:PHE:CD1	3:I:338:LYS:HD3	2.45	0.51
3:L:96:TYR:O	3:L:99:SER:HB2	2.11	0.51
3:L:109:TYR:HD1	3:L:110:LEU:HD23	1.75	0.51
2:B:387:THR:C	2:B:389:ASP:H	2.12	0.51
2:B:421:GLN:HG2	2:B:445:TYR:CD1	2.46	0.51
3:C:157:ALA:HA	3:C:161:ALA:HB3	1.93	0.51
3:C:181:TYR:CG	3:C:181:TYR:O	2.63	0.51
2:E:326:TYR:OH	2:E:351:ASN:ND2	2.44	0.51
2:E:456:PRO:O	2:E:457:PHE:O	2.28	0.51
2:H:310:LEU:H	2:H:325:HIS:CE1	2.29	0.51
1:J:122:LEU:HD21	3:L:98:ALA:HA	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:156:THR:O	2:K:158:ASN:N	2.43	0.51
2:K:391:ARG:HG2	2:K:391:ARG:NH1	2.24	0.51
2:K:434:GLY:O	2:K:436:VAL:HG13	2.10	0.51
2:E:242:MET:HA	2:E:247:GLY:HA3	1.92	0.51
2:E:373:MET:HA	2:E:373:MET:CE	2.41	0.51
1:G:159:ARG:CZ	2:H:418:TRP:CE3	2.94	0.51
3:I:340:HIS:H	4:S:1:GLY:HA2	1.74	0.51
3:L:359:THR:OG1	3:L:362:GLY:HA2	2.10	0.51
2:B:311:LEU:HD11	2:B:323:LYS:HB2	1.93	0.51
2:E:406:ARG:HE	4:N:3:ARG:HB2	1.74	0.51
1:G:167:ARG:HD2	1:G:168:ALA:N	2.26	0.51
2:H:210:GLU:OE1	2:H:212:GLU:N	2.33	0.51
2:H:213:GLU:OE2	2:H:217:LYS:NZ	2.36	0.51
2:H:411:ASN:HD22	2:H:434:GLY:H	1.58	0.51
3:I:169:ILE:CD1	3:I:171:PRO:HD3	2.29	0.51
3:I:189:ASN:CG	3:I:391:ARG:HE	2.13	0.51
2:K:311:LEU:HD21	2:K:313:GLU:OE2	2.10	0.51
2:K:405:ASN:O	2:K:406:ARG:C	2.49	0.51
1:A:124:ARG:N	1:A:124:ARG:CD	2.73	0.51
1:A:158:ILE:CG2	1:A:159:ARG:N	2.74	0.51
1:A:190:ALA:C	1:A:191:LYS:HZ3	2.14	0.51
2:B:218:GLY:CA	3:C:210:GLN:HE21	2.23	0.51
3:C:202:VAL:HG21	3:C:225:GLU:O	2.11	0.51
1:D:168:ALA:HA	2:E:189:GLN:HE22	1.75	0.51
2:E:202:ASN:ND2	3:F:219:SER:HB3	2.26	0.51
2:E:223:GLU:CB	2:E:287:GLY:HA2	2.40	0.51
2:E:391:ARG:HG2	2:E:391:ARG:NH1	2.25	0.51
2:H:218:GLY:CA	3:I:210:GLN:HE21	2.23	0.51
2:H:236:TYR:CE2	2:H:298:LYS:HD3	2.46	0.51
3:L:295:PHE:CE2	3:L:305:THR:HG21	2.46	0.51
3:L:295:PHE:CE2	4:T:2:PRO:HD3	2.45	0.51
3:L:355:SER:C	3:L:357:ALA:N	2.64	0.51
2:B:325:HIS:O	2:B:345:TYR:HA	2.11	0.50
2:B:340:ILE:HD12	2:B:403:TRP:CE3	2.46	0.50
2:B:434:GLY:O	2:B:436:VAL:HG13	2.10	0.50
1:D:126:VAL:O	1:D:129:LYS:N	2.44	0.50
1:G:151:GLU:OE2	1:G:173:VAL:CG1	2.59	0.50
2:H:205:VAL:HG21	3:I:215:PHE:O	2.12	0.50
2:H:246:ASN:HB2	2:H:455:ARG:HH12	1.76	0.50
2:K:333:ASN:HB3	2:K:336:ASN:ND2	2.26	0.50
2:K:402:TRP:CH2	2:K:412:PRO:HG2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:HG12	3:C:114:TYR:CE1	2.46	0.50
2:B:449:LYS:NZ	2:B:449:LYS:HB3	2.26	0.50
1:D:127:ILE:HG23	1:D:128:GLU:N	2.25	0.50
2:E:245:GLU:O	2:E:246:ASN:HB2	2.11	0.50
3:F:295:PHE:CE2	3:F:305:THR:HG21	2.47	0.50
1:G:159:ARG:O	2:H:259:SER:N	2.44	0.50
2:H:173:GLU:O	2:H:175:LEU:N	2.44	0.50
2:H:179:ILE:O	2:H:179:ILE:HG22	2.11	0.50
2:H:180:GLN:C	2:H:182:LEU:H	2.14	0.50
2:H:345:TYR:HB3	2:H:354:MET:CE	2.40	0.50
2:H:411:ASN:CB	2:H:436:VAL:HG22	2.39	0.50
2:H:449:LYS:NZ	2:H:449:LYS:HB3	2.27	0.50
3:I:197:ARG:HB2	3:I:382:THR:HB	1.93	0.50
3:I:279:ALA:HB2	3:L:308:ASN:ND2	2.26	0.50
2:K:373:MET:CG	2:K:405:ASN:HB2	2.36	0.50
2:K:397:GLU:C	2:K:399:GLY:H	2.14	0.50
2:B:204:PRO:HA	3:C:217:HIS:CB	2.41	0.50
3:C:273:LYS:HE3	3:C:319:ASN:CG	2.32	0.50
3:C:381:LYS:O	3:C:382:THR:OG1	2.26	0.50
3:C:387:ILE:HG12	3:C:388:PRO:N	2.25	0.50
3:F:276:LEU:HD23	3:F:276:LEU:C	2.31	0.50
3:F:389:PHE:O	3:F:390:ASN:C	2.49	0.50
2:H:193:CYS:HB3	3:I:134:GLN:CD	2.32	0.50
2:H:299:ILE:C	2:H:301:GLN:N	2.63	0.50
2:H:326:TYR:O	2:H:328:GLY:N	2.45	0.50
1:J:127:ILE:HG22	1:J:128:GLU:N	2.27	0.50
2:K:242:MET:HA	2:K:247:GLY:HA3	1.93	0.50
3:L:204:PHE:C	3:L:206:LYS:N	2.61	0.50
2:B:158:ASN:C	2:B:162:PRO:HG2	2.31	0.50
2:B:350:GLY:O	2:B:352:ALA:N	2.44	0.50
3:C:191:TRP:CH2	3:C:247:ARG:HD3	2.46	0.50
2:E:211:CYS:SG	2:E:250:THR:HA	2.51	0.50
3:F:93:ILE:O	3:F:95:LYS:N	2.45	0.50
3:F:330:ASP:HB3	3:F:343:HIS:HE1	1.76	0.50
1:G:141:ARG:HB3	1:G:141:ARG:HH11	1.76	0.50
1:G:191:LYS:O	1:G:192:ASP:HB3	2.12	0.50
3:I:131:LEU:HD23	3:I:132:GLU:N	2.26	0.50
3:I:166:LEU:HD11	3:I:219:SER:O	2.11	0.50
2:B:173:GLU:C	2:B:175:LEU:H	2.15	0.50
2:B:173:GLU:O	2:B:176:ARG:N	2.45	0.50
3:C:287:GLY:O	3:C:369:TRP:NE1	2.34	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:ILE:HG23	1:G:189:ILE:O	2.12	0.50
2:H:229:PRO:O	2:H:230:ASP:C	2.49	0.50
2:H:351:ASN:CG	2:H:354:MET:HB2	2.32	0.50
3:I:202:VAL:O	3:I:203:ASP:C	2.49	0.50
2:K:355:ASP:HA	2:K:369:ILE:CD1	2.42	0.50
3:L:354:TYR:O	3:L:376:TRP:HB3	2.11	0.50
3:L:389:PHE:O	3:L:390:ASN:C	2.49	0.50
2:B:229:PRO:O	2:B:230:ASP:C	2.49	0.50
1:G:167:ARG:HD2	1:G:167:ARG:C	2.32	0.50
3:I:235:LEU:HD12	3:I:235:LEU:N	2.25	0.50
3:I:310:MET:O	3:I:335:TRP:CD1	2.64	0.50
2:B:326:TYR:O	2:B:328:GLY:N	2.45	0.50
2:B:342:VAL:O	2:B:371:ASN:ND2	2.45	0.50
3:C:107:ILE:HG23	3:C:108:ARG:N	2.27	0.50
3:C:193:VAL:HA	3:C:385:LYS:HB3	1.93	0.50
3:C:197:ARG:NH2	3:C:348:TYR:HB2	2.27	0.50
2:E:264:ARG:HG2	3:F:136:GLN:NE2	2.25	0.50
3:F:109:TYR:CE1	3:F:113:ILE:HD11	2.46	0.50
2:H:249:TRP:HB3	2:H:453:LYS:HB2	1.94	0.50
2:H:317:TRP:CE3	2:H:448:ARG:HD3	2.47	0.50
3:I:264:MET:CE	3:L:279:ALA:HA	2.41	0.50
3:I:287:GLY:HA3	3:I:371:THR:HB	1.93	0.50
1:J:128:GLU:HA	1:J:131:GLN:OE1	2.12	0.50
1:A:127:ILE:C	1:A:130:VAL:HG12	2.32	0.50
2:B:242:MET:HA	2:B:247:GLY:CA	2.42	0.50
2:B:408:HIS:NE2	2:B:436:VAL:HG21	2.27	0.50
3:C:171:PRO:O	3:C:174:ALA:HB3	2.12	0.50
1:D:169:LEU:H	2:E:189:GLN:NE2	2.10	0.50
1:D:191:LYS:O	1:D:192:ASP:HB2	2.11	0.50
2:E:266:TRP:HA	2:E:377:THR:HG21	1.93	0.50
1:G:159:ARG:O	1:G:161:CYS:N	2.44	0.50
1:G:161:CYS:O	1:G:163:GLY:N	2.41	0.50
2:H:264:ARG:HD2	2:H:268:PRO:HB3	1.94	0.50
2:H:360:LEU:O	2:H:361:MET:HG2	2.12	0.50
3:I:272:ASP:O	3:I:273:LYS:CB	2.59	0.50
2:K:164:ASN:O	2:K:168:LEU:HD23	2.11	0.50
2:K:280:THR:OG1	2:K:288:LEU:HG	2.12	0.50
2:K:405:ASN:O	2:K:407:CYS:N	2.45	0.50
3:L:97:GLU:HA	3:L:100:ILE:CG1	2.41	0.50
3:L:105:SER:O	3:L:108:ARG:N	2.45	0.50
3:L:227:TRP:HE1	3:L:230:ASN:ND2	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG23	1:A:174:ASP:N	2.27	0.50
1:A:185:LEU:HD13	1:A:185:LEU:O	2.12	0.50
2:B:179:ILE:CD1	3:C:117:ASN:ND2	2.75	0.50
2:B:185:ASP:C	2:B:187:SER:H	2.15	0.50
2:B:246:ASN:HB2	2:B:455:ARG:HH12	1.77	0.50
2:B:384:GLY:C	2:B:406:ARG:HB2	2.32	0.50
3:C:97:GLU:O	3:C:101:LEU:HB2	2.12	0.50
3:C:209:ILE:O	3:C:209:ILE:HG22	2.10	0.50
3:C:334:TRP:CH2	3:C:344:LEU:HB2	2.47	0.50
3:C:353:THR:HA	3:C:377:TYR:HA	1.94	0.50
2:H:316:ASP:HB2	2:H:445:TYR:CE2	2.42	0.50
2:H:398:ASP:CA	2:H:433:ASP:HB3	2.39	0.50
2:H:421:GLN:HG2	2:H:445:TYR:CD1	2.47	0.50
3:I:154:GLN:NE2	3:I:190:GLY:H	2.09	0.50
3:I:191:TRP:HH2	3:I:247:ARG:HH11	1.59	0.50
3:I:280:TYR:HD2	3:I:281:PHE:O	1.94	0.50
3:I:317:ASN:HD22	3:I:317:ASN:C	2.16	0.50
2:K:264:ARG:HG2	2:K:264:ARG:NH1	2.25	0.50
3:L:391:ARG:HB2	3:L:391:ARG:HH11	1.73	0.50
1:A:191:LYS:HD2	1:A:191:LYS:N	2.27	0.49
2:B:165:LEU:CD1	3:C:106:SER:O	2.59	0.49
2:B:169:ARG:HH12	3:C:109:TYR:HD2	1.58	0.49
3:C:261:ASP:O	3:C:262:TYR:CG	2.65	0.49
3:C:293:PHE:CA	3:C:302:LYS:HG3	2.42	0.49
3:C:336:MET:HE1	3:C:340:HIS:CD2	2.47	0.49
1:D:148:LYS:HG3	1:D:178:TYR:CG	2.47	0.49
2:E:203:ILE:HG21	2:E:226:LEU:HD22	1.93	0.49
2:E:216:ARG:HH11	2:E:216:ARG:HB3	1.73	0.49
3:F:100:ILE:CG2	3:F:103:HIS:HB2	2.42	0.49
3:F:223:THR:O	3:F:224:THR:HB	2.12	0.49
3:F:227:TRP:NE1	3:F:230:ASN:ND2	2.60	0.49
3:F:311:GLN:O	3:F:335:TRP:HA	2.12	0.49
1:J:136:LEU:HD11	3:L:110:LEU:HB2	1.94	0.49
2:K:436:VAL:HG12	2:K:445:TYR:O	2.12	0.49
3:L:200:GLY:H	3:L:225:GLU:CD	2.14	0.49
2:B:157:VAL:O	2:B:157:VAL:HG23	2.12	0.49
2:B:362:GLY:O	2:B:365:ARG:N	2.45	0.49
3:C:331:GLY:O	3:C:332:SER:HB3	2.12	0.49
3:C:390:ASN:OD1	3:C:391:ARG:HG3	2.12	0.49
2:H:428:LYS:C	2:H:429:HIS:HD2	2.14	0.49
3:L:236:ILE:HG22	3:L:386:ILE:HD11	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:365:ASN:HD22	3:L:365:ASN:N	2.02	0.49
3:L:391:ARG:HH11	3:L:391:ARG:CB	2.25	0.49
2:B:169:ARG:HH22	3:C:109:TYR:HD2	1.56	0.49
2:B:398:ASP:HA	2:B:433:ASP:HB2	1.92	0.49
3:C:280:TYR:HD2	3:C:281:PHE:O	1.95	0.49
1:D:130:VAL:O	1:D:133:ILE:HB	2.12	0.49
2:E:155:GLU:O	2:E:156:THR:C	2.51	0.49
2:E:402:TRP:CH2	2:E:412:PRO:HG2	2.47	0.49
3:F:325:ASN:C	3:F:325:ASN:ND2	2.62	0.49
1:G:169:LEU:HD12	1:G:171:ARG:HB3	1.94	0.49
2:H:287:GLY:C	2:H:288:LEU:HD23	2.33	0.49
2:H:340:ILE:HD12	2:H:403:TRP:CE3	2.47	0.49
2:K:238:VAL:HG23	2:K:294:LEU:HD13	1.94	0.49
3:L:276:LEU:HD23	3:L:276:LEU:C	2.33	0.49
2:E:224:MET:SD	2:E:237:ARG:HD3	2.52	0.49
2:H:156:THR:O	2:H:161:ILE:HB	2.12	0.49
3:I:163:GLN:HA	3:I:163:GLN:NE2	2.21	0.49
3:I:331:GLY:O	3:I:332:SER:HB3	2.11	0.49
3:I:394:ILE:HG23	3:I:395:GLY:N	2.26	0.49
1:A:158:ILE:HG21	1:A:171:ARG:HE	1.77	0.49
2:B:161:ILE:HB	2:B:162:PRO:HD3	1.94	0.49
3:C:114:TYR:O	3:C:116:SER:N	2.45	0.49
3:C:344:LEU:HD22	3:C:382:THR:HG21	1.95	0.49
2:E:234:LYS:C	2:E:234:LYS:HD3	2.32	0.49
2:E:340:ILE:HG21	2:E:403:TRP:CG	2.47	0.49
3:F:204:PHE:C	3:F:206:LYS:N	2.62	0.49
3:F:227:TRP:HZ3	3:F:384:MET:HE2	1.76	0.49
3:F:318:ASP:OD1	3:F:320:ASP:OD2	2.30	0.49
1:G:184:GLN:HE21	1:G:185:LEU:HB2	1.77	0.49
2:H:227:ILE:CD1	2:H:238:VAL:HG11	2.42	0.49
2:H:256:GLN:CA	2:H:449:LYS:HG2	2.41	0.49
2:H:310:LEU:HD12	2:H:311:LEU:N	2.27	0.49
3:I:107:ILE:O	3:I:108:ARG:C	2.50	0.49
3:I:219:SER:HB3	3:I:224:THR:HG21	1.95	0.49
2:K:216:ARG:HB2	2:K:216:ARG:HH11	1.59	0.49
3:L:242:ILE:HG22	3:L:243:PRO:HD2	1.93	0.49
3:L:290:PHE:HD1	3:L:307:HIS:ND1	2.09	0.49
3:L:307:HIS:O	3:L:308:ASN:C	2.50	0.49
2:B:165:LEU:HD13	3:C:110:LEU:CD2	2.42	0.49
2:B:412:PRO:CB	2:B:450:MET:HE1	2.42	0.49
3:C:295:PHE:H	3:C:301:ASP:HB3	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:VAL:O	1:D:144:LEU:HD12	2.13	0.49
2:E:411:ASN:HB3	2:E:434:GLY:O	2.13	0.49
3:F:355:SER:C	3:F:357:ALA:N	2.66	0.49
3:I:281:PHE:CD2	3:I:288:ASP:HB2	2.47	0.49
1:J:144:LEU:HD13	1:J:182:GLN:HG2	1.95	0.49
1:J:185:LEU:CD1	1:J:189:ILE:HD11	2.42	0.49
3:L:197:ARG:NE	3:L:204:PHE:CE1	2.80	0.49
3:L:311:GLN:O	3:L:335:TRP:HA	2.13	0.49
3:L:325:ASN:C	3:L:325:ASN:ND2	2.62	0.49
1:A:144:LEU:CG	1:A:182:GLN:HG2	2.42	0.49
2:B:175:LEU:O	2:B:175:LEU:HD23	2.12	0.49
2:B:301:GLN:NE2	2:B:301:GLN:C	2.66	0.49
3:C:171:PRO:CG	3:C:236:ILE:HG22	2.42	0.49
3:C:219:SER:OG	3:C:224:THR:HG21	2.13	0.49
3:C:264:MET:HE3	3:F:279:ALA:HA	1.94	0.49
3:C:340:HIS:HE1	3:C:364:ASP:OD2	1.96	0.49
2:E:213:GLU:O	2:E:217:LYS:HG3	2.12	0.49
2:H:422:TYR:CE1	2:H:444:TRP:HA	2.48	0.49
3:I:97:GLU:O	3:I:100:ILE:HG13	2.12	0.49
3:I:287:GLY:O	3:I:369:TRP:NE1	2.36	0.49
3:I:318:ASP:OD2	3:I:325:ASN:HB2	2.12	0.49
1:A:188:VAL:C	1:A:189:ILE:HD12	2.33	0.49
3:C:245:ALA:HA	3:C:265:PHE:HB2	1.95	0.49
3:C:272:ASP:O	3:C:273:LYS:CB	2.60	0.49
3:C:344:LEU:HD22	3:C:382:THR:CG2	2.42	0.49
3:F:243:PRO:HB2	3:F:389:PHE:HB3	1.95	0.49
1:G:139:ASN:HB3	3:I:114:TYR:OH	2.12	0.49
2:H:226:LEU:O	2:H:226:LEU:HD12	2.13	0.49
3:I:120:LYS:O	3:I:123:ASN:HB2	2.13	0.49
2:K:408:HIS:CD2	2:K:411:ASN:HB2	2.48	0.49
3:L:199:ASP:OD1	3:L:201:SER:HB3	2.12	0.49
2:B:236:TYR:CB	2:B:298:LYS:HZ3	2.24	0.49
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.77	0.49
3:C:189:ASN:CG	3:C:391:ARG:HE	2.15	0.49
2:E:351:ASN:C	2:E:351:ASN:ND2	2.66	0.49
3:F:224:THR:O	3:F:226:PHE:CD1	2.66	0.49
2:H:204:PRO:HA	3:I:217:HIS:CB	2.43	0.49
2:H:236:TYR:CB	2:H:298:LYS:HZ3	2.26	0.49
2:H:276:VAL:O	2:H:276:VAL:HG12	2.12	0.49
2:H:310:LEU:HD12	2:H:310:LEU:C	2.34	0.49
2:K:253:GLN:OE1	2:K:255:ARG:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:350:GLN:C	3:L:352:GLY:H	2.16	0.49
1:A:188:VAL:O	1:A:189:ILE:HD12	2.13	0.49
2:B:166:ARG:O	2:B:170:SER:HB2	2.12	0.49
2:B:210:GLU:HA	2:B:227:ILE:CB	2.34	0.49
2:B:326:TYR:OH	2:B:353:LEU:HB2	2.12	0.49
2:B:422:TYR:CE1	2:B:444:TRP:HA	2.48	0.49
3:C:235:LEU:HD12	3:C:235:LEU:N	2.26	0.49
2:E:162:PRO:HG3	3:F:103:HIS:CE1	2.47	0.49
2:E:270:LYS:HG3	2:E:338:TYR:OH	2.12	0.49
3:F:218:LEU:HD21	3:F:226:PHE:CE2	2.48	0.49
2:H:299:ILE:C	2:H:301:GLN:H	2.16	0.49
2:H:326:TYR:OH	2:H:353:LEU:HB2	2.12	0.49
2:H:333:ASN:C	2:H:335:ALA:N	2.67	0.49
3:I:191:TRP:CH2	3:I:247:ARG:HD3	2.48	0.49
3:L:216:GLY:O	3:L:217:HIS:CD2	2.65	0.49
2:B:164:ASN:N	2:B:166:ARG:HE	2.10	0.48
2:B:205:VAL:HG21	3:C:215:PHE:O	2.13	0.48
2:B:252:ILE:HG23	2:B:299:ILE:HG12	1.94	0.48
2:E:234:LYS:HG2	2:E:235:PRO:HD2	1.94	0.48
2:E:385:TRP:HZ3	2:E:397:GLU:OE2	1.95	0.48
3:F:92:GLU:HG2	3:F:93:ILE:H	1.76	0.48
3:I:202:VAL:HG21	3:I:225:GLU:O	2.13	0.48
2:K:224:MET:SD	2:K:237:ARG:HD3	2.53	0.48
2:B:317:TRP:CE3	2:B:448:ARG:HD3	2.48	0.48
2:B:399:GLY:H	2:B:433:ASP:HB2	1.79	0.48
3:C:97:GLU:C	3:C:99:SER:N	2.65	0.48
3:C:310:MET:O	3:C:335:TRP:CD1	2.65	0.48
1:D:131:GLN:HG3	1:D:132:HIS:H	1.78	0.48
1:D:176:LYS:HE2	1:D:176:LYS:HB2	1.68	0.48
2:E:223:GLU:HA	2:E:287:GLY:HA2	1.95	0.48
3:F:238:THR:HG22	3:F:266:LYS:CE	2.41	0.48
2:H:189:GLN:O	2:H:193:CYS:SG	2.71	0.48
2:H:262:PHE:HB3	2:H:269:TYR:OH	2.12	0.48
2:H:317:TRP:CH2	2:H:418:TRP:HA	2.49	0.48
3:I:245:ALA:HA	3:I:265:PHE:HB2	1.95	0.48
2:K:237:ARG:HH11	2:K:237:ARG:HG3	1.77	0.48
2:K:266:TRP:HA	2:K:377:THR:HG21	1.94	0.48
1:A:128:GLU:HA	1:A:131:GLN:CD	2.34	0.48
2:B:262:PHE:HB3	2:B:269:TYR:OH	2.13	0.48
2:B:316:ASP:HB2	2:B:445:TYR:CE2	2.45	0.48
3:C:196:LYS:HE3	3:C:198:LEU:HD11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:280:THR:OG1	2:E:288:LEU:HG	2.13	0.48
1:G:133:ILE:C	1:G:135:LEU:H	2.14	0.48
2:H:252:ILE:CG2	2:H:299:ILE:HG12	2.43	0.48
3:I:117:ASN:HD22	3:I:117:ASN:H	1.52	0.48
3:I:275:ARG:HB2	3:I:311:GLN:HG2	1.95	0.48
2:K:234:LYS:HD3	2:K:235:PRO:O	2.13	0.48
2:K:293:TRP:HE1	2:K:296:ASN:ND2	2.10	0.48
3:L:216:GLY:HA3	3:L:226:PHE:HA	1.95	0.48
2:B:236:TYR:CD2	2:B:298:LYS:HD3	2.48	0.48
3:C:169:ILE:CD1	3:C:171:PRO:HD3	2.31	0.48
2:E:310:LEU:HB3	2:E:326:TYR:HB2	1.95	0.48
2:H:362:GLY:O	2:H:365:ARG:N	2.47	0.48
3:I:276:LEU:CD2	3:I:276:LEU:H	2.26	0.48
3:I:304:PHE:CB	3:I:338:LYS:HB3	2.43	0.48
3:I:353:THR:HA	3:I:377:TYR:HA	1.96	0.48
1:J:126:VAL:HG13	1:J:127:ILE:H	1.78	0.48
3:L:205:LYS:HZ2	3:L:331:GLY:HA2	1.77	0.48
3:L:261:ASP:HB2	3:L:282:ALA:HB3	1.94	0.48
3:L:314:THR:HG22	3:L:333:GLY:HA3	1.95	0.48
2:B:161:ILE:O	2:B:166:ARG:CZ	2.62	0.48
2:B:176:ARG:C	2:B:178:LYS:H	2.17	0.48
2:B:267:ASP:O	2:B:270:LYS:N	2.47	0.48
3:C:166:LEU:C	3:C:167:TYR:CD1	2.86	0.48
3:C:383:THR:O	3:C:384:MET:HG3	2.13	0.48
1:D:143:GLN:O	1:D:147:MET:HG2	2.13	0.48
2:E:280:THR:O	2:E:281:ASP:C	2.51	0.48
3:F:166:LEU:CD2	3:F:218:LEU:HB3	2.43	0.48
3:I:337:ASN:C	3:I:339:CYS:N	2.64	0.48
1:J:140:VAL:CG1	1:J:141:ARG:N	2.76	0.48
3:L:94:MET:HB3	3:L:96:TYR:HE2	1.78	0.48
3:L:320:ASP:HB3	3:L:336:MET:HB2	1.95	0.48
3:C:96:TYR:O	3:C:99:SER:N	2.46	0.48
3:F:145:ILE:HD13	3:F:168:PHE:CE2	2.44	0.48
3:F:198:LEU:N	3:F:198:LEU:HD12	2.28	0.48
3:F:391:ARG:HB2	3:F:391:ARG:HH11	1.75	0.48
3:I:394:ILE:C	3:I:396:GLU:H	2.17	0.48
2:B:177:SER:CA	2:B:180:GLN:HG2	2.42	0.48
2:B:276:VAL:O	2:B:276:VAL:HG12	2.13	0.48
2:B:428:LYS:C	2:B:429:HIS:HD2	2.16	0.48
2:E:253:GLN:OE1	2:E:255:ARG:HG2	2.14	0.48
2:H:326:TYR:C	2:H:328:GLY:H	2.17	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:336:ASN:O	2:H:337:LYS:C	2.51	0.48
3:I:238:THR:HG22	3:I:266:LYS:CG	2.44	0.48
1:J:141:ARG:NH1	1:J:186:GLU:OE2	2.44	0.48
2:K:373:MET:CG	2:K:405:ASN:HD22	2.26	0.48
3:L:243:PRO:HB2	3:L:389:PHE:HB3	1.96	0.48
2:B:249:TRP:HB3	2:B:453:LYS:HB2	1.96	0.48
2:B:300:SER:OG	2:B:332:GLN:O	2.31	0.48
2:B:356:GLY:O	2:B:439:ASN:OD1	2.30	0.48
2:B:442:GLY:O	2:B:444:TRP:N	2.47	0.48
3:C:272:ASP:O	3:C:311:GLN:NE2	2.45	0.48
2:E:355:ASP:O	2:E:365:ARG:HD3	2.14	0.48
1:G:127:ILE:O	1:G:131:GLN:HB2	2.14	0.48
3:I:96:TYR:CD1	3:I:96:TYR:C	2.87	0.48
3:I:100:ILE:C	3:I:102:THR:H	2.16	0.48
3:I:295:PHE:H	3:I:301:ASP:HB3	1.78	0.48
1:J:167:ARG:HB2	2:K:192:TYR:CG	2.49	0.48
2:K:318:LYS:NZ	2:K:441:LYS:NZ	2.61	0.48
3:C:120:LYS:O	3:C:123:ASN:HB2	2.13	0.48
3:C:197:ARG:HB2	3:C:382:THR:HB	1.96	0.48
3:F:216:GLY:HA3	3:F:226:PHE:HA	1.95	0.48
3:F:275:ARG:HA	3:F:311:GLN:HA	1.95	0.48
3:F:304:PHE:C	3:F:306:SER:H	2.17	0.48
3:I:390:ASN:OD1	3:I:391:ARG:HG3	2.13	0.48
1:J:143:GLN:NE2	3:L:117:ASN:CB	2.77	0.48
1:J:186:GLU:OE1	1:J:189:ILE:HD12	2.14	0.48
2:K:278:THR:O	2:K:288:LEU:HB2	2.14	0.48
2:K:351:ASN:HD21	2:K:354:MET:HB2	1.79	0.48
2:B:252:ILE:CG2	2:B:299:ILE:HG12	2.43	0.48
2:B:351:ASN:CG	2:B:354:MET:HB2	2.34	0.48
2:B:385:TRP:CE3	4:M:3:ARG:HG3	2.48	0.48
3:C:263:ALA:HB1	3:C:264:MET:SD	2.54	0.48
1:D:148:LYS:O	1:D:151:GLU:HB3	2.14	0.48
3:F:172:LEU:CD1	3:F:240:SER:HB3	2.37	0.48
3:F:391:ARG:HH11	3:F:391:ARG:CB	2.27	0.48
2:H:161:ILE:HG21	3:I:103:HIS:HE1	1.74	0.48
2:H:177:SER:OG	2:H:178:LYS:N	2.47	0.48
2:H:350:GLY:O	2:H:352:ALA:N	2.47	0.48
3:I:94:MET:HG3	3:I:94:MET:O	2.14	0.48
3:I:167:TYR:N	3:I:167:TYR:HD1	2.12	0.48
3:I:394:ILE:HG13	3:I:396:GLU:H	1.77	0.48
1:J:156:ILE:HG22	1:J:157:LYS:HZ2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:251:GLU:CD	3:L:381:LYS:HD2	2.34	0.48
2:B:156:THR:CA	2:B:160:ASN:HB2	2.44	0.47
1:D:123:LYS:O	1:D:125:LYS:N	2.47	0.47
1:D:188:VAL:HG11	2:E:164:ASN:HA	1.96	0.47
2:H:252:ILE:HG23	2:H:299:ILE:HG12	1.95	0.47
2:H:342:VAL:O	2:H:371:ASN:ND2	2.47	0.47
2:H:398:ASP:HA	2:H:433:ASP:HB2	1.93	0.47
2:H:412:PRO:HG3	2:H:450:MET:CE	2.44	0.47
3:I:219:SER:HB2	3:I:220:PRO:HD2	1.95	0.47
3:I:243:PRO:HB2	3:I:389:PHE:HB3	1.95	0.47
1:J:138:LYS:HB2	1:J:138:LYS:HZ2	1.79	0.47
2:K:204:PRO:O	2:K:205:VAL:O	2.32	0.47
2:K:351:ASN:ND2	2:K:351:ASN:C	2.67	0.47
3:L:261:ASP:O	3:L:262:TYR:CD2	2.67	0.47
1:A:128:GLU:HA	1:A:131:GLN:OE1	2.14	0.47
2:B:165:LEU:CB	2:B:166:ARG:NH2	2.76	0.47
1:D:143:GLN:NE2	3:F:117:ASN:CB	2.76	0.47
1:D:161:CYS:C	1:D:163:GLY:N	2.65	0.47
2:E:170:SER:O	2:E:171:ILE:C	2.53	0.47
2:E:180:GLN:HG3	2:E:181:LYS:H	1.77	0.47
3:F:290:PHE:HD1	3:F:307:HIS:ND1	2.11	0.47
2:H:267:ASP:O	2:H:270:LYS:N	2.47	0.47
3:I:113:ILE:HD12	3:I:113:ILE:H	1.77	0.47
3:I:336:MET:HE1	3:I:340:HIS:HD2	1.79	0.47
2:K:367:MET:O	2:K:405:ASN:O	2.32	0.47
3:L:246:LEU:HG	3:L:247:ARG:H	1.78	0.47
3:L:304:PHE:C	3:L:306:SER:H	2.17	0.47
2:B:176:ARG:O	2:B:180:GLN:CD	2.52	0.47
2:B:238:VAL:CG2	2:B:239:TYR:H	2.27	0.47
3:C:198:LEU:CD2	3:C:223:THR:HA	2.45	0.47
3:C:207:ASN:OD1	3:C:210:GLN:HG3	2.13	0.47
1:D:151:GLU:OE2	2:E:182:LEU:HD21	2.13	0.47
2:E:167:VAL:O	2:E:168:LEU:C	2.50	0.47
3:F:109:TYR:O	3:F:112:GLU:HB2	2.14	0.47
1:G:133:ILE:C	1:G:135:LEU:N	2.67	0.47
2:H:183:GLU:O	2:H:183:GLU:CD	2.53	0.47
2:H:249:TRP:CZ2	2:H:455:ARG:CZ	2.97	0.47
3:I:133:ALA:HA	3:I:136:GLN:CG	2.44	0.47
3:I:370:ALA:HA	3:I:373:LYS:O	2.14	0.47
2:K:280:THR:O	2:K:281:ASP:C	2.52	0.47
3:L:185:ASP:OD2	3:L:187:SER:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:198:LEU:HD12	3:L:198:LEU:N	2.29	0.47
2:B:161:ILE:HG22	2:B:166:ARG:NH1	2.28	0.47
2:B:167:VAL:HG23	2:B:167:VAL:O	2.13	0.47
2:B:253:GLN:HB2	2:B:293:TRP:HE3	1.76	0.47
2:B:287:GLY:C	2:B:288:LEU:HD23	2.35	0.47
3:C:168:PHE:CE1	3:C:179:LEU:HD13	2.50	0.47
1:D:124:ARG:H	1:D:124:ARG:CD	2.18	0.47
2:E:203:ILE:HD12	2:E:203:ILE:H	1.77	0.47
2:E:333:ASN:HB3	2:E:336:ASN:ND2	2.29	0.47
1:G:119:ILE:O	1:G:119:ILE:HG12	2.14	0.47
3:I:109:TYR:O	3:I:112:GLU:N	2.48	0.47
3:I:295:PHE:H	3:I:301:ASP:CB	2.27	0.47
1:J:128:GLU:O	1:J:129:LYS:C	2.53	0.47
2:K:187:SER:HA	2:K:190:MET:HE3	1.95	0.47
3:L:109:TYR:CD1	3:L:110:LEU:HD23	2.49	0.47
3:L:227:TRP:NE1	3:L:230:ASN:ND2	2.63	0.47
1:A:124:ARG:CD	1:A:124:ARG:H	2.27	0.47
2:B:249:TRP:CZ2	2:B:455:ARG:CZ	2.97	0.47
2:B:351:ASN:O	2:B:355:ASP:HB2	2.14	0.47
3:C:103:HIS:HA	3:C:106:SER:CB	2.44	0.47
3:F:208:TRP:HA	3:F:314:THR:HG21	1.97	0.47
3:F:292:GLY:HA2	3:F:305:THR:O	2.13	0.47
3:F:313:SER:HB3	3:F:319:ASN:H	1.80	0.47
1:G:155:ASP:HA	1:G:171:ARG:NH1	2.30	0.47
2:H:173:GLU:C	2:H:175:LEU:N	2.68	0.47
2:H:224:MET:HB2	2:H:286:CYS:HB2	1.95	0.47
3:I:165:GLY:C	3:I:166:LEU:HD23	2.35	0.47
3:I:166:LEU:HD23	3:I:166:LEU:N	2.29	0.47
3:I:387:ILE:HG12	3:I:388:PRO:N	2.28	0.47
1:J:125:LYS:O	1:J:128:GLU:HB2	2.15	0.47
2:K:201:CYS:O	3:L:143:VAL:HG21	2.14	0.47
3:L:131:LEU:O	3:L:134:GLN:N	2.36	0.47
2:B:266:TRP:HB3	2:B:267:ASP:H	1.54	0.47
2:B:411:ASN:HD22	2:B:434:GLY:H	1.63	0.47
3:C:105:SER:C	3:C:107:ILE:N	2.66	0.47
3:C:145:ILE:HD12	3:C:145:ILE:O	2.15	0.47
3:F:194:PHE:CE2	3:F:384:MET:CB	2.97	0.47
2:H:266:TRP:HB3	2:H:267:ASP:H	1.55	0.47
3:I:103:HIS:C	3:I:105:SER:N	2.67	0.47
3:I:252:ASP:C	3:I:254:ASN:H	2.18	0.47
2:K:340:ILE:HG21	2:K:403:TRP:CG	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:385:TRP:HZ3	2:K:397:GLU:OE2	1.97	0.47
1:A:146:ASP:O	1:A:146:ASP:OD2	2.33	0.47
1:A:151:GLU:O	1:A:154:ILE:HG22	2.13	0.47
2:B:172:LEU:HD11	3:C:113:ILE:HG22	1.95	0.47
2:B:299:ILE:C	2:B:301:GLN:H	2.18	0.47
2:B:336:ASN:O	2:B:337:LYS:C	2.52	0.47
2:B:345:TYR:HB3	2:B:354:MET:CE	2.44	0.47
2:B:368:THR:HB	2:B:409:ALA:HB2	1.97	0.47
3:C:165:GLY:C	3:C:166:LEU:HD23	2.35	0.47
3:C:198:LEU:HD12	3:C:198:LEU:N	2.29	0.47
3:C:276:LEU:H	3:C:276:LEU:CD2	2.28	0.47
1:D:169:LEU:HD22	1:D:170:ALA:O	2.14	0.47
3:F:216:GLY:O	3:F:217:HIS:CD2	2.67	0.47
3:F:244:TYR:CE2	3:F:388:PRO:HG3	2.49	0.47
3:F:307:HIS:O	3:F:308:ASN:C	2.52	0.47
3:F:333:GLY:O	3:F:334:TRP:HB2	2.14	0.47
3:F:334:TRP:CZ3	3:F:344:LEU:HB2	2.50	0.47
1:G:154:ILE:HG22	1:G:171:ARG:NH1	2.30	0.47
1:G:167:ARG:HH12	1:G:169:LEU:HD23	1.80	0.47
2:H:226:LEU:O	2:H:227:ILE:C	2.53	0.47
2:H:276:VAL:O	2:H:277:ALA:CB	2.62	0.47
2:H:311:LEU:HD11	2:H:323:LYS:HB2	1.97	0.47
3:I:175:ASN:O	3:I:176:GLN:C	2.53	0.47
3:I:263:ALA:HB1	3:I:264:MET:SD	2.55	0.47
1:J:167:ARG:NH1	1:J:168:ALA:H	2.13	0.47
2:K:205:VAL:O	2:K:206:VAL:C	2.53	0.47
2:K:313:GLU:HB3	2:K:323:LYS:HG3	1.96	0.47
3:L:166:LEU:CD2	3:L:218:LEU:HB3	2.45	0.47
1:A:159:ARG:NH2	2:B:418:TRP:CD2	2.83	0.47
2:B:161:ILE:CG2	2:B:166:ARG:HH12	2.28	0.47
2:B:284:ASN:ND2	2:B:284:ASN:N	2.63	0.47
3:C:175:ASN:O	3:C:176:GLN:C	2.54	0.47
1:D:166:SER:HB2	2:E:195:THR:O	2.15	0.47
2:E:181:LYS:O	2:E:184:SER:HB3	2.15	0.47
1:G:149:ARG:HG2	2:H:426:MET:O	2.15	0.47
3:I:198:LEU:HD12	3:I:198:LEU:N	2.30	0.47
3:C:355:SER:C	3:C:357:ALA:H	2.18	0.47
2:H:242:MET:HA	2:H:247:GLY:HA3	1.97	0.47
2:H:351:ASN:O	2:H:355:ASP:HB2	2.15	0.47
2:H:442:GLY:C	2:H:444:TRP:H	2.18	0.47
3:I:298:ASP:N	3:I:301:ASP:OD1	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:VAL:CG1	1:J:127:ILE:H	2.28	0.47
1:J:191:LYS:NZ	1:J:191:LYS:CB	2.77	0.47
2:K:326:TYR:CD1	2:K:342:VAL:HB	2.50	0.47
3:L:172:LEU:CD1	3:L:240:SER:HB3	2.38	0.47
3:L:194:PHE:CE2	3:L:384:MET:CB	2.98	0.47
1:A:169:LEU:HD13	1:A:170:ALA:H	1.76	0.47
2:B:333:ASN:C	2:B:335:ALA:N	2.68	0.47
2:B:397:GLU:O	2:B:398:ASP:C	2.53	0.47
1:D:142:ALA:O	1:D:145:VAL:HB	2.15	0.47
2:E:205:VAL:O	2:E:206:VAL:C	2.53	0.47
2:H:310:LEU:CD1	2:H:312:ILE:HG13	2.37	0.47
2:H:351:ASN:C	2:H:351:ASN:HD22	2.18	0.47
2:H:359:GLN:O	2:H:359:GLN:CG	2.63	0.47
3:I:344:LEU:C	3:I:346:GLY:N	2.69	0.47
1:J:139:ASN:HB3	3:L:114:TYR:CZ	2.50	0.47
1:J:141:ARG:O	1:J:142:ALA:C	2.51	0.47
2:K:405:ASN:C	2:K:407:CYS:H	2.16	0.47
4:R:2:PRO:O	4:R:3:ARG:HD3	2.15	0.47
3:C:172:LEU:HD12	3:C:172:LEU:N	2.24	0.46
3:C:259:THR:H	3:C:286:ALA:HB2	1.79	0.46
3:C:311:GLN:OE1	3:C:319:ASN:HB3	2.15	0.46
1:D:180:ASP:O	1:D:184:GLN:HB2	2.15	0.46
1:D:186:GLU:OE1	1:D:189:ILE:HD12	2.15	0.46
3:F:290:PHE:HA	3:F:307:HIS:ND1	2.30	0.46
2:H:304:ARG:HH11	2:H:304:ARG:HG3	1.79	0.46
2:K:326:TYR:OH	2:K:351:ASN:ND2	2.48	0.46
3:L:312:PHE:HD1	3:L:335:TRP:CD1	2.33	0.46
3:L:313:SER:HB3	3:L:319:ASN:H	1.80	0.46
3:C:243:PRO:HB2	3:C:389:PHE:HB3	1.97	0.46
3:C:287:GLY:CA	3:C:371:THR:HB	2.45	0.46
1:D:185:LEU:HB2	2:E:171:ILE:HD11	1.97	0.46
1:G:120:GLU:OE1	1:G:124:ARG:NH2	2.48	0.46
2:H:363:GLU:O	2:H:367:MET:HG2	2.16	0.46
3:I:208:TRP:O	3:I:210:GLN:N	2.48	0.46
3:I:253:TRP:CD2	3:I:380:LYS:HB2	2.51	0.46
2:K:412:PRO:O	2:K:413:ASN:CB	2.50	0.46
3:L:203:ASP:OD2	3:L:205:LYS:HB2	2.16	0.46
1:A:161:CYS:HB3	1:A:165:CYS:SG	2.55	0.46
1:A:167:ARG:NH1	1:A:169:LEU:HD23	2.16	0.46
2:B:197:CYS:O	3:C:140:LYS:N	2.42	0.46
2:B:210:GLU:CD	2:B:212:GLU:HB3	2.35	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:208:TRP:CA	3:C:314:THR:HG21	2.44	0.46
3:C:219:SER:HB2	3:C:220:PRO:HD2	1.97	0.46
3:C:237:SER:O	3:C:266:LYS:HG3	2.15	0.46
2:E:432:ASP:HB3	2:E:444:TRP:CH2	2.50	0.46
3:F:172:LEU:H	3:F:239:GLN:HE21	1.63	0.46
3:F:203:ASP:OD2	3:F:205:LYS:HB2	2.16	0.46
3:F:355:SER:C	3:F:357:ALA:H	2.17	0.46
1:G:158:ILE:HG13	2:H:189:GLN:HG2	1.97	0.46
2:H:284:ASN:H	2:H:284:ASN:ND2	2.06	0.46
2:H:326:TYR:C	2:H:328:GLY:N	2.69	0.46
2:H:360:LEU:HD22	5:H:470:NAG:H83	1.96	0.46
3:I:236:ILE:O	3:I:236:ILE:HG13	2.14	0.46
3:I:259:THR:H	3:I:286:ALA:HB2	1.80	0.46
2:K:242:MET:C	2:K:247:GLY:HA3	2.35	0.46
2:B:256:GLN:HE21	2:B:449:LYS:CE	2.18	0.46
2:B:266:TRP:NE1	2:B:380:ARG:CZ	2.78	0.46
2:B:386:LEU:O	2:B:386:LEU:HD13	2.15	0.46
3:C:243:PRO:HB3	3:C:264:MET:HE3	1.97	0.46
3:C:252:ASP:C	3:C:254:ASN:H	2.18	0.46
2:E:182:LEU:O	2:E:186:VAL:HG23	2.14	0.46
3:F:350:GLN:C	3:F:352:GLY:H	2.19	0.46
2:H:185:ASP:C	2:H:187:SER:H	2.18	0.46
2:H:359:GLN:NE2	2:H:359:GLN:N	2.62	0.46
3:I:198:LEU:CD2	3:I:223:THR:HA	2.45	0.46
3:I:340:HIS:HE1	3:I:364:ASP:OD2	1.98	0.46
3:L:322:PHE:CE2	3:L:324:GLY:HA3	2.50	0.46
3:L:355:SER:C	3:L:357:ALA:H	2.17	0.46
2:B:284:ASN:HD22	2:B:284:ASN:N	2.05	0.46
3:C:116:SER:O	3:C:120:LYS:N	2.37	0.46
1:D:128:GLU:O	1:D:131:GLN:HG2	2.16	0.46
1:G:184:GLN:OE1	2:H:167:VAL:HG22	2.15	0.46
2:H:356:GLY:O	2:H:439:ASN:OD1	2.34	0.46
3:I:124:LEU:N	3:I:124:LEU:CD1	2.77	0.46
3:I:392:LEU:O	3:I:393:THR:HB	2.16	0.46
1:J:144:LEU:CD2	2:K:175:LEU:HD21	2.44	0.46
2:K:243:ASN:O	2:K:244:THR:C	2.53	0.46
3:L:246:LEU:HD13	3:L:265:PHE:CD2	2.50	0.46
2:B:226:LEU:O	2:B:226:LEU:HD12	2.16	0.46
2:B:236:TYR:O	2:B:236:TYR:CD1	2.69	0.46
3:C:166:LEU:HD23	3:C:166:LEU:N	2.31	0.46
3:C:382:THR:O	3:C:382:THR:CG2	2.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:278:THR:O	2:E:288:LEU:HB2	2.16	0.46
1:G:165:CYS:O	1:G:166:SER:O	2.34	0.46
2:H:365:ARG:O	2:H:368:THR:HG23	2.15	0.46
2:H:368:THR:HB	2:H:409:ALA:HB2	1.98	0.46
2:H:373:MET:HE3	2:H:374:PHE:H	1.80	0.46
3:I:162:LYS:HE3	3:I:186:GLY:HA2	1.96	0.46
1:J:149:ARG:O	1:J:152:VAL:CG2	2.64	0.46
1:J:178:TYR:CZ	2:K:178:LYS:HD3	2.51	0.46
2:K:351:ASN:OD1	2:K:354:MET:HB2	2.16	0.46
3:L:329:GLN:HE21	3:L:361:ASN:HD22	1.64	0.46
2:B:158:ASN:OD1	3:C:100:ILE:HG21	2.16	0.46
2:B:264:ARG:HD2	2:B:268:PRO:HB3	1.98	0.46
2:B:334:GLU:HG3	2:B:338:TYR:CE2	2.51	0.46
3:C:163:GLN:CA	3:C:163:GLN:NE2	2.78	0.46
3:C:195:GLN:OE1	3:C:197:ARG:HG2	2.15	0.46
3:C:238:THR:HG22	3:C:266:LYS:CG	2.46	0.46
3:C:248:VAL:HG22	3:C:384:MET:HG2	1.98	0.46
2:E:204:PRO:O	2:E:205:VAL:O	2.34	0.46
3:F:252:ASP:C	3:F:254:ASN:H	2.19	0.46
3:F:305:THR:CB	3:F:341:ALA:HB2	2.45	0.46
2:H:190:MET:HB2	3:I:131:LEU:HD12	1.98	0.46
2:H:236:TYR:O	2:H:236:TYR:CD1	2.69	0.46
2:K:155:GLU:O	2:K:157:VAL:N	2.49	0.46
2:K:327:GLY:HA3	2:K:344:LYS:CB	2.43	0.46
1:A:144:LEU:HD11	1:A:182:GLN:CG	2.46	0.46
1:A:188:VAL:HG11	2:B:167:VAL:HG21	1.97	0.46
2:B:242:MET:HA	2:B:247:GLY:HA3	1.98	0.46
3:C:118:ASN:ND2	3:C:118:ASN:N	2.60	0.46
3:C:148:ILE:HD13	3:C:156:ILE:CG2	2.46	0.46
3:C:156:ILE:HA	3:C:159:LYS:CD	2.45	0.46
3:C:258:SER:O	3:C:259:THR:HB	2.16	0.46
3:C:344:LEU:C	3:C:346:GLY:N	2.69	0.46
2:E:432:ASP:HB3	2:E:444:TRP:CZ3	2.51	0.46
3:F:236:ILE:HG22	3:F:386:ILE:HD11	1.96	0.46
3:F:261:ASP:HB2	3:F:282:ALA:HB3	1.97	0.46
3:I:195:GLN:OE1	3:I:197:ARG:HG2	2.15	0.46
2:K:182:LEU:O	2:K:186:VAL:HG23	2.15	0.46
3:L:107:ILE:O	3:L:107:ILE:HD13	2.16	0.46
3:L:153:CYS:HA	3:L:156:ILE:HD12	1.97	0.46
3:L:246:LEU:HD12	3:L:386:ILE:HG22	1.96	0.46
3:L:275:ARG:HA	3:L:311:GLN:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:330:ASP:HB3	3:L:343:HIS:HE1	1.80	0.46
2:B:365:ARG:HG2	2:B:366:THR:N	2.30	0.46
1:D:140:VAL:CG1	1:D:141:ARG:H	2.29	0.46
2:E:435:VAL:O	2:E:446:SER:HA	2.16	0.46
3:F:242:ILE:HG23	3:F:243:PRO:HD2	1.97	0.46
3:F:320:ASP:OD1	3:F:326:CYS:SG	2.73	0.46
3:F:384:MET:HB2	3:F:384:MET:HE3	1.80	0.46
1:G:140:VAL:HG12	3:I:114:TYR:CE1	2.51	0.46
3:I:248:VAL:O	3:I:248:VAL:HG12	2.16	0.46
3:I:272:ASP:O	3:I:311:GLN:NE2	2.47	0.46
3:I:322:PHE:CG	3:I:323:GLU:N	2.84	0.46
1:A:136:LEU:HA	1:A:139:ASN:HB2	1.98	0.46
1:A:154:ILE:CG2	1:A:155:ASP:N	2.79	0.46
2:B:157:VAL:O	2:B:158:ASN:CB	2.60	0.46
2:B:345:TYR:CZ	2:B:351:ASN:N	2.84	0.46
3:C:248:VAL:O	3:C:259:THR:HA	2.16	0.46
1:D:123:LYS:C	1:D:125:LYS:N	2.69	0.46
2:E:318:LYS:NZ	2:E:441:LYS:NZ	2.64	0.46
2:H:210:GLU:CD	2:H:212:GLU:HB3	2.35	0.46
2:H:267:ASP:O	2:H:268:PRO:C	2.54	0.46
2:H:357:ALA:CA	2:H:439:ASN:HD21	2.17	0.46
3:I:137:GLU:HB3	3:I:138:PRO:HD2	1.98	0.46
3:I:339:CYS:HB2	4:S:1:GLY:O	2.16	0.46
2:K:183:GLU:HG2	3:L:124:LEU:HG	1.98	0.46
2:K:434:GLY:O	2:K:436:VAL:N	2.49	0.46
1:A:190:ALA:C	1:A:191:LYS:HD2	2.36	0.45
2:B:210:GLU:CD	2:B:212:GLU:H	2.16	0.45
3:C:340:HIS:ND1	3:C:368:ILE:HD11	2.31	0.45
2:E:214:ILE:CD1	2:E:227:ILE:HG22	2.45	0.45
2:E:374:PHE:O	2:E:403:TRP:HA	2.16	0.45
2:E:408:HIS:CD2	2:E:411:ASN:HB2	2.52	0.45
3:F:154:GLN:C	3:F:156:ILE:N	2.69	0.45
3:F:162:LYS:HE3	3:F:186:GLY:CA	2.45	0.45
3:F:229:GLY:O	3:F:233:ILE:CG1	2.62	0.45
1:G:167:ARG:NE	2:H:192:TYR:CD2	2.77	0.45
2:H:236:TYR:CD2	2:H:298:LYS:HD3	2.52	0.45
2:H:309:GLU:O	2:H:454:ILE:HB	2.16	0.45
3:L:252:ASP:C	3:L:254:ASN:H	2.19	0.45
3:L:318:ASP:OD1	3:L:320:ASP:OD2	2.35	0.45
2:B:226:LEU:O	2:B:227:ILE:C	2.55	0.45
2:B:299:ILE:O	2:B:301:GLN:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:300:SER:HA	2:B:331:VAL:HB	1.97	0.45
2:B:300:SER:HG	2:B:332:GLN:C	2.20	0.45
2:B:349:ALA:O	2:B:440:TRP:HB2	2.16	0.45
2:B:369:ILE:O	2:B:405:ASN:HB3	2.15	0.45
3:C:96:TYR:O	3:C:98:ALA:N	2.49	0.45
3:C:320:ASP:OD2	3:C:322:PHE:HB3	2.16	0.45
3:C:389:PHE:C	3:C:391:ARG:N	2.69	0.45
2:E:326:TYR:CD1	2:E:342:VAL:HB	2.51	0.45
2:E:367:MET:HB2	2:E:406:ARG:HB3	1.98	0.45
2:E:397:GLU:C	2:E:399:GLY:N	2.68	0.45
1:G:189:ILE:O	1:G:189:ILE:HG13	2.15	0.45
2:H:447:MET:H	2:H:447:MET:HG2	1.43	0.45
3:I:207:ASN:OD1	3:I:210:GLN:HG3	2.16	0.45
3:I:389:PHE:C	3:I:391:ARG:N	2.69	0.45
1:A:147:MET:CE	3:C:121:ILE:HD11	2.46	0.45
2:B:224:MET:HB2	2:B:286:CYS:HB2	1.98	0.45
2:B:267:ASP:O	2:B:268:PRO:C	2.54	0.45
3:C:322:PHE:CG	3:C:323:GLU:N	2.84	0.45
2:E:159:SER:O	2:E:160:ASN:HB2	2.16	0.45
2:E:234:LYS:HD3	2:E:235:PRO:O	2.16	0.45
3:F:242:ILE:HG22	3:F:243:PRO:HD2	1.96	0.45
1:G:146:ASP:O	1:G:146:ASP:OD2	2.34	0.45
2:H:300:SER:OG	2:H:332:GLN:O	2.33	0.45
2:H:366:THR:O	2:H:369:ILE:HG13	2.17	0.45
3:I:156:ILE:HA	3:I:159:LYS:CD	2.46	0.45
3:I:166:LEU:C	3:I:167:TYR:CD1	2.89	0.45
2:K:203:ILE:HG21	2:K:226:LEU:HD22	1.98	0.45
2:K:204:PRO:HA	3:L:217:HIS:CD2	2.51	0.45
2:K:223:GLU:CB	2:K:287:GLY:HA2	2.46	0.45
3:L:154:GLN:HE21	3:L:158:ASN:ND2	2.13	0.45
3:L:384:MET:HB2	3:L:384:MET:HE3	1.77	0.45
1:A:136:LEU:CD2	1:A:139:ASN:HD22	2.29	0.45
2:B:164:ASN:O	2:B:168:LEU:HB2	2.17	0.45
2:B:187:SER:HA	2:B:190:MET:CB	2.40	0.45
2:B:209:LYS:HG2	2:B:229:PRO:HA	1.97	0.45
3:C:204:PHE:CE1	3:C:225:GLU:HB3	2.50	0.45
3:C:326:CYS:O	3:C:327:ALA:C	2.55	0.45
2:E:204:PRO:HA	3:F:217:HIS:CD2	2.50	0.45
3:F:281:PHE:CG	3:F:288:ASP:HB2	2.52	0.45
3:I:204:PHE:CE1	3:I:225:GLU:HB3	2.50	0.45
3:I:326:CYS:O	3:I:327:ALA:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:229:GLY:O	3:L:233:ILE:CG1	2.63	0.45
1:A:187:GLN:O	1:A:189:ILE:N	2.41	0.45
3:C:158:ASN:OD1	3:C:188:GLY:O	2.34	0.45
3:C:253:TRP:O	3:C:254:ASN:CG	2.55	0.45
3:C:372:TRP:CE2	3:C:373:LYS:NZ	2.85	0.45
1:D:126:VAL:O	1:D:128:GLU:N	2.50	0.45
2:E:222:SER:O	2:E:223:GLU:HB3	2.16	0.45
2:E:373:MET:CG	2:E:405:ASN:HD22	2.28	0.45
3:F:168:PHE:HD1	3:F:177:GLN:CG	2.29	0.45
2:H:250:THR:O	2:H:252:ILE:CD1	2.65	0.45
2:H:358:SER:C	2:H:360:LEU:H	2.19	0.45
2:H:440:TRP:CE3	2:H:447:MET:HE1	2.52	0.45
3:I:261:ASP:N	3:I:261:ASP:OD1	2.49	0.45
3:I:307:HIS:O	3:I:310:MET:HB2	2.16	0.45
1:J:127:ILE:CG2	1:J:128:GLU:N	2.79	0.45
1:J:176:LYS:HE3	1:J:176:LYS:HB2	1.76	0.45
3:L:154:GLN:HA	3:L:190:GLY:HA3	1.98	0.45
3:L:290:PHE:HA	3:L:307:HIS:ND1	2.32	0.45
3:L:336:MET:SD	3:L:340:HIS:HD2	2.40	0.45
3:L:385:LYS:HG3	3:L:385:LYS:O	2.16	0.45
1:A:181:GLN:HE21	2:B:174:ASN:HB2	1.81	0.45
2:B:237:ARG:NH2	3:C:143:VAL:HG23	2.21	0.45
2:B:337:LYS:O	2:B:339:GLN:N	2.49	0.45
3:C:295:PHE:H	3:C:301:ASP:CB	2.30	0.45
2:E:257:ASP:CG	2:E:259:SER:HG	2.20	0.45
1:G:144:LEU:HD21	1:G:182:GLN:CG	2.42	0.45
1:G:147:MET:HE2	2:H:179:ILE:CG1	2.37	0.45
2:H:223:GLU:O	2:H:225:TYR:HD1	1.99	0.45
2:H:346:ARG:CB	2:H:346:ARG:NH1	2.77	0.45
3:I:197:ARG:NH2	3:I:348:TYR:HB2	2.32	0.45
3:I:235:LEU:O	3:I:239:GLN:HG3	2.16	0.45
1:J:159:ARG:HD3	2:K:258:GLY:H	1.81	0.45
2:K:183:GLU:HA	3:L:124:LEU:HD21	1.98	0.45
2:K:296:ASN:HD22	2:K:296:ASN:HA	1.56	0.45
2:K:351:ASN:ND2	2:K:354:MET:HB2	2.32	0.45
2:K:370:HIS:CE1	2:K:402:TRP:HE1	2.35	0.45
1:A:128:GLU:C	1:A:130:VAL:H	2.18	0.45
2:B:191:GLU:O	2:B:193:CYS:N	2.42	0.45
3:C:196:LYS:HA	3:C:383:THR:HA	1.98	0.45
3:F:203:ASP:O	3:F:206:LYS:CE	2.65	0.45
3:F:209:ILE:O	3:F:213:GLU:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:322:PHE:CB	3:F:338:LYS:HD2	2.46	0.45
2:H:340:ILE:O	2:H:340:ILE:HG23	2.16	0.45
2:H:409:ALA:O	2:H:438:MET:HB2	2.17	0.45
3:I:111:GLN:O	3:I:111:GLN:CG	2.62	0.45
3:I:250:LEU:CD1	3:I:382:THR:HA	2.39	0.45
3:I:264:MET:O	3:I:265:PHE:O	2.34	0.45
3:L:145:ILE:HD13	3:L:168:PHE:CE2	2.50	0.45
3:L:192:THR:HG23	3:L:386:ILE:CG1	2.47	0.45
3:L:207:ASN:N	3:L:210:GLN:OE1	2.46	0.45
1:A:174:ASP:OD2	1:A:177:ASP:HB2	2.17	0.45
2:B:199:VAL:HG23	3:C:141:ASP:OD1	2.16	0.45
2:B:268:PRO:O	2:B:273:PHE:HD2	2.00	0.45
2:B:364:ASN:HD22	5:B:470:NAG:C7	2.28	0.45
3:C:124:LEU:HG	3:C:124:LEU:O	2.16	0.45
2:E:311:LEU:HD21	2:E:313:GLU:OE2	2.16	0.45
3:F:96:TYR:N	3:F:96:TYR:CD1	2.73	0.45
3:F:236:ILE:O	3:F:244:TYR:CE1	2.70	0.45
3:F:246:LEU:HD13	3:F:265:PHE:CD2	2.51	0.45
1:G:128:GLU:OE1	1:G:129:LYS:NZ	2.49	0.45
1:G:131:GLN:HA	1:G:134:GLN:NE2	2.32	0.45
2:H:337:LYS:O	2:H:339:GLN:N	2.49	0.45
1:J:182:GLN:O	1:J:186:GLU:HG2	2.17	0.45
2:K:370:HIS:CE1	2:K:408:HIS:HB2	2.52	0.45
2:B:256:GLN:CB	2:B:449:LYS:HE2	2.38	0.45
2:B:317:TRP:CH2	2:B:448:ARG:HD3	2.51	0.45
2:B:346:ARG:CB	2:B:346:ARG:NH1	2.78	0.45
3:C:96:TYR:O	3:C:97:GLU:C	2.55	0.45
3:C:235:LEU:O	3:C:239:GLN:HG3	2.16	0.45
3:C:246:LEU:HD21	3:C:248:VAL:CG2	2.47	0.45
3:C:252:ASP:HB2	3:C:377:TYR:OH	2.17	0.45
2:E:235:PRO:HG2	3:F:168:PHE:CE1	2.45	0.45
3:F:227:TRP:CE2	3:F:230:ASN:ND2	2.85	0.45
1:G:131:GLN:HA	1:G:134:GLN:HE21	1.82	0.45
1:G:140:VAL:HG23	1:G:141:ARG:N	2.31	0.45
2:H:242:MET:SD	2:H:248:GLY:CA	3.02	0.45
3:I:208:TRP:CA	3:I:314:THR:HG21	2.46	0.45
2:K:264:ARG:HG2	3:L:136:GLN:NE2	2.31	0.45
2:K:397:GLU:C	2:K:399:GLY:N	2.70	0.45
3:L:113:ILE:O	3:L:114:TYR:C	2.53	0.45
3:L:196:LYS:O	3:L:225:GLU:HA	2.17	0.45
3:L:314:THR:O	3:L:315:TRP:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:339:CYS:O	3:L:340:HIS:HB3	2.17	0.45
2:B:328:GLY:HA3	2:B:343:ASN:OD1	2.17	0.45
2:B:340:ILE:HG23	2:B:340:ILE:O	2.16	0.45
2:B:389:ASP:OD1	2:B:390:PRO:HD2	2.17	0.45
2:E:242:MET:C	2:E:247:GLY:HA3	2.37	0.45
3:F:98:ALA:C	3:F:100:ILE:H	2.20	0.45
3:F:270:GLU:HB2	3:F:274:TYR:CZ	2.53	0.45
2:H:334:GLU:HG3	2:H:338:TYR:CE2	2.52	0.45
2:K:318:LYS:NZ	2:K:441:LYS:HZ3	2.15	0.45
3:L:227:TRP:CE2	3:L:230:ASN:ND2	2.85	0.45
2:B:294:LEU:O	2:B:295:GLY:C	2.54	0.44
2:B:301:GLN:HE21	2:B:302:LEU:HD23	1.81	0.44
3:C:356:LYS:HA	3:C:359:THR:CG2	2.48	0.44
3:F:200:GLY:H	3:F:225:GLU:CD	2.19	0.44
3:F:322:PHE:CE2	3:F:324:GLY:HA3	2.52	0.44
3:F:349:TYR:HB2	3:F:378:SER:HB3	1.98	0.44
1:G:151:GLU:HG3	1:G:152:VAL:N	2.31	0.44
2:H:175:LEU:C	2:H:175:LEU:HD12	2.37	0.44
2:H:209:LYS:HG2	2:H:229:PRO:HA	1.98	0.44
2:H:215:ILE:HA	2:H:219:GLY:O	2.17	0.44
2:H:353:LEU:HD23	2:H:370:HIS:CD2	2.53	0.44
3:I:128:VAL:O	3:I:129:ALA:C	2.56	0.44
3:I:204:PHE:HE2	3:I:227:TRP:HB2	1.81	0.44
3:I:355:SER:C	3:I:357:ALA:H	2.20	0.44
1:J:139:ASN:O	3:L:114:TYR:CE1	2.70	0.44
1:J:167:ARG:CZ	1:J:167:ARG:CA	2.86	0.44
2:K:236:TYR:CD2	2:K:298:LYS:HE2	2.51	0.44
3:L:209:ILE:O	3:L:213:GLU:HG2	2.16	0.44
3:L:242:ILE:HG23	3:L:243:PRO:HD2	1.98	0.44
1:A:140:VAL:O	1:A:141:ARG:C	2.56	0.44
2:B:209:LYS:NZ	2:B:209:LYS:CB	2.80	0.44
2:B:296:ASN:HB3	2:B:338:TYR:CZ	2.52	0.44
2:B:329:PHE:CZ	2:B:331:VAL:HG23	2.52	0.44
2:B:447:MET:H	2:B:447:MET:HG2	1.47	0.44
3:C:184:ILE:HG22	3:C:185:ASP:N	2.32	0.44
3:C:315:TRP:CE3	3:C:328:GLU:HG2	2.52	0.44
3:F:95:LYS:HG3	3:F:95:LYS:O	2.17	0.44
3:F:192:THR:HG23	3:F:386:ILE:CG1	2.47	0.44
3:F:192:THR:CG2	3:F:386:ILE:HG13	2.46	0.44
2:H:169:ARG:NH2	3:I:109:TYR:CD2	2.84	0.44
2:H:373:MET:HG3	2:H:405:ASN:HB2	1.97	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:163:GLN:CA	3:I:163:GLN:NE2	2.80	0.44
3:I:171:PRO:HD2	3:I:174:ALA:CB	2.46	0.44
2:K:234:LYS:HG2	2:K:235:PRO:HD2	1.98	0.44
1:A:164:SER:CB	3:C:137:GLU:O	2.65	0.44
1:A:184:GLN:NE2	1:A:185:LEU:HB2	2.29	0.44
2:B:153:ILE:O	2:B:155:GLU:N	2.47	0.44
2:B:294:LEU:CD2	2:B:298:LYS:HB2	2.47	0.44
2:B:351:ASN:C	2:B:351:ASN:HD22	2.20	0.44
3:C:107:ILE:CG2	3:C:108:ARG:N	2.80	0.44
1:D:162:ARG:O	1:D:162:ARG:CG	2.65	0.44
3:F:206:LYS:HB3	3:F:210:GLN:OE1	2.17	0.44
3:F:312:PHE:HD1	3:F:335:TRP:CD1	2.35	0.44
2:H:393:GLN:O	2:H:395:SER:N	2.51	0.44
3:I:179:LEU:O	3:I:218:LEU:HD11	2.17	0.44
3:I:253:TRP:CE2	3:I:380:LYS:HB2	2.53	0.44
1:J:149:ARG:O	1:J:152:VAL:HG23	2.17	0.44
2:K:239:TYR:HB3	2:K:251:VAL:HB	1.99	0.44
2:K:276:VAL:HA	2:K:292:TYR:CD1	2.52	0.44
3:L:322:PHE:CD2	4:T:3:ARG:HG3	2.52	0.44
3:L:383:THR:O	3:L:383:THR:OG1	2.35	0.44
2:B:166:ARG:H	2:B:166:ARG:HE	1.59	0.44
2:B:179:ILE:HG13	2:B:179:ILE:H	1.62	0.44
2:B:317:TRP:CH2	2:B:418:TRP:HA	2.53	0.44
2:B:385:TRP:HB2	2:B:406:ARG:HA	2.00	0.44
3:C:133:ALA:HA	3:C:136:GLN:CG	2.47	0.44
3:C:271:ALA:C	3:C:273:LYS:N	2.71	0.44
3:F:230:ASN:C	3:F:232:LYS:N	2.70	0.44
3:F:273:LYS:HA	3:F:273:LYS:HD3	1.78	0.44
1:G:128:GLU:OE2	1:G:129:LYS:HG2	2.17	0.44
2:H:176:ARG:CZ	2:H:176:ARG:HB3	2.47	0.44
2:H:185:ASP:HA	2:H:188:ALA:CB	2.48	0.44
2:H:345:TYR:CZ	2:H:351:ASN:N	2.86	0.44
3:I:158:ASN:OD1	3:I:188:GLY:O	2.35	0.44
3:I:178:PHE:CZ	3:I:232:LYS:HG2	2.52	0.44
3:I:227:TRP:HE1	3:I:230:ASN:ND2	2.15	0.44
2:K:242:MET:HA	2:K:247:GLY:CA	2.48	0.44
2:K:375:PHE:CD1	2:K:376:SER:N	2.85	0.44
3:L:145:ILE:HG21	3:L:168:PHE:CD2	2.52	0.44
3:L:154:GLN:C	3:L:156:ILE:N	2.70	0.44
3:L:292:GLY:HA2	3:L:305:THR:O	2.17	0.44
1:A:126:VAL:O	1:A:127:ILE:C	2.55	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:TYR:CD1	2:B:152:TYR:N	2.85	0.44
3:C:250:LEU:HD12	3:C:250:LEU:HA	1.85	0.44
3:C:258:SER:O	3:C:259:THR:CB	2.65	0.44
2:E:161:ILE:O	2:E:162:PRO:C	2.55	0.44
1:G:125:LYS:O	1:G:126:VAL:HG23	2.17	0.44
2:H:270:LYS:HG3	2:H:338:TYR:OH	2.17	0.44
2:H:296:ASN:HA	2:H:299:ILE:HD12	1.99	0.44
2:K:375:PHE:HD1	2:K:376:SER:N	2.16	0.44
3:L:197:ARG:O	3:L:381:LYS:HG2	2.17	0.44
1:A:148:LYS:HE2	1:A:148:LYS:HB3	1.74	0.44
2:B:152:TYR:O	2:B:155:GLU:HG3	2.18	0.44
2:B:161:ILE:CB	2:B:162:PRO:HD3	2.48	0.44
2:B:191:GLU:C	2:B:193:CYS:N	2.67	0.44
3:C:270:GLU:O	3:C:271:ALA:O	2.36	0.44
3:F:127:LYS:O	3:F:130:GLN:N	2.50	0.44
3:F:269:PRO:C	3:F:273:LYS:O	2.56	0.44
3:F:270:GLU:HA	3:F:273:LYS:O	2.17	0.44
1:G:121:VAL:HG12	1:G:124:ARG:NE	2.28	0.44
1:G:148:LYS:HE2	2:H:425:ASP:O	2.17	0.44
1:G:163:GLY:O	3:I:138:PRO:HA	2.17	0.44
1:G:174:ASP:HB3	1:G:177:ASP:HB3	1.99	0.44
2:H:268:PRO:O	2:H:273:PHE:HD2	2.01	0.44
3:I:204:PHE:CE2	3:I:227:TRP:HB2	2.53	0.44
3:I:212:LYS:HG3	3:I:274:TYR:OH	2.17	0.44
3:I:293:PHE:CA	3:I:302:LYS:HG3	2.47	0.44
3:I:356:LYS:HA	3:I:359:THR:CG2	2.48	0.44
3:L:238:THR:HG22	3:L:266:LYS:CE	2.46	0.44
1:A:157:LYS:O	1:A:160:SER:HB3	2.18	0.44
1:A:176:LYS:O	1:A:176:LYS:HG3	2.16	0.44
2:B:155:GLU:C	2:B:157:VAL:N	2.70	0.44
2:B:223:GLU:O	2:B:225:TYR:HD1	2.00	0.44
2:B:326:TYR:HE1	2:B:354:MET:HG3	1.83	0.44
2:B:326:TYR:C	2:B:328:GLY:N	2.71	0.44
2:B:363:GLU:O	2:B:367:MET:HG2	2.18	0.44
2:B:422:TYR:N	2:B:422:TYR:CD1	2.86	0.44
3:C:261:ASP:N	3:C:261:ASP:OD1	2.51	0.44
1:D:182:GLN:O	1:D:186:GLU:HG2	2.18	0.44
3:F:295:PHE:CE2	4:P:1:GLY:HA2	2.52	0.44
3:F:313:SER:O	3:F:333:GLY:HA2	2.18	0.44
3:F:344:LEU:HA	3:F:344:LEU:HD23	1.72	0.44
2:H:213:GLU:CG	2:H:217:LYS:HE3	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:171:PRO:HB2	3:I:174:ALA:CB	2.24	0.44
3:I:196:LYS:HA	3:I:383:THR:HA	1.99	0.44
3:I:256:ARG:NH1	3:I:256:ARG:CG	2.81	0.44
1:A:128:GLU:HA	1:A:131:GLN:CG	2.46	0.44
2:B:210:GLU:O	2:B:212:GLU:N	2.51	0.44
2:B:405:ASN:O	2:B:405:ASN:CG	2.56	0.44
3:C:296:GLY:O	3:C:298:ASP:N	2.50	0.44
2:E:243:ASN:O	2:E:244:THR:C	2.55	0.44
2:E:293:TRP:HE1	2:E:296:ASN:ND2	2.15	0.44
2:E:425:ASP:OD1	2:E:425:ASP:N	2.49	0.44
3:F:154:GLN:HA	3:F:190:GLY:HA3	1.99	0.44
2:H:294:LEU:CD2	2:H:298:LYS:HB2	2.48	0.44
3:I:148:ILE:HD13	3:I:156:ILE:CG2	2.48	0.44
3:I:320:ASP:OD2	3:I:322:PHE:HB3	2.17	0.44
3:I:367:ILE:HB	3:I:379:MET:N	2.31	0.44
1:J:131:GLN:HE21	1:J:132:HIS:N	2.16	0.44
3:L:281:PHE:CG	3:L:288:ASP:HB2	2.53	0.44
2:B:206:VAL:HG13	2:B:206:VAL:O	2.18	0.44
3:C:179:LEU:O	3:C:218:LEU:HD11	2.18	0.44
3:C:227:TRP:NE1	3:C:230:ASN:ND2	2.65	0.44
3:C:246:LEU:CB	3:C:265:PHE:CD1	3.01	0.44
3:C:264:MET:O	3:C:265:PHE:O	2.35	0.44
3:C:334:TRP:NE1	3:C:342:GLY:O	2.51	0.44
1:D:137:GLN:C	1:D:140:VAL:HG12	2.38	0.44
2:E:455:ARG:HG3	2:E:456:PRO:HD2	2.00	0.44
3:F:246:LEU:HG	3:F:247:ARG:H	1.83	0.44
3:F:340:HIS:CE1	3:F:368:ILE:HD11	2.53	0.44
2:H:262:PHE:N	2:H:262:PHE:CD1	2.86	0.44
2:H:362:GLY:O	2:H:363:GLU:C	2.56	0.44
3:I:149:THR:O	3:I:159:LYS:NZ	2.49	0.44
3:I:172:LEU:HD12	3:I:172:LEU:N	2.27	0.44
3:L:236:ILE:O	3:L:244:TYR:CE1	2.71	0.44
1:A:159:ARG:C	1:A:161:CYS:H	2.21	0.43
2:B:187:SER:C	2:B:189:GLN:H	2.20	0.43
2:B:242:MET:SD	2:B:248:GLY:CA	3.04	0.43
3:C:94:MET:C	3:C:96:TYR:N	2.71	0.43
3:C:162:LYS:HE3	3:C:186:GLY:HA2	1.99	0.43
3:C:171:PRO:HD2	3:C:174:ALA:CB	2.47	0.43
2:E:157:VAL:HG12	3:F:100:ILE:HG21	2.00	0.43
2:E:239:TYR:HB3	2:E:251:VAL:HB	1.99	0.43
1:G:179:GLU:HG2	1:G:182:GLN:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:237:ARG:NH2	3:I:143:VAL:HG23	2.24	0.43
2:H:329:PHE:CZ	2:H:331:VAL:HG23	2.53	0.43
3:I:100:ILE:O	3:I:100:ILE:HD12	2.18	0.43
3:I:206:LYS:HG3	3:I:215:PHE:CG	2.53	0.43
3:I:312:PHE:CE1	3:I:333:GLY:O	2.71	0.43
1:J:144:LEU:HD13	1:J:182:GLN:HG3	2.00	0.43
3:L:98:ALA:O	3:L:101:LEU:HD23	2.18	0.43
3:L:172:LEU:H	3:L:239:GLN:HE21	1.66	0.43
1:A:184:GLN:HE22	1:A:185:LEU:HD23	1.83	0.43
2:B:276:VAL:O	2:B:277:ALA:CB	2.66	0.43
2:B:330:THR:OG1	2:B:341:SER:HB2	2.19	0.43
2:B:338:TYR:O	2:B:339:GLN:C	2.56	0.43
2:B:374:PHE:O	2:B:403:TRP:HA	2.17	0.43
2:E:204:PRO:O	2:E:205:VAL:C	2.55	0.43
2:E:214:ILE:HD11	2:E:227:ILE:HG22	1.99	0.43
3:F:197:ARG:O	3:F:381:LYS:HG2	2.18	0.43
2:H:167:VAL:HG12	2:H:168:LEU:N	2.32	0.43
2:H:186:VAL:O	2:H:190:MET:HB2	2.18	0.43
3:I:168:PHE:CE1	3:I:179:LEU:HD13	2.53	0.43
3:I:246:LEU:CB	3:I:265:PHE:CD1	3.01	0.43
2:K:163:THR:O	2:K:163:THR:HG22	2.18	0.43
2:K:237:ARG:HG3	2:K:237:ARG:NH1	2.33	0.43
2:K:304:ARG:C	2:K:306:GLY:H	2.21	0.43
3:L:162:LYS:HE3	3:L:186:GLY:CA	2.47	0.43
2:B:199:VAL:N	3:C:140:LYS:O	2.50	0.43
3:C:97:GLU:O	3:C:99:SER:N	2.48	0.43
3:C:178:PHE:CZ	3:C:232:LYS:HG2	2.52	0.43
1:D:188:VAL:HG21	2:E:167:VAL:HG21	2.00	0.43
2:E:296:ASN:HD22	2:E:296:ASN:HA	1.57	0.43
3:F:169:ILE:O	3:F:177:GLN:HB2	2.17	0.43
2:H:152:TYR:CD1	2:H:152:TYR:N	2.86	0.43
2:H:362:GLY:O	2:H:364:ASN:N	2.51	0.43
3:I:105:SER:HA	3:I:108:ARG:HB3	2.00	0.43
3:I:298:ASP:OD2	3:I:300:SER:HB2	2.18	0.43
3:L:192:THR:CG2	3:L:386:ILE:HG13	2.48	0.43
3:L:194:PHE:HB2	3:L:228:LEU:HB3	2.00	0.43
3:L:198:LEU:HB3	3:L:381:LYS:HG2	1.99	0.43
3:L:230:ASN:C	3:L:232:LYS:N	2.71	0.43
3:L:334:TRP:CZ3	3:L:344:LEU:HB2	2.54	0.43
3:L:349:TYR:HB2	3:L:378:SER:HB3	1.99	0.43
4:R:3:ARG:CB	4:R:4:PRO:CD	2.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LEU:HD23	2:B:370:HIS:CD2	2.53	0.43
3:C:107:ILE:O	3:C:110:LEU:HB2	2.19	0.43
3:C:198:LEU:C	3:C:348:TYR:OH	2.56	0.43
3:C:256:ARG:NH1	3:C:256:ARG:CG	2.81	0.43
3:F:207:ASN:N	3:F:210:GLN:OE1	2.47	0.43
3:F:230:ASN:O	3:F:232:LYS:N	2.51	0.43
1:G:129:LYS:C	1:G:133:ILE:HD13	2.38	0.43
1:G:151:GLU:OE1	2:H:182:LEU:HD11	2.17	0.43
2:H:284:ASN:ND2	2:H:284:ASN:N	2.66	0.43
2:H:358:SER:O	2:H:360:LEU:N	2.43	0.43
3:I:154:GLN:HG2	3:I:388:PRO:HG2	2.00	0.43
3:I:248:VAL:O	3:I:259:THR:HA	2.19	0.43
3:I:258:SER:O	3:I:259:THR:HB	2.18	0.43
2:K:381:ASP:O	2:K:382:ASN:OD1	2.36	0.43
3:L:95:LYS:O	3:L:95:LYS:HG2	2.18	0.43
2:B:326:TYR:C	2:B:328:GLY:H	2.22	0.43
2:B:398:ASP:CA	2:B:433:ASP:CB	2.88	0.43
2:B:401:GLY:O	2:B:402:TRP:HB2	2.18	0.43
1:D:131:GLN:O	1:D:134:GLN:HG2	2.18	0.43
2:E:210:GLU:OE1	2:E:212:GLU:HB3	2.18	0.43
2:E:217:LYS:HE3	3:F:213:GLU:CD	2.39	0.43
2:E:370:HIS:NE2	2:E:408:HIS:HA	2.34	0.43
2:H:197:CYS:O	3:I:140:LYS:N	2.44	0.43
2:H:214:ILE:HD13	2:H:225:TYR:CD2	2.48	0.43
2:H:299:ILE:O	2:H:301:GLN:N	2.52	0.43
2:H:333:ASN:O	2:H:335:ALA:N	2.52	0.43
2:H:349:ALA:O	2:H:440:TRP:HB2	2.19	0.43
2:H:365:ARG:O	2:H:368:THR:N	2.51	0.43
3:I:276:LEU:H	3:I:276:LEU:HD23	1.84	0.43
3:L:204:PHE:O	3:L:206:LYS:N	2.50	0.43
3:L:248:VAL:O	3:L:259:THR:HA	2.17	0.43
3:L:344:LEU:HA	3:L:344:LEU:HD23	1.72	0.43
1:A:126:VAL:O	1:A:128:GLU:N	2.51	0.43
2:B:412:PRO:HG3	2:B:450:MET:CE	2.47	0.43
2:B:417:TYR:HB2	2:B:446:SER:CB	2.49	0.43
3:C:253:TRP:CD2	3:C:380:LYS:HB2	2.54	0.43
2:E:376:SER:HB3	2:E:382:ASN:H	1.84	0.43
3:F:383:THR:O	3:F:383:THR:OG1	2.36	0.43
2:H:210:GLU:CD	2:H:212:GLU:H	2.19	0.43
1:J:130:VAL:HA	1:J:133:ILE:CG2	2.47	0.43
3:L:269:PRO:C	3:L:273:LYS:O	2.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:270:GLU:HB2	3:L:274:TYR:CZ	2.54	0.43
3:L:279:ALA:O	3:L:280:TYR:HB3	2.18	0.43
3:L:304:PHE:O	3:L:337:ASN:HB3	2.18	0.43
2:B:345:TYR:HB2	2:B:354:MET:HE2	2.00	0.43
2:B:411:ASN:CB	2:B:436:VAL:HG22	2.43	0.43
2:B:442:GLY:C	2:B:444:TRP:H	2.22	0.43
3:C:212:LYS:HG3	3:C:274:TYR:OH	2.18	0.43
1:D:128:GLU:O	1:D:129:LYS:C	2.55	0.43
2:E:161:ILE:HB	2:E:162:PRO:HD3	2.01	0.43
2:E:370:HIS:CE1	2:E:408:HIS:HB2	2.54	0.43
3:F:203:ASP:O	3:F:206:LYS:CG	2.66	0.43
3:F:284:GLY:C	3:F:286:ALA:H	2.22	0.43
3:F:304:PHE:O	3:F:337:ASN:HB3	2.18	0.43
2:H:222:SER:O	2:H:223:GLU:HB3	2.19	0.43
2:H:281:ASP:OD1	2:H:281:ASP:N	2.52	0.43
2:H:300:SER:HA	2:H:331:VAL:HB	1.99	0.43
3:I:120:LYS:O	3:I:124:LEU:HD13	2.18	0.43
3:I:233:ILE:O	3:I:237:SER:HB2	2.19	0.43
3:I:271:ALA:C	3:I:273:LYS:N	2.72	0.43
3:I:339:CYS:HB3	4:S:1:GLY:N	2.33	0.43
2:K:166:ARG:HD3	2:K:166:ARG:HA	1.90	0.43
2:K:313:GLU:CD	2:K:323:LYS:HZ3	2.22	0.43
3:L:168:PHE:CD1	3:L:177:GLN:HG3	2.52	0.43
3:L:313:SER:O	3:L:333:GLY:HA2	2.19	0.43
2:B:184:SER:C	2:B:186:VAL:N	2.72	0.43
2:B:365:ARG:O	2:B:368:THR:HG23	2.19	0.43
3:C:239:GLN:C	3:C:241:ALA:H	2.21	0.43
1:D:131:GLN:O	1:D:134:GLN:N	2.50	0.43
2:E:161:ILE:N	2:E:162:PRO:CD	2.82	0.43
2:E:215:ILE:HG23	2:E:216:ARG:N	2.34	0.43
3:F:248:VAL:O	3:F:259:THR:HA	2.18	0.43
2:H:152:TYR:C	2:H:154:ASP:N	2.72	0.43
2:H:295:GLY:O	2:H:299:ILE:HG13	2.18	0.43
2:H:371:ASN:C	2:H:373:MET:H	2.22	0.43
3:I:253:TRP:O	3:I:254:ASN:CG	2.57	0.43
3:I:297:ASP:HB3	4:S:4:PRO:HG3	2.00	0.43
3:L:243:PRO:HB2	3:L:389:PHE:CB	2.49	0.43
3:L:304:PHE:CD1	3:L:338:LYS:CB	3.01	0.43
1:A:189:ILE:O	1:A:190:ALA:HB3	2.18	0.43
3:C:250:LEU:CD1	3:C:382:THR:HA	2.40	0.43
1:G:140:VAL:CA	3:I:114:TYR:HE1	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:155:GLU:C	2:H:157:VAL:N	2.70	0.43
2:H:280:THR:O	2:H:281:ASP:C	2.56	0.43
2:H:326:TYR:CZ	2:H:353:LEU:HB2	2.54	0.43
3:I:204:PHE:CD2	3:I:215:PHE:CZ	3.07	0.43
3:I:246:LEU:HD21	3:I:248:VAL:CG2	2.49	0.43
3:I:269:PRO:O	3:I:271:ALA:N	2.52	0.43
3:I:273:LYS:NZ	3:I:317:ASN:HD21	2.17	0.43
2:K:164:ASN:C	2:K:166:ARG:N	2.72	0.43
2:K:176:ARG:C	2:K:178:LYS:H	2.22	0.43
2:K:432:ASP:HB3	2:K:444:TRP:CH2	2.53	0.43
3:L:121:ILE:O	3:L:125:LYS:HG3	2.18	0.43
1:A:128:GLU:O	1:A:130:VAL:N	2.42	0.43
1:A:128:GLU:C	1:A:131:GLN:HG2	2.38	0.43
2:B:257:ASP:OD2	2:B:257:ASP:N	2.52	0.43
2:B:398:ASP:OD1	2:B:408:HIS:CE1	2.72	0.43
2:B:438:MET:O	2:B:440:TRP:N	2.52	0.43
3:C:191:TRP:CH2	3:C:247:ARG:CD	3.02	0.43
2:E:242:MET:HA	2:E:247:GLY:CA	2.49	0.43
2:E:304:ARG:C	2:E:306:GLY:H	2.21	0.43
2:E:381:ASP:O	2:E:382:ASN:OD1	2.37	0.43
3:F:145:ILE:HG21	3:F:168:PHE:CD2	2.54	0.43
2:H:160:ASN:O	2:H:164:ASN:HB2	2.18	0.43
2:H:206:VAL:O	2:H:206:VAL:HG13	2.19	0.43
2:H:209:LYS:NZ	2:H:209:LYS:CB	2.81	0.43
2:H:239:TYR:OH	2:H:289:PRO:HD3	2.19	0.43
3:I:145:ILE:O	3:I:145:ILE:HD12	2.19	0.43
3:I:326:CYS:SG	3:I:339:CYS:N	2.91	0.43
1:J:179:GLU:O	1:J:180:ASP:C	2.57	0.43
2:K:295:GLY:O	2:K:299:ILE:N	2.49	0.43
2:K:394:CYS:O	2:K:397:GLU:O	2.37	0.43
1:A:145:VAL:O	1:A:145:VAL:HG12	2.18	0.42
1:A:167:ARG:NH2	2:B:192:TYR:CD2	2.87	0.42
2:B:173:GLU:C	2:B:175:LEU:N	2.73	0.42
2:B:213:GLU:CG	2:B:217:LYS:HE3	2.47	0.42
2:B:358:SER:O	2:B:360:LEU:N	2.51	0.42
2:B:358:SER:C	2:B:360:LEU:H	2.21	0.42
3:C:103:HIS:O	3:C:105:SER:N	2.52	0.42
3:C:126:GLU:C	3:C:128:VAL:N	2.69	0.42
2:H:374:PHE:O	2:H:403:TRP:HA	2.18	0.42
2:H:399:GLY:H	2:H:433:ASP:HB2	1.84	0.42
3:I:258:SER:O	3:I:259:THR:CB	2.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:356:LYS:HB3	3:I:356:LYS:HE2	1.77	0.42
2:K:203:ILE:N	2:K:203:ILE:CD1	2.78	0.42
2:K:321:LYS:HB2	2:K:321:LYS:HZ3	1.83	0.42
3:L:244:TYR:CE2	3:L:388:PRO:HG3	2.53	0.42
2:B:190:MET:CB	3:C:131:LEU:HD12	2.49	0.42
2:B:304:ARG:HG3	2:B:304:ARG:NH1	2.34	0.42
3:C:208:TRP:O	3:C:210:GLN:N	2.52	0.42
1:D:171:ARG:HD2	2:E:185:ASP:OD2	2.19	0.42
2:E:203:ILE:HA	2:E:204:PRO:HD3	1.84	0.42
2:E:229:PRO:CG	2:E:301:GLN:HE22	2.29	0.42
2:E:386:LEU:HD13	2:E:387:THR:N	2.34	0.42
2:E:410:ALA:C	2:E:412:PRO:HD3	2.40	0.42
3:F:196:LYS:HG3	3:F:383:THR:HG22	2.01	0.42
3:I:150:GLY:N	3:I:156:ILE:HG12	2.34	0.42
3:I:242:ILE:CG2	3:I:243:PRO:HD2	2.49	0.42
3:I:334:TRP:NE1	3:I:342:GLY:O	2.53	0.42
3:L:230:ASN:HD22	3:L:233:ILE:HD12	1.84	0.42
1:A:124:ARG:O	1:A:126:VAL:N	2.51	0.42
1:A:141:ARG:HD2	1:A:186:GLU:OE1	2.19	0.42
1:A:144:LEU:CD1	1:A:182:GLN:HG2	2.48	0.42
2:B:304:ARG:HH22	2:B:333:ASN:CB	2.31	0.42
3:C:197:ARG:HH22	3:C:348:TYR:N	2.17	0.42
3:F:197:ARG:NE	3:F:204:PHE:CZ	2.87	0.42
3:F:338:LYS:O	4:P:2:PRO:HA	2.19	0.42
1:G:126:VAL:C	1:G:128:GLU:H	2.20	0.42
2:H:152:TYR:C	2:H:154:ASP:H	2.22	0.42
2:H:199:VAL:HG23	3:I:141:ASP:OD1	2.19	0.42
2:H:296:ASN:HB3	2:H:338:TYR:CZ	2.54	0.42
2:H:360:LEU:HA	5:H:470:NAG:H81	2.01	0.42
3:I:287:GLY:CA	3:I:371:THR:HB	2.49	0.42
2:K:186:VAL:O	2:K:190:MET:HE3	2.20	0.42
3:L:114:TYR:HD2	3:L:115:ASN:ND2	2.18	0.42
3:L:167:TYR:CD1	3:L:182:CYS:HB2	2.54	0.42
3:L:284:GLY:C	3:L:286:ALA:H	2.23	0.42
2:B:294:LEU:CD2	2:B:298:LYS:HD2	2.49	0.42
2:B:365:ARG:O	2:B:368:THR:N	2.52	0.42
2:B:385:TRP:CA	2:B:406:ARG:HB2	2.50	0.42
3:C:110:LEU:HD12	3:C:110:LEU:N	2.34	0.42
3:C:206:LYS:HG3	3:C:215:PHE:CG	2.54	0.42
3:C:328:GLU:O	3:C:331:GLY:N	2.51	0.42
1:D:141:ARG:HA	1:D:144:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:364:ASN:O	2:E:368:THR:HG23	2.19	0.42
2:E:367:MET:O	2:E:405:ASN:O	2.37	0.42
3:F:305:THR:HB	3:F:341:ALA:CB	2.48	0.42
2:H:160:ASN:N	2:H:160:ASN:HD22	2.18	0.42
2:H:230:ASP:O	2:H:233:VAL:HG12	2.19	0.42
2:H:257:ASP:OD2	2:H:257:ASP:N	2.52	0.42
2:H:294:LEU:O	2:H:295:GLY:C	2.57	0.42
3:I:148:ILE:N	3:I:148:ILE:HD12	2.35	0.42
3:I:250:LEU:HD12	3:I:250:LEU:HA	1.86	0.42
3:L:127:LYS:O	3:L:130:GLN:N	2.44	0.42
1:A:128:GLU:CA	1:A:131:GLN:HG2	2.49	0.42
1:A:140:VAL:HG12	3:C:114:TYR:CD1	2.54	0.42
2:B:179:ILE:HD13	3:C:117:ASN:ND2	2.34	0.42
2:B:184:SER:O	2:B:186:VAL:N	2.52	0.42
2:B:359:GLN:NE2	2:B:359:GLN:N	2.66	0.42
2:B:409:ALA:O	2:B:438:MET:HB2	2.19	0.42
3:C:191:TRP:C	3:C:192:THR:HG22	2.40	0.42
3:C:307:HIS:O	3:C:310:MET:HB2	2.20	0.42
3:C:367:ILE:HB	3:C:379:MET:N	2.32	0.42
2:E:370:HIS:CE1	2:E:402:TRP:HE1	2.38	0.42
2:E:394:CYS:O	2:E:397:GLU:O	2.37	0.42
3:F:359:THR:OG1	3:F:362:GLY:HA2	2.19	0.42
2:H:284:ASN:HD22	2:H:284:ASN:N	2.09	0.42
3:I:298:ASP:O	3:I:301:ASP:OD1	2.37	0.42
1:J:139:ASN:O	3:L:114:TYR:HE1	2.03	0.42
2:K:225:TYR:CE1	2:K:242:MET:HE2	2.54	0.42
2:K:245:GLU:O	2:K:246:ASN:HB2	2.18	0.42
3:L:322:PHE:HB2	3:L:338:LYS:HA	2.00	0.42
1:A:126:VAL:HG12	1:A:127:ILE:N	2.35	0.42
1:A:150:LEU:O	1:A:150:LEU:HD12	2.20	0.42
1:A:168:ALA:HA	2:B:189:GLN:CD	2.40	0.42
2:B:153:ILE:C	2:B:155:GLU:N	2.72	0.42
2:B:230:ASP:O	2:B:233:VAL:HG12	2.19	0.42
2:B:295:GLY:O	2:B:299:ILE:HG13	2.19	0.42
2:B:385:TRP:CD1	2:B:406:ARG:NH1	2.87	0.42
3:C:156:ILE:C	3:C:158:ASN:N	2.72	0.42
3:C:164:SER:HB2	3:C:183:GLU:HA	2.00	0.42
3:C:307:HIS:CE1	3:C:341:ALA:H	2.38	0.42
3:C:340:HIS:CE1	3:C:364:ASP:OD2	2.72	0.42
3:F:117:ASN:O	3:F:121:ILE:CG1	2.62	0.42
3:F:194:PHE:HB2	3:F:228:LEU:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:198:LEU:HB3	3:F:381:LYS:HG2	2.01	0.42
2:H:366:THR:HA	2:H:369:ILE:HG13	2.00	0.42
3:I:198:LEU:C	3:I:348:TYR:OH	2.57	0.42
2:K:204:PRO:O	2:K:205:VAL:C	2.57	0.42
2:K:235:PRO:HG2	3:L:168:PHE:CE1	2.49	0.42
2:K:309:GLU:OE1	2:K:325:HIS:CE1	2.72	0.42
1:A:120:GLU:OE1	1:A:122:LEU:HB3	2.20	0.42
1:A:132:HIS:O	1:A:133:ILE:C	2.56	0.42
3:C:154:GLN:HG2	3:C:388:PRO:HG2	2.02	0.42
3:C:171:PRO:HB2	3:C:174:ALA:CB	2.25	0.42
3:C:298:ASP:N	3:C:301:ASP:OD1	2.52	0.42
2:E:236:TYR:CG	2:E:298:LYS:HE2	2.55	0.42
3:F:95:LYS:O	3:F:95:LYS:CG	2.67	0.42
1:G:147:MET:HE2	2:H:179:ILE:HG23	2.02	0.42
2:H:371:ASN:OD1	2:H:372:GLY:N	2.52	0.42
3:I:113:ILE:H	3:I:113:ILE:CD1	2.33	0.42
3:I:372:TRP:CE2	3:I:373:LYS:NZ	2.88	0.42
2:K:215:ILE:HG23	2:K:216:ARG:N	2.35	0.42
2:K:373:MET:CE	2:K:374:PHE:H	2.33	0.42
1:A:140:VAL:HG23	1:A:141:ARG:N	2.34	0.42
1:A:148:LYS:HZ1	2:B:425:ASP:CB	2.33	0.42
2:B:399:GLY:N	2:B:433:ASP:HB2	2.34	0.42
2:B:421:GLN:HA	2:B:444:TRP:O	2.20	0.42
1:D:185:LEU:HD13	1:D:189:ILE:HD11	2.02	0.42
3:F:143:VAL:HA	3:F:220:PRO:HG2	2.02	0.42
3:F:196:LYS:O	3:F:225:GLU:HA	2.20	0.42
1:G:169:LEU:HD13	1:G:170:ALA:C	2.40	0.42
2:H:166:ARG:HD3	2:H:166:ARG:HA	1.87	0.42
2:H:330:THR:OG1	2:H:341:SER:HB2	2.20	0.42
3:I:334:TRP:HH2	3:I:344:LEU:HD12	1.84	0.42
3:I:340:HIS:CE1	3:I:364:ASP:OD2	2.72	0.42
2:K:217:LYS:HE3	3:L:213:GLU:CD	2.40	0.42
2:K:374:PHE:O	2:K:403:TRP:HA	2.20	0.42
3:L:246:LEU:HD13	3:L:265:PHE:CZ	2.55	0.42
2:B:215:ILE:HA	2:B:219:GLY:O	2.20	0.42
3:C:193:VAL:HA	3:C:385:LYS:CB	2.50	0.42
3:C:263:ALA:HB2	3:C:280:TYR:CE1	2.54	0.42
2:E:191:GLU:O	2:E:193:CYS:N	2.52	0.42
2:E:201:CYS:O	3:F:143:VAL:HG21	2.20	0.42
2:E:325:HIS:N	2:E:346:ARG:O	2.45	0.42
1:G:144:LEU:HD11	1:G:181:GLN:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ARG:O	2:H:259:SER:HA	2.20	0.42
1:G:175:LEU:O	1:G:179:GLU:HB2	2.20	0.42
2:H:252:ILE:HG12	2:H:452:MET:O	2.19	0.42
3:I:154:GLN:OE1	3:I:190:GLY:N	2.53	0.42
3:I:156:ILE:C	3:I:158:ASN:N	2.73	0.42
3:I:239:GLN:C	3:I:241:ALA:H	2.22	0.42
1:J:130:VAL:HA	1:J:133:ILE:HG22	2.02	0.42
2:K:361:MET:HB2	5:K:470:NAG:C8	2.49	0.42
3:L:194:PHE:HE2	3:L:384:MET:CB	2.33	0.42
3:L:333:GLY:O	3:L:334:TRP:HB2	2.19	0.42
1:A:158:ILE:HA	1:A:158:ILE:HD12	1.75	0.42
3:C:250:LEU:HD23	3:C:372:TRP:CE3	2.54	0.42
3:C:394:ILE:C	3:C:396:GLU:N	2.73	0.42
1:D:136:LEU:HD13	3:F:111:GLN:NE2	2.35	0.42
2:E:321:LYS:HB2	2:E:321:LYS:HZ3	1.84	0.42
2:E:456:PRO:O	2:E:457:PHE:C	2.58	0.42
3:F:243:PRO:HB2	3:F:389:PHE:CB	2.50	0.42
3:F:367:ILE:HB	3:F:378:SER:OG	2.20	0.42
2:H:238:VAL:CG2	2:H:239:TYR:H	2.33	0.42
2:H:448:ARG:HD2	2:H:448:ARG:HA	1.82	0.42
3:I:184:ILE:HG22	3:I:185:ASP:N	2.34	0.42
3:I:191:TRP:C	3:I:192:THR:HG22	2.41	0.42
2:K:340:ILE:HG12	2:K:341:SER:N	2.35	0.42
1:A:139:ASN:HB3	3:C:114:TYR:OH	2.19	0.41
1:A:144:LEU:O	1:A:144:LEU:HG	2.20	0.41
2:B:322:VAL:HB	2:B:348:THR:OG1	2.19	0.41
2:B:326:TYR:CZ	2:B:353:LEU:HB2	2.55	0.41
2:B:359:GLN:O	2:B:359:GLN:CG	2.67	0.41
2:B:362:GLY:O	2:B:363:GLU:C	2.59	0.41
3:C:143:VAL:HG12	3:C:220:PRO:CD	2.42	0.41
3:C:153:CYS:CB	3:C:191:TRP:O	2.67	0.41
3:C:298:ASP:OD2	3:C:300:SER:HB2	2.20	0.41
3:C:370:ALA:HA	3:C:373:LYS:O	2.20	0.41
1:D:181:GLN:OE1	2:E:174:ASN:ND2	2.53	0.41
2:E:215:ILE:CG2	2:E:216:ARG:N	2.83	0.41
2:E:252:ILE:HG12	2:E:454:ILE:HG12	2.02	0.41
2:E:310:LEU:HD21	2:E:312:ILE:CD1	2.50	0.41
2:E:434:GLY:O	2:E:436:VAL:N	2.53	0.41
3:F:261:ASP:O	3:F:262:TYR:CD2	2.73	0.41
2:H:180:GLN:C	2:H:182:LEU:N	2.74	0.41
3:I:289:ALA:HB2	3:I:371:THR:OG1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:156:THR:C	2:K:158:ASN:H	2.22	0.41
2:K:456:PRO:O	2:K:457:PHE:C	2.58	0.41
3:L:101:LEU:HD12	3:L:104:ASP:HB2	2.02	0.41
3:L:203:ASP:O	3:L:206:LYS:CG	2.67	0.41
3:L:203:ASP:O	3:L:206:LYS:CE	2.68	0.41
3:L:203:ASP:O	3:L:206:LYS:HE3	2.21	0.41
2:B:222:SER:O	2:B:223:GLU:HB3	2.20	0.41
2:B:266:TRP:CE3	2:B:266:TRP:CA	3.03	0.41
3:C:169:ILE:HG12	3:C:180:VAL:CG1	2.50	0.41
3:C:312:PHE:CE1	3:C:333:GLY:O	2.73	0.41
3:C:394:ILE:HG12	3:C:396:GLU:O	2.20	0.41
2:E:203:ILE:N	2:E:203:ILE:CD1	2.78	0.41
3:F:194:PHE:HE2	3:F:384:MET:CB	2.33	0.41
3:F:227:TRP:CZ3	3:F:384:MET:HE2	2.54	0.41
3:F:314:THR:O	3:F:315:TRP:C	2.56	0.41
1:G:173:VAL:O	1:G:173:VAL:HG23	2.20	0.41
2:H:304:ARG:HH22	2:H:333:ASN:CB	2.32	0.41
2:H:315:GLU:CB	2:H:321:LYS:HB3	2.44	0.41
2:H:385:TRP:CZ3	4:Q:3:ARG:HG3	2.55	0.41
3:I:164:SER:HB2	3:I:183:GLU:HA	2.01	0.41
3:I:288:ASP:OD1	3:I:291:ASP:HB2	2.20	0.41
1:A:161:CYS:C	1:A:163:GLY:N	2.73	0.41
2:B:173:GLU:O	2:B:176:ARG:HB3	2.20	0.41
2:B:184:SER:O	2:B:185:ASP:C	2.58	0.41
2:B:253:GLN:HB2	2:B:293:TRP:CZ3	2.55	0.41
2:B:266:TRP:CZ2	2:B:380:ARG:NE	2.88	0.41
2:B:280:THR:O	2:B:281:ASP:C	2.57	0.41
3:C:93:ILE:C	3:C:95:LYS:H	2.23	0.41
3:C:253:TRP:CE2	3:C:380:LYS:HB2	2.55	0.41
3:C:269:PRO:O	3:C:271:ALA:N	2.53	0.41
1:D:131:GLN:HA	1:D:134:GLN:HG2	2.02	0.41
2:E:309:GLU:OE1	2:E:325:HIS:CE1	2.73	0.41
3:F:233:ILE:HG13	3:F:233:ILE:H	1.65	0.41
3:F:299:PRO:O	3:F:301:ASP:N	2.46	0.41
3:F:322:PHE:HA	3:F:338:LYS:HD2	2.01	0.41
2:K:203:ILE:H	2:K:203:ILE:CD1	2.33	0.41
3:L:310:MET:C	3:L:311:GLN:O	2.56	0.41
3:L:325:ASN:O	3:L:326:CYS:C	2.57	0.41
3:L:340:HIS:CE1	3:L:368:ILE:HD11	2.55	0.41
3:L:359:THR:HA	3:L:360:PRO:HD3	1.74	0.41
2:B:162:PRO:HA	2:B:166:ARG:CD	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:VAL:C	2:B:200:SER:HG	2.23	0.41
2:B:207:SER:OG	2:B:208:GLY:N	2.52	0.41
2:B:254:ASN:HD21	2:B:256:GLN:NE2	2.17	0.41
3:C:171:PRO:O	3:C:172:LEU:C	2.59	0.41
3:C:248:VAL:O	3:C:248:VAL:HG12	2.21	0.41
3:C:288:ASP:OD1	3:C:291:ASP:HB2	2.20	0.41
1:D:159:ARG:O	1:D:159:ARG:CG	2.69	0.41
1:G:185:LEU:O	1:G:189:ILE:HB	2.19	0.41
2:H:246:ASN:HB2	2:H:455:ARG:NH1	2.35	0.41
3:I:153:CYS:CB	3:I:191:TRP:O	2.68	0.41
1:J:167:ARG:HB2	2:K:192:TYR:CB	2.50	0.41
3:L:117:ASN:O	3:L:121:ILE:CG1	2.63	0.41
3:L:205:LYS:NZ	3:L:331:GLY:HA2	2.34	0.41
3:L:325:ASN:ND2	3:L:327:ALA:HB3	2.28	0.41
2:B:236:TYR:HB2	2:B:298:LYS:HZ3	1.85	0.41
2:B:255:ARG:NH1	2:B:262:PHE:CD1	2.88	0.41
2:B:373:MET:HE3	2:B:374:PHE:H	1.85	0.41
3:C:110:LEU:O	3:C:112:GLU:N	2.53	0.41
2:E:232:SER:O	2:E:233:VAL:HB	2.21	0.41
2:E:265:LYS:HB3	2:E:379:ASP:OD2	2.21	0.41
2:E:301:GLN:HE21	2:E:301:GLN:HB3	1.54	0.41
3:F:336:MET:SD	3:F:340:HIS:HD2	2.43	0.41
1:G:190:ALA:O	1:G:191:LYS:HB2	2.20	0.41
2:H:179:ILE:HD13	3:I:117:ASN:HB3	2.03	0.41
2:H:190:MET:O	2:H:190:MET:SD	2.78	0.41
2:H:211:CYS:O	2:H:242:MET:HE1	2.20	0.41
2:H:296:ASN:O	2:H:299:ILE:N	2.53	0.41
2:H:301:GLN:HE21	2:H:302:LEU:HD23	1.85	0.41
2:H:398:ASP:OD1	2:H:408:HIS:CE1	2.73	0.41
3:I:196:LYS:CE	3:I:198:LEU:HD21	2.39	0.41
3:I:248:VAL:HG22	3:I:384:MET:HG2	2.02	0.41
1:J:171:ARG:HH21	1:J:173:VAL:HG22	1.85	0.41
2:K:161:ILE:O	2:K:164:ASN:HB3	2.21	0.41
2:K:254:ASN:O	2:K:291:GLU:HA	2.21	0.41
1:A:124:ARG:C	1:A:126:VAL:N	2.72	0.41
1:A:167:ARG:NE	2:B:192:TYR:CD2	2.89	0.41
2:B:173:GLU:HA	2:B:176:ARG:CB	2.49	0.41
2:B:250:THR:O	2:B:252:ILE:CD1	2.69	0.41
2:B:448:ARG:HD2	2:B:448:ARG:HA	1.85	0.41
3:C:150:GLY:N	3:C:156:ILE:HG12	2.36	0.41
3:C:233:ILE:O	3:C:237:SER:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ASP:OD2	3:C:392:LEU:HD11	2.20	0.41
3:C:377:TYR:CD2	3:C:377:TYR:C	2.94	0.41
2:E:205:VAL:HG12	2:E:206:VAL:H	1.78	0.41
2:E:313:GLU:HB3	2:E:323:LYS:HG3	2.02	0.41
2:H:184:SER:O	2:H:188:ALA:N	2.54	0.41
2:H:314:MET:HB3	2:H:450:MET:HG3	2.02	0.41
2:H:397:GLU:O	2:H:398:ASP:C	2.59	0.41
3:I:101:LEU:O	3:I:104:ASP:N	2.54	0.41
3:I:169:ILE:HG12	3:I:180:VAL:CG1	2.50	0.41
3:I:235:LEU:H	3:I:235:LEU:CD1	2.28	0.41
3:I:311:GLN:OE1	3:I:319:ASN:HB3	2.21	0.41
1:J:171:ARG:HH21	1:J:173:VAL:CG2	2.34	0.41
2:K:222:SER:O	2:K:223:GLU:HB3	2.20	0.41
3:L:97:GLU:HA	3:L:100:ILE:CD1	2.51	0.41
3:L:169:ILE:O	3:L:177:GLN:HB2	2.19	0.41
2:B:186:VAL:O	2:B:186:VAL:HG13	2.20	0.41
2:B:254:ASN:ND2	2:B:256:GLN:OE1	2.54	0.41
3:C:156:ILE:HA	3:C:159:LYS:HD3	2.03	0.41
3:C:239:GLN:HB2	3:C:239:GLN:HE21	1.53	0.41
3:C:258:SER:OG	3:C:372:TRP:CE2	2.73	0.41
2:E:241:ASP:O	2:E:247:GLY:HA2	2.21	0.41
2:H:310:LEU:HB2	2:H:454:ILE:HG22	2.03	0.41
2:H:324:ALA:HB1	2:H:345:TYR:HE1	1.86	0.41
2:H:357:ALA:HA	2:H:439:ASN:CG	2.39	0.41
2:H:369:ILE:O	2:H:405:ASN:HB3	2.19	0.41
2:H:422:TYR:N	2:H:422:TYR:CD1	2.89	0.41
3:I:93:ILE:HD12	3:I:93:ILE:N	2.35	0.41
3:I:107:ILE:O	3:I:109:TYR:N	2.53	0.41
3:I:156:ILE:HA	3:I:159:LYS:HD3	2.03	0.41
1:J:122:LEU:HA	1:J:122:LEU:HD23	1.80	0.41
1:J:176:LYS:O	1:J:179:GLU:N	2.54	0.41
2:K:211:CYS:SG	2:K:250:THR:HG23	2.61	0.41
3:L:154:GLN:OE1	3:L:190:GLY:N	2.46	0.41
3:L:273:LYS:HA	3:L:273:LYS:HD3	1.81	0.41
3:L:367:ILE:HB	3:L:378:SER:OG	2.21	0.41
2:B:173:GLU:C	2:B:176:ARG:H	2.23	0.41
2:B:257:ASP:O	2:B:291:GLU:OE1	2.38	0.41
2:B:333:ASN:O	2:B:335:ALA:N	2.54	0.41
3:C:149:THR:O	3:C:159:LYS:NZ	2.50	0.41
3:C:191:TRP:CZ3	3:C:385:LYS:HE2	2.56	0.41
3:C:206:LYS:HB3	3:C:210:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLN:O	1:D:184:GLN:HB3	2.21	0.41
2:E:375:PHE:CD1	2:E:376:SER:N	2.88	0.41
3:F:284:GLY:O	3:F:286:ALA:N	2.45	0.41
3:F:295:PHE:CZ	4:P:1:GLY:HA2	2.56	0.41
3:F:314:THR:O	3:F:316:ASP:N	2.54	0.41
2:H:266:TRP:CE3	2:H:266:TRP:CA	3.03	0.41
2:H:389:ASP:OD1	2:H:390:PRO:HD2	2.21	0.41
3:I:315:TRP:CE3	3:I:328:GLU:HG2	2.55	0.41
3:I:322:PHE:CD1	3:I:338:LYS:HG3	2.51	0.41
2:K:217:LYS:HB3	3:L:213:GLU:HG3	2.02	0.41
2:K:341:SER:HA	2:K:371:ASN:OD1	2.20	0.41
3:L:192:THR:HG23	3:L:386:ILE:HG12	2.02	0.41
3:L:233:ILE:HG13	3:L:233:ILE:H	1.65	0.41
3:L:265:PHE:CZ	3:L:267:VAL:HG23	2.56	0.41
1:A:126:VAL:C	1:A:128:GLU:N	2.74	0.41
1:A:174:ASP:OD2	1:A:177:ASP:CB	2.69	0.41
2:B:227:ILE:HG12	2:B:238:VAL:HG11	2.02	0.41
2:B:254:ASN:HD21	2:B:256:GLN:HE22	1.69	0.41
2:B:266:TRP:CE2	2:B:380:ARG:NE	2.89	0.41
2:B:366:THR:HA	2:B:369:ILE:HG13	2.02	0.41
3:C:124:LEU:O	3:C:128:VAL:HG23	2.21	0.41
3:C:296:GLY:O	3:C:297:ASP:C	2.58	0.41
1:D:137:GLN:NE2	1:D:189:ILE:HA	2.36	0.41
1:D:188:VAL:HB	2:E:164:ASN:CG	2.41	0.41
2:E:225:TYR:CE1	2:E:242:MET:HE2	2.56	0.41
2:E:408:HIS:CE1	4:N:1:GLY:N	2.89	0.41
3:F:92:GLU:CG	3:F:93:ILE:H	2.32	0.41
3:F:154:GLN:HE21	3:F:158:ASN:ND2	2.18	0.41
3:F:288:ASP:O	3:F:371:THR:HG21	2.20	0.41
1:G:147:MET:CE	3:I:121:ILE:HD11	2.51	0.41
1:G:158:ILE:HA	1:G:158:ILE:HD12	1.80	0.41
1:G:184:GLN:NE2	1:G:185:LEU:N	2.68	0.41
2:H:202:ASN:O	2:H:204:PRO:HD3	2.20	0.41
2:H:398:ASP:CA	2:H:433:ASP:CB	2.91	0.41
3:I:252:ASP:OD1	3:I:256:ARG:O	2.38	0.41
2:K:223:GLU:HA	2:K:287:GLY:HA2	2.03	0.41
3:L:107:ILE:HG23	3:L:108:ARG:N	2.36	0.41
3:L:198:LEU:CA	3:L:381:LYS:HG2	2.51	0.41
2:B:171:ILE:O	2:B:175:LEU:HB3	2.21	0.41
2:B:176:ARG:HD2	2:B:179:ILE:CD1	2.50	0.41
2:B:179:ILE:HD11	3:C:117:ASN:ND2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:TYR:CB	2:B:298:LYS:NZ	2.84	0.41
2:B:281:ASP:OD1	2:B:281:ASP:N	2.53	0.41
2:B:371:ASN:C	2:B:373:MET:H	2.24	0.41
3:C:111:GLN:HG2	3:C:111:GLN:O	2.21	0.41
3:C:230:ASN:HA	3:C:233:ILE:HB	2.03	0.41
3:C:310:MET:HE2	3:C:321:LYS:HE3	2.03	0.41
2:E:191:GLU:C	2:E:193:CYS:H	2.24	0.41
3:F:115:ASN:N	3:F:115:ASN:HD22	2.19	0.41
3:F:211:TYR:CE2	3:F:333:GLY:HA3	2.56	0.41
3:F:293:PHE:HD2	3:F:370:ALA:HB1	1.86	0.41
2:H:317:TRP:CH2	2:H:448:ARG:HD3	2.55	0.41
3:I:191:TRP:CH2	3:I:247:ARG:CD	3.04	0.41
3:I:336:MET:HE1	3:I:340:HIS:CD2	2.56	0.41
1:J:137:GLN:NE2	1:J:189:ILE:HA	2.35	0.41
2:K:316:ASP:OD1	2:K:320:ASP:O	2.38	0.41
3:L:196:LYS:HG3	3:L:383:THR:HG22	2.03	0.41
3:L:205:LYS:HG2	3:L:331:GLY:CA	2.51	0.41
3:L:270:GLU:HA	3:L:273:LYS:O	2.21	0.41
1:A:142:ALA:O	1:A:146:ASP:N	2.54	0.40
1:A:167:ARG:HH21	2:B:192:TYR:HD2	1.69	0.40
2:B:223:GLU:HG2	2:B:225:TYR:HE1	1.85	0.40
2:B:322:VAL:HG21	2:B:349:ALA:HA	2.03	0.40
2:B:362:GLY:O	2:B:364:ASN:N	2.54	0.40
3:C:101:LEU:HD22	3:C:101:LEU:HA	1.93	0.40
3:C:356:LYS:HE2	3:C:356:LYS:HB3	1.78	0.40
3:F:310:MET:C	3:F:311:GLN:O	2.56	0.40
3:F:329:GLN:HE21	3:F:361:ASN:HD22	1.70	0.40
2:H:207:SER:OG	2:H:208:GLY:N	2.53	0.40
2:H:326:TYR:HE1	2:H:354:MET:HG3	1.87	0.40
3:I:96:TYR:CD1	3:I:97:GLU:N	2.89	0.40
3:I:171:PRO:O	3:I:172:LEU:C	2.60	0.40
2:K:156:THR:HG22	2:K:157:VAL:N	2.36	0.40
2:K:215:ILE:CG2	2:K:216:ARG:N	2.85	0.40
3:L:191:TRP:CE3	3:L:386:ILE:O	2.74	0.40
3:C:114:TYR:C	3:C:116:SER:H	2.24	0.40
2:E:238:VAL:HG23	2:E:294:LEU:HD13	2.02	0.40
2:E:375:PHE:HD1	2:E:376:SER:N	2.20	0.40
3:F:205:LYS:HG2	3:F:331:GLY:CA	2.51	0.40
3:F:251:GLU:HG3	3:F:257:THR:CG2	2.51	0.40
1:G:140:VAL:HG12	3:I:114:TYR:HD1	1.86	0.40
2:H:205:VAL:H	3:I:217:HIS:HA	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:338:TYR:O	2:H:339:GLN:C	2.58	0.40
2:H:453:LYS:H	2:H:453:LYS:HG2	1.79	0.40
1:J:124:ARG:HG2	1:J:124:ARG:NH1	2.36	0.40
1:J:132:HIS:C	1:J:134:GLN:H	2.24	0.40
2:K:210:GLU:OE1	2:K:212:GLU:HB3	2.21	0.40
2:K:338:TYR:O	2:K:339:GLN:C	2.60	0.40
2:K:402:TRP:CG	2:K:403:TRP:N	2.89	0.40
3:L:105:SER:O	3:L:106:SER:C	2.60	0.40
3:L:299:PRO:O	3:L:301:ASP:N	2.45	0.40
1:A:184:GLN:NE2	1:A:185:LEU:N	2.69	0.40
2:B:252:ILE:HG12	2:B:452:MET:O	2.20	0.40
2:B:324:ALA:HB1	2:B:345:TYR:HE1	1.86	0.40
3:C:191:TRP:HH2	3:C:247:ARG:CD	2.34	0.40
3:C:289:ALA:HB2	3:C:371:THR:OG1	2.22	0.40
1:D:122:LEU:CD2	3:F:98:ALA:HB2	2.52	0.40
2:E:156:THR:HA	2:E:160:ASN:HB3	2.03	0.40
2:E:328:GLY:HA3	2:E:343:ASN:OD1	2.22	0.40
3:F:246:LEU:HB2	3:F:265:PHE:CB	2.51	0.40
2:H:153:ILE:O	2:H:156:THR:HG23	2.21	0.40
2:H:175:LEU:HD12	2:H:179:ILE:HD11	2.03	0.40
2:H:199:VAL:N	3:I:140:LYS:O	2.53	0.40
2:H:223:GLU:HB3	2:H:287:GLY:HA2	1.98	0.40
2:H:266:TRP:CZ2	2:H:380:ARG:NE	2.89	0.40
2:H:310:LEU:CA	2:H:454:ILE:HG22	2.47	0.40
2:H:385:TRP:CE3	4:Q:3:ARG:HG3	2.57	0.40
2:H:421:GLN:HA	2:H:444:TRP:O	2.22	0.40
3:I:250:LEU:HD23	3:I:372:TRP:CE3	2.55	0.40
3:I:252:ASP:HB2	3:I:377:TYR:OH	2.22	0.40
3:L:341:ALA:HB1	3:L:370:ALA:HB3	2.03	0.40
1:A:144:LEU:HD11	1:A:182:GLN:CA	2.52	0.40
2:B:357:ALA:CA	2:B:439:ASN:HD21	2.21	0.40
2:B:393:GLN:O	2:B:395:SER:N	2.55	0.40
3:C:235:LEU:H	3:C:235:LEU:CD1	2.27	0.40
2:E:225:TYR:HB3	2:E:226:LEU:H	1.64	0.40
2:E:302:LEU:O	2:E:305:MET:HB3	2.22	0.40
3:F:204:PHE:O	3:F:206:LYS:N	2.53	0.40
3:F:307:HIS:O	3:F:310:MET:HB2	2.22	0.40
3:F:359:THR:HA	3:F:360:PRO:HD3	1.76	0.40
2:H:210:GLU:OE1	2:H:212:GLU:CB	2.69	0.40
2:H:304:ARG:HG3	2:H:304:ARG:NH1	2.37	0.40
3:I:310:MET:HA	3:I:310:MET:CE	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:328:GLU:O	3:I:331:GLY:N	2.53	0.40
3:I:377:TYR:CD2	3:I:377:TYR:C	2.95	0.40
2:K:190:MET:HG3	3:L:131:LEU:HD13	2.04	0.40
2:K:265:LYS:HB3	2:K:379:ASP:OD2	2.21	0.40
3:L:227:TRP:CZ3	3:L:384:MET:HE2	2.54	0.40
3:L:386:ILE:O	3:L:387:ILE:HB	2.21	0.40
1:A:132:HIS:O	1:A:135:LEU:N	2.53	0.40
1:A:140:VAL:HA	1:A:143:GLN:HB2	2.04	0.40
2:B:163:THR:O	2:B:167:VAL:CG2	2.70	0.40
2:B:177:SER:C	2:B:180:GLN:HG2	2.42	0.40
3:C:196:LYS:O	3:C:225:GLU:HA	2.22	0.40
3:C:204:PHE:CE2	3:C:227:TRP:HB2	2.56	0.40
3:F:154:GLN:HE21	3:F:158:ASN:CG	2.25	0.40
3:F:246:LEU:HD12	3:F:386:ILE:HG22	2.03	0.40
2:H:165:LEU:HD13	2:H:165:LEU:HA	1.88	0.40
2:H:191:GLU:C	2:H:193:CYS:N	2.72	0.40
2:H:236:TYR:HB2	2:H:298:LYS:HZ3	1.87	0.40
3:I:237:SER:O	3:I:266:LYS:HG3	2.22	0.40
2:K:263:GLY:HA2	2:K:400:GLY:HA2	2.03	0.40
3:L:230:ASN:O	3:L:232:LYS:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	72/87 (83%)	44 (61%)	15 (21%)	13 (18%)	0 0
1	D	69/87 (79%)	50 (72%)	15 (22%)	4 (6%)	1 5
1	G	72/87 (83%)	44 (61%)	14 (19%)	14 (19%)	0 0
1	J	77/87 (88%)	55 (71%)	18 (23%)	4 (5%)	2 6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	305/328 (93%)	186 (61%)	76 (25%)	43 (14%)	0	0
2	E	302/328 (92%)	235 (78%)	41 (14%)	26 (9%)	1	2
2	H	305/328 (93%)	196 (64%)	64 (21%)	45 (15%)	0	0
2	K	303/328 (92%)	236 (78%)	47 (16%)	20 (7%)	1	3
3	C	303/323 (94%)	167 (55%)	86 (28%)	50 (16%)	0	0
3	F	298/323 (92%)	207 (70%)	69 (23%)	22 (7%)	1	2
3	I	303/323 (94%)	170 (56%)	81 (27%)	52 (17%)	0	0
3	L	298/323 (92%)	207 (70%)	68 (23%)	23 (8%)	1	2
4	M	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
4	N	3/5 (60%)	0	2 (67%)	1 (33%)	0	0
4	O	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
4	P	3/5 (60%)	1 (33%)	1 (33%)	1 (33%)	0	0
4	Q	3/5 (60%)	1 (33%)	1 (33%)	1 (33%)	0	0
4	R	3/5 (60%)	0	2 (67%)	1 (33%)	0	0
4	S	3/5 (60%)	3 (100%)	0	0	100	100
4	T	3/5 (60%)	1 (33%)	1 (33%)	1 (33%)	0	0
All	All	2731/2992 (91%)	1806 (66%)	604 (22%)	321 (12%)	0	1

All (321) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	SER
1	A	190	ALA
2	B	227	ILE
2	B	230	ASP
2	B	259	SER
2	B	266	TRP
2	B	295	GLY
2	B	338	TYR
2	B	339	GLN
2	B	351	ASN
2	B	366	THR
2	B	447	MET
3	C	162	LYS
3	C	164	SER
3	C	203	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	218	LEU
3	C	219	SER
3	C	221	THR
3	C	224	THR
3	C	259	THR
3	C	271	ALA
3	C	273	LYS
3	C	317	ASN
2	E	156	THR
2	E	160	ASN
2	E	164	ASN
2	E	205	VAL
2	E	206	VAL
2	E	229	PRO
2	E	233	VAL
2	E	235	PRO
2	E	399	GLY
3	F	104	ASP
3	F	159	LYS
3	F	240	SER
3	F	241	ALA
3	F	371	THR
3	F	374	THR
3	F	389	PHE
3	F	390	ASN
1	G	124	ARG
1	G	125	LYS
1	G	126	VAL
1	G	164	SER
1	G	166	SER
2	H	163	THR
2	H	167	VAL
2	H	174	ASN
2	H	182	LEU
2	H	227	ILE
2	H	230	ASP
2	H	266	TRP
2	H	295	GLY
2	H	338	TYR
2	H	351	ASN
2	H	366	THR
2	H	435	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	443	SER
2	H	447	MET
3	I	97	GLU
3	I	162	LYS
3	I	164	SER
3	I	203	ASP
3	I	218	LEU
3	I	219	SER
3	I	221	THR
3	I	224	THR
3	I	248	VAL
3	I	259	THR
3	I	271	ALA
3	I	273	LYS
3	I	317	ASN
3	I	339	CYS
1	J	151	GLU
2	K	156	THR
2	K	205	VAL
2	K	206	VAL
2	K	229	PRO
2	K	233	VAL
2	K	235	PRO
2	K	399	GLY
3	L	159	LYS
3	L	240	SER
3	L	241	ALA
3	L	371	THR
3	L	374	THR
3	L	389	PHE
3	L	390	ASN
1	A	162	ARG
1	A	185	LEU
1	A	188	VAL
2	B	153	ILE
2	B	199	VAL
2	B	211	CYS
2	B	231	SER
2	B	256	GLN
2	B	320	ASP
2	B	362	GLY
2	B	365	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	394	CYS
2	B	399	GLY
2	B	424	TRP
2	B	435	VAL
2	B	443	SER
3	C	115	ASN
3	C	151	LYS
3	C	161	ALA
3	C	205	LYS
3	C	248	VAL
3	C	265	PHE
3	C	284	GLY
3	C	297	ASP
3	C	370	ALA
3	C	372	TRP
3	C	390	ASN
1	D	124	ARG
1	D	162	ARG
2	E	157	VAL
2	E	301	GLN
2	E	398	ASP
2	E	405	ASN
2	E	406	ARG
3	F	161	ALA
3	F	234	HIS
3	F	285	ASP
3	F	325	ASN
1	G	121	VAL
1	G	130	VAL
1	G	160	SER
1	G	162	ARG
1	G	191	LYS
2	H	170	SER
2	H	211	CYS
2	H	231	SER
2	H	256	GLN
2	H	259	SER
2	H	320	ASP
2	H	339	GLN
2	H	362	GLY
2	H	365	ARG
2	H	394	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	399	GLY
2	H	424	TRP
3	I	98	ALA
3	I	100	ILE
3	I	111	GLN
3	I	118	ASN
3	I	126	GLU
3	I	151	LYS
3	I	161	ALA
3	I	265	PHE
3	I	284	GLY
3	I	370	ALA
3	I	372	TRP
3	I	390	ASN
2	K	157	VAL
2	K	164	ASN
2	K	247	GLY
2	K	398	ASP
2	K	407	CYS
3	L	161	ALA
3	L	285	ASP
3	L	315	TRP
3	L	325	ASN
3	L	339	CYS
1	A	125	LYS
1	A	130	VAL
1	A	160	SER
2	B	158	ASN
2	B	192	TYR
2	B	202	ASN
2	B	281	ASP
2	B	284	ASN
2	B	355	ASP
2	B	359	GLN
2	B	439	ASN
3	C	194	PHE
3	C	208	TRP
3	C	220	PRO
3	C	332	SER
3	C	369	TRP
1	D	127	ILE
1	D	151	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	223	GLU
2	E	256	GLN
3	F	132	GLU
3	F	224	THR
3	F	278	TYR
3	F	298	ASP
1	G	151	GLU
2	H	162	PRO
2	H	192	TYR
2	H	199	VAL
2	H	277	ALA
2	H	281	ASP
2	H	284	ASN
2	H	355	ASP
2	H	359	GLN
3	I	115	ASN
3	I	205	LYS
3	I	208	TRP
3	I	209	ILE
3	I	220	PRO
3	I	297	ASP
3	I	331	GLY
3	I	332	SER
3	I	369	TRP
1	J	162	ARG
2	K	256	GLN
2	K	301	GLN
2	K	405	ASN
3	L	100	ILE
3	L	224	THR
3	L	234	HIS
3	L	278	TYR
3	L	298	ASP
3	L	323	GLU
4	P	2	PRO
1	A	151	GLU
1	A	163	GLY
1	A	174	ASP
2	B	154	ASP
2	B	182	LEU
2	B	277	ALA
2	B	327	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	334	GLU
2	B	388	SER
3	C	104	ASP
3	C	157	ALA
3	C	209	ILE
3	C	222	GLY
3	C	243	PRO
3	C	251	GLU
3	C	331	GLY
3	C	341	ALA
3	C	382	THR
2	E	170	SER
2	E	171	ILE
2	E	192	TYR
3	F	172	LEU
3	F	198	LEU
3	F	323	GLU
1	G	120	GLU
2	H	317	TRP
2	H	327	GLY
2	H	334	GLU
2	H	388	SER
2	H	407	CYS
2	H	439	ASN
3	I	108	ARG
3	I	157	ALA
3	I	171	PRO
3	I	178	PHE
3	I	194	PHE
3	I	222	GLY
3	I	251	GLU
3	I	264	MET
3	I	341	ALA
2	K	223	GLU
3	L	132	GLU
3	L	171	PRO
1	A	173	VAL
2	B	162	PRO
2	B	235	PRO
2	B	267	ASP
3	C	97	GLU
3	C	98	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	127	LYS
3	C	171	PRO
3	C	172	LEU
3	C	193	VAL
3	C	270	GLU
2	E	281	ASP
2	E	383	ASP
1	G	122	LEU
2	H	179	ILE
2	H	202	ASN
3	I	243	PRO
3	I	270	GLU
3	I	382	THR
2	K	305	MET
2	K	435	VAL
3	L	198	LEU
3	L	353	THR
4	N	2	PRO
2	B	317	TRP
3	C	111	GLN
3	C	178	PHE
3	C	264	MET
2	E	247	GLY
2	E	302	LEU
2	E	305	MET
3	F	175	ASN
2	H	235	PRO
3	I	360	PRO
2	K	170	SER
3	L	279	ALA
4	R	2	PRO
3	C	128	VAL
3	F	171	PRO
1	G	189	ILE
2	H	267	ASP
2	H	276	VAL
3	I	128	VAL
3	I	193	VAL
1	J	133	ILE
2	K	161	ILE
4	Q	2	PRO
2	B	276	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	360	PRO
3	C	387	ILE
2	E	435	VAL
3	I	188	GLY
3	C	188	GLY
2	E	414	GLY
1	J	152	VAL
4	T	2	PRO
2	B	186	VAL
3	F	138	PRO
3	I	387	ILE
1	A	127	ILE

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	69/82 (84%)	58 (84%)	11 (16%)	2 7
1	D	66/82 (80%)	57 (86%)	9 (14%)	3 11
1	G	69/82 (84%)	60 (87%)	9 (13%)	4 12
1	J	74/82 (90%)	62 (84%)	12 (16%)	2 7
2	B	265/286 (93%)	235 (89%)	30 (11%)	6 18
2	E	262/286 (92%)	233 (89%)	29 (11%)	6 19
2	H	265/286 (93%)	236 (89%)	29 (11%)	6 19
2	K	263/286 (92%)	234 (89%)	29 (11%)	6 19
3	C	257/269 (96%)	229 (89%)	28 (11%)	6 19
3	F	253/269 (94%)	221 (87%)	32 (13%)	4 13
3	I	257/269 (96%)	228 (89%)	29 (11%)	6 18
3	L	253/269 (94%)	218 (86%)	35 (14%)	3 10
4	M	3/3 (100%)	3 (100%)	0	100 100
4	N	3/3 (100%)	3 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	O	3/3 (100%)	3 (100%)	0	100	100
4	P	3/3 (100%)	3 (100%)	0	100	100
4	Q	3/3 (100%)	3 (100%)	0	100	100
4	R	3/3 (100%)	3 (100%)	0	100	100
4	S	3/3 (100%)	3 (100%)	0	100	100
4	T	3/3 (100%)	3 (100%)	0	100	100
All	All	2377/2572 (92%)	2095 (88%)	282 (12%)	5	15

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	144	LEU
1	A	155	ASP
1	A	159	ARG
1	A	167	ARG
1	A	171	ARG
1	A	172	GLU
1	A	178	TYR
1	A	179	GLU
1	A	185	LEU
1	A	186	GLU
2	B	153	ILE
2	B	155	GLU
2	B	166	ARG
2	B	172	LEU
2	B	180	GLN
2	B	189	GLN
2	B	190	MET
2	B	194	ARG
2	B	210	GLU
2	B	253	GLN
2	B	256	GLN
2	B	261	ASP
2	B	266	TRP
2	B	267	ASP
2	B	281	ASP
2	B	284	ASN
2	B	285	TYR
2	B	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	310	LEU
2	B	315	GLU
2	B	316	ASP
2	B	323	LYS
2	B	346	ARG
2	B	351	ASN
2	B	359	GLN
2	B	376	SER
2	B	387	THR
2	B	422	TYR
2	B	439	ASN
2	B	447	MET
3	C	96	TYR
3	C	101	LEU
3	C	103	HIS
3	C	118	ASN
3	C	134	GLN
3	C	148	ILE
3	C	163	GLN
3	C	166	LEU
3	C	167	TYR
3	C	192	THR
3	C	217	HIS
3	C	230	ASN
3	C	232	LYS
3	C	235	LEU
3	C	239	GLN
3	C	246	LEU
3	C	261	ASP
3	C	264	MET
3	C	276	LEU
3	C	294	ASP
3	C	315	TRP
3	C	317	ASN
3	C	323	GLU
3	C	329	GLN
3	C	335	TRP
3	C	365	ASN
3	C	377	TYR
3	C	383	THR
1	D	124	ARG
1	D	132	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	135	LEU
1	D	143	GLN
1	D	148	LYS
1	D	161	CYS
1	D	167	ARG
1	D	169	LEU
1	D	182	GLN
2	E	154	ASP
2	E	157	VAL
2	E	158	ASN
2	E	164	ASN
2	E	180	GLN
2	E	191	GLU
2	E	194	ARG
2	E	195	THR
2	E	210	GLU
2	E	221	THR
2	E	253	GLN
2	E	257	ASP
2	E	264	ARG
2	E	271	GLN
2	E	279	ASN
2	E	301	GLN
2	E	323	LYS
2	E	340	ILE
2	E	348	THR
2	E	351	ASN
2	E	359	GLN
2	E	366	THR
2	E	375	PHE
2	E	376	SER
2	E	386	LEU
2	E	391	ARG
2	E	395	SER
2	E	398	ASP
2	E	433	ASP
3	F	96	TYR
3	F	102	THR
3	F	106	SER
3	F	107	ILE
3	F	124	LEU
3	F	147	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	148	ILE
3	F	164	SER
3	F	171	PRO
3	F	173	LYS
3	F	176	GLN
3	F	194	PHE
3	F	198	LEU
3	F	202	VAL
3	F	205	LYS
3	F	221	THR
3	F	225	GLU
3	F	239	GLN
3	F	250	LEU
3	F	259	THR
3	F	264	MET
3	F	278	TYR
3	F	285	ASP
3	F	290	PHE
3	F	294	ASP
3	F	297	ASP
3	F	313	SER
3	F	325	ASN
3	F	354	TYR
3	F	365	ASN
3	F	383	THR
3	F	389	PHE
1	G	122	LEU
1	G	128	GLU
1	G	137	GLN
1	G	141	ARG
1	G	155	ASP
1	G	164	SER
1	G	179	GLU
1	G	182	GLN
1	G	186	GLU
2	H	155	GLU
2	H	161	ILE
2	H	166	ARG
2	H	175	LEU
2	H	182	LEU
2	H	190	MET
2	H	194	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	210	GLU
2	H	253	GLN
2	H	256	GLN
2	H	261	ASP
2	H	266	TRP
2	H	267	ASP
2	H	281	ASP
2	H	284	ASN
2	H	285	TYR
2	H	301	GLN
2	H	310	LEU
2	H	315	GLU
2	H	323	LYS
2	H	346	ARG
2	H	351	ASN
2	H	359	GLN
2	H	376	SER
2	H	387	THR
2	H	422	TYR
2	H	425	ASP
2	H	439	ASN
2	H	447	MET
3	I	117	ASN
3	I	121	ILE
3	I	125	LYS
3	I	134	GLN
3	I	145	ILE
3	I	148	ILE
3	I	163	GLN
3	I	166	LEU
3	I	167	TYR
3	I	192	THR
3	I	217	HIS
3	I	230	ASN
3	I	232	LYS
3	I	235	LEU
3	I	239	GLN
3	I	246	LEU
3	I	257	THR
3	I	261	ASP
3	I	264	MET
3	I	276	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	294	ASP
3	I	315	TRP
3	I	317	ASN
3	I	323	GLU
3	I	329	GLN
3	I	335	TRP
3	I	365	ASN
3	I	377	TYR
3	I	383	THR
1	J	118	ARG
1	J	131	GLN
1	J	132	HIS
1	J	134	GLN
1	J	135	LEU
1	J	138	LYS
1	J	157	LYS
1	J	161	CYS
1	J	167	ARG
1	J	169	LEU
1	J	188	VAL
1	J	191	LYS
2	K	157	VAL
2	K	165	LEU
2	K	166	ARG
2	K	167	VAL
2	K	180	GLN
2	K	191	GLU
2	K	194	ARG
2	K	195	THR
2	K	210	GLU
2	K	221	THR
2	K	253	GLN
2	K	257	ASP
2	K	264	ARG
2	K	279	ASN
2	K	301	GLN
2	K	323	LYS
2	K	340	ILE
2	K	348	THR
2	K	351	ASN
2	K	359	GLN
2	K	363	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	366	THR
2	K	375	PHE
2	K	376	SER
2	K	386	LEU
2	K	391	ARG
2	K	395	SER
2	K	398	ASP
2	K	433	ASP
3	L	95	LYS
3	L	96	TYR
3	L	102	THR
3	L	104	ASP
3	L	106	SER
3	L	107	ILE
3	L	109	TYR
3	L	147	ASP
3	L	148	ILE
3	L	164	SER
3	L	171	PRO
3	L	173	LYS
3	L	176	GLN
3	L	194	PHE
3	L	198	LEU
3	L	202	VAL
3	L	205	LYS
3	L	211	TYR
3	L	221	THR
3	L	225	GLU
3	L	239	GLN
3	L	250	LEU
3	L	259	THR
3	L	264	MET
3	L	276	LEU
3	L	278	TYR
3	L	285	ASP
3	L	290	PHE
3	L	294	ASP
3	L	297	ASP
3	L	313	SER
3	L	325	ASN
3	L	365	ASN
3	L	383	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	389	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	HIS
1	A	139	ASN
1	A	143	GLN
1	A	181	GLN
1	A	182	GLN
1	A	184	GLN
2	B	164	ASN
2	B	174	ASN
2	B	253	GLN
2	B	254	ASN
2	B	256	GLN
2	B	296	ASN
2	B	301	GLN
2	B	351	ASN
2	B	359	GLN
2	B	405	ASN
2	B	411	ASN
2	B	421	GLN
2	B	429	HIS
2	B	439	ASN
3	C	118	ASN
3	C	119	GLN
3	C	134	GLN
3	C	158	ASN
3	C	163	GLN
3	C	177	GLN
3	C	210	GLN
3	C	230	ASN
3	C	317	ASN
3	C	329	GLN
3	C	340	HIS
3	C	365	ASN
1	D	134	GLN
1	D	137	GLN
1	D	143	GLN
1	D	187	GLN
2	E	158	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	174	ASN
2	E	189	GLN
2	E	256	GLN
2	E	279	ASN
2	E	284	ASN
2	E	296	ASN
2	E	301	GLN
2	E	325	HIS
2	E	333	ASN
2	E	336	ASN
2	E	351	ASN
2	E	405	ASN
2	E	408	HIS
2	E	421	GLN
2	E	439	ASN
3	F	103	HIS
3	F	111	GLN
3	F	115	ASN
3	F	119	GLN
3	F	136	GLN
3	F	158	ASN
3	F	163	GLN
3	F	217	HIS
3	F	230	ASN
3	F	254	ASN
3	F	308	ASN
3	F	311	GLN
3	F	317	ASN
3	F	319	ASN
3	F	325	ASN
3	F	329	GLN
3	F	365	ASN
1	G	134	GLN
1	G	182	GLN
1	G	184	GLN
2	H	174	ASN
2	H	189	GLN
2	H	253	GLN
2	H	254	ASN
2	H	256	GLN
2	H	296	ASN
2	H	301	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	351	ASN
2	H	359	GLN
2	H	405	ASN
2	H	411	ASN
2	H	421	GLN
2	H	429	HIS
2	H	439	ASN
3	I	103	HIS
3	I	111	GLN
3	I	117	ASN
3	I	119	GLN
3	I	123	ASN
3	I	136	GLN
3	I	158	ASN
3	I	163	GLN
3	I	177	GLN
3	I	210	GLN
3	I	230	ASN
3	I	317	ASN
3	I	329	GLN
3	I	340	HIS
3	I	345	ASN
3	I	365	ASN
1	J	131	GLN
1	J	137	GLN
1	J	139	ASN
1	J	143	GLN
1	J	181	GLN
1	J	184	GLN
1	J	187	GLN
2	K	160	ASN
2	K	189	GLN
2	K	256	GLN
2	K	271	GLN
2	K	296	ASN
2	K	301	GLN
2	K	325	HIS
2	K	336	ASN
2	K	351	ASN
2	K	405	ASN
2	K	421	GLN
2	K	439	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	L	111	GLN
3	L	115	ASN
3	L	136	GLN
3	L	158	ASN
3	L	163	GLN
3	L	217	HIS
3	L	230	ASN
3	L	254	ASN
3	L	308	ASN
3	L	311	GLN
3	L	317	ASN
3	L	319	ASN
3	L	325	ASN
3	L	329	GLN
3	L	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	470	2	14,14,15	0.78	0	17,19,21	0.78	1 (5%)
5	NAG	H	470	2	14,14,15	0.70	0	17,19,21	0.97	1 (5%)
5	NAG	K	470	2	14,14,15	0.50	0	17,19,21	0.94	1 (5%)
5	NAG	E	470	2	14,14,15	0.61	0	17,19,21	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	470	2	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	H	470	2	-	6/6/23/26	0/1/1/1
5	NAG	K	470	2	-	4/6/23/26	0/1/1/1
5	NAG	E	470	2	1/1/5/7	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	470	NAG	C2-N2-C7	-2.50	119.34	122.90
5	B	470	NAG	C2-N2-C7	-2.11	119.89	122.90
5	K	470	NAG	C2-N2-C7	-2.04	120.00	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	470	NAG	C1
5	E	470	NAG	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	470	NAG	C8-C7-N2-C2
5	E	470	NAG	O7-C7-N2-C2
5	H	470	NAG	C8-C7-N2-C2
5	H	470	NAG	O7-C7-N2-C2
5	K	470	NAG	C8-C7-N2-C2
5	K	470	NAG	O7-C7-N2-C2
5	B	470	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	470	NAG	O7-C7-N2-C2
5	K	470	NAG	C4-C5-C6-O6
5	K	470	NAG	O5-C5-C6-O6
5	H	470	NAG	O5-C5-C6-O6
5	H	470	NAG	C1-C2-N2-C7
5	B	470	NAG	O5-C5-C6-O6
5	E	470	NAG	C4-C5-C6-O6
5	H	470	NAG	C3-C2-N2-C7
5	H	470	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	470	NAG	1	0
5	H	470	NAG	4	0
5	K	470	NAG	3	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	74/87 (85%)	-0.05	2 (2%) 54 50	62, 83, 105, 111	0
1	D	71/87 (81%)	-0.34	0 100 100	29, 56, 89, 96	0
1	G	74/87 (85%)	-0.17	2 (2%) 54 50	62, 81, 100, 115	0
1	J	79/87 (90%)	-0.34	0 100 100	35, 58, 108, 122	0
2	B	307/328 (93%)	-0.26	3 (0%) 82 82	42, 76, 99, 108	0
2	E	304/328 (92%)	-0.43	0 100 100	27, 51, 79, 99	0
2	H	307/328 (93%)	-0.29	4 (1%) 77 77	42, 76, 99, 107	0
2	K	305/328 (92%)	-0.45	0 100 100	25, 51, 80, 97	0
3	C	305/323 (94%)	-0.09	12 (3%) 39 35	49, 83, 107, 116	0
3	F	300/323 (92%)	-0.35	1 (0%) 94 94	39, 66, 92, 116	0
3	I	305/323 (94%)	-0.14	12 (3%) 39 35	54, 84, 109, 136	0
3	L	300/323 (92%)	-0.37	0 100 100	36, 66, 91, 117	0
4	M	4/5 (80%)	0.54	1 (25%) 0 0	63, 64, 65, 97	0
4	N	4/5 (80%)	0.19	0 100 100	41, 48, 60, 86	0
4	O	4/5 (80%)	0.24	0 100 100	90, 94, 99, 106	0
4	P	4/5 (80%)	-0.21	0 100 100	64, 73, 79, 93	0
4	Q	4/5 (80%)	0.10	0 100 100	63, 64, 64, 94	0
4	R	4/5 (80%)	-0.38	0 100 100	44, 50, 62, 87	0
4	S	4/5 (80%)	0.03	0 100 100	89, 100, 101, 104	0
4	T	4/5 (80%)	-0.35	0 100 100	66, 73, 74, 91	0
All	All	2763/2992 (92%)	-0.29	37 (1%) 77 77	25, 71, 100, 136	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	344	LEU	5.1
3	I	236	ILE	4.0
3	I	344	LEU	3.9
3	C	241	ALA	3.9
1	A	169	LEU	3.8
3	C	236	ILE	3.6
4	M	4	PRO	3.5
3	C	305	THR	3.3
3	C	165	GLY	3.2
3	I	180	VAL	3.0
1	G	137	GLN	2.9
2	H	168	LEU	2.9
3	I	235	LEU	2.8
2	H	206	VAL	2.8
2	H	445	TYR	2.8
2	B	353	LEU	2.8
3	I	149	THR	2.7
3	C	357	ALA	2.7
2	B	445	TYR	2.6
3	C	266	LYS	2.6
3	I	168	PHE	2.6
3	I	191	TRP	2.6
3	I	178	PHE	2.5
2	B	158	ASN	2.4
3	C	265	PHE	2.4
3	I	289	ALA	2.4
3	C	341	ALA	2.3
3	C	389	PHE	2.3
3	C	240	SER	2.2
1	A	127	ILE	2.2
3	C	191	TRP	2.1
1	G	127	ILE	2.1
2	H	338	TYR	2.1
3	I	179	LEU	2.0
3	I	313	SER	2.0
3	I	293	PHE	2.0
3	F	179	LEU	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	470	14/15	0.78	0.25	94,105,117,117	0
5	NAG	B	470	14/15	0.84	0.12	60,83,88,91	0
6	CA	E	3	1/1	0.84	0.09	90,90,90,90	0
6	CA	K	3	1/1	0.86	0.07	89,89,89,89	0
5	NAG	E	470	14/15	0.90	0.19	68,77,92,92	0
6	CA	E	2	1/1	0.91	0.17	57,57,57,57	0
6	CA	I	1	1/1	0.92	0.22	76,76,76,76	0
5	NAG	K	470	14/15	0.92	0.17	65,75,82,89	0
6	CA	F	1	1/1	0.93	0.15	54,54,54,54	0
6	CA	H	2	1/1	0.93	0.18	83,83,83,83	0
6	CA	B	2	1/1	0.94	0.19	90,90,90,90	0
6	CA	C	1	1/1	0.94	0.15	78,78,78,78	0
6	CA	K	2	1/1	0.96	0.22	60,60,60,60	0
6	CA	L	1	1/1	0.97	0.09	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.