Full wwPDB X-ray Structure Validation Report

Aug 2, 2016 – 09:14 PM EDT

PDB ID	:	1HT1
Title	:	Nucleotide-Dependent Conformational Changes in a Protease-Associated ATPase HslU
Authors	:	Wang, J.; Song, J.J.; Seong, I.S.; Franklin, M.C.; Kamtekar, S.; Eom, S.H.; Chung, C.H.
Deposited on	:	2000-12-27
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

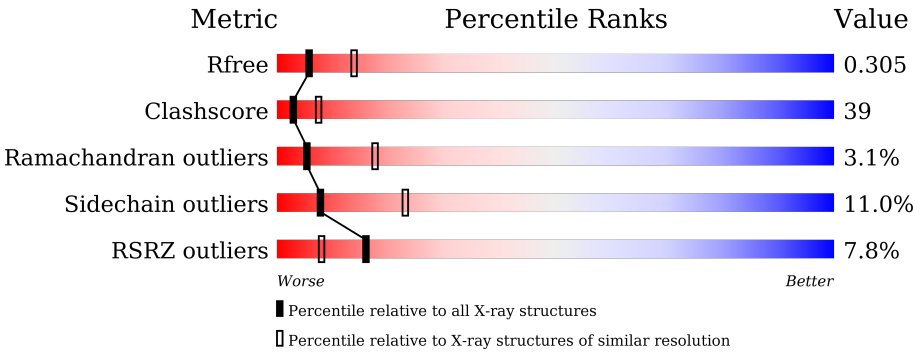
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.80 Å.

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



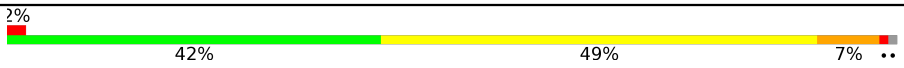
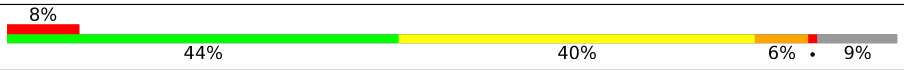
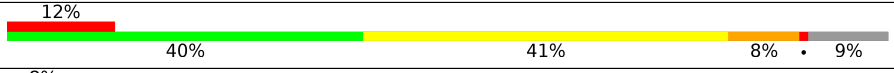
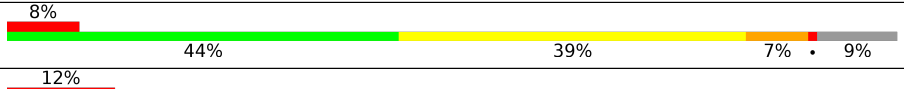
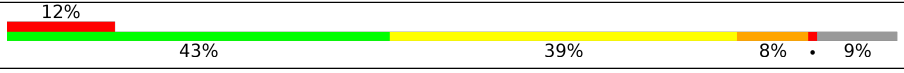
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	175	2% 54% 42%
1	B	175	7% 38% 54% 7%
1	C	175	8% 37% 53% 9%
1	D	175	4% 53% 39% 7%
1	V	175	7% 34% 56% 9%
1	X	175	2% 52% 40% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Y	175	
1	Z	175	
2	E	449	
2	F	449	
2	G	449	
2	I	449	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23636 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 HEAT SHOCK LOCUS HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	D	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	V	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	X	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	A	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	B	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	Z	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			
1	Y	174	Total	C	N	O	S	0	0	0
			1328	834	237	253	4			

- Molecule 2 is a protein called HEAT SHOCK LOCUS HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	F	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	G	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			
2	I	408	Total	C	N	O	S	0	0	0
			3226	2014	577	625	10			

There are 28 discrepancies between the modelled and reference sequences:

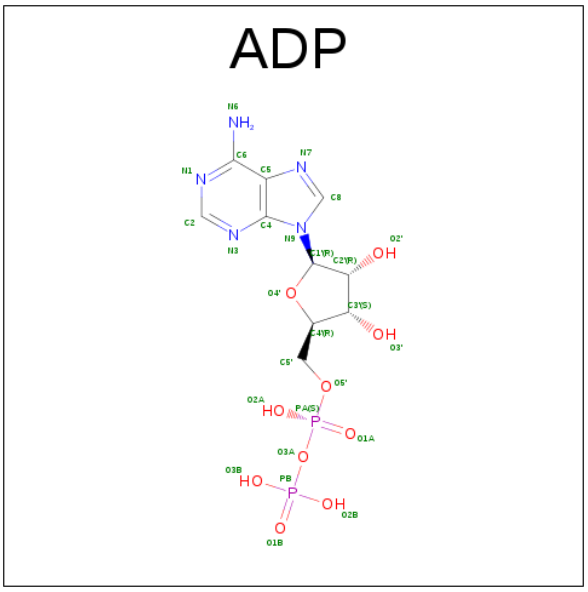
Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
E	1	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
F	1	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
G	1	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-5	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-4	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-3	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-2	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	-1	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	0	HIS	-	EXPRESSION TAG	UNP P0A6H5
I	1	HIS	-	EXPRESSION TAG	UNP P0A6H5

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

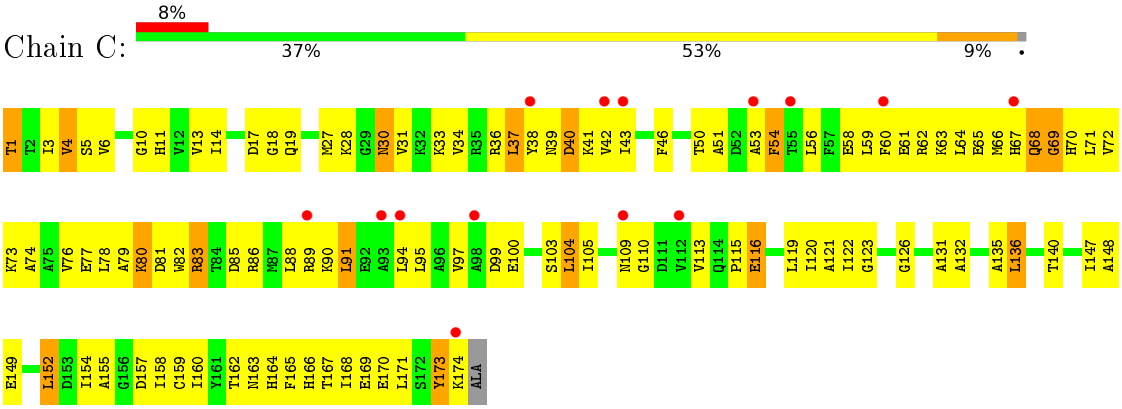


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

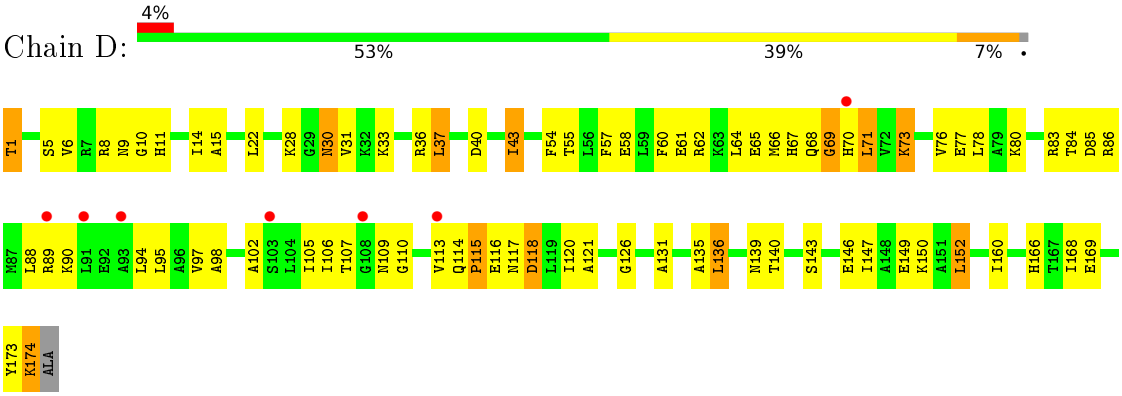
3 Residue-property plots (i)

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

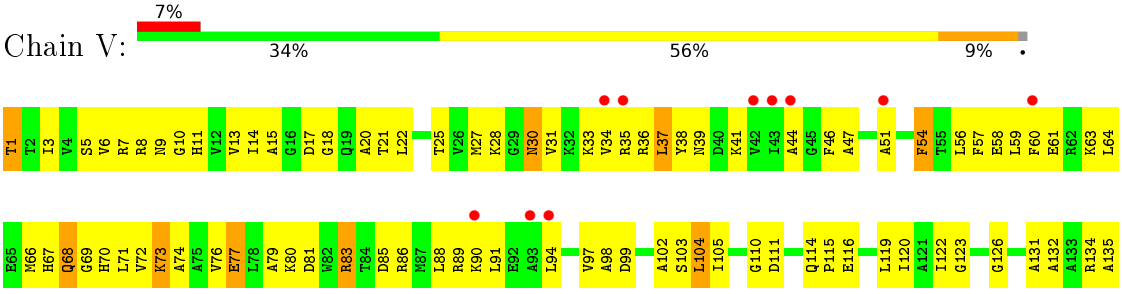
- Molecule 1: HEAT SHOCK LOCUS HSLV

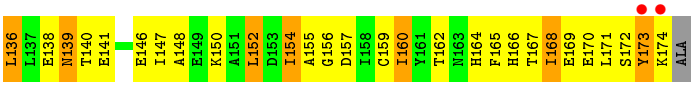


- Molecule 1: HEAT SHOCK LOCUS HSLV



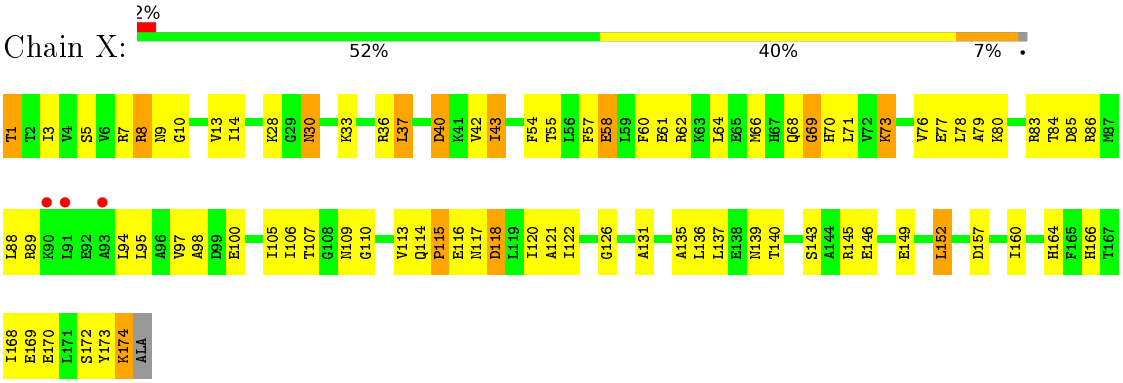
- Molecule 1: HEAT SHOCK LOCUS HSLV





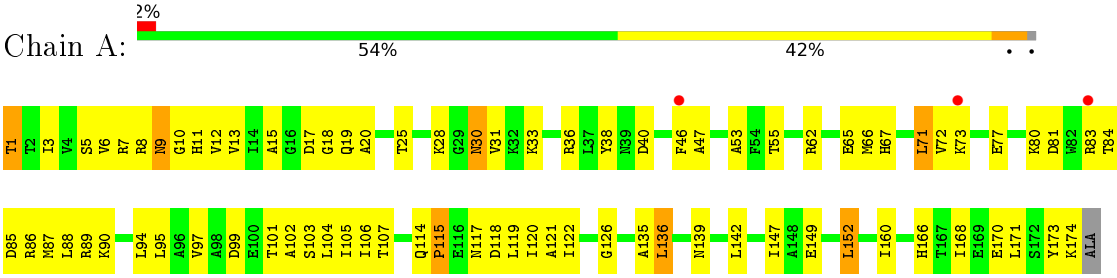
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain X:



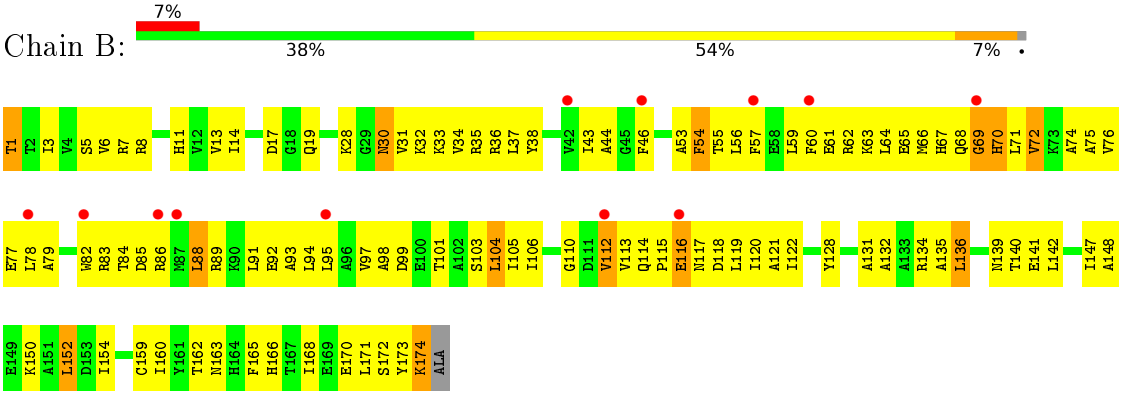
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain A:



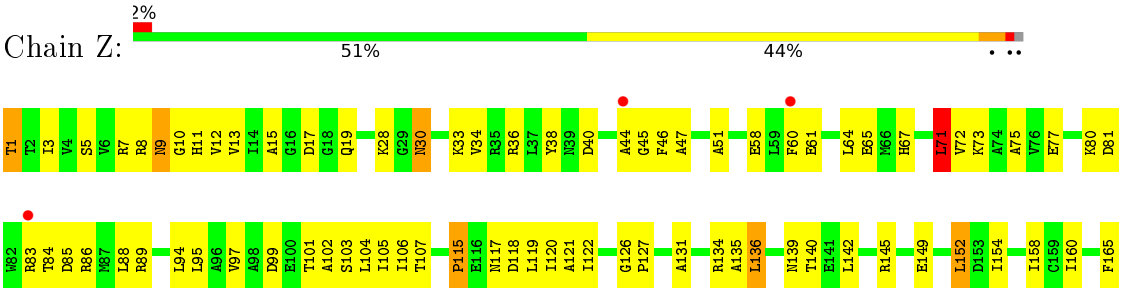
• Molecule 1: HEAT SHOCK LOCUS HSLV

Chain B:

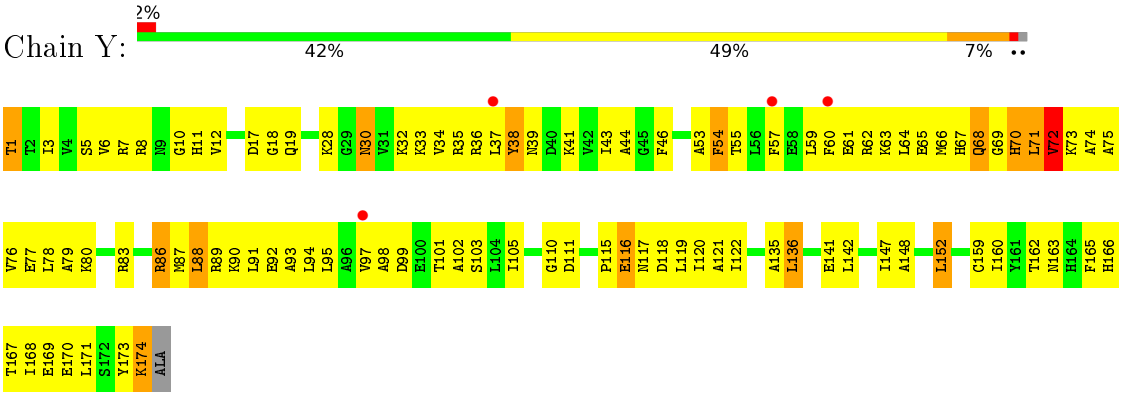


• Molecule 1: HEAT SHOCK LOCUS HSLV

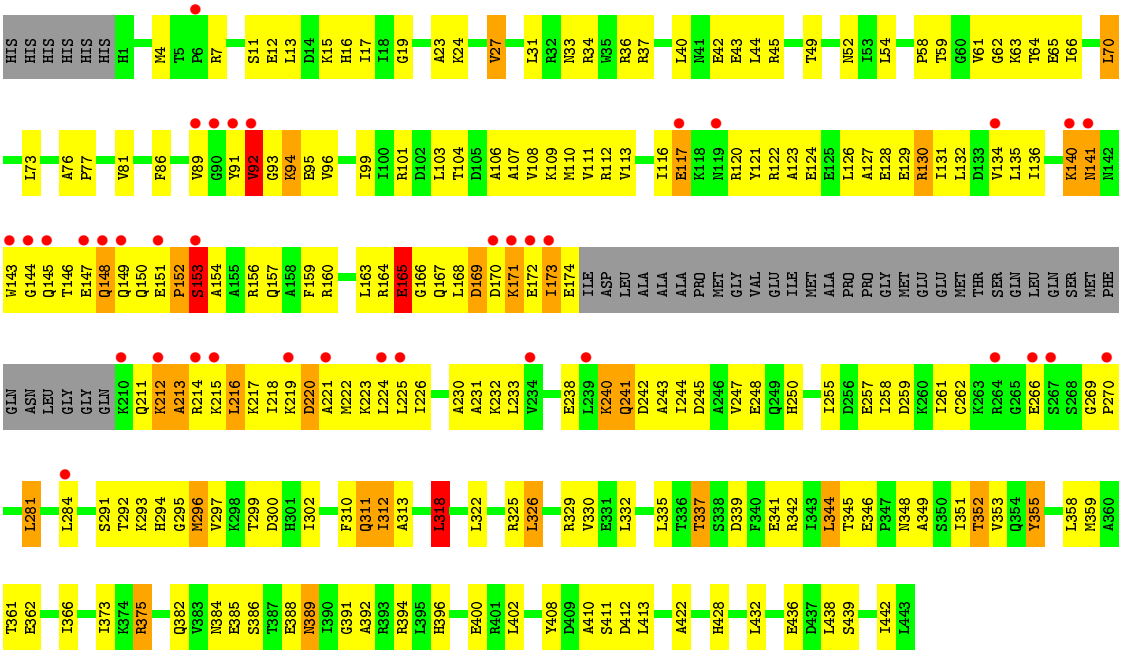
Chain Z:



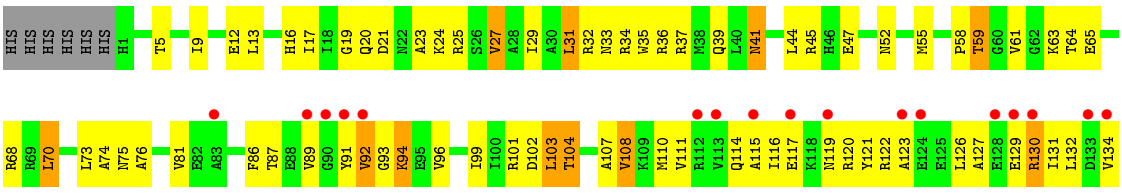
• Molecule 1: HEAT SHOCK LOCUS HSLV

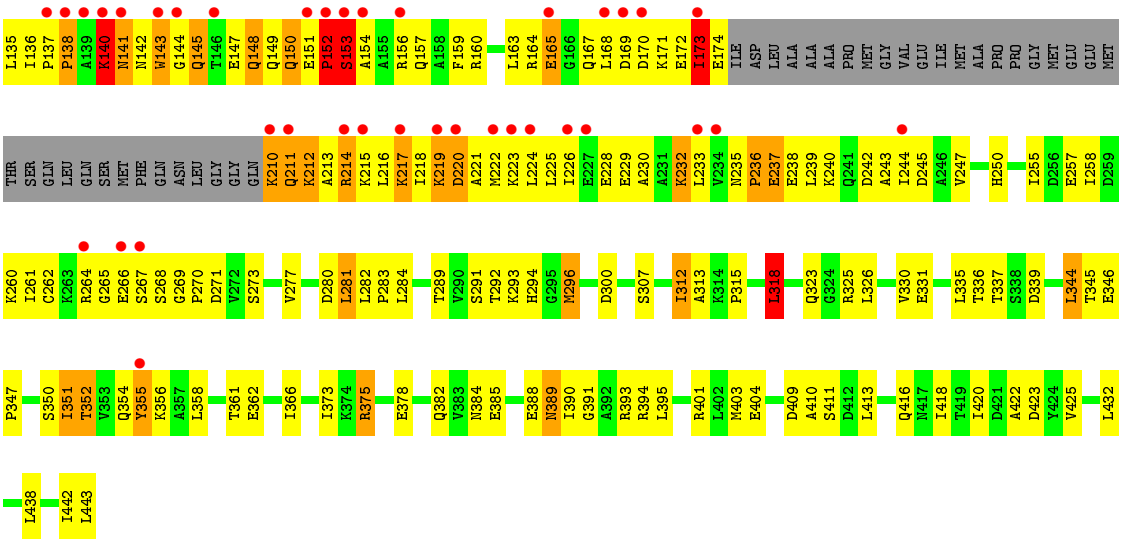


• Molecule 2: HEAT SHOCK LOCUS HSLU



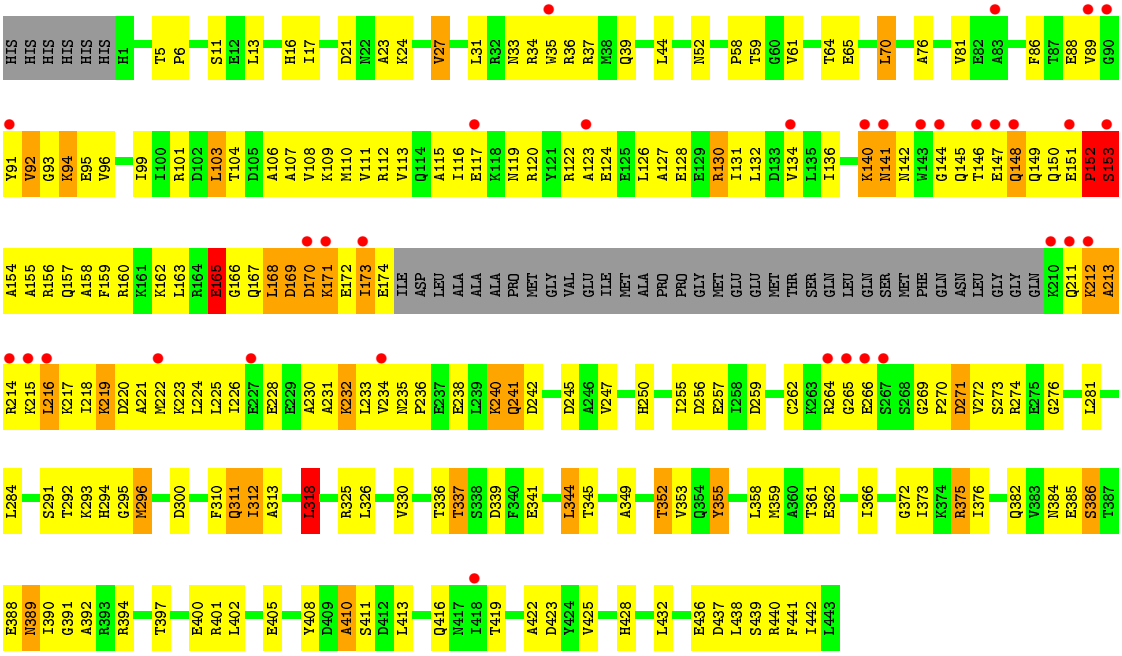
• Molecule 2: HEAT SHOCK LOCUS HSLU





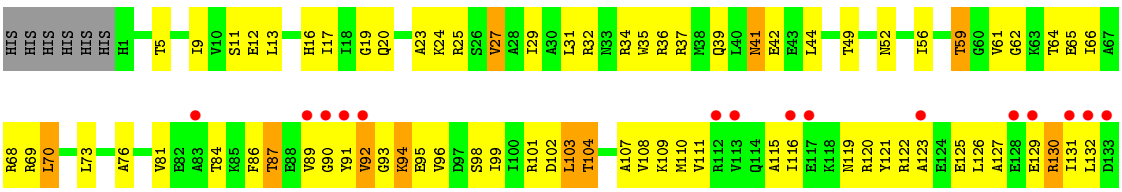
• Molecule 2: HEAT SHOCK LOCUS HSLU

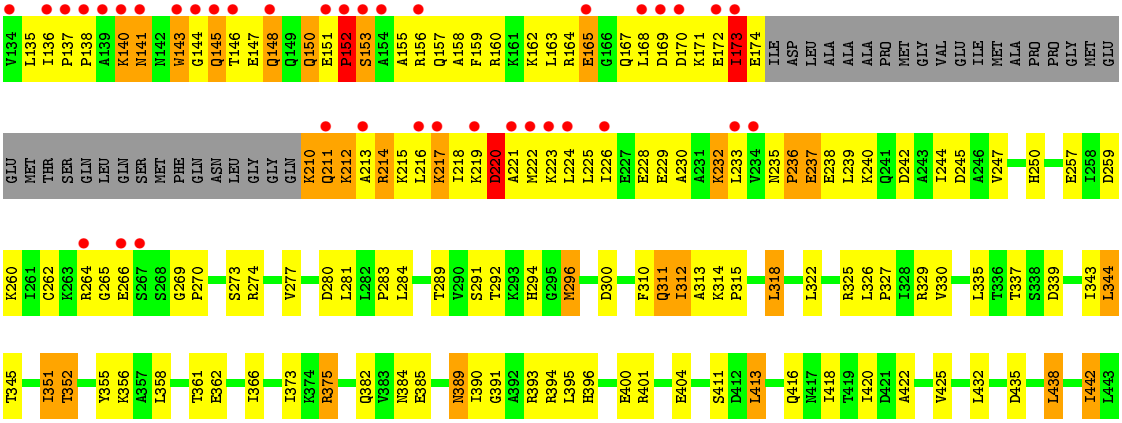
Chain G:



• Molecule 2: HEAT SHOCK LOCUS HSLU

Chain I:




V134 L135 I136 P137 P138 A139 K140 N141 N142 W143 G144 Q145 T146 E147 Q148 Q149 Q150 E151 P152 S153 A154 A155 R156 Q157 A158 F159 R160 K161 K162 L163 R164 E165 G166 Q167 L168 D169 D170 K171 E172 I173 E174 ILE ASP LEU ALA ALA PRO MET GLY VAL GLU ILE MET ALA PRO PRO GLY MET GLU
GLU MET THR SER GLN LEU GLN SER MET PHE GLN ASN LEU GLY GLY GLN K210 Q211 K212 A213 R214 K215 L216 K217 I218 K219 D220 A221 M222 K223 L224 L225 I226 E227 E228 E229 A230 A231 K232 L233 V234 N235 P236 E237 E238 L239 K240 Q241 D242 A243 I244 D245 A246 V247 H250 E257 I258 D259
K260 I261 C262 K263 R264 G265 E266 S267 S268 G269 P270 S273 R274 V277 D280 L281 L282 P283 L284 T289 V290 S291 T292 K293 H294 G295 M296 D300 F310 Q311 I312 A313 K314 P315 L318 L322 R325 L326 P327 I328 R329 V330 L335 T336 T337 S338 D339 I343 L344
T345 I351 T352 Y355 K356 A357 I358 T361 E362 I366 I373 K374 R375 Q382 V383 N384 E385 N389 I390 G391 A392 R393 R394 L395 H396 E400 R401 E404 S411 D412 I413 Q416 N417 I418 T419 I420 D421 A422 V425 L432 D435 L438 I442 L443

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	172.02Å 172.02Å 276.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.62 – 2.80 29.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.62-2.80) 92.5 (29.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.261 , 0.309 0.256 , 0.305	Depositor DCC
R_{free} test set	10933 reflections (11.26%)	DCC
Wilson B-factor (Å^2)	67.6	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23636	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4024e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.46	0/1345	0.72	0/1817
1	B	0.41	0/1345	0.66	0/1817
1	C	0.44	0/1345	0.66	0/1817
1	D	0.37	0/1345	0.65	0/1817
1	V	0.45	0/1345	0.64	0/1817
1	X	0.36	0/1345	0.64	0/1817
1	Y	0.41	0/1345	0.67	0/1817
1	Z	0.46	0/1345	0.72	0/1817
2	E	0.42	0/3266	0.69	3/4400 (0.1%)
2	F	0.45	1/3266 (0.0%)	0.69	2/4400 (0.0%)
2	G	0.43	1/3266 (0.0%)	0.69	4/4400 (0.1%)
2	I	0.42	0/3266	0.68	2/4400 (0.0%)
All	All	0.43	2/23824 (0.0%)	0.68	11/32136 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	219	LYS	C-N	5.58	1.46	1.34
2	F	152	PRO	CA-C	-5.43	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	318	LEU	CA-CB-CG	6.46	130.16	115.30
2	I	220	ASP	CB-CA-C	-6.40	97.59	110.40
2	G	318	LEU	CA-CB-CG	6.35	129.90	115.30
2	G	152	PRO	C-N-CA	-5.99	106.72	121.70
2	F	152	PRO	CA-N-CD	-5.91	103.23	111.50
2	G	153	SER	C-N-CA	5.65	135.82	121.70
2	E	152	PRO	CA-N-CD	-5.51	103.79	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	152	PRO	CA-N-CD	-5.29	104.10	111.50
2	E	153	SER	CB-CA-C	5.29	120.14	110.10
2	I	152	PRO	CA-N-CD	-5.28	104.10	111.50
2	F	318	LEU	CA-CB-CG	5.20	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1328	0	1348	96	0
1	B	1328	0	1348	126	0
1	C	1328	0	1348	140	0
1	D	1328	0	1348	87	0
1	V	1328	0	1348	143	0
1	X	1328	0	1348	98	0
1	Y	1328	0	1348	121	0
1	Z	1328	0	1348	101	0
2	E	3226	0	3294	260	1
2	F	3226	0	3293	265	1
2	G	3226	0	3294	280	0
2	I	3226	0	3293	303	0
3	E	27	0	12	3	0
3	F	27	0	12	3	0
3	G	27	0	12	3	0
3	I	27	0	12	4	0
All	All	23636	0	24006	1871	1

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 39.

All (1871) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:PRO:O	2:E:154:ALA:CA	1.83	1.25
2:E:152:PRO:C	2:E:154:ALA:H	1.27	1.15
2:E:152:PRO:C	2:E:154:ALA:N	1.80	1.12
1:B:135:ALA:HB1	1:Z:136:LEU:HD13	1.21	1.12
2:F:216:LEU:HG	2:F:221:ALA:HB2	1.25	1.11
1:D:83:ARG:HB3	1:D:83:ARG:NH1	1.71	1.06
2:E:152:PRO:O	2:E:153:SER:C	1.88	1.04
1:X:83:ARG:NH1	1:X:83:ARG:HB3	1.71	1.04
1:C:115:PRO:HG3	1:C:120:ILE:HG12	1.38	1.02
1:C:105:ILE:HD11	1:C:120:ILE:CG2	1.91	1.01
1:Y:83:ARG:HD2	1:Y:110:GLY:HA3	1.39	1.01
1:A:160:ILE:HD11	1:Z:19:GLN:NE2	1.75	1.01
2:G:152:PRO:HB2	2:G:156:ARG:HB2	1.36	1.00
2:E:174:GLU:HB3	2:E:211:GLN:HG3	1.44	1.00
2:E:212:LYS:HD3	2:E:216:LEU:HD21	1.40	0.99
2:E:152:PRO:HB2	2:E:156:ARG:HB2	1.42	0.99
1:V:15:ALA:HB2	1:V:168:ILE:HG23	1.47	0.97
2:E:170:ASP:HA	2:E:217:LYS:HA	1.46	0.97
2:F:217:LYS:O	2:F:221:ALA:N	1.98	0.96
2:G:130:ARG:HB2	2:G:130:ARG:NH2	1.80	0.96
1:Z:80:LYS:HA	1:Z:83:ARG:NH1	1.79	0.96
2:E:312:ILE:HD13	2:E:312:ILE:H	1.31	0.96
2:E:104:THR:HG21	2:E:292:THR:HG21	1.48	0.96
2:F:27:VAL:HG13	2:F:70:LEU:HG	1.48	0.96
2:G:174:GLU:HB3	2:G:211:GLN:HG3	1.47	0.95
1:X:83:ARG:HB3	1:X:83:ARG:HH11	1.23	0.95
2:E:130:ARG:HD2	2:E:225:LEU:HD11	1.49	0.95
2:E:130:ARG:NH2	2:E:130:ARG:HB2	1.82	0.94
2:G:92:VAL:HG21	2:I:92:VAL:HA	1.49	0.94
1:V:105:ILE:HD11	1:V:120:ILE:CG2	1.98	0.93
2:F:216:LEU:CG	2:F:221:ALA:HB2	1.98	0.92
2:G:212:LYS:HD3	2:G:216:LEU:HD21	1.51	0.92
1:C:105:ILE:HD11	1:C:120:ILE:HG21	1.49	0.92
2:I:122:ARG:HH11	2:I:126:LEU:HD23	1.32	0.92
2:G:168:LEU:HG	2:G:219:LYS:HD3	1.48	0.92
1:X:30:ASN:H	1:X:30:ASN:HD22	1.17	0.92
2:I:91:TYR:O	2:I:92:VAL:HG13	1.71	0.91
1:A:83:ARG:HH11	1:A:83:ARG:HG2	1.33	0.91
2:I:312:ILE:H	2:I:312:ILE:HD13	1.32	0.91
1:V:79:ALA:HB1	1:V:110:GLY:HA2	1.53	0.91
2:I:148:GLN:HA	2:I:151:GLU:HG3	1.53	0.90
1:D:174:LYS:HA	1:D:174:LYS:NZ	1.87	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:152:LEU:HD13	1:V:166:HIS:ND1	1.85	0.90
2:E:152:PRO:O	2:E:154:ALA:N	0.76	0.90
1:A:90:LYS:NZ	1:B:89:ARG:NH2	2.20	0.90
1:C:13:VAL:HG12	1:C:170:GLU:HA	1.52	0.89
2:G:94:LYS:HA	2:G:94:LYS:HE2	1.54	0.89
1:D:135:ALA:HB1	1:V:136:LEU:HD13	1.54	0.89
1:B:104:LEU:HD12	1:B:112:VAL:HG12	1.55	0.89
1:V:105:ILE:HD11	1:V:120:ILE:HG23	1.53	0.88
2:F:171:LYS:NZ	2:F:218:ILE:HD11	1.88	0.88
2:E:132:LEU:HD11	2:E:160:ARG:HG3	1.55	0.88
2:E:145:GLN:HB2	2:E:148:GLN:HB2	1.55	0.88
1:Z:10:GLY:HA3	1:Z:174:LYS:HA	1.55	0.88
1:B:140:THR:CG2	1:Z:140:THR:HG22	2.04	0.88
2:G:312:ILE:H	2:G:312:ILE:HD13	1.39	0.88
1:Y:63:LYS:HA	1:Y:66:MET:HE3	1.56	0.87
1:Z:80:LYS:HA	1:Z:83:ARG:HH12	1.36	0.87
1:C:136:LEU:HD13	1:X:135:ALA:HB1	1.54	0.87
2:F:94:LYS:HE2	2:F:94:LYS:HA	1.54	0.87
1:C:158:ILE:O	1:V:25:THR:HA	1.73	0.87
1:C:152:LEU:HD13	1:C:166:HIS:ND1	1.90	0.86
1:X:174:LYS:HA	1:X:174:LYS:NZ	1.90	0.86
2:E:94:LYS:HE2	2:E:94:LYS:HA	1.55	0.86
2:E:299:THR:HA	2:E:302:ILE:HD13	1.57	0.86
1:B:136:LEU:HD13	1:Z:135:ALA:HB1	1.58	0.86
1:B:86:ARG:HA	1:B:89:ARG:NE	1.90	0.86
2:E:153:SER:HA	2:E:157:GLN:HG2	1.58	0.85
1:B:1:THR:HB	1:B:33:LYS:HZ3	1.39	0.85
1:A:19:GLN:NE2	1:Z:160:ILE:HD11	1.90	0.85
2:I:217:LYS:O	2:I:221:ALA:HB2	1.77	0.85
1:D:83:ARG:HB3	1:D:83:ARG:HH11	1.36	0.85
2:E:89:VAL:HG12	2:E:93:GLY:HA3	1.60	0.84
2:G:104:THR:HG21	2:G:292:THR:HG21	1.59	0.84
2:F:122:ARG:HH11	2:F:126:LEU:HD23	1.41	0.84
2:G:211:GLN:HG2	2:G:212:LYS:H	1.41	0.84
1:Y:72:VAL:O	1:Y:76:VAL:HG23	1.77	0.84
1:A:85:ASP:O	1:A:89:ARG:HB2	1.77	0.84
1:C:71:LEU:HG	1:C:99:ASP:OD1	1.76	0.83
2:I:174:GLU:HA	2:I:213:ALA:H	1.43	0.83
1:B:140:THR:HG22	1:Z:140:THR:HG22	1.61	0.83
2:I:351:ILE:HD13	2:I:351:ILE:H	1.40	0.83
1:B:135:ALA:HB1	1:Z:136:LEU:CD1	2.08	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:224:LEU:O	2:I:228:GLU:HB2	1.78	0.83
2:F:312:ILE:H	2:F:312:ILE:HD13	1.42	0.83
2:I:356:LYS:HG3	2:I:366:ILE:HG22	1.61	0.82
2:I:217:LYS:O	2:I:221:ALA:CB	2.27	0.82
1:B:72:VAL:O	1:B:76:VAL:HG23	1.79	0.82
2:F:145:GLN:HB2	2:F:148:GLN:HG2	1.61	0.82
1:B:1:THR:HB	1:B:33:LYS:NZ	1.94	0.82
1:C:158:ILE:CG2	1:V:25:THR:HB	2.08	0.82
2:I:132:LEU:HD11	2:I:160:ARG:HG3	1.60	0.82
1:D:136:LEU:HD13	1:V:135:ALA:HB1	1.58	0.82
1:B:86:ARG:HA	1:B:89:ARG:CZ	2.09	0.82
1:C:86:ARG:HA	1:C:89:ARG:NH1	1.95	0.81
2:G:109:LYS:HD3	2:I:296:MET:HB3	1.61	0.81
1:D:43:ILE:H	1:D:43:ILE:HD13	1.45	0.81
1:A:160:ILE:HD11	1:Z:19:GLN:HE22	1.45	0.81
2:F:91:TYR:O	2:F:92:VAL:HG13	1.81	0.81
1:B:63:LYS:HA	1:B:66:MET:HE3	1.62	0.81
2:G:150:GLN:O	2:G:153:SER:HB2	1.81	0.81
2:I:171:LYS:NZ	2:I:218:ILE:HD11	1.95	0.81
1:Y:60:PHE:CD1	1:Y:78:LEU:HD22	2.16	0.81
2:E:211:GLN:HG2	2:E:212:LYS:H	1.45	0.81
2:I:27:VAL:HG13	2:I:70:LEU:HG	1.62	0.81
1:B:57:PHE:O	1:B:61:GLU:HG3	1.82	0.80
2:G:174:GLU:HA	2:G:212:LYS:HB3	1.62	0.80
2:G:92:VAL:CG2	2:I:92:VAL:HA	2.12	0.80
1:V:115:PRO:HG3	1:V:120:ILE:HG13	1.64	0.80
1:A:1:THR:HB	1:A:33:LYS:HZ3	1.47	0.80
1:C:54:PHE:O	1:C:58:GLU:HB2	1.82	0.80
2:F:224:LEU:O	2:F:228:GLU:HB2	1.82	0.80
1:D:28:LYS:HE2	1:D:30:ASN:ND2	1.97	0.80
1:A:80:LYS:HA	1:A:83:ARG:NH1	1.98	0.79
2:I:19:GLY:O	2:I:24:LYS:HE3	1.83	0.79
2:E:344:LEU:O	2:E:352:THR:HB	1.82	0.79
2:G:92:VAL:HG21	2:I:92:VAL:HG12	1.63	0.79
2:E:389:ASN:C	2:E:389:ASN:HD22	1.85	0.79
1:A:90:LYS:HZ1	1:B:89:ARG:NH2	1.80	0.79
2:G:344:LEU:O	2:G:352:THR:HB	1.82	0.79
1:C:28:LYS:HE2	1:C:30:ASN:ND2	1.97	0.79
2:F:384:ASN:ND2	2:F:394:ARG:HE	1.81	0.79
1:Z:10:GLY:HA2	1:Z:173:TYR:CE1	2.17	0.79
2:F:151:GLU:HB2	2:F:152:PRO:CD	2.13	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:172:GLU:HB3	2:I:215:LYS:HD2	1.65	0.79
2:I:312:ILE:CD1	2:I:312:ILE:H	1.96	0.78
1:B:134:ARG:HG2	1:Z:154:ILE:HD12	1.65	0.78
2:G:130:ARG:HH21	2:G:130:ARG:HB2	1.43	0.78
1:C:115:PRO:HB2	1:C:119:LEU:O	1.83	0.78
1:Y:1:THR:HB	1:Y:33:LYS:NZ	1.99	0.78
2:F:312:ILE:H	2:F:312:ILE:CD1	1.96	0.78
2:I:108:VAL:HA	2:I:111:VAL:HG22	1.64	0.78
1:Y:170:GLU:HG2	1:Y:171:LEU:H	1.47	0.78
2:F:351:ILE:HD13	2:F:351:ILE:H	1.46	0.78
2:G:173:ILE:HG12	2:G:212:LYS:HD2	1.65	0.78
2:F:211:GLN:HE21	2:F:212:LYS:H	1.29	0.77
1:D:139:ASN:HD22	1:V:136:LEU:HD11	1.49	0.77
1:A:10:GLY:HA2	1:A:173:TYR:CE1	2.19	0.77
2:E:174:GLU:HA	2:E:212:LYS:HB3	1.65	0.77
2:E:103:LEU:HD22	2:E:247:VAL:HG22	1.65	0.77
2:F:389:ASN:ND2	2:F:391:GLY:H	1.83	0.77
2:F:135:LEU:HG	2:F:171:LYS:HE2	1.67	0.77
1:X:60:PHE:HB2	1:X:78:LEU:HD22	1.67	0.77
2:I:89:VAL:HG12	2:I:93:GLY:HA3	1.67	0.77
1:Y:105:ILE:HD11	1:Y:120:ILE:HG23	1.67	0.77
1:B:28:LYS:NZ	1:B:30:ASN:HD21	1.82	0.77
2:F:393:ARG:HG2	2:F:393:ARG:HH11	1.49	0.77
2:E:147:GLU:HA	2:E:150:GLN:HG3	1.67	0.77
2:F:130:ARG:HG2	2:F:225:LEU:HD11	1.66	0.76
2:F:375:ARG:CZ	2:F:422:ALA:HB1	2.14	0.76
2:F:64:THR:HB	3:F:1450:ADP:O2A	1.84	0.76
2:F:174:GLU:HA	2:F:213:ALA:H	1.49	0.76
2:I:147:GLU:HG2	2:I:150:GLN:NE2	2.00	0.76
2:E:91:TYR:O	2:E:92:VAL:HG13	1.86	0.76
2:G:173:ILE:HD11	2:G:221:ALA:HB1	1.68	0.76
1:D:30:ASN:H	1:D:30:ASN:HD22	1.31	0.76
2:G:152:PRO:HB3	2:G:156:ARG:H	1.49	0.76
1:A:67:HIS:HD2	1:A:73:LYS:HD2	1.49	0.76
1:V:27:MET:SD	1:X:113:VAL:HG21	2.25	0.76
1:X:13:VAL:HG12	1:X:170:GLU:HG3	1.66	0.76
2:G:89:VAL:HA	2:G:93:GLY:N	2.00	0.75
2:G:389:ASN:ND2	2:G:391:GLY:H	1.84	0.75
2:G:397:THR:HG22	2:I:327:PRO:HA	1.66	0.75
1:A:13:VAL:HG12	1:A:170:GLU:HG3	1.67	0.75
1:B:71:LEU:HG	1:B:99:ASP:OD1	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:145:GLN:HB2	2:G:148:GLN:HB2	1.67	0.75
1:C:71:LEU:HD21	1:C:97:VAL:HG11	1.69	0.75
2:E:130:ARG:HH21	2:E:130:ARG:HB2	1.51	0.75
2:F:171:LYS:HZ2	2:F:218:ILE:HD11	1.52	0.75
2:E:116:ILE:O	2:E:120:ARG:HB2	1.87	0.75
2:F:173:ILE:HG12	2:F:212:LYS:HD2	1.68	0.75
2:F:218:ILE:C	2:F:220:ASP:H	1.89	0.75
1:C:105:ILE:HD11	1:C:120:ILE:HG23	1.68	0.74
2:E:291:SER:HA	2:E:296:MET:HE2	1.69	0.74
2:F:123:ALA:HA	2:F:127:ALA:HB3	1.68	0.74
2:E:64:THR:HB	3:E:450:ADP:O2A	1.87	0.74
2:F:235:ASN:OD1	2:F:238:GLU:HB2	1.87	0.74
2:F:172:GLU:HB3	2:F:215:LYS:HD2	1.68	0.74
2:G:312:ILE:H	2:G:312:ILE:CD1	2.00	0.74
1:X:30:ASN:ND2	1:X:30:ASN:H	1.85	0.74
1:X:37:LEU:HD23	1:X:57:PHE:HB3	1.69	0.74
1:V:115:PRO:HB2	1:V:119:LEU:O	1.87	0.74
1:C:135:ALA:HB1	1:X:136:LEU:HD13	1.69	0.74
2:F:217:LYS:HB2	2:F:217:LYS:NZ	2.03	0.74
1:B:60:PHE:CD1	1:B:78:LEU:HD22	2.22	0.74
2:I:94:LYS:HE2	2:I:94:LYS:HA	1.69	0.74
1:X:43:ILE:HD13	1:X:43:ILE:H	1.53	0.74
2:E:171:LYS:HG3	2:E:218:ILE:HD11	1.70	0.74
2:I:389:ASN:ND2	2:I:391:GLY:H	1.86	0.74
1:Z:67:HIS:CD2	1:Z:73:LYS:HD2	2.22	0.74
2:E:152:PRO:CB	2:E:156:ARG:HB2	2.17	0.74
2:E:384:ASN:ND2	2:E:394:ARG:HE	1.86	0.74
2:I:153:SER:HB3	2:I:157:GLN:OE1	1.88	0.74
1:C:160:ILE:HG23	1:V:160:ILE:HG23	1.70	0.74
1:X:105:ILE:HD11	1:X:120:ILE:HG23	1.69	0.74
2:E:312:ILE:CD1	2:E:312:ILE:H	1.98	0.74
2:G:291:SER:HA	2:G:296:MET:HE2	1.69	0.73
2:G:92:VAL:HG21	2:I:92:VAL:CG1	2.17	0.73
2:G:150:GLN:C	2:G:153:SER:OG	2.27	0.73
2:I:217:LYS:HG3	2:I:218:ILE:H	1.51	0.73
1:C:71:LEU:HD21	1:C:97:VAL:CG1	2.17	0.73
1:V:132:ALA:HB2	1:V:154:ILE:HG21	1.70	0.73
2:G:169:ASP:OD1	2:G:218:ILE:HD12	1.88	0.73
2:G:389:ASN:C	2:G:389:ASN:HD22	1.91	0.73
1:V:138:GLU:C	1:V:139:ASN:HD22	1.92	0.73
2:F:223:LYS:HA	2:F:226:ILE:HG12	1.70	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:345:THR:CG2	2:G:373:ILE:HD13	2.18	0.73
1:X:95:LEU:HB2	1:X:106:ILE:HB	1.69	0.73
1:C:132:ALA:HB2	1:C:154:ILE:HG21	1.70	0.73
1:B:17:ASP:HA	1:B:165:PHE:O	1.89	0.73
2:F:81:VAL:HG11	2:F:99:ILE:HG12	1.71	0.73
1:C:86:ARG:HG3	1:C:89:ARG:HH22	1.52	0.72
2:I:344:LEU:O	2:I:352:THR:HB	1.89	0.72
1:Y:71:LEU:HG	1:Y:99:ASP:OD1	1.89	0.72
2:I:81:VAL:HG11	2:I:99:ILE:HG12	1.71	0.72
1:B:28:LYS:HZ2	1:B:30:ASN:HD21	1.35	0.72
2:G:122:ARG:CZ	2:G:126:LEU:HD21	2.20	0.72
2:G:64:THR:HB	3:G:2450:ADP:O2A	1.88	0.72
1:A:90:LYS:HZ2	1:B:89:ARG:NH2	1.88	0.72
1:C:70:HIS:CE1	1:C:72:VAL:HB	2.25	0.72
1:D:28:LYS:HE2	1:D:30:ASN:HD21	1.54	0.72
2:I:345:THR:CG2	2:I:373:ILE:HD13	2.20	0.72
1:V:54:PHE:O	1:V:58:GLU:HB2	1.90	0.72
1:A:10:GLY:HA3	1:A:174:LYS:HA	1.69	0.72
1:A:83:ARG:NH1	1:A:83:ARG:HG2	1.99	0.72
2:G:140:LYS:O	2:G:141:ASN:HB2	1.89	0.72
2:G:91:TYR:HD1	2:I:91:TYR:CD2	2.08	0.72
1:X:152:LEU:HD13	1:X:166:HIS:ND1	2.04	0.72
2:E:359:MET:HG3	2:E:366:ILE:HG13	1.71	0.72
2:G:432:LEU:HD12	2:G:432:LEU:H	1.55	0.72
1:Y:57:PHE:O	1:Y:61:GLU:HG3	1.89	0.72
1:Y:86:ARG:HA	1:Y:89:ARG:CZ	2.20	0.72
2:E:345:THR:CG2	2:E:373:ILE:HD13	2.19	0.72
1:C:158:ILE:HG22	1:V:25:THR:HB	1.72	0.72
1:C:46:PHE:CE2	1:C:53:ALA:HB2	2.25	0.72
1:V:90:LYS:HZ1	1:X:89:ARG:NH1	1.88	0.72
1:Y:36:ARG:O	1:Y:37:LEU:HD23	1.89	0.71
1:D:60:PHE:HB2	1:D:78:LEU:HD22	1.69	0.71
2:I:41:ASN:HD22	2:I:41:ASN:C	1.92	0.71
1:V:71:LEU:HG	1:V:99:ASP:OD1	1.89	0.71
2:I:108:VAL:HG21	2:I:294:HIS:HD2	1.55	0.71
1:C:160:ILE:CG2	1:V:160:ILE:HG23	2.19	0.71
2:I:384:ASN:ND2	2:I:394:ARG:HE	1.87	0.71
1:Z:85:ASP:O	1:Z:89:ARG:HB2	1.89	0.71
2:I:173:ILE:HG12	2:I:212:LYS:HD2	1.72	0.71
1:C:80:LYS:HZ2	1:C:80:LYS:HB3	1.55	0.71
1:D:37:LEU:HD13	1:D:57:PHE:HB3	1.70	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:148:GLN:OE1	2:F:151:GLU:HG3	1.91	0.71
1:C:136:LEU:HD11	1:X:139:ASN:HD22	1.56	0.71
1:B:104:LEU:CD1	1:B:112:VAL:HG12	2.19	0.71
2:G:168:LEU:HA	2:G:219:LYS:HB3	1.73	0.71
2:E:117:GLU:HG3	2:E:120:ARG:NH2	2.04	0.71
2:E:312:ILE:HG12	2:E:313:ALA:H	1.56	0.71
1:B:134:ARG:HG2	1:Z:154:ILE:CD1	2.21	0.71
2:G:150:GLN:CA	2:G:153:SER:OG	2.39	0.71
1:C:17:ASP:HA	1:C:165:PHE:O	1.91	0.71
2:G:130:ARG:HD2	2:G:225:LEU:HD11	1.71	0.71
2:E:389:ASN:ND2	2:E:391:GLY:H	1.89	0.70
2:E:27:VAL:HG13	2:E:70:LEU:HG	1.71	0.70
1:Y:86:ARG:HA	1:Y:89:ARG:NE	2.05	0.70
2:I:242:ASP:HA	2:I:245:ASP:OD1	1.91	0.70
1:Y:28:LYS:NZ	1:Y:30:ASN:ND2	2.39	0.70
2:F:89:VAL:HG11	2:F:94:LYS:O	1.90	0.70
2:F:257:GLU:HB2	2:F:260:LYS:HG3	1.74	0.70
1:B:152:LEU:HD13	1:B:166:HIS:ND1	2.07	0.70
2:G:170:ASP:HA	2:G:217:LYS:HA	1.72	0.70
1:D:30:ASN:H	1:D:30:ASN:ND2	1.90	0.70
2:E:216:LEU:HD23	2:E:216:LEU:H	1.57	0.70
1:D:174:LYS:HZ2	1:D:174:LYS:HA	1.56	0.69
2:F:152:PRO:HB2	2:F:156:ARG:HB2	1.72	0.69
1:A:90:LYS:HZ1	1:B:89:ARG:HH22	1.37	0.69
1:V:51:ALA:HB3	1:X:110:GLY:O	1.91	0.69
2:F:315:PRO:O	2:F:318:LEU:HB2	1.91	0.69
2:G:108:VAL:HG21	2:G:294:HIS:CD2	2.26	0.69
1:C:94:LEU:HB3	1:C:122:ILE:HD12	1.73	0.69
1:D:95:LEU:HB2	1:D:106:ILE:HB	1.72	0.69
2:G:132:LEU:HD11	2:G:160:ARG:HG2	1.74	0.69
2:I:151:GLU:HB2	2:I:152:PRO:CD	2.23	0.69
1:Z:1:THR:HB	1:Z:33:LYS:HZ3	1.57	0.69
1:Y:28:LYS:NZ	1:Y:30:ASN:HD21	1.89	0.69
1:A:28:LYS:HD2	1:B:113:VAL:HG13	1.75	0.69
2:I:64:THR:HB	3:I:3450:ADP:O2A	1.92	0.69
2:E:124:GLU:HA	2:E:127:ALA:HB3	1.72	0.69
2:G:150:GLN:O	2:G:153:SER:CB	2.41	0.69
2:F:242:ASP:HA	2:F:245:ASP:OD1	1.91	0.69
2:G:150:GLN:HA	2:G:153:SER:OG	1.93	0.69
1:V:3:ILE:HD12	1:V:122:ILE:HD11	1.73	0.69
1:Z:117:ASN:O	1:Z:118:ASP:HB2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:169:ASP:OD1	2:E:218:ILE:HD12	1.93	0.69
2:G:345:THR:HG21	2:G:373:ILE:HD13	1.75	0.69
2:I:170:ASP:HA	2:I:217:LYS:HA	1.75	0.69
2:E:219:LYS:O	2:E:223:LYS:HG3	1.93	0.68
2:G:91:TYR:O	2:G:92:VAL:HG13	1.92	0.68
2:I:236:PRO:HG2	2:I:237:GLU:H	1.58	0.68
2:E:293:LYS:HG3	2:E:294:HIS:CD2	2.28	0.68
2:F:130:ARG:NH2	2:F:229:GLU:HG3	2.07	0.68
2:I:223:LYS:HA	2:I:226:ILE:HG12	1.75	0.68
1:V:79:ALA:HB1	1:V:110:GLY:CA	2.24	0.68
2:E:173:ILE:N	2:E:173:ILE:HD13	2.08	0.68
2:I:239:LEU:HD23	2:I:240:LYS:N	2.07	0.68
2:G:124:GLU:HA	2:G:127:ALA:HB3	1.74	0.68
2:I:174:GLU:HB3	2:I:211:GLN:HB2	1.75	0.68
2:G:173:ILE:N	2:G:173:ILE:HD13	2.08	0.68
2:I:163:LEU:HD11	2:I:222:MET:CE	2.24	0.68
2:E:108:VAL:HG21	2:E:294:HIS:ND1	2.07	0.68
2:E:214:ARG:HG2	2:E:215:LYS:N	2.09	0.68
1:C:79:ALA:HB1	1:C:110:GLY:HA2	1.76	0.68
2:F:96:VAL:HG11	2:F:281:LEU:HD12	1.74	0.68
2:G:122:ARG:O	2:G:126:LEU:HD23	1.93	0.68
1:Z:77:GLU:O	1:Z:80:LYS:HB2	1.93	0.68
1:A:8:ARG:NH1	1:A:142:LEU:O	2.24	0.68
1:D:10:GLY:HA2	1:D:173:TYR:CE1	2.29	0.68
2:F:25:ARG:O	2:F:29:ILE:HG12	1.92	0.68
2:G:220:ASP:HA	2:G:223:LYS:HD2	1.75	0.68
1:X:86:ARG:HA	1:X:89:ARG:NH1	2.09	0.68
1:A:135:ALA:HB1	1:Y:136:LEU:HD13	1.75	0.68
1:A:80:LYS:HA	1:A:83:ARG:HH12	1.57	0.68
2:E:150:GLN:O	2:E:153:SER:OG	2.12	0.68
2:E:375:ARG:CZ	2:E:422:ALA:HB1	2.23	0.67
1:C:158:ILE:HG23	1:V:25:THR:HB	1.74	0.67
1:X:55:THR:O	1:X:58:GLU:HB2	1.94	0.67
1:B:28:LYS:NZ	1:B:30:ASN:ND2	2.42	0.67
2:G:223:LYS:HA	2:G:226:ILE:HG12	1.76	0.67
1:V:30:ASN:ND2	1:V:30:ASN:H	1.92	0.67
2:F:344:LEU:O	2:F:352:THR:HB	1.94	0.67
1:X:36:ARG:NH1	1:X:40:ASP:O	2.28	0.67
2:E:131:ILE:HD11	2:E:218:ILE:HG12	1.75	0.67
2:E:153:SER:CA	2:E:157:GLN:HG2	2.25	0.67
2:G:171:LYS:HB2	2:G:218:ILE:HG13	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:216:LEU:HD23	2:G:216:LEU:H	1.60	0.67
2:G:52:ASN:HB2	2:G:325:ARG:O	1.94	0.67
1:Y:8:ARG:NH1	1:Y:142:LEU:O	2.26	0.67
1:C:73:LYS:HD3	1:C:76:VAL:HG11	1.77	0.67
2:I:291:SER:HA	2:I:296:MET:HE2	1.76	0.67
1:C:51:ALA:HB3	1:D:110:GLY:O	1.95	0.67
1:D:143:SER:OG	1:D:146:GLU:HG3	1.94	0.67
1:D:174:LYS:HZ3	1:D:174:LYS:HA	1.56	0.67
2:E:136:ILE:O	2:E:136:ILE:HG22	1.94	0.67
2:I:108:VAL:HG21	2:I:294:HIS:CD2	2.30	0.67
1:B:8:ARG:NH1	1:B:142:LEU:O	2.27	0.67
1:D:36:ARG:NH1	1:D:40:ASP:O	2.24	0.67
2:G:152:PRO:HB2	2:G:156:ARG:CB	2.19	0.67
2:F:151:GLU:HB2	2:F:152:PRO:HD2	1.76	0.66
2:E:122:ARG:O	2:E:126:LEU:HD23	1.95	0.66
2:G:174:GLU:HA	2:G:213:ALA:H	1.60	0.66
1:C:27:MET:SD	1:D:113:VAL:HG21	2.36	0.66
2:E:174:GLU:CB	2:E:211:GLN:HG3	2.23	0.66
2:F:236:PRO:HG2	2:F:237:GLU:H	1.60	0.66
2:F:389:ASN:HD22	2:F:391:GLY:H	1.41	0.66
1:V:73:LYS:HA	1:V:76:VAL:HG12	1.77	0.66
1:V:83:ARG:HG3	1:V:83:ARG:HH11	1.60	0.66
1:Z:51:ALA:CB	1:Y:111:ASP:OD2	2.43	0.66
1:Y:65:GLU:HG2	2:I:143:TRP:CD1	2.30	0.66
1:B:56:LEU:HD13	1:B:95:LEU:HD11	1.77	0.66
2:E:361:THR:HG21	2:F:36:ARG:HA	1.78	0.66
2:G:174:GLU:HB3	2:G:211:GLN:CG	2.22	0.66
1:D:83:ARG:HB3	1:D:83:ARG:CZ	2.26	0.66
2:E:147:GLU:HA	2:E:150:GLN:CG	2.24	0.66
1:V:37:LEU:HD23	1:V:37:LEU:N	2.10	0.66
1:X:143:SER:OG	1:X:146:GLU:HG3	1.95	0.66
1:A:1:THR:HB	1:A:33:LYS:NZ	2.10	0.66
2:G:242:ASP:HA	2:G:245:ASP:OD1	1.96	0.66
2:G:432:LEU:HD12	2:G:432:LEU:N	2.10	0.66
2:I:217:LYS:NZ	2:I:217:LYS:HB2	2.11	0.66
2:E:89:VAL:HA	2:E:93:GLY:N	2.11	0.66
2:G:91:TYR:HB2	2:I:90:GLY:O	1.96	0.66
1:C:86:ARG:HA	1:C:89:ARG:HH12	1.59	0.65
1:X:174:LYS:HA	1:X:174:LYS:HZ3	1.60	0.65
1:A:19:GLN:HE22	1:Z:160:ILE:HD11	1.59	0.65
2:G:92:VAL:HG21	2:I:92:VAL:CA	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:65:GLU:HG2	2:I:143:TRP:NE1	2.12	0.65
1:Y:17:ASP:HA	1:Y:165:PHE:O	1.96	0.65
2:G:131:ILE:HD11	2:G:218:ILE:HG12	1.78	0.65
2:G:136:ILE:O	2:G:136:ILE:HG22	1.96	0.65
2:G:131:ILE:HD11	2:G:218:ILE:CD1	2.25	0.65
1:V:3:ILE:HB	1:V:122:ILE:HG12	1.79	0.65
2:E:103:LEU:HD13	2:E:247:VAL:HG13	1.78	0.65
2:I:135:LEU:CD2	2:I:171:LYS:HE2	2.27	0.65
2:I:262:CYS:SG	2:I:318:LEU:HD13	2.37	0.65
1:A:86:ARG:HA	1:A:89:ARG:CZ	2.26	0.65
1:D:64:LEU:O	1:D:69:GLY:N	2.30	0.65
2:E:174:GLU:HB3	2:E:211:GLN:CG	2.24	0.65
2:E:293:LYS:HG3	2:E:294:HIS:HD2	1.62	0.65
2:E:312:ILE:HG12	2:E:313:ALA:N	2.11	0.65
2:F:218:ILE:C	2:F:220:ASP:N	2.50	0.65
1:Z:67:HIS:HD2	1:Z:73:LYS:HD2	1.60	0.65
1:A:67:HIS:CD2	1:A:73:LYS:HD2	2.31	0.65
1:Y:28:LYS:HZ2	1:Y:30:ASN:HD21	1.43	0.65
2:F:174:GLU:HB3	2:F:211:GLN:HB2	1.77	0.65
2:I:235:ASN:HB2	2:I:236:PRO:HD2	1.79	0.65
2:I:257:GLU:HB2	2:I:260:LYS:HG3	1.78	0.65
1:X:174:LYS:HZ2	1:X:174:LYS:HA	1.60	0.65
1:A:28:LYS:NZ	1:A:30:ASN:ND2	2.45	0.64
2:F:211:GLN:HE21	2:F:212:LYS:N	1.95	0.64
2:F:27:VAL:CG1	2:F:70:LEU:HG	2.25	0.64
1:C:6:VAL:HG21	1:C:147:ILE:HG22	1.80	0.64
2:F:130:ARG:HH21	2:F:229:GLU:HG3	1.61	0.64
2:F:375:ARG:HB3	2:F:425:VAL:HG11	1.80	0.64
2:G:103:LEU:HD22	2:G:247:VAL:HG22	1.79	0.64
2:G:384:ASN:ND2	2:G:394:ARG:HE	1.95	0.64
1:Z:65:GLU:OE1	2:G:141:ASN:HB3	1.96	0.64
1:A:65:GLU:HG2	2:E:143:TRP:HE1	1.62	0.64
2:E:211:GLN:HG2	2:E:212:LYS:N	2.12	0.64
1:A:87:MET:CE	1:B:84:THR:HG23	2.27	0.64
2:F:108:VAL:C	2:F:110:MET:H	2.01	0.64
2:I:130:ARG:NH2	2:I:229:GLU:HG3	2.12	0.64
1:V:30:ASN:HD22	1:V:30:ASN:H	1.43	0.64
1:V:3:ILE:HD11	1:V:46:PHE:O	1.98	0.64
1:Z:13:VAL:HG12	1:Z:170:GLU:HG3	1.80	0.64
1:B:105:ILE:HD11	1:B:120:ILE:HG23	1.79	0.64
1:B:59:LEU:HG	1:B:78:LEU:CD1	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:THR:HB	1:D:33:LYS:HZ3	1.61	0.64
2:E:89:VAL:HG12	2:E:93:GLY:CA	2.27	0.64
2:I:122:ARG:NH1	2:I:126:LEU:HD23	2.10	0.64
1:C:56:LEU:HD13	1:C:95:LEU:HD11	1.80	0.64
1:Y:152:LEU:HD13	1:Y:166:HIS:ND1	2.12	0.64
2:F:41:ASN:C	2:F:41:ASN:HD22	2.01	0.64
2:G:211:GLN:HG2	2:G:212:LYS:N	2.11	0.64
1:V:71:LEU:HD21	1:V:97:VAL:CG1	2.28	0.64
1:Z:84:THR:HG23	1:Z:85:ASP:H	1.62	0.64
2:F:135:LEU:HD13	2:F:159:PHE:HD2	1.63	0.63
2:F:151:GLU:CB	2:F:152:PRO:CD	2.74	0.63
2:F:211:GLN:NE2	2:F:212:LYS:H	1.96	0.63
2:I:147:GLU:CG	2:I:150:GLN:NE2	2.61	0.63
1:V:17:ASP:O	1:V:33:LYS:HD2	1.97	0.63
1:Z:105:ILE:CD1	1:Z:120:ILE:HG23	2.29	0.63
2:E:214:ARG:HD3	2:E:216:LEU:HD22	1.80	0.63
2:G:89:VAL:HG12	2:G:93:GLY:C	2.19	0.63
2:G:91:TYR:O	2:G:92:VAL:HG22	1.99	0.63
1:Y:60:PHE:HD1	1:Y:78:LEU:HD22	1.63	0.63
1:A:77:GLU:O	1:A:80:LYS:HB2	1.98	0.63
2:E:345:THR:HG21	2:E:373:ILE:HD13	1.81	0.63
2:I:96:VAL:HG11	2:I:281:LEU:HD12	1.80	0.63
1:C:83:ARG:HH11	1:C:83:ARG:HG3	1.64	0.63
2:G:152:PRO:CB	2:G:156:ARG:H	2.10	0.63
2:G:359:MET:HG3	2:G:366:ILE:HG13	1.80	0.63
2:I:140:LYS:H	2:I:140:LYS:HD3	1.63	0.63
2:E:168:LEU:HD23	2:E:219:LYS:HB3	1.81	0.63
2:I:123:ALA:HA	2:I:127:ALA:HB3	1.80	0.63
2:I:223:LYS:N	2:I:223:LYS:HD2	2.14	0.63
2:I:86:PHE:O	2:I:89:VAL:HG22	1.98	0.63
1:Y:136:LEU:HB3	1:Y:147:ILE:CD1	2.28	0.63
2:G:174:GLU:CB	2:G:211:GLN:HG3	2.25	0.63
2:I:20:GLN:O	2:I:24:LYS:HG3	1.99	0.63
2:E:130:ARG:CD	2:E:225:LEU:HD11	2.26	0.63
2:F:140:LYS:HD3	2:F:140:LYS:H	1.63	0.63
2:F:351:ILE:N	2:F:351:ILE:HD13	2.14	0.63
1:Y:70:HIS:HE1	1:Y:72:VAL:HB	1.64	0.63
1:B:38:TYR:HB2	1:B:64:LEU:HD12	1.81	0.63
1:C:36:ARG:NE	1:C:169:GLU:OE1	2.31	0.63
2:G:171:LYS:HG3	2:G:218:ILE:HD11	1.81	0.62
1:V:105:ILE:HD11	1:V:120:ILE:HG21	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:147:GLU:HA	2:G:150:GLN:HG3	1.81	0.62
2:I:212:LYS:HB2	2:I:212:LYS:NZ	2.14	0.62
1:D:136:LEU:CD1	1:V:135:ALA:HB1	2.29	0.62
2:F:131:ILE:HG21	2:F:222:MET:HE1	1.81	0.62
1:D:152:LEU:HD13	1:D:166:HIS:CE1	2.35	0.62
2:E:122:ARG:CZ	2:E:126:LEU:HD21	2.30	0.62
2:F:312:ILE:HD13	2:F:312:ILE:N	2.14	0.62
1:Y:28:LYS:HZ1	1:Y:30:ASN:ND2	1.97	0.62
1:C:170:GLU:HG3	1:C:171:LEU:H	1.65	0.62
2:F:218:ILE:O	2:F:222:MET:HB3	1.98	0.62
1:X:149:GLU:HG2	1:X:168:ILE:HD11	1.82	0.62
2:G:170:ASP:HB3	2:G:217:LYS:HD3	1.79	0.62
2:I:153:SER:C	2:I:157:GLN:HB2	2.19	0.62
1:V:6:VAL:HG21	1:V:147:ILE:HG22	1.80	0.62
1:V:86:ARG:HA	1:V:89:ARG:CZ	2.29	0.62
1:X:73:LYS:HZ1	1:X:77:GLU:HG3	1.64	0.62
1:A:47:ALA:HB3	1:A:94:LEU:HB2	1.82	0.62
1:B:131:ALA:HB3	1:Z:131:ALA:HB3	1.80	0.62
2:G:214:ARG:HD3	2:G:216:LEU:HD22	1.80	0.62
1:A:117:ASN:O	1:A:118:ASP:HB2	1.99	0.62
2:I:12:GLU:HG2	2:I:73:LEU:HD13	1.82	0.62
1:B:154:ILE:CD1	1:Z:134:ARG:HG2	2.29	0.62
2:E:173:ILE:HD11	2:E:221:ALA:CB	2.30	0.62
2:F:393:ARG:HG2	2:F:393:ARG:NH1	2.13	0.62
2:G:440:ARG:HD3	2:I:314:LYS:HD3	1.81	0.62
2:F:89:VAL:HA	2:F:92:VAL:C	2.19	0.61
1:X:62:ARG:O	1:X:66:MET:HB2	1.99	0.61
2:E:140:LYS:O	2:E:141:ASN:HB2	1.98	0.61
2:F:220:ASP:O	2:F:224:LEU:HD23	2.00	0.61
1:V:34:VAL:HB	1:V:167:THR:HG22	1.82	0.61
2:F:102:ASP:C	2:F:104:THR:H	2.03	0.61
1:Y:53:ALA:O	1:Y:55:THR:N	2.33	0.61
1:Z:80:LYS:O	1:Z:84:THR:HG22	1.99	0.61
2:F:167:GLN:O	2:F:168:LEU:HB3	2.00	0.61
2:G:375:ARG:CZ	2:G:422:ALA:HB1	2.30	0.61
2:I:132:LEU:HA	2:I:135:LEU:HD12	1.83	0.61
2:I:375:ARG:HB3	2:I:425:VAL:HG11	1.82	0.61
2:I:432:LEU:N	2:I:432:LEU:HD12	2.15	0.61
1:Z:10:GLY:HA3	1:Z:174:LYS:CA	2.27	0.61
1:C:38:TYR:CG	1:C:64:LEU:HD13	2.35	0.61
2:I:132:LEU:HD23	2:I:135:LEU:HD12	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:HD23	1:C:74:ALA:CB	2.30	0.61
2:E:292:THR:HG22	2:E:294:HIS:H	1.66	0.61
2:I:217:LYS:HG3	2:I:218:ILE:N	2.16	0.61
1:V:47:ALA:HB3	1:V:94:LEU:HB2	1.83	0.61
1:Y:141:GLU:HA	1:Y:141:GLU:OE2	1.99	0.61
1:A:15:ALA:HB1	1:A:152:LEU:HD12	1.80	0.61
1:V:70:HIS:HE1	1:V:72:VAL:HB	1.66	0.61
1:X:60:PHE:CZ	1:X:97:VAL:HG11	2.35	0.61
1:Y:1:THR:HB	1:Y:33:LYS:HZ2	1.64	0.61
1:D:94:LEU:CD2	1:D:107:THR:HG22	2.29	0.61
2:E:58:PRO:HG2	2:E:61:VAL:HG11	1.81	0.61
2:I:116:ILE:O	2:I:120:ARG:HB2	2.00	0.61
1:V:46:PHE:HB3	1:V:57:PHE:CZ	2.36	0.61
1:V:71:LEU:HD21	1:V:97:VAL:HG11	1.81	0.61
1:B:136:LEU:CD1	1:Z:135:ALA:HB1	2.31	0.61
1:C:152:LEU:HB3	1:C:166:HIS:CE1	2.35	0.61
2:E:109:LYS:HG3	2:E:109:LYS:O	2.01	0.61
2:E:432:LEU:HD12	2:E:432:LEU:H	1.66	0.61
2:F:116:ILE:O	2:F:120:ARG:HB2	2.01	0.61
1:A:136:LEU:HD13	1:Y:135:ALA:HB1	1.82	0.61
2:F:103:LEU:CD1	2:F:247:VAL:HG13	2.31	0.61
2:G:362:GLU:HG2	2:G:410:ALA:HB1	1.81	0.61
2:I:389:ASN:HD22	2:I:391:GLY:H	1.47	0.61
1:Z:1:THR:HB	1:Z:33:LYS:NZ	2.15	0.61
1:V:28:LYS:HE2	1:V:30:ASN:ND2	2.15	0.60
2:E:432:LEU:N	2:E:432:LEU:HD12	2.15	0.60
2:G:91:TYR:CD1	2:I:91:TYR:CD2	2.89	0.60
1:Y:1:THR:HB	1:Y:33:LYS:HZ3	1.64	0.60
2:F:108:VAL:HA	2:F:111:VAL:HG22	1.83	0.60
2:F:147:GLU:O	2:F:151:GLU:HG2	2.00	0.60
2:I:269:GLY:N	2:I:270:PRO:HD2	2.16	0.60
1:B:115:PRO:HG3	1:B:120:ILE:HG12	1.82	0.60
2:F:127:ALA:HA	2:F:130:ARG:NH2	2.16	0.60
2:G:262:CYS:SG	2:G:318:LEU:HD13	2.41	0.60
1:C:59:LEU:HD11	1:C:63:LYS:HE2	1.84	0.60
1:D:105:ILE:HD11	1:D:120:ILE:HG23	1.83	0.60
2:G:96:VAL:HG11	2:G:281:LEU:HD12	1.84	0.60
2:I:389:ASN:HD22	2:I:389:ASN:C	2.05	0.60
1:V:81:ASP:HB3	1:V:88:LEU:CD1	2.31	0.60
2:F:291:SER:HA	2:F:296:MET:HE2	1.82	0.60
2:F:413:LEU:O	2:F:416:GLN:HG3	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:140:LYS:H	2:G:140:LYS:HD3	1.67	0.60
2:F:217:LYS:O	2:F:220:ASP:HB2	2.02	0.60
2:G:152:PRO:CB	2:G:156:ARG:HB2	2.22	0.60
2:I:344:LEU:HD13	2:I:395:LEU:HD13	1.82	0.60
2:E:311:GLN:HE21	2:E:311:GLN:CA	2.12	0.60
2:F:262:CYS:SG	2:F:318:LEU:HD13	2.42	0.60
2:F:101:ARG:O	2:F:104:THR:HB	2.02	0.60
2:F:358:LEU:O	2:F:361:THR:HB	2.01	0.60
2:F:432:LEU:N	2:F:432:LEU:HD12	2.16	0.60
1:B:141:GLU:OE2	1:B:141:GLU:HA	2.02	0.59
1:D:152:LEU:HD13	1:D:166:HIS:ND1	2.17	0.59
2:E:151:GLU:HB2	2:E:152:PRO:CD	2.30	0.59
2:F:220:ASP:O	2:F:224:LEU:N	2.27	0.59
2:I:108:VAL:C	2:I:110:MET:H	2.03	0.59
1:V:17:ASP:HA	1:V:165:PHE:O	2.02	0.59
1:V:5:SER:HB3	1:V:120:ILE:HB	1.83	0.59
1:B:170:GLU:HG2	1:B:171:LEU:H	1.67	0.59
1:C:10:GLY:HA3	1:C:174:LYS:HA	1.84	0.59
2:E:152:PRO:O	2:E:154:ALA:C	2.39	0.59
2:E:173:ILE:HG12	2:E:212:LYS:HD2	1.84	0.59
2:G:173:ILE:HD11	2:G:221:ALA:CB	2.31	0.59
1:A:87:MET:HE1	1:B:84:THR:HG23	1.82	0.59
1:C:86:ARG:HG3	1:C:89:ARG:NH2	2.17	0.59
2:E:169:ASP:O	2:E:218:ILE:HG13	2.03	0.59
2:G:88:GLU:CD	2:I:90:GLY:HA2	2.23	0.59
1:B:64:LEU:HD23	1:B:74:ALA:CB	2.32	0.59
1:C:37:LEU:N	1:C:37:LEU:HD23	2.16	0.59
2:G:142:ASN:CB	2:G:149:GLN:HE22	2.15	0.59
1:X:79:ALA:HB1	1:X:110:GLY:HA2	1.83	0.59
1:Y:86:ARG:HA	1:Y:89:ARG:NH1	2.16	0.59
1:Y:53:ALA:C	1:Y:55:THR:H	2.04	0.59
2:F:123:ALA:HA	2:F:127:ALA:CB	2.31	0.59
1:Y:67:HIS:CD2	1:Y:73:LYS:HD2	2.38	0.59
2:I:375:ARG:CZ	2:I:422:ALA:HB1	2.33	0.59
1:V:86:ARG:HA	1:V:89:ARG:NH1	2.17	0.59
1:X:152:LEU:HD22	1:X:166:HIS:HE1	1.68	0.59
1:C:3:ILE:O	1:C:121:ALA:HA	2.03	0.59
2:E:389:ASN:HD22	2:E:391:GLY:H	1.48	0.59
2:G:116:ILE:O	2:G:120:ARG:HB2	2.02	0.59
2:I:214:ARG:HE	2:I:216:LEU:HB3	1.67	0.59
2:E:131:ILE:O	2:E:134:VAL:HG12	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:257:GLU:HG3	2:E:257:GLU:O	2.03	0.58
2:F:170:ASP:HB3	2:F:217:LYS:HD3	1.84	0.58
2:G:168:LEU:HD12	2:G:219:LYS:HB3	1.84	0.58
2:G:27:VAL:HG13	2:G:70:LEU:HG	1.85	0.58
2:E:167:GLN:NE2	2:E:168:LEU:HG	2.18	0.58
1:C:132:ALA:CB	1:C:154:ILE:HG21	2.33	0.58
1:D:37:LEU:N	1:D:37:LEU:HD23	2.18	0.58
2:F:52:ASN:HB2	2:F:325:ARG:O	2.04	0.58
2:I:217:LYS:O	2:I:221:ALA:HB3	2.01	0.58
2:I:130:ARG:HH21	2:I:229:GLU:HG3	1.68	0.58
1:B:154:ILE:HD12	1:Z:134:ARG:CG	2.33	0.58
1:C:28:LYS:HD3	1:C:31:VAL:HG22	1.84	0.58
2:E:86:PHE:O	2:E:89:VAL:HG22	2.03	0.58
2:F:132:LEU:HD11	2:F:160:ARG:HG2	1.85	0.58
2:F:232:LYS:N	2:F:232:LYS:HZ1	2.01	0.58
2:I:101:ARG:O	2:I:104:THR:HB	2.02	0.58
2:I:312:ILE:HG12	2:I:313:ALA:N	2.19	0.58
1:V:73:LYS:NZ	1:V:77:GLU:HG2	2.18	0.58
1:D:62:ARG:O	1:D:66:MET:HB2	2.04	0.58
2:G:122:ARG:NH1	2:G:126:LEU:HD21	2.19	0.58
2:G:174:GLU:CA	2:G:212:LYS:HB3	2.34	0.58
2:I:12:GLU:HG2	2:I:73:LEU:CD1	2.34	0.58
1:Z:88:LEU:HD12	1:Z:88:LEU:H	1.69	0.58
2:I:217:LYS:CG	2:I:218:ILE:H	2.11	0.58
1:B:36:ARG:O	1:B:37:LEU:HD23	2.03	0.58
1:C:157:ASP:OD2	1:C:164:HIS:NE2	2.34	0.58
1:D:64:LEU:HB3	1:D:69:GLY:HA2	1.85	0.58
1:Y:168:ILE:N	1:Y:168:ILE:HD12	2.18	0.58
1:Z:86:ARG:HA	1:Z:89:ARG:NH2	2.18	0.58
2:I:135:LEU:HD23	2:I:171:LYS:HE2	1.86	0.58
1:Y:60:PHE:HE1	1:Y:75:ALA:HA	1.69	0.58
2:G:231:ALA:C	2:G:233:LEU:H	2.06	0.58
2:I:130:ARG:HG2	2:I:225:LEU:HD11	1.84	0.58
2:I:27:VAL:CG1	2:I:70:LEU:HG	2.33	0.58
1:V:54:PHE:HD1	1:X:76:VAL:HG21	1.69	0.58
1:A:152:LEU:HD13	1:A:166:HIS:ND1	2.19	0.57
2:E:337:THR:O	2:E:341:GLU:HG3	2.03	0.57
2:G:214:ARG:HG2	2:G:215:LYS:N	2.19	0.57
1:V:70:HIS:CE1	1:V:72:VAL:HB	2.39	0.57
2:F:235:ASN:HB2	2:F:236:PRO:HD2	1.86	0.57
2:G:389:ASN:HD22	2:G:391:GLY:H	1.49	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:103:LEU:CD1	2:I:247:VAL:HG13	2.34	0.57
2:I:89:VAL:HG11	2:I:94:LYS:O	2.03	0.57
1:V:136:LEU:HB3	1:V:147:ILE:CD1	2.34	0.57
1:V:139:ASN:HD22	1:V:139:ASN:N	2.02	0.57
1:X:100:GLU:OE2	1:X:173:TYR:HB2	2.04	0.57
1:Y:72:VAL:O	1:Y:75:ALA:HB3	2.03	0.57
1:C:159:CYS:HB3	1:C:162:THR:HB	1.86	0.57
2:E:4:MET:HE1	2:E:73:LEU:HD11	1.86	0.57
2:I:127:ALA:HA	2:I:130:ARG:NH2	2.18	0.57
1:Y:46:PHE:CE2	1:Y:53:ALA:HB2	2.39	0.57
2:G:359:MET:CE	2:I:36:ARG:NH1	2.67	0.57
2:I:401:ARG:NH2	2:I:442:ILE:HG13	2.19	0.57
1:C:168:ILE:N	1:C:168:ILE:HD12	2.19	0.57
2:E:134:VAL:CG1	2:E:171:LYS:HD3	2.34	0.57
2:F:108:VAL:HG21	2:F:294:HIS:HD2	1.69	0.57
2:F:356:LYS:HA	2:F:366:ILE:HG22	1.86	0.57
1:C:73:LYS:O	1:C:76:VAL:HG12	2.05	0.57
2:G:312:ILE:N	2:G:312:ILE:HD13	2.15	0.57
1:V:170:GLU:HG3	1:V:171:LEU:H	1.70	0.57
1:B:46:PHE:CE2	1:B:53:ALA:HB2	2.40	0.57
2:I:168:LEU:O	2:I:217:LYS:HD2	2.04	0.57
1:C:73:LYS:HA	1:C:76:VAL:HG12	1.87	0.57
2:E:147:GLU:CA	2:E:150:GLN:HG3	2.34	0.57
2:I:219:LYS:HA	2:I:219:LYS:HE3	1.85	0.57
2:I:89:VAL:HA	2:I:92:VAL:C	2.24	0.57
1:Z:152:LEU:HD13	1:Z:166:HIS:CE1	2.40	0.57
1:Z:12:VAL:HG12	1:Z:171:LEU:HB3	1.86	0.57
1:C:17:ASP:O	1:C:33:LYS:HD2	2.05	0.57
2:F:151:GLU:HB2	2:F:152:PRO:HD3	1.87	0.57
2:G:122:ARG:NE	2:G:126:LEU:HD21	2.20	0.57
1:B:128:TYR:O	1:Z:131:ALA:HB1	2.05	0.57
2:I:89:VAL:HA	2:I:92:VAL:O	2.04	0.57
2:F:174:GLU:HA	2:F:212:LYS:HB3	1.86	0.56
2:F:239:LEU:HD23	2:F:240:LYS:N	2.19	0.56
1:X:30:ASN:N	1:X:30:ASN:HD22	1.86	0.56
1:Z:51:ALA:HB2	1:Y:111:ASP:OD2	2.05	0.56
1:A:55:THR:OG1	1:B:83:ARG:NH2	2.36	0.56
1:A:88:LEU:CD1	1:A:88:LEU:H	2.18	0.56
2:E:262:CYS:SG	2:E:318:LEU:HD13	2.45	0.56
2:F:210:LYS:N	2:F:210:LYS:HD3	2.19	0.56
2:F:58:PRO:HG2	2:F:61:VAL:HG11	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:312:ILE:HG12	2:G:313:ALA:N	2.20	0.56
2:G:441:PHE:HD1	2:I:56:ILE:HD13	1.69	0.56
1:V:39:ASN:O	1:V:41:LYS:HG3	2.06	0.56
1:Y:99:ASP:OD2	1:Y:101:THR:HB	2.04	0.56
1:Z:115:PRO:HG3	1:Z:120:ILE:HG12	1.87	0.56
1:D:10:GLY:HA2	1:D:173:TYR:CZ	2.40	0.56
2:E:130:ARG:HB2	2:E:130:ARG:CZ	2.35	0.56
2:E:12:GLU:OE1	2:E:15:LYS:HE2	2.06	0.56
2:F:217:LYS:HZ2	2:F:217:LYS:HB2	1.69	0.56
2:G:88:GLU:HB3	2:I:90:GLY:HA2	1.87	0.56
1:Z:36:ARG:NH1	1:Z:40:ASP:O	2.38	0.56
1:C:67:HIS:NE2	1:C:77:GLU:HG3	2.20	0.56
2:E:389:ASN:ND2	2:E:389:ASN:C	2.58	0.56
2:F:229:GLU:OE2	2:F:232:LYS:HD2	2.05	0.56
2:G:432:LEU:CD1	2:G:432:LEU:H	2.17	0.56
1:X:152:LEU:HD13	1:X:166:HIS:CE1	2.40	0.56
2:E:52:ASN:HB2	2:E:325:ARG:O	2.05	0.56
2:F:108:VAL:C	2:F:110:MET:N	2.59	0.56
2:F:76:ALA:HB1	2:F:250:HIS:O	2.04	0.56
2:G:130:ARG:CD	2:G:225:LEU:HD11	2.35	0.56
2:I:210:LYS:N	2:I:210:LYS:HD3	2.20	0.56
2:G:91:TYR:HB3	2:I:91:TYR:HA	1.88	0.56
1:Z:105:ILE:HD11	1:Z:120:ILE:HG23	1.86	0.56
1:D:1:THR:HB	1:D:33:LYS:NZ	2.20	0.56
2:F:65:GLU:HG3	3:F:1450:ADP:H2'	1.87	0.56
2:G:361:THR:HG21	2:I:36:ARG:HA	1.86	0.56
2:I:76:ALA:HB1	2:I:250:HIS:O	2.06	0.56
2:E:77:PRO:HB2	2:E:103:LEU:HD21	1.88	0.56
2:G:34:ARG:CZ	2:G:250:HIS:HA	2.36	0.56
1:Y:38:TYR:HB2	1:Y:64:LEU:HD12	1.87	0.56
1:Y:62:ARG:HA	1:Y:65:GLU:HG3	1.88	0.56
1:Z:88:LEU:CD1	1:Z:88:LEU:H	2.19	0.56
2:I:96:VAL:HG12	2:I:284:LEU:HD11	1.88	0.56
1:B:19:GLN:HB2	1:B:163:ASN:ND2	2.21	0.56
1:C:64:LEU:HA	1:C:74:ALA:CB	2.36	0.56
2:E:216:LEU:HD23	2:E:216:LEU:N	2.21	0.56
2:I:158:ALA:HB1	2:I:162:LYS:NZ	2.21	0.56
1:A:36:ARG:NH1	1:A:40:ASP:O	2.36	0.56
1:B:154:ILE:HD12	1:Z:134:ARG:HB3	1.87	0.56
2:G:145:GLN:C	2:G:147:GLU:H	2.09	0.56
2:G:311:GLN:CA	2:G:311:GLN:HE21	2.19	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:88:GLU:CD	2:I:90:GLY:CA	2.74	0.56
2:E:232:LYS:NZ	2:E:232:LYS:HB3	2.21	0.56
2:F:173:ILE:HD13	2:F:173:ILE:N	2.20	0.56
2:F:163:LEU:HD11	2:F:222:MET:CE	2.35	0.56
1:X:105:ILE:CD1	1:X:120:ILE:HG23	2.36	0.56
1:B:62:ARG:O	1:B:66:MET:HG3	2.06	0.55
2:E:152:PRO:HB3	2:E:156:ARG:H	1.72	0.55
1:V:136:LEU:HB3	1:V:147:ILE:HD12	1.88	0.55
1:Y:98:ALA:CB	1:Y:103:SER:HB3	2.36	0.55
1:Z:149:GLU:HG2	1:Z:168:ILE:HD11	1.88	0.55
1:B:154:ILE:HD12	1:Z:134:ARG:HG2	1.86	0.55
2:G:58:PRO:HG2	2:G:61:VAL:HG11	1.89	0.55
2:I:103:LEU:HD13	2:I:247:VAL:HG22	1.88	0.55
1:X:86:ARG:CG	1:X:89:ARG:HH22	2.19	0.55
1:D:55:THR:O	1:D:58:GLU:HB3	2.07	0.55
2:E:151:GLU:CB	2:E:152:PRO:CD	2.84	0.55
2:E:173:ILE:HD11	2:E:221:ALA:HB1	1.88	0.55
2:E:27:VAL:CG1	2:E:70:LEU:HG	2.36	0.55
2:F:135:LEU:HD22	2:F:159:PHE:CE2	2.41	0.55
2:I:221:ALA:O	2:I:225:LEU:HD23	2.05	0.55
1:C:85:ASP:O	1:C:89:ARG:HB2	2.06	0.55
1:D:28:LYS:HG2	1:D:31:VAL:HG22	1.89	0.55
1:D:83:ARG:CB	1:D:83:ARG:HH11	2.14	0.55
2:G:147:GLU:HA	2:G:150:GLN:CG	2.35	0.55
2:G:130:ARG:CG	2:G:225:LEU:HD11	2.36	0.55
2:I:135:LEU:HB3	2:I:159:PHE:CD2	2.41	0.55
1:A:6:VAL:HG21	1:A:147:ILE:HG22	1.86	0.55
1:V:63:LYS:HD2	1:V:77:GLU:HB3	1.88	0.55
1:Z:15:ALA:HB1	1:Z:152:LEU:HD12	1.87	0.55
1:B:72:VAL:O	1:B:75:ALA:HB3	2.06	0.55
2:E:269:GLY:N	2:E:270:PRO:HD2	2.21	0.55
2:F:153:SER:N	2:F:156:ARG:HB3	2.21	0.55
2:F:216:LEU:CD2	2:F:221:ALA:HB2	2.36	0.55
2:F:225:LEU:HA	2:F:228:GLU:CB	2.37	0.55
2:F:345:THR:CG2	2:F:373:ILE:HD12	2.36	0.55
2:I:25:ARG:O	2:I:29:ILE:HG12	2.07	0.55
1:V:132:ALA:CB	1:V:154:ILE:HG21	2.35	0.55
1:A:28:LYS:HZ2	1:A:30:ASN:ND2	2.04	0.55
2:E:92:VAL:HG21	2:F:91:TYR:C	2.27	0.55
2:F:269:GLY:N	2:F:270:PRO:HD2	2.21	0.55
2:F:32:ARG:O	2:F:36:ARG:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:10:GLY:HA2	1:X:173:TYR:CE1	2.42	0.55
1:D:6:VAL:HG21	1:D:147:ILE:HG22	1.88	0.55
2:G:109:LYS:HB2	2:I:296:MET:HG2	1.87	0.55
2:I:151:GLU:HB2	2:I:152:PRO:HD3	1.89	0.55
2:I:235:ASN:OD1	2:I:238:GLU:HB2	2.07	0.55
2:E:96:VAL:HG12	2:E:284:LEU:HD11	1.89	0.55
2:G:147:GLU:O	2:G:150:GLN:HG3	2.07	0.55
2:G:382:GLN:O	2:G:386:SER:HB3	2.07	0.55
1:V:63:LYS:HA	1:V:66:MET:HE3	1.89	0.55
1:V:67:HIS:CD2	1:V:73:LYS:HE2	2.42	0.55
1:V:83:ARG:CG	1:V:83:ARG:HH11	2.19	0.55
2:E:174:GLU:HA	2:E:213:ALA:H	1.72	0.55
2:F:270:PRO:O	2:F:273:SER:HB3	2.06	0.55
2:F:89:VAL:HG12	2:F:93:GLY:CA	2.36	0.55
2:I:122:ARG:CZ	2:I:122:ARG:HA	2.37	0.55
2:I:167:GLN:O	2:I:168:LEU:HB3	2.05	0.55
2:I:393:ARG:NH2	3:I:3450:ADP:O1B	2.40	0.55
1:X:1:THR:HB	1:X:33:LYS:NZ	2.22	0.55
1:X:83:ARG:HB3	1:X:83:ARG:CZ	2.36	0.55
1:Z:8:ARG:NH1	1:Z:142:LEU:O	2.32	0.55
1:Z:28:LYS:NZ	1:Z:30:ASN:ND2	2.55	0.55
2:E:131:ILE:HD11	2:E:218:ILE:CD1	2.37	0.54
2:G:124:GLU:HA	2:G:127:ALA:CB	2.37	0.54
2:I:140:LYS:O	2:I:141:ASN:HB3	2.07	0.54
2:I:432:LEU:H	2:I:432:LEU:HD12	1.71	0.54
1:A:28:LYS:HD2	1:B:113:VAL:CG1	2.36	0.54
1:B:140:THR:CG2	1:Z:140:THR:CG2	2.84	0.54
1:B:168:ILE:HD12	1:B:168:ILE:N	2.23	0.54
2:E:150:GLN:O	2:E:153:SER:CB	2.54	0.54
1:X:85:ASP:HB3	1:X:88:LEU:HB2	1.88	0.54
1:X:86:ARG:HG2	1:X:89:ARG:HH22	1.71	0.54
1:V:38:TYR:N	1:V:61:GLU:OE1	2.40	0.54
1:V:83:ARG:CZ	1:V:83:ARG:HB3	2.37	0.54
1:X:64:LEU:O	1:X:69:GLY:N	2.36	0.54
2:E:140:LYS:HD3	2:E:140:LYS:H	1.72	0.54
2:E:312:ILE:N	2:E:312:ILE:HD13	2.12	0.54
2:F:59:THR:O	2:F:61:VAL:HG13	2.07	0.54
2:F:91:TYR:O	2:F:92:VAL:HG22	2.07	0.54
2:G:131:ILE:HD11	2:G:218:ILE:CG1	2.38	0.54
2:G:358:LEU:O	2:G:361:THR:HB	2.08	0.54
1:Y:70:HIS:CE1	1:Y:73:LYS:H	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASP:OD2	1:B:101:THR:HB	2.07	0.54
2:E:112:ARG:HH11	2:E:112:ARG:HG3	1.72	0.54
2:F:35:TRP:O	2:F:39:GLN:HG2	2.08	0.54
1:X:1:THR:HB	1:X:33:LYS:HZ3	1.73	0.54
1:A:152:LEU:HD13	1:A:166:HIS:CE1	2.42	0.54
1:B:53:ALA:O	1:B:55:THR:N	2.40	0.54
2:E:63:LYS:HD3	2:E:332:LEU:HD13	1.88	0.54
2:F:131:ILE:HD11	2:F:218:ILE:HD13	1.88	0.54
2:F:264:ARG:NE	2:F:265:GLY:H	2.05	0.54
2:I:108:VAL:C	2:I:110:MET:N	2.61	0.54
2:I:214:ARG:NE	2:I:216:LEU:HB3	2.23	0.54
2:I:171:LYS:HZ3	2:I:218:ILE:HD11	1.73	0.54
1:Y:43:ILE:HG12	1:Y:98:ALA:O	2.07	0.54
1:Z:88:LEU:HD12	1:Z:88:LEU:N	2.21	0.54
1:C:3:ILE:HD11	1:C:46:PHE:O	2.08	0.54
2:E:108:VAL:C	2:E:110:MET:H	2.11	0.54
2:E:408:TYR:HD1	2:F:29:ILE:HD11	1.73	0.54
2:F:212:LYS:NZ	2:F:212:LYS:HB2	2.23	0.54
2:G:86:PHE:O	2:G:89:VAL:HG22	2.07	0.54
1:B:6:VAL:HG12	1:B:7:ARG:N	2.22	0.54
2:F:292:THR:C	2:F:294:HIS:H	2.11	0.54
1:V:90:LYS:NZ	1:X:89:ARG:NH1	2.56	0.54
1:Z:95:LEU:HB2	1:Z:106:ILE:HB	1.90	0.54
2:F:103:LEU:O	2:F:107:ALA:HB2	2.08	0.54
2:F:135:LEU:CG	2:F:171:LYS:HE2	2.35	0.54
2:I:358:LEU:O	2:I:361:THR:HB	2.06	0.54
1:B:86:ARG:HA	1:B:89:ARG:NH1	2.23	0.53
1:C:6:VAL:HG21	1:C:147:ILE:CG2	2.38	0.53
2:E:230:ALA:O	2:E:233:LEU:HB3	2.08	0.53
1:V:141:GLU:OE2	1:V:141:GLU:HA	2.07	0.53
1:V:159:CYS:HB3	1:V:162:THR:HB	1.90	0.53
1:Y:98:ALA:HB2	1:Y:103:SER:HB3	1.90	0.53
1:A:10:GLY:HA3	1:A:174:LYS:CA	2.37	0.53
2:I:393:ARG:HH11	2:I:393:ARG:HG2	1.72	0.53
1:X:14:ILE:HD12	1:X:43:ILE:HG12	1.90	0.53
1:A:12:VAL:HG12	1:A:171:LEU:HB3	1.90	0.53
1:A:88:LEU:HD12	1:A:88:LEU:H	1.74	0.53
1:C:154:ILE:HG22	1:C:155:ALA:N	2.23	0.53
2:E:167:GLN:HE22	2:E:168:LEU:HG	1.73	0.53
2:E:344:LEU:HD23	2:E:373:ILE:HG23	1.89	0.53
2:F:223:LYS:HD2	2:F:223:LYS:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:217:LYS:HG3	2:G:219:LYS:HZ3	1.72	0.53
1:V:1:THR:HB	1:V:33:LYS:NZ	2.23	0.53
2:F:147:GLU:HG2	2:F:150:GLN:HE21	1.72	0.53
2:G:257:GLU:O	2:G:257:GLU:HG3	2.08	0.53
1:Y:115:PRO:HG3	1:Y:120:ILE:HG12	1.90	0.53
1:Y:64:LEU:HD23	1:Y:74:ALA:CB	2.38	0.53
2:F:23:ALA:HB1	2:F:55:MET:HE3	1.90	0.53
2:F:257:GLU:HB2	2:F:260:LYS:CG	2.39	0.53
2:G:408:TYR:HB2	2:I:29:ILE:HD11	1.91	0.53
1:X:73:LYS:NZ	1:X:77:GLU:HG3	2.23	0.53
2:F:151:GLU:CB	2:F:152:PRO:HD3	2.39	0.53
2:G:116:ILE:O	2:G:116:ILE:HG22	2.08	0.53
2:I:103:LEU:O	2:I:107:ALA:HB2	2.09	0.53
1:X:86:ARG:HA	1:X:89:ARG:HH12	1.73	0.53
1:B:60:PHE:HD1	1:B:78:LEU:HD22	1.73	0.53
2:F:89:VAL:HG12	2:F:93:GLY:HA3	1.90	0.53
2:G:173:ILE:HG12	2:G:212:LYS:CD	2.38	0.53
1:V:3:ILE:HB	1:V:122:ILE:CG1	2.37	0.53
1:V:71:LEU:HD13	1:V:71:LEU:C	2.29	0.53
2:F:135:LEU:HB3	2:F:159:PHE:CD2	2.43	0.53
1:V:94:LEU:HB3	1:V:122:ILE:HD12	1.89	0.53
1:X:109:ASN:O	1:X:110:GLY:C	2.46	0.53
1:Z:60:PHE:CE2	1:Z:97:VAL:HG21	2.44	0.53
1:V:6:VAL:HG21	1:V:147:ILE:CG2	2.39	0.53
1:V:86:ARG:HA	1:V:89:ARG:NH2	2.24	0.53
1:Y:10:GLY:HA2	1:Y:173:TYR:CZ	2.44	0.53
2:E:322:LEU:O	2:E:326:LEU:HD22	2.09	0.53
2:F:140:LYS:O	2:F:141:ASN:HB3	2.09	0.53
2:I:345:THR:CG2	2:I:373:ILE:CD1	2.87	0.53
1:Y:79:ALA:O	1:Y:83:ARG:HG2	2.09	0.53
2:F:108:VAL:HG21	2:F:294:HIS:CD2	2.44	0.52
2:G:126:LEU:O	2:G:130:ARG:NH2	2.40	0.52
2:G:150:GLN:O	2:G:153:SER:OG	2.27	0.52
2:G:232:LYS:NZ	2:G:232:LYS:HB3	2.24	0.52
2:I:130:ARG:CG	2:I:225:LEU:HD11	2.39	0.52
2:I:173:ILE:N	2:I:173:ILE:HD13	2.25	0.52
1:V:28:LYS:CE	1:V:30:ASN:ND2	2.72	0.52
1:Y:10:GLY:HA2	1:Y:173:TYR:CE1	2.44	0.52
1:X:115:PRO:HG3	1:X:120:ILE:HG12	1.91	0.52
1:Z:149:GLU:OE1	1:Z:168:ILE:HD11	2.09	0.52
1:Z:38:TYR:HE1	1:Z:65:GLU:HG2	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:VAL:HG12	1:C:170:GLU:CA	2.33	0.52
1:C:36:ARG:C	1:C:37:LEU:HD23	2.29	0.52
2:E:172:GLU:HG3	2:E:214:ARG:O	2.08	0.52
2:E:358:LEU:O	2:E:361:THR:HB	2.08	0.52
2:F:432:LEU:H	2:F:432:LEU:HD12	1.74	0.52
2:F:86:PHE:O	2:F:89:VAL:HG22	2.08	0.52
2:I:312:ILE:HD13	2:I:312:ILE:N	2.12	0.52
1:V:64:LEU:HD23	1:V:74:ALA:CB	2.39	0.52
1:A:10:GLY:HA2	1:A:173:TYR:CZ	2.43	0.52
2:E:217:LYS:HG3	2:E:219:LYS:NZ	2.24	0.52
2:G:134:VAL:HG21	2:G:172:GLU:O	2.08	0.52
2:G:292:THR:HG22	2:G:293:LYS:N	2.24	0.52
2:E:140:LYS:HD3	2:E:140:LYS:N	2.25	0.52
2:E:257:GLU:O	2:E:257:GLU:CG	2.57	0.52
2:F:21:ASP:HA	2:F:24:LYS:HD2	1.91	0.52
2:F:366:ILE:HD12	2:F:418:ILE:HB	1.90	0.52
2:G:359:MET:HE1	2:I:36:ARG:NH1	2.24	0.52
2:I:366:ILE:HG13	2:I:420:ILE:CD1	2.39	0.52
1:V:148:ALA:O	1:V:152:LEU:HB2	2.10	0.52
1:C:168:ILE:HG22	1:C:169:GLU:N	2.25	0.52
1:D:85:ASP:HB3	1:D:88:LEU:HB2	1.92	0.52
2:I:211:GLN:NE2	2:I:212:LYS:H	2.08	0.52
2:G:401:ARG:NH2	2:I:329:ARG:O	2.42	0.52
2:I:362:GLU:HG3	2:I:411:SER:HA	1.90	0.52
1:C:140:THR:HG22	1:X:140:THR:HG22	1.92	0.52
1:Z:7:ARG:HB2	1:Z:12:VAL:HG23	1.91	0.52
1:B:136:LEU:HB3	1:B:147:ILE:CD1	2.39	0.52
2:F:362:GLU:HG3	2:F:411:SER:HA	1.92	0.52
2:G:128:GLU:O	2:G:131:ILE:HG22	2.10	0.52
2:G:292:THR:HB	2:G:295:GLY:O	2.10	0.52
2:I:140:LYS:HD3	2:I:140:LYS:N	2.25	0.52
1:V:36:ARG:C	1:V:37:LEU:HD23	2.30	0.52
1:Z:10:GLY:HA2	1:Z:173:TYR:CZ	2.44	0.52
1:A:33:LYS:HA	1:A:46:PHE:CE1	2.45	0.52
2:E:131:ILE:HD11	2:E:218:ILE:CG1	2.40	0.52
2:E:311:GLN:NE2	2:E:311:GLN:CA	2.72	0.52
2:E:76:ALA:HB1	2:E:250:HIS:O	2.09	0.52
2:F:356:LYS:HA	2:F:366:ILE:CG2	2.40	0.52
2:G:362:GLU:HG2	2:G:410:ALA:CB	2.39	0.52
2:G:405:GLU:HG3	2:G:428:HIS:CE1	2.45	0.52
2:I:174:GLU:HA	2:I:212:LYS:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ILE:CD1	1:A:120:ILE:HG23	2.40	0.52
1:A:149:GLU:HG2	1:A:168:ILE:HD11	1.91	0.52
1:A:88:LEU:HD12	1:A:88:LEU:N	2.25	0.52
2:G:130:ARG:HB2	2:G:130:ARG:CZ	2.40	0.52
1:V:13:VAL:HG12	1:V:170:GLU:HA	1.92	0.52
2:E:122:ARG:NH1	2:E:126:LEU:HD21	2.24	0.52
2:E:311:GLN:N	2:E:311:GLN:HE21	2.08	0.52
2:F:23:ALA:HA	2:F:330:VAL:HG21	1.92	0.52
1:V:152:LEU:HD13	1:V:166:HIS:CE1	2.45	0.52
1:X:70:HIS:ND1	1:X:73:LYS:HB2	2.24	0.52
1:V:90:LYS:HZ1	1:X:89:ARG:HH11	1.58	0.52
2:F:136:ILE:HD11	2:F:159:PHE:CZ	2.45	0.51
1:Z:8:ARG:O	1:Z:11:HIS:HB2	2.10	0.51
1:A:66:MET:HB3	1:A:67:HIS:ND1	2.25	0.51
1:B:30:ASN:C	1:B:30:ASN:HD22	2.13	0.51
2:E:151:GLU:HB2	2:E:152:PRO:HD2	1.91	0.51
2:G:151:GLU:CB	2:G:152:PRO:CD	2.88	0.51
2:I:89:VAL:HG12	2:I:93:GLY:CA	2.38	0.51
2:E:168:LEU:HD22	2:E:219:LYS:HD3	1.92	0.51
2:F:147:GLU:CG	2:F:150:GLN:NE2	2.73	0.51
2:I:147:GLU:O	2:I:151:GLU:HG2	2.10	0.51
1:D:70:HIS:ND1	1:D:73:LYS:HB2	2.25	0.51
2:E:432:LEU:H	2:E:432:LEU:CD1	2.23	0.51
2:G:269:GLY:N	2:G:270:PRO:HD2	2.25	0.51
2:G:96:VAL:CG1	2:G:281:LEU:HD12	2.40	0.51
2:I:132:LEU:HD11	2:I:160:ARG:CG	2.36	0.51
2:I:136:ILE:HD11	2:I:159:PHE:CZ	2.46	0.51
1:B:128:TYR:CE1	1:Z:127:PRO:HB2	2.45	0.51
2:E:95:GLU:H	2:E:95:GLU:CD	2.14	0.51
2:F:135:LEU:CD2	2:F:171:LYS:HE2	2.40	0.51
2:F:225:LEU:HA	2:F:228:GLU:HB3	1.91	0.51
2:G:108:VAL:HG21	2:G:294:HIS:HD2	1.73	0.51
2:G:89:VAL:HG12	2:G:93:GLY:CA	2.41	0.51
2:I:102:ASP:C	2:I:104:THR:H	2.14	0.51
2:I:158:ALA:HB1	2:I:162:LYS:HZ2	1.73	0.51
2:I:211:GLN:HE21	2:I:212:LYS:N	2.09	0.51
2:I:315:PRO:O	2:I:318:LEU:HB2	2.10	0.51
2:I:62:GLY:O	2:I:66:ILE:HG13	2.11	0.51
1:V:90:LYS:NZ	1:X:84:THR:O	2.44	0.51
1:A:95:LEU:HB2	1:A:106:ILE:HB	1.91	0.51
1:A:10:GLY:HA2	1:A:173:TYR:CD1	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HE2	1:B:114:GLN:O	2.10	0.51
1:B:60:PHE:CE2	1:B:97:VAL:HG21	2.45	0.51
1:C:90:LYS:HE2	1:D:89:ARG:CZ	2.40	0.51
2:E:132:LEU:HB3	2:E:156:ARG:NH1	2.26	0.51
2:F:168:LEU:O	2:F:217:LYS:HD2	2.11	0.51
2:F:384:ASN:HD21	2:F:390:ILE:HG12	1.76	0.51
2:G:171:LYS:HE3	2:G:172:GLU:N	2.26	0.51
1:Y:95:LEU:HD12	1:Y:95:LEU:N	2.25	0.51
1:C:136:LEU:HB3	1:C:147:ILE:CD1	2.41	0.51
1:D:105:ILE:CD1	1:D:120:ILE:HG23	2.39	0.51
2:I:211:GLN:HE21	2:I:212:LYS:H	1.56	0.51
2:I:163:LEU:HD11	2:I:222:MET:HE3	1.92	0.51
2:I:311:GLN:CA	2:I:311:GLN:HE21	2.23	0.51
1:C:5:SER:HA	1:C:13:VAL:O	2.11	0.51
1:C:73:LYS:CD	1:C:76:VAL:HG11	2.40	0.51
2:I:108:VAL:HA	2:I:111:VAL:CG2	2.37	0.51
1:D:109:ASN:O	1:D:110:GLY:C	2.49	0.51
2:G:212:LYS:CD	2:G:216:LEU:HD21	2.33	0.51
2:I:123:ALA:HA	2:I:127:ALA:CB	2.40	0.51
1:X:94:LEU:CD2	1:X:107:THR:HG22	2.40	0.51
1:Y:19:GLN:HB2	1:Y:163:ASN:ND2	2.26	0.51
1:D:30:ASN:ND2	1:D:30:ASN:N	2.54	0.50
2:E:63:LYS:HG2	2:E:332:LEU:HD22	1.92	0.50
1:Z:5:SER:HB3	1:Z:120:ILE:HB	1.92	0.50
1:B:154:ILE:CD1	1:Z:134:ARG:CG	2.89	0.50
1:B:79:ALA:HB1	1:B:110:GLY:HA2	1.93	0.50
1:C:62:ARG:HA	1:C:65:GLU:OE2	2.11	0.50
2:F:218:ILE:O	2:F:220:ASP:N	2.45	0.50
2:G:337:THR:O	2:G:341:GLU:HG3	2.11	0.50
1:V:103:SER:HB3	1:V:120:ILE:HD11	1.93	0.50
1:A:115:PRO:CG	1:A:119:LEU:O	2.60	0.50
1:C:28:LYS:CE	1:C:30:ASN:ND2	2.70	0.50
2:E:259:ASP:HB3	2:E:310:PHE:CZ	2.46	0.50
2:F:143:TRP:HB2	2:F:148:GLN:HE21	1.76	0.50
2:G:112:ARG:HH11	2:G:112:ARG:HG3	1.76	0.50
2:G:234:VAL:O	2:G:236:PRO:HD3	2.11	0.50
2:I:163:LEU:HD11	2:I:222:MET:HE1	1.93	0.50
1:C:103:SER:HB3	1:C:120:ILE:HD11	1.94	0.50
1:Y:3:ILE:HB	1:Y:122:ILE:CG1	2.42	0.50
1:Z:149:GLU:OE2	1:Z:166:HIS:HD2	1.94	0.50
1:D:73:LYS:NZ	1:D:77:GLU:HG2	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:134:VAL:HG21	2:F:172:GLU:O	2.12	0.50
2:F:17:ILE:N	2:F:17:ILE:HD12	2.26	0.50
1:X:64:LEU:HB3	1:X:69:GLY:HA2	1.94	0.50
1:D:43:ILE:HD13	1:D:43:ILE:N	2.21	0.50
2:E:171:LYS:HE3	2:E:172:GLU:N	2.26	0.50
2:F:389:ASN:HD22	2:F:389:ASN:C	2.14	0.50
2:F:401:ARG:NH2	2:F:442:ILE:HG13	2.26	0.50
2:I:217:LYS:HB2	2:I:217:LYS:HZ3	1.76	0.50
1:A:103:SER:O	1:A:104:LEU:HB3	2.12	0.50
1:A:102:ALA:HB1	1:A:114:GLN:OE1	2.11	0.50
2:F:362:GLU:HG2	2:F:410:ALA:CB	2.42	0.50
2:I:164:ARG:O	2:I:165:GLU:HB3	2.11	0.50
2:I:216:LEU:HD11	2:I:221:ALA:HA	1.94	0.50
2:I:432:LEU:H	2:I:432:LEU:CD1	2.25	0.50
1:X:149:GLU:CG	1:X:168:ILE:HD11	2.42	0.50
1:B:65:GLU:OE2	2:F:143:TRP:CD1	2.65	0.50
2:E:147:GLU:O	2:E:150:GLN:HG3	2.11	0.50
2:G:165:GLU:HG2	2:G:166:GLY:N	2.26	0.50
2:G:382:GLN:HA	2:G:382:GLN:NE2	2.27	0.50
2:G:91:TYR:C	2:G:92:VAL:HG22	2.32	0.50
2:I:130:ARG:CD	2:I:225:LEU:HD11	2.42	0.50
1:Y:12:VAL:HG12	1:Y:171:LEU:HB3	1.94	0.50
1:B:59:LEU:HD12	1:B:59:LEU:O	2.12	0.50
1:C:1:THR:HB	1:C:33:LYS:NZ	2.27	0.50
1:C:63:LYS:HA	1:C:66:MET:HE3	1.94	0.50
1:D:149:GLU:HG2	1:D:168:ILE:HD11	1.94	0.50
2:E:408:TYR:HB2	2:F:29:ILE:HD11	1.93	0.50
2:I:145:GLN:HE21	2:I:145:GLN:CA	2.24	0.50
2:I:119:ASN:ND2	2:I:233:LEU:HD23	2.27	0.50
2:I:94:LYS:HZ2	2:I:98:SER:HB3	1.76	0.50
1:X:68:GLN:O	1:X:70:HIS:N	2.45	0.50
1:Z:51:ALA:HB3	1:Y:111:ASP:OD2	2.11	0.50
1:Z:17:ASP:HA	1:Z:165:PHE:O	2.12	0.50
1:Z:77:GLU:HA	1:Z:80:LYS:HD2	1.94	0.50
1:A:65:GLU:HG2	2:E:143:TRP:NE1	2.26	0.49
1:C:173:TYR:CD2	1:C:173:TYR:N	2.80	0.49
2:F:89:VAL:HG12	2:F:93:GLY:C	2.32	0.49
2:I:95:GLU:CD	2:I:95:GLU:H	2.16	0.49
1:V:11:HIS:HA	1:V:171:LEU:O	2.12	0.49
1:D:140:THR:HG22	1:V:140:THR:CG2	2.42	0.49
1:B:28:LYS:HD3	1:B:31:VAL:HG22	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LYS:HB3	1:C:80:LYS:NZ	2.26	0.49
2:F:147:GLU:HG2	2:F:150:GLN:NE2	2.27	0.49
2:I:115:ALA:O	2:I:119:ASN:HB2	2.13	0.49
2:I:73:LEU:O	2:I:73:LEU:HG	2.12	0.49
1:V:28:LYS:HD3	1:V:31:VAL:HG22	1.94	0.49
1:Y:35:ARG:O	1:Y:169:GLU:HG3	2.13	0.49
1:Z:84:THR:HG23	1:Z:85:ASP:N	2.26	0.49
1:B:92:GLU:O	1:B:93:ALA:HB2	2.12	0.49
1:C:37:LEU:HD23	1:C:42:VAL:O	2.12	0.49
1:D:14:ILE:HD12	1:D:43:ILE:HG12	1.92	0.49
2:E:170:ASP:HB3	2:E:217:LYS:HD3	1.95	0.49
2:F:130:ARG:CG	2:F:225:LEU:HD11	2.39	0.49
2:F:258:ILE:HG22	2:F:307:SER:O	2.12	0.49
2:I:169:ASP:O	2:I:218:ILE:HG13	2.11	0.49
2:I:345:THR:HG21	2:I:373:ILE:CD1	2.43	0.49
2:G:361:THR:HG22	2:I:35:TRP:CZ3	2.47	0.49
2:I:35:TRP:O	2:I:39:GLN:HG2	2.12	0.49
1:D:117:ASN:O	1:D:118:ASP:HB2	2.10	0.49
1:D:71:LEU:HD21	1:D:97:VAL:CG1	2.42	0.49
2:G:65:GLU:HG3	3:G:2450:ADP:H2'	1.94	0.49
1:X:86:ARG:HA	1:X:89:ARG:CZ	2.42	0.49
1:Y:39:ASN:O	1:Y:41:LYS:HG3	2.12	0.49
2:E:124:GLU:HA	2:E:127:ALA:CB	2.39	0.49
2:E:292:THR:HB	2:E:295:GLY:O	2.12	0.49
2:F:123:ALA:CA	2:F:127:ALA:HB3	2.38	0.49
2:F:393:ARG:NH2	3:F:1450:ADP:O1B	2.45	0.49
2:F:119:ASN:ND2	2:F:233:LEU:HD23	2.27	0.49
2:I:132:LEU:HD23	2:I:135:LEU:CD1	2.42	0.49
2:I:270:PRO:O	2:I:274:ARG:HD2	2.12	0.49
1:B:82:TRP:HE1	1:B:91:LEU:HB2	1.78	0.49
1:B:88:LEU:HD12	1:B:91:LEU:HD11	1.93	0.49
1:D:150:LYS:HD3	1:V:139:ASN:OD1	2.13	0.49
2:F:132:LEU:HD11	2:F:160:ARG:CG	2.41	0.49
2:G:93:GLY:O	2:G:94:LYS:C	2.51	0.49
2:I:171:LYS:O	2:I:215:LYS:HD2	2.12	0.49
2:I:212:LYS:HB2	2:I:212:LYS:HZ2	1.78	0.49
2:I:103:LEU:HD13	2:I:247:VAL:HG13	1.94	0.49
2:I:34:ARG:CZ	2:I:250:HIS:HA	2.42	0.49
1:A:8:ARG:O	1:A:11:HIS:HB2	2.13	0.49
1:C:94:LEU:HD13	1:C:122:ILE:HB	1.93	0.49
1:C:54:PHE:CD1	1:D:76:VAL:HG21	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:408:TYR:CD1	2:F:29:ILE:HD11	2.46	0.49
2:I:366:ILE:HD12	2:I:418:ILE:HB	1.93	0.49
1:X:117:ASN:O	1:X:118:ASP:HB2	2.12	0.49
1:X:89:ARG:HH11	1:X:89:ARG:HB2	1.77	0.49
1:B:86:ARG:HA	1:B:89:ARG:HE	1.75	0.49
2:E:134:VAL:HG13	2:E:171:LYS:HD3	1.94	0.49
2:E:255:ILE:HD13	2:E:281:LEU:HD21	1.93	0.49
2:F:86:PHE:HB2	2:F:277:VAL:HG13	1.94	0.49
2:G:436:GLU:O	2:G:439:SER:HB2	2.12	0.49
2:G:89:VAL:HA	2:G:93:GLY:CA	2.42	0.49
2:I:220:ASP:O	2:I:224:LEU:HD23	2.12	0.49
2:I:413:LEU:O	2:I:416:GLN:HG3	2.12	0.49
1:Y:6:VAL:HG12	1:Y:7:ARG:N	2.28	0.49
1:A:160:ILE:HG13	1:Z:160:ILE:O	2.12	0.49
1:B:69:GLY:O	1:B:71:LEU:N	2.45	0.49
1:C:71:LEU:HD21	1:C:97:VAL:HG12	1.93	0.49
2:E:77:PRO:HB3	2:E:107:ALA:HB2	1.95	0.49
2:G:131:ILE:CD1	2:G:218:ILE:HG12	2.42	0.49
2:G:140:LYS:O	2:G:141:ASN:CB	2.59	0.49
2:G:23:ALA:HA	2:G:330:VAL:HG21	1.95	0.49
2:G:33:ASN:ND2	2:G:36:ARG:HD2	2.27	0.49
2:I:122:ARG:NE	2:I:122:ARG:HA	2.28	0.49
2:I:229:GLU:OE2	2:I:232:LYS:HD2	2.12	0.49
2:I:435:ASP:CG	2:I:438:LEU:HB2	2.33	0.49
1:V:59:LEU:HD11	1:V:63:LYS:HE2	1.95	0.49
1:X:83:ARG:CB	1:X:83:ARG:HH11	2.10	0.49
1:Z:34:VAL:HG13	1:Z:44:ALA:O	2.13	0.49
1:Z:86:ARG:HG2	1:Z:89:ARG:HH22	1.77	0.49
2:E:211:GLN:O	2:E:212:LYS:HB2	2.13	0.49
2:E:173:ILE:HD11	2:E:221:ALA:HB2	1.95	0.49
2:I:32:ARG:O	2:I:36:ARG:HG3	2.13	0.49
1:X:73:LYS:NZ	1:X:77:GLU:CG	2.75	0.49
1:Y:36:ARG:NE	1:Y:169:GLU:OE2	2.44	0.49
1:B:117:ASN:O	1:B:118:ASP:HB2	2.13	0.48
1:D:61:GLU:O	1:D:65:GLU:HG2	2.12	0.48
2:F:218:ILE:HG23	2:F:222:MET:HB2	1.95	0.48
2:I:171:LYS:HZ2	2:I:218:ILE:HD11	1.72	0.48
1:V:157:ASP:OD2	1:V:164:HIS:NE2	2.33	0.48
2:E:150:GLN:O	2:E:153:SER:HB2	2.14	0.48
2:F:172:GLU:O	2:F:173:ILE:HG23	2.13	0.48
2:G:264:ARG:NE	2:G:265:GLY:H	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:135:LEU:HD22	2:I:159:PHE:CD2	2.48	0.48
2:I:396:HIS:O	2:I:400:GLU:HB2	2.14	0.48
2:G:88:GLU:CG	2:I:90:GLY:HA2	2.43	0.48
1:V:73:LYS:HD2	1:V:76:VAL:CG1	2.43	0.48
1:Y:170:GLU:CG	1:Y:171:LEU:H	2.23	0.48
1:Z:3:ILE:HB	1:Z:122:ILE:HG12	1.95	0.48
1:A:80:LYS:O	1:A:81:ASP:C	2.50	0.48
1:B:28:LYS:HZ1	1:B:30:ASN:ND2	2.10	0.48
1:B:44:ALA:HB2	1:B:97:VAL:HG23	1.94	0.48
1:D:5:SER:HB3	1:D:120:ILE:HB	1.95	0.48
2:E:222:MET:O	2:E:226:ILE:HG12	2.14	0.48
2:E:23:ALA:HA	2:E:330:VAL:HG21	1.94	0.48
2:E:408:TYR:HA	2:F:29:ILE:CD1	2.43	0.48
2:F:12:GLU:HG2	2:F:73:LEU:HD11	1.94	0.48
2:G:270:PRO:HB2	2:G:274:ARG:HD2	1.95	0.48
2:I:151:GLU:CB	2:I:152:PRO:CD	2.88	0.48
1:D:131:ALA:HB3	1:V:131:ALA:HB3	1.95	0.48
1:X:30:ASN:ND2	1:X:30:ASN:N	2.50	0.48
1:Y:170:GLU:HG2	1:Y:171:LEU:N	2.21	0.48
1:B:85:ASP:O	1:B:89:ARG:HG3	2.14	0.48
2:F:12:GLU:HG2	2:F:73:LEU:CD1	2.42	0.48
2:G:130:ARG:HD2	2:G:225:LEU:CD1	2.42	0.48
2:G:231:ALA:C	2:G:233:LEU:N	2.67	0.48
2:I:311:GLN:NE2	2:I:311:GLN:HA	2.28	0.48
1:Y:7:ARG:NE	1:Y:118:ASP:OD2	2.42	0.48
1:B:132:ALA:HB1	1:Z:135:ALA:HB2	1.93	0.48
1:A:7:ARG:HB2	1:A:12:VAL:HG23	1.95	0.48
1:C:11:HIS:HE1	1:C:174:LYS:NZ	2.11	0.48
2:E:160:ARG:HH12	2:E:164:ARG:NH2	2.11	0.48
2:F:115:ALA:O	2:F:119:ASN:HB2	2.13	0.48
2:F:153:SER:HA	2:F:157:GLN:H	1.79	0.48
2:F:268:SER:HA	2:F:271:ASP:OD2	2.12	0.48
2:G:108:VAL:HA	2:G:111:VAL:HG22	1.96	0.48
2:G:109:LYS:O	2:G:113:VAL:HG23	2.14	0.48
2:G:222:MET:O	2:G:226:ILE:HG12	2.13	0.48
1:X:5:SER:HB3	1:X:120:ILE:HB	1.95	0.48
1:X:43:ILE:HD11	1:X:98:ALA:HB3	1.96	0.48
1:B:98:ALA:CB	1:B:103:SER:HB3	2.42	0.48
1:B:94:LEU:HB3	1:B:122:ILE:HD12	1.95	0.48
1:D:30:ASN:HD22	1:D:30:ASN:N	1.96	0.48
2:E:174:GLU:CA	2:E:212:LYS:HB3	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:342:ARG:NH2	2:E:346:GLU:OE2	2.37	0.48
2:F:351:ILE:CD1	2:F:351:ILE:H	2.24	0.48
2:I:216:LEU:HG	2:I:221:ALA:HB2	1.96	0.48
2:I:335:LEU:HD22	2:I:339:ASP:HB3	1.96	0.48
2:E:153:SER:C	2:E:157:GLN:HG2	2.33	0.48
2:E:258:ILE:O	2:E:261:ILE:HG12	2.14	0.48
2:E:408:TYR:CB	2:F:29:ILE:HD11	2.43	0.48
2:F:223:LYS:HA	2:F:226:ILE:CG1	2.41	0.48
2:G:103:LEU:HD13	2:G:247:VAL:HG13	1.96	0.48
2:I:223:LYS:HA	2:I:226:ILE:CG1	2.43	0.48
1:Z:121:ALA:HB1	1:Z:126:GLY:O	2.14	0.48
1:B:38:TYR:HB2	1:B:64:LEU:CD1	2.43	0.48
2:E:292:THR:HG22	2:E:293:LYS:N	2.27	0.48
2:F:163:LEU:HD21	2:F:222:MET:HE1	1.94	0.48
1:V:80:LYS:C	1:V:80:LYS:HD2	2.34	0.48
1:Y:3:ILE:HB	1:Y:122:ILE:HG12	1.96	0.48
2:F:152:PRO:CB	2:F:156:ARG:HB2	2.41	0.48
1:X:145:ARG:NE	1:X:170:GLU:OE1	2.40	0.48
1:X:37:LEU:N	1:X:37:LEU:HD12	2.28	0.48
1:Z:86:ARG:HA	1:Z:89:ARG:CZ	2.43	0.48
1:A:139:ASN:HD22	1:Y:136:LEU:HD11	1.78	0.48
1:A:5:SER:HB3	1:A:120:ILE:HB	1.96	0.48
1:C:115:PRO:CB	1:C:119:LEU:O	2.57	0.48
1:C:70:HIS:HE1	1:C:72:VAL:HB	1.73	0.48
2:E:91:TYR:C	2:E:92:VAL:HG22	2.33	0.48
2:F:34:ARG:CZ	2:F:250:HIS:HA	2.44	0.48
2:G:312:ILE:HG12	2:G:313:ALA:H	1.79	0.48
1:V:8:ARG:HG2	1:V:9:ASN:ND2	2.29	0.48
1:X:10:GLY:HA2	1:X:173:TYR:CZ	2.48	0.48
1:X:8:ARG:HG2	1:X:9:ASN:ND2	2.29	0.48
1:A:121:ALA:HB1	1:A:126:GLY:O	2.14	0.47
1:B:98:ALA:HB2	1:B:103:SER:HB3	1.95	0.47
1:C:83:ARG:CG	1:C:83:ARG:HH11	2.25	0.47
2:G:372:GLY:O	2:G:376:ILE:HG13	2.14	0.47
2:I:151:GLU:HB2	2:I:152:PRO:HD2	1.96	0.47
2:I:59:THR:O	2:I:61:VAL:HG13	2.14	0.47
1:C:136:LEU:CD1	1:X:135:ALA:HB1	2.36	0.47
1:B:13:VAL:HG12	1:B:170:GLU:HG3	1.96	0.47
1:B:71:LEU:HD13	1:B:71:LEU:C	2.34	0.47
1:C:14:ILE:O	1:C:34:VAL:HG11	2.14	0.47
2:E:212:LYS:NZ	2:E:212:LYS:HB2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:102:ASP:C	2:F:104:THR:N	2.67	0.47
2:F:103:LEU:HD13	2:F:247:VAL:HG22	1.96	0.47
2:I:219:LYS:O	2:I:223:LYS:HD3	2.14	0.47
2:I:23:ALA:HA	2:I:330:VAL:HG21	1.95	0.47
1:Y:136:LEU:HB3	1:Y:147:ILE:HD12	1.94	0.47
1:Y:44:ALA:HB2	1:Y:97:VAL:HG23	1.96	0.47
1:Y:62:ARG:O	1:Y:66:MET:HG3	2.14	0.47
1:C:68:GLN:O	1:C:70:HIS:N	2.48	0.47
1:D:8:ARG:O	1:D:11:HIS:HB2	2.14	0.47
2:E:19:GLY:O	2:E:24:LYS:HE3	2.14	0.47
2:E:348:ASN:O	2:E:349:ALA:HB3	2.15	0.47
2:F:267:SER:O	2:F:271:ASP:OD2	2.31	0.47
2:G:148:GLN:HA	2:G:151:GLU:HG2	1.95	0.47
1:V:146:GLU:O	1:V:150:LYS:HG3	2.14	0.47
1:B:64:LEU:HD23	1:B:74:ALA:HB3	1.95	0.47
1:C:59:LEU:HG	1:C:78:LEU:HD13	1.95	0.47
2:E:86:PHE:HA	2:E:89:VAL:HG13	1.95	0.47
2:F:160:ARG:HG2	2:F:160:ARG:HH11	1.80	0.47
2:I:17:ILE:HD12	2:I:17:ILE:N	2.29	0.47
2:I:344:LEU:CD1	2:I:395:LEU:HD13	2.43	0.47
1:V:85:ASP:HB3	1:V:88:LEU:HD12	1.96	0.47
1:Y:33:LYS:HA	1:Y:46:PHE:CE1	2.50	0.47
1:D:15:ALA:HB1	1:D:152:LEU:HD12	1.97	0.47
1:D:86:ARG:HA	1:D:89:ARG:NH1	2.29	0.47
2:E:109:LYS:O	2:E:113:VAL:HG23	2.15	0.47
2:E:362:GLU:HG3	2:E:411:SER:HA	1.95	0.47
2:F:211:GLN:O	2:F:212:LYS:HB2	2.15	0.47
2:F:335:LEU:HD22	2:F:339:ASP:HB3	1.95	0.47
2:G:130:ARG:HG2	2:G:225:LEU:HD11	1.97	0.47
1:V:115:PRO:CB	1:V:119:LEU:O	2.61	0.47
1:V:30:ASN:N	1:V:30:ASN:HD22	2.04	0.47
1:A:25:THR:HA	1:Z:158:ILE:O	2.14	0.47
1:A:18:GLY:HA2	1:A:33:LYS:HE3	1.97	0.47
1:C:69:GLY:O	1:C:71:LEU:N	2.48	0.47
2:F:312:ILE:HG12	2:F:313:ALA:N	2.29	0.47
2:I:163:LEU:HD21	2:I:222:MET:HE1	1.96	0.47
1:A:62:ARG:CD	2:E:141:ASN:HD21	2.28	0.47
1:B:3:ILE:HB	1:B:122:ILE:HG12	1.97	0.47
1:B:70:HIS:HE1	1:B:72:VAL:HB	1.80	0.47
1:C:60:PHE:HB2	1:C:78:LEU:HD22	1.96	0.47
1:A:65:GLU:OE1	2:E:143:TRP:NE1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:442:ILE:CG2	2:E:442:ILE:O	2.63	0.47
2:F:142:ASN:ND2	2:F:149:GLN:NE2	2.63	0.47
2:I:167:GLN:HB2	2:I:218:ILE:CG2	2.44	0.47
2:G:359:MET:HE3	2:I:36:ARG:NH1	2.30	0.47
1:V:173:TYR:CD2	1:V:173:TYR:N	2.83	0.47
1:Y:92:GLU:O	1:Y:93:ALA:HB2	2.14	0.47
1:C:64:LEU:HA	1:C:74:ALA:HB2	1.97	0.47
2:E:108:VAL:C	2:E:110:MET:N	2.68	0.47
2:I:270:PRO:O	2:I:273:SER:HB3	2.15	0.47
1:V:170:GLU:CG	1:V:171:LEU:N	2.78	0.47
1:Y:34:VAL:HB	1:Y:167:THR:HG22	1.97	0.47
1:A:99:ASP:OD1	1:A:101:THR:N	2.42	0.47
1:C:60:PHE:CZ	1:C:97:VAL:HG11	2.50	0.47
1:D:28:LYS:CE	1:D:30:ASN:HD21	2.27	0.47
2:E:149:GLN:C	2:E:151:GLU:H	2.17	0.47
2:E:62:GLY:O	2:E:66:ILE:HG13	2.15	0.47
2:F:153:SER:CA	2:F:156:ARG:HB3	2.45	0.47
2:F:169:ASP:O	2:F:218:ILE:HG13	2.15	0.47
2:F:280:ASP:O	2:F:283:PRO:HD2	2.14	0.47
2:F:318:LEU:O	2:F:323:GLN:NE2	2.41	0.47
2:G:170:ASP:CB	2:G:217:LYS:HD3	2.45	0.47
2:I:280:ASP:O	2:I:283:PRO:HD2	2.15	0.47
1:B:70:HIS:CE1	1:B:72:VAL:HB	2.50	0.47
1:D:152:LEU:HD22	1:D:166:HIS:HE1	1.80	0.47
2:F:219:LYS:C	2:F:223:LYS:HD3	2.35	0.47
2:G:131:ILE:O	2:G:134:VAL:HG12	2.15	0.47
2:I:389:ASN:HD22	2:I:390:ILE:N	2.12	0.47
1:V:7:ARG:HH21	1:V:103:SER:N	2.13	0.47
1:V:83:ARG:NH1	1:V:83:ARG:CG	2.78	0.47
1:X:121:ALA:HB1	1:X:126:GLY:O	2.15	0.47
1:Y:60:PHE:CE2	1:Y:97:VAL:HG21	2.50	0.47
1:A:30:ASN:ND2	1:A:30:ASN:H	2.13	0.47
1:C:81:ASP:HB3	1:C:88:LEU:CD1	2.45	0.47
2:G:108:VAL:C	2:G:110:MET:N	2.68	0.47
2:G:211:GLN:O	2:G:212:LYS:HB2	2.14	0.47
2:G:336:THR:O	2:G:339:ASP:HB2	2.15	0.47
2:G:344:LEU:HD23	2:G:373:ILE:HG23	1.97	0.47
2:I:155:ALA:O	2:I:159:PHE:HD1	1.97	0.47
2:I:236:PRO:O	2:I:238:GLU:N	2.41	0.47
1:A:28:LYS:HZ3	1:A:30:ASN:ND2	2.12	0.46
1:D:86:ARG:O	1:D:90:LYS:HE3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:PRO:HB2	2:E:156:ARG:CB	2.27	0.46
2:F:145:GLN:HB2	2:F:148:GLN:CG	2.40	0.46
1:V:169:GLU:OE1	1:V:169:GLU:HA	2.15	0.46
1:V:91:LEU:O	1:V:91:LEU:HD12	2.14	0.46
1:Z:71:LEU:HD21	1:Z:99:ASP:HB3	1.97	0.46
2:E:12:GLU:CD	2:E:15:LYS:HE2	2.35	0.46
2:F:174:GLU:CA	2:F:212:LYS:HB3	2.44	0.46
2:F:432:LEU:H	2:F:432:LEU:CD1	2.28	0.46
2:G:362:GLU:HG3	2:G:411:SER:HA	1.97	0.46
2:I:211:GLN:O	2:I:212:LYS:HB2	2.15	0.46
1:C:4:VAL:HA	1:C:120:ILE:O	2.16	0.46
2:F:148:GLN:HA	2:F:151:GLU:CG	2.45	0.46
1:V:71:LEU:HD21	1:V:97:VAL:HG12	1.97	0.46
1:Y:174:LYS:HD2	1:Y:174:LYS:N	2.30	0.46
1:Y:79:ALA:HB1	1:Y:110:GLY:HA2	1.96	0.46
1:Z:152:LEU:HD13	1:Z:166:HIS:ND1	2.31	0.46
1:Z:30:ASN:H	1:Z:30:ASN:ND2	2.14	0.46
1:B:136:LEU:HD11	1:Z:139:ASN:HD22	1.79	0.46
1:C:67:HIS:CE1	1:C:77:GLU:HG3	2.50	0.46
1:D:168:ILE:HG22	1:D:169:GLU:N	2.30	0.46
2:F:122:ARG:CZ	2:F:122:ARG:HA	2.46	0.46
2:G:108:VAL:C	2:G:110:MET:H	2.19	0.46
2:G:165:GLU:HG2	2:G:166:GLY:H	1.81	0.46
2:G:392:ALA:HB3	3:G:2450:ADP:C8	2.50	0.46
2:I:220:ASP:O	2:I:224:LEU:HB2	2.16	0.46
1:Y:70:HIS:CE1	1:Y:72:VAL:HB	2.48	0.46
1:B:79:ALA:HB2	1:B:106:ILE:HG23	1.97	0.46
2:E:382:GLN:O	2:E:386:SER:HB3	2.16	0.46
2:F:264:ARG:CZ	2:F:265:GLY:H	2.28	0.46
2:F:346:GLU:HB2	2:F:347:PRO:HD3	1.98	0.46
2:G:147:GLU:CA	2:G:150:GLN:HG3	2.44	0.46
2:I:129:GLU:HB2	2:I:130:ARG:NH1	2.31	0.46
1:X:60:PHE:HZ	1:X:97:VAL:HG11	1.77	0.46
1:Y:63:LYS:HD2	1:Y:77:GLU:HB3	1.96	0.46
1:Z:17:ASP:O	1:Z:33:LYS:HD2	2.16	0.46
1:C:136:LEU:HB3	1:C:147:ILE:HD12	1.97	0.46
1:C:18:GLY:C	1:C:163:ASN:HD21	2.19	0.46
1:C:64:LEU:HD23	1:C:74:ALA:HB3	1.97	0.46
1:D:149:GLU:CD	1:D:168:ILE:HD11	2.36	0.46
2:F:388:GLU:OE2	2:F:388:GLU:N	2.49	0.46
2:G:145:GLN:HB2	2:G:148:GLN:CB	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:89:VAL:HG12	2:G:93:GLY:HA3	1.98	0.46
2:I:174:GLU:CA	2:I:212:LYS:HB3	2.46	0.46
1:V:58:GLU:O	1:V:61:GLU:HB2	2.16	0.46
1:Z:149:GLU:HG2	1:Z:168:ILE:CD1	2.45	0.46
1:C:170:GLU:CG	1:C:171:LEU:H	2.28	0.46
1:C:64:LEU:HA	1:C:74:ALA:HB1	1.97	0.46
2:F:255:ILE:HD13	2:F:281:LEU:HD21	1.97	0.46
2:F:63:LYS:HE2	2:F:307:SER:OG	2.15	0.46
2:G:255:ILE:HD13	2:G:281:LEU:HD21	1.97	0.46
2:I:102:ASP:C	2:I:104:THR:N	2.69	0.46
1:V:90:LYS:HZ1	1:X:89:ARG:HD3	1.80	0.46
1:X:13:VAL:CG1	1:X:170:GLU:HG3	2.43	0.46
1:X:37:LEU:H	1:X:37:LEU:HD12	1.81	0.46
1:B:53:ALA:C	1:B:55:THR:H	2.19	0.46
1:A:87:MET:HE3	1:B:84:THR:HG23	1.96	0.46
2:F:164:ARG:O	2:F:165:GLU:HB3	2.16	0.46
2:F:344:LEU:HD21	2:F:395:LEU:HD22	1.98	0.46
2:G:152:PRO:HB3	2:G:156:ARG:N	2.26	0.46
2:I:292:THR:C	2:I:294:HIS:H	2.20	0.46
1:Y:68:GLN:O	1:Y:70:HIS:N	2.49	0.46
1:B:103:SER:C	1:B:104:LEU:HD23	2.36	0.46
1:B:34:VAL:HG13	1:B:44:ALA:O	2.15	0.46
1:D:115:PRO:HG3	1:D:120:ILE:HG12	1.98	0.46
2:G:212:LYS:NZ	2:G:212:LYS:HB2	2.30	0.46
2:G:259:ASP:HB3	2:G:310:PHE:CZ	2.51	0.46
1:Z:149:GLU:CG	1:Z:168:ILE:HD11	2.46	0.46
1:C:121:ALA:HB1	1:C:126:GLY:O	2.15	0.46
1:C:67:HIS:O	1:C:68:GLN:C	2.54	0.46
2:E:34:ARG:CZ	2:E:250:HIS:HA	2.45	0.46
1:Y:88:LEU:HD12	1:Y:91:LEU:HD11	1.97	0.46
1:B:117:ASN:C	1:B:119:LEU:N	2.69	0.45
1:C:34:VAL:HB	1:C:167:THR:HG22	1.98	0.45
1:D:67:HIS:O	1:D:68:GLN:C	2.54	0.45
1:D:86:ARG:HA	1:D:89:ARG:NH2	2.31	0.45
2:F:145:GLN:CA	2:F:145:GLN:HE21	2.28	0.45
2:G:217:LYS:CB	2:G:219:LYS:HZ3	2.28	0.45
2:I:356:LYS:CG	2:I:366:ILE:HG22	2.40	0.45
1:V:68:GLN:O	1:V:70:HIS:N	2.49	0.45
1:C:83:ARG:HG3	1:C:109:ASN:O	2.17	0.45
2:E:135:LEU:O	2:E:136:ILE:HG12	2.16	0.45
2:E:355:TYR:HE2	2:E:400:GLU:OE2	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:311:GLN:HA	2:G:311:GLN:HE21	1.81	0.45
2:I:96:VAL:HG12	2:I:284:LEU:CD1	2.46	0.45
1:D:86:ARG:HA	1:D:89:ARG:CZ	2.46	0.45
2:E:145:GLN:HG3	2:E:148:GLN:HG3	1.98	0.45
2:E:388:GLU:O	2:E:394:ARG:NH2	2.49	0.45
2:I:135:LEU:HD22	2:I:159:PHE:HD2	1.80	0.45
2:I:420:ILE:HD12	2:I:420:ILE:N	2.31	0.45
1:Y:6:VAL:HG21	1:Y:147:ILE:HG22	1.98	0.45
1:Z:33:LYS:HA	1:Z:46:PHE:CE1	2.52	0.45
1:B:154:ILE:HD12	1:Z:134:ARG:CB	2.47	0.45
2:E:311:GLN:HA	2:E:311:GLN:NE2	2.32	0.45
2:E:335:LEU:HD22	2:E:339:ASP:HB3	1.96	0.45
2:E:81:VAL:HG11	2:E:99:ILE:HG12	1.97	0.45
1:V:64:LEU:HD23	1:V:74:ALA:HB2	1.98	0.45
1:Y:5:SER:HB3	1:Y:120:ILE:HB	1.98	0.45
1:Y:95:LEU:H	1:Y:95:LEU:HD12	1.82	0.45
1:B:11:HIS:CE1	1:B:172:SER:OG	2.69	0.45
1:B:63:LYS:HD2	1:B:77:GLU:HB3	1.98	0.45
1:C:170:GLU:CG	1:C:171:LEU:N	2.80	0.45
1:C:39:ASN:O	1:C:41:LYS:N	2.50	0.45
1:C:56:LEU:HD21	1:C:91:LEU:HD13	1.98	0.45
1:D:60:PHE:CZ	1:D:97:VAL:HG11	2.51	0.45
2:F:31:LEU:HD11	2:F:74:ALA:HB2	1.98	0.45
2:G:142:ASN:HB2	2:G:149:GLN:NE2	2.32	0.45
2:I:52:ASN:HB2	2:I:325:ARG:O	2.17	0.45
2:I:65:GLU:HG3	3:I:3450:ADP:H2'	1.99	0.45
1:V:134:ARG:HD2	1:V:138:GLU:OE1	2.16	0.45
1:V:154:ILE:HG22	1:V:155:ALA:N	2.30	0.45
1:Y:63:LYS:HD3	1:Y:66:MET:CE	2.46	0.45
1:Y:71:LEU:HD13	1:Y:72:VAL:N	2.32	0.45
1:Z:145:ARG:NE	1:Z:170:GLU:OE1	2.43	0.45
1:B:148:ALA:O	1:B:152:LEU:HB2	2.16	0.45
1:D:84:THR:O	1:D:89:ARG:NH1	2.49	0.45
2:E:217:LYS:HG3	2:E:219:LYS:HZ1	1.80	0.45
2:E:382:GLN:HA	2:E:382:GLN:NE2	2.31	0.45
2:G:272:VAL:O	2:G:276:GLY:N	2.50	0.45
2:I:311:GLN:CA	2:I:311:GLN:NE2	2.80	0.45
1:V:73:LYS:O	1:V:77:GLU:HB2	2.17	0.45
1:X:57:PHE:O	1:X:61:GLU:HB2	2.16	0.45
1:Y:53:ALA:C	1:Y:55:THR:N	2.70	0.45
1:Y:59:LEU:O	1:Y:59:LEU:HD12	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:SER:HB3	1:B:120:ILE:HB	1.98	0.45
1:B:159:CYS:HB3	1:B:162:THR:HB	1.98	0.45
1:C:148:ALA:O	1:C:152:LEU:HB2	2.16	0.45
1:D:73:LYS:HZ2	1:D:77:GLU:HG2	1.82	0.45
2:E:165:GLU:HG2	2:E:166:GLY:N	2.32	0.45
2:E:244:ILE:HG22	2:E:245:ASP:N	2.32	0.45
2:F:129:GLU:HB2	2:F:130:ARG:NH1	2.31	0.45
2:G:91:TYR:HD1	2:I:91:TYR:HD2	1.62	0.45
2:I:16:HIS:HB2	2:I:17:ILE:HD12	1.98	0.45
1:B:117:ASN:C	1:B:119:LEU:H	2.20	0.45
2:E:242:ASP:HA	2:E:245:ASP:OD1	2.16	0.45
2:F:104:THR:HA	2:F:107:ALA:HB3	1.98	0.45
2:G:76:ALA:HB1	2:G:250:HIS:O	2.17	0.45
2:I:130:ARG:HD2	2:I:225:LEU:HD11	1.99	0.45
2:G:91:TYR:CB	2:I:91:TYR:HA	2.47	0.45
1:X:152:LEU:HD23	1:X:152:LEU:O	2.17	0.45
1:Y:70:HIS:ND1	1:Y:73:LYS:HB2	2.32	0.45
2:E:355:TYR:CE2	2:E:400:GLU:OE2	2.70	0.45
2:F:216:LEU:HG	2:F:221:ALA:CB	2.18	0.45
2:F:232:LYS:N	2:F:232:LYS:NZ	2.64	0.45
2:F:356:LYS:HG3	2:F:366:ILE:HG22	1.99	0.45
2:G:174:GLU:HB3	2:G:211:GLN:HB2	1.99	0.45
2:G:219:LYS:O	2:G:223:LYS:HE3	2.17	0.45
2:G:271:ASP:HA	2:G:274:ARG:HB2	1.98	0.45
2:G:432:LEU:CD1	2:G:432:LEU:N	2.78	0.45
2:I:129:GLU:HB2	2:I:130:ARG:HH11	1.81	0.45
2:I:145:GLN:C	2:I:147:GLU:H	2.20	0.45
2:I:322:LEU:HD12	2:I:322:LEU:HA	1.84	0.45
1:Y:152:LEU:HD13	1:Y:166:HIS:CE1	2.51	0.45
1:A:149:GLU:HG2	1:A:168:ILE:CD1	2.47	0.45
1:B:95:LEU:N	1:B:95:LEU:HD12	2.31	0.45
2:F:350:SER:O	2:F:354:GLN:HG3	2.17	0.45
2:G:441:PHE:HA	2:I:315:PRO:HG2	1.99	0.45
2:G:81:VAL:HG11	2:G:99:ILE:HG12	1.99	0.45
1:X:37:LEU:CD2	1:X:57:PHE:HB3	2.43	0.45
2:E:170:ASP:CB	2:E:217:LYS:HD3	2.47	0.44
2:F:375:ARG:NH2	2:F:422:ALA:HB1	2.32	0.44
2:G:109:LYS:HG3	2:G:109:LYS:O	2.15	0.44
2:G:33:ASN:HD22	2:G:36:ARG:HD2	1.82	0.44
2:G:442:ILE:CG2	2:G:442:ILE:O	2.65	0.44
2:I:432:LEU:N	2:I:432:LEU:CD1	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:435:ASP:OD1	2:I:438:LEU:HD12	2.17	0.44
2:I:12:GLU:CG	2:I:73:LEU:HD13	2.47	0.44
1:Y:38:TYR:CD2	1:Y:41:LYS:HD2	2.52	0.44
1:Z:33:LYS:O	1:Z:45:GLY:HA2	2.17	0.44
1:B:150:LYS:O	1:B:154:ILE:HG12	2.18	0.44
2:G:153:SER:N	2:G:156:ARG:HB3	2.32	0.44
2:G:216:LEU:HD23	2:G:216:LEU:N	2.29	0.44
2:I:132:LEU:HB3	2:I:156:ARG:CZ	2.47	0.44
2:G:92:VAL:CG2	2:I:92:VAL:CG1	2.92	0.44
1:A:84:THR:HG23	1:A:85:ASP:N	2.33	0.44
2:E:240:LYS:HD3	2:E:241:GLN:N	2.32	0.44
2:F:153:SER:HA	2:F:156:ARG:HB3	1.98	0.44
2:G:101:ARG:O	2:G:104:THR:HB	2.17	0.44
2:G:153:SER:HA	2:G:157:GLN:HG3	1.99	0.44
2:G:16:HIS:HB2	2:G:17:ILE:HD12	1.99	0.44
2:G:134:VAL:CG1	2:G:171:LYS:HD3	2.46	0.44
2:I:119:ASN:CG	2:I:233:LEU:HD23	2.37	0.44
1:Y:8:ARG:HH12	1:Y:141:GLU:C	2.20	0.44
1:C:38:TYR:N	1:C:61:GLU:OE1	2.48	0.44
2:F:21:ASP:O	2:F:24:LYS:HB2	2.17	0.44
2:G:270:PRO:O	2:G:273:SER:N	2.51	0.44
2:G:35:TRP:O	2:G:39:GLN:HG2	2.17	0.44
2:G:95:GLU:CD	2:G:95:GLU:H	2.20	0.44
2:I:217:LYS:CG	2:I:218:ILE:N	2.78	0.44
1:V:5:SER:HB3	1:V:120:ILE:HD13	1.97	0.44
1:Y:19:GLN:N	1:Y:163:ASN:ND2	2.66	0.44
1:Y:32:LYS:HE3	1:Y:32:LYS:HB2	1.74	0.44
1:Z:13:VAL:CG1	1:Z:170:GLU:HG3	2.44	0.44
1:C:19:GLN:HB2	1:C:163:ASN:ND2	2.32	0.44
1:D:8:ARG:HG2	1:D:9:ASN:ND2	2.33	0.44
2:I:218:ILE:C	2:I:220:ASP:N	2.70	0.44
2:I:312:ILE:CG1	2:I:313:ALA:N	2.80	0.44
1:V:98:ALA:HA	1:V:102:ALA:O	2.18	0.44
1:V:35:ARG:HD3	1:V:57:PHE:CD2	2.52	0.44
1:Y:6:VAL:HG21	1:Y:147:ILE:CG2	2.47	0.44
1:B:32:LYS:HE3	1:B:32:LYS:HB2	1.76	0.44
1:C:5:SER:HB3	1:C:120:ILE:HB	2.00	0.44
1:C:62:ARG:O	1:C:65:GLU:HB2	2.18	0.44
1:D:121:ALA:HB1	1:D:126:GLY:O	2.17	0.44
2:E:148:GLN:OE1	2:E:151:GLU:HG3	2.18	0.44
2:E:89:VAL:HG12	2:E:93:GLY:C	2.37	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:LYS:NZ	2:F:101:ARG:HH12	2.15	0.44
2:G:151:GLU:HB2	2:G:152:PRO:HD2	1.99	0.44
2:G:292:THR:HG22	2:G:294:HIS:H	1.83	0.44
2:I:159:PHE:O	2:I:163:LEU:HB2	2.18	0.44
1:C:73:LYS:HA	1:C:76:VAL:CG1	2.47	0.44
2:E:128:GLU:O	2:E:129:GLU:C	2.56	0.44
2:E:140:LYS:O	2:E:141:ASN:CB	2.65	0.44
2:E:436:GLU:O	2:E:439:SER:HB2	2.18	0.44
2:F:122:ARG:NE	2:F:122:ARG:HA	2.33	0.44
2:I:131:ILE:HD11	2:I:218:ILE:HD13	2.00	0.44
2:I:269:GLY:N	2:I:270:PRO:CD	2.81	0.44
2:I:41:ASN:HD21	2:I:44:LEU:H	1.66	0.44
1:X:10:GLY:O	1:X:172:SER:HA	2.18	0.44
1:X:28:LYS:HG2	1:X:30:ASN:ND2	2.32	0.44
1:A:101:THR:O	1:A:102:ALA:HB2	2.18	0.44
2:F:389:ASN:HD22	2:F:390:ILE:N	2.16	0.44
2:F:96:VAL:HG12	2:F:284:LEU:HD11	1.99	0.44
2:F:96:VAL:HG21	2:F:280:ASP:HB3	2.00	0.44
2:G:231:ALA:O	2:G:233:LEU:N	2.51	0.44
2:G:358:LEU:CD2	2:I:36:ARG:HB3	2.48	0.44
2:I:123:ALA:C	2:I:127:ALA:HB3	2.38	0.44
1:V:5:SER:O	1:V:119:LEU:HD12	2.18	0.44
1:Y:66:MET:C	1:Y:67:HIS:ND1	2.71	0.44
1:Y:71:LEU:CD1	1:Y:72:VAL:N	2.80	0.44
1:Z:47:ALA:HB3	1:Z:94:LEU:HB2	1.99	0.44
1:A:149:GLU:OE1	1:A:168:ILE:HD11	2.18	0.44
1:C:6:VAL:HG11	1:C:147:ILE:HG21	1.99	0.44
1:C:86:ARG:HA	1:C:89:ARG:CZ	2.48	0.44
2:E:214:ARG:CG	2:E:215:LYS:N	2.81	0.44
2:E:442:ILE:O	2:E:442:ILE:HG22	2.16	0.44
2:F:167:GLN:O	2:F:168:LEU:CB	2.66	0.44
2:F:219:LYS:HE3	2:F:219:LYS:HA	1.99	0.44
2:I:220:ASP:HB3	2:I:224:LEU:HD23	2.00	0.44
2:G:358:LEU:HD22	2:I:36:ARG:HB2	1.99	0.44
1:V:170:GLU:HG3	1:V:171:LEU:N	2.32	0.44
1:Y:63:LYS:CA	1:Y:66:MET:HE3	2.37	0.44
2:E:106:ALA:O	2:E:110:MET:HB2	2.18	0.43
2:I:289:THR:CG2	2:I:296:MET:HG3	2.48	0.43
1:V:18:GLY:O	1:V:31:VAL:HG23	2.17	0.43
1:C:28:LYS:HE2	1:C:30:ASN:HD22	1.76	0.43
1:C:37:LEU:HD11	1:C:60:PHE:HD2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:TYR:CE1	1:C:64:LEU:HB3	2.53	0.43
2:E:135:LEU:HB3	2:E:159:PHE:CD2	2.53	0.43
2:E:312:ILE:CG1	2:E:313:ALA:H	2.28	0.43
2:E:438:LEU:O	2:E:438:LEU:HD23	2.18	0.43
2:F:244:ILE:HD12	2:F:244:ILE:N	2.33	0.43
2:F:375:ARG:HA	2:F:378:GLU:HB2	2.00	0.43
2:I:123:ALA:O	2:I:127:ALA:HB3	2.18	0.43
2:I:240:LYS:HE2	2:I:240:LYS:HB3	1.85	0.43
2:I:312:ILE:HG12	2:I:313:ALA:H	1.82	0.43
1:Z:36:ARG:HD3	1:Z:40:ASP:OD1	2.19	0.43
1:B:7:ARG:NE	1:B:118:ASP:OD2	2.45	0.43
1:A:65:GLU:OE1	2:E:141:ASN:O	2.35	0.43
2:E:132:LEU:HB3	2:E:156:ARG:CZ	2.48	0.43
2:E:231:ALA:C	2:E:233:LEU:H	2.20	0.43
2:E:362:GLU:HG2	2:E:410:ALA:CB	2.49	0.43
2:F:108:VAL:HA	2:F:111:VAL:CG2	2.47	0.43
2:F:217:LYS:HB2	2:F:217:LYS:HZ3	1.82	0.43
2:G:215:LYS:O	2:G:215:LYS:HG3	2.19	0.43
2:G:355:TYR:HE2	2:G:400:GLU:OE2	2.01	0.43
1:V:86:ARG:HG3	1:V:89:ARG:NH2	2.33	0.43
1:Y:86:ARG:HA	1:Y:89:ARG:HE	1.80	0.43
1:B:65:GLU:HB3	2:F:143:TRP:HA	2.01	0.43
2:G:106:ALA:HB2	2:I:289:THR:HB	2.00	0.43
2:G:163:LEU:O	2:G:163:LEU:HG	2.18	0.43
2:G:358:LEU:HD23	2:I:36:ARG:HB3	1.98	0.43
2:G:88:GLU:CB	2:I:90:GLY:HA2	2.49	0.43
1:A:3:ILE:HB	1:A:122:ILE:HG12	2.00	0.43
1:C:60:PHE:HZ	1:C:71:LEU:CD2	2.32	0.43
2:E:322:LEU:HD12	2:E:322:LEU:HA	1.87	0.43
2:F:16:HIS:HB2	2:F:17:ILE:HD12	2.01	0.43
2:G:155:ALA:O	2:G:159:PHE:HD1	2.01	0.43
1:V:37:LEU:N	1:V:37:LEU:CD2	2.80	0.43
1:V:37:LEU:HD11	1:V:60:PHE:HD2	1.84	0.43
1:A:1:THR:HA	1:A:17:ASP:OD1	2.18	0.43
1:D:43:ILE:HD13	1:D:98:ALA:O	2.19	0.43
2:E:212:LYS:C	2:E:214:ARG:H	2.22	0.43
2:F:131:ILE:HG23	2:F:132:LEU:N	2.34	0.43
2:F:96:VAL:CG1	2:F:281:LEU:HD12	2.45	0.43
2:F:41:ASN:C	2:F:41:ASN:ND2	2.71	0.43
2:G:224:LEU:O	2:G:228:GLU:HG3	2.19	0.43
2:I:123:ALA:CA	2:I:127:ALA:HB3	2.45	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:160:ARG:HH11	2:I:160:ARG:HG2	1.82	0.43
2:I:235:ASN:HB2	2:I:236:PRO:CD	2.47	0.43
1:X:149:GLU:OE1	1:X:166:HIS:CD2	2.72	0.43
1:Y:98:ALA:HB2	1:Y:103:SER:CB	2.48	0.43
1:A:38:TYR:HE1	1:A:65:GLU:HG2	1.84	0.43
1:C:54:PHE:HD1	1:D:76:VAL:HG21	1.82	0.43
2:F:108:VAL:O	2:F:110:MET:N	2.52	0.43
2:G:223:LYS:HA	2:G:226:ILE:CG1	2.45	0.43
2:G:355:TYR:CE2	2:G:400:GLU:OE2	2.71	0.43
2:I:384:ASN:HD21	2:I:390:ILE:HG12	1.84	0.43
2:I:390:ILE:HG13	2:I:393:ARG:HB2	2.01	0.43
1:V:152:LEU:HB3	1:V:166:HIS:CE1	2.53	0.43
1:X:89:ARG:CB	1:X:89:ARG:HH11	2.32	0.43
1:Y:90:LYS:HD2	1:Y:90:LYS:H	1.84	0.43
1:Z:115:PRO:CG	1:Z:119:LEU:O	2.67	0.43
1:B:136:LEU:HD11	1:Z:135:ALA:O	2.18	0.43
1:B:152:LEU:HD13	1:B:166:HIS:CE1	2.54	0.43
1:B:95:LEU:H	1:B:95:LEU:HD12	1.83	0.43
1:C:160:ILE:CG2	1:V:160:ILE:CG2	2.93	0.43
1:D:86:ARG:HG2	1:D:89:ARG:HH22	1.83	0.43
2:E:109:LYS:HD3	2:F:296:MET:HB3	2.01	0.43
2:E:217:LYS:CB	2:E:219:LYS:HZ3	2.31	0.43
2:F:20:GLN:O	2:F:24:LYS:HG3	2.18	0.43
2:F:336:THR:O	2:F:339:ASP:HB2	2.18	0.43
2:G:361:THR:CG2	2:I:35:TRP:CZ3	3.02	0.43
2:I:223:LYS:N	2:I:223:LYS:CD	2.82	0.43
1:X:168:ILE:HG22	1:X:169:GLU:N	2.33	0.43
1:Y:73:LYS:O	1:Y:73:LYS:HD3	2.18	0.43
1:Z:61:GLU:HA	1:Z:64:LEU:HD12	2.00	0.43
1:B:63:LYS:CA	1:B:66:MET:HE3	2.41	0.43
1:C:63:LYS:HD3	1:C:66:MET:HE1	2.01	0.43
1:D:149:GLU:CG	1:D:168:ILE:HD11	2.49	0.43
2:E:128:GLU:O	2:E:131:ILE:HG22	2.19	0.43
2:F:432:LEU:N	2:F:432:LEU:CD1	2.81	0.43
2:G:34:ARG:NH2	2:G:250:HIS:HA	2.34	0.43
2:I:94:LYS:NZ	2:I:101:ARG:HH12	2.16	0.43
2:I:259:ASP:HB3	2:I:310:PHE:CZ	2.54	0.43
1:D:102:ALA:HB1	1:D:114:GLN:OE1	2.19	0.43
1:B:65:GLU:HG2	2:F:143:TRP:CD1	2.54	0.43
2:G:311:GLN:HA	2:G:311:GLN:NE2	2.33	0.43
2:I:5:THR:O	2:I:9:ILE:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:17:ASP:OD1	1:V:33:LYS:NZ	2.45	0.43
1:V:73:LYS:HZ1	1:V:77:GLU:HG2	1.82	0.43
1:Y:78:LEU:C	1:Y:80:LYS:N	2.72	0.43
1:Z:81:ASP:HA	1:Z:84:THR:CG2	2.48	0.43
1:A:46:PHE:CD2	1:A:53:ALA:HB2	2.54	0.42
1:A:94:LEU:CD2	1:A:107:THR:HG22	2.50	0.42
1:B:173:TYR:O	1:B:174:LYS:HB2	2.19	0.42
2:E:65:GLU:HG3	3:E:450:ADP:H2'	2.00	0.42
2:F:136:ILE:O	2:F:138:PRO:HD3	2.19	0.42
2:F:5:THR:O	2:F:9:ILE:HG12	2.18	0.42
2:G:126:LEU:HD22	2:G:126:LEU:N	2.34	0.42
2:G:240:LYS:HD3	2:G:241:GLN:N	2.34	0.42
2:I:125:GLU:C	2:I:127:ALA:H	2.23	0.42
2:I:339:ASP:O	2:I:343:ILE:HG13	2.18	0.42
2:I:84:THR:O	2:I:87:THR:OG1	2.35	0.42
1:Y:61:GLU:O	1:Y:65:GLU:HG3	2.20	0.42
1:Z:101:THR:O	1:Z:102:ALA:HB2	2.19	0.42
1:A:99:ASP:C	1:A:99:ASP:OD1	2.57	0.42
2:E:16:HIS:HB2	2:E:17:ILE:HD12	2.01	0.42
2:E:168:LEU:CD2	2:E:219:LYS:HD3	2.49	0.42
2:G:256:ASP:O	2:G:257:GLU:HG2	2.20	0.42
2:I:148:GLN:C	2:I:150:GLN:H	2.23	0.42
2:E:150:GLN:C	2:E:153:SER:OG	2.57	0.42
2:F:145:GLN:C	2:F:147:GLU:H	2.22	0.42
2:I:264:ARG:NE	2:I:265:GLY:H	2.17	0.42
1:V:14:ILE:HD12	1:V:44:ALA:HA	2.00	0.42
1:X:157:ASP:OD2	1:X:164:HIS:NE2	2.52	0.42
1:C:11:HIS:HA	1:C:171:LEU:O	2.19	0.42
1:C:168:ILE:CG2	1:C:169:GLU:N	2.83	0.42
1:D:114:GLN:HA	1:D:115:PRO:HD2	1.86	0.42
1:D:22:LEU:HD23	1:D:22:LEU:C	2.40	0.42
2:E:123:ALA:O	2:E:127:ALA:HB2	2.20	0.42
2:E:148:GLN:HA	2:E:151:GLU:HG2	2.02	0.42
2:E:131:ILE:CD1	2:E:218:ILE:HG12	2.47	0.42
2:G:17:ILE:HD12	2:G:17:ILE:N	2.34	0.42
2:G:389:ASN:C	2:G:389:ASN:ND2	2.63	0.42
1:X:152:LEU:HD22	1:X:166:HIS:CE1	2.50	0.42
1:B:98:ALA:HB2	1:B:103:SER:CB	2.49	0.42
1:C:131:ALA:HB3	1:X:131:ALA:HB3	2.02	0.42
1:D:57:PHE:O	1:D:61:GLU:HB2	2.20	0.42
2:I:109:LYS:O	2:I:109:LYS:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:437:ASP:OD2	2:I:314:LYS:HE3	2.19	0.42
1:Y:94:LEU:HA	1:Y:94:LEU:HD23	1.91	0.42
1:A:86:ARG:HA	1:A:89:ARG:NH2	2.35	0.42
1:B:13:VAL:HG12	1:B:170:GLU:HA	2.01	0.42
2:E:101:ARG:O	2:E:104:THR:HB	2.19	0.42
2:E:77:PRO:HB2	2:E:103:LEU:CD2	2.49	0.42
2:E:116:ILE:HG22	2:E:116:ILE:O	2.19	0.42
2:E:220:ASP:O	2:E:224:LEU:HD23	2.20	0.42
2:F:225:LEU:HA	2:F:228:GLU:HB2	2.02	0.42
2:F:33:ASN:ND2	2:F:36:ARG:HD2	2.34	0.42
2:G:134:VAL:HG13	2:G:171:LYS:HD3	2.02	0.42
2:I:145:GLN:HA	2:I:145:GLN:NE2	2.34	0.42
1:Y:148:ALA:O	1:Y:152:LEU:HB2	2.19	0.42
1:A:160:ILE:O	1:Z:160:ILE:HG13	2.20	0.42
1:D:136:LEU:HD11	1:V:135:ALA:O	2.19	0.42
2:E:326:LEU:O	2:E:329:ARG:NE	2.48	0.42
2:G:230:ALA:O	2:G:233:LEU:HB3	2.20	0.42
2:I:170:ASP:HB2	2:I:216:LEU:O	2.19	0.42
1:V:35:ARG:C	1:V:36:ARG:HG3	2.39	0.42
1:X:89:ARG:CB	1:X:89:ARG:NH1	2.83	0.42
1:Y:117:ASN:C	1:Y:119:LEU:N	2.71	0.42
1:Y:168:ILE:HD12	1:Y:168:ILE:H	1.84	0.42
1:Y:63:LYS:HD3	1:Y:66:MET:HE3	2.00	0.42
1:Y:79:ALA:HB1	1:Y:110:GLY:O	2.20	0.42
1:A:105:ILE:HD11	1:A:120:ILE:HG23	2.02	0.42
1:A:81:ASP:HA	1:A:84:THR:CG2	2.49	0.42
1:B:3:ILE:O	1:B:121:ALA:HA	2.19	0.42
1:C:42:VAL:HG11	1:C:60:PHE:HE2	1.84	0.42
1:C:46:PHE:CD2	1:C:53:ALA:HB2	2.54	0.42
1:C:82:TRP:CZ3	1:C:95:LEU:HD13	2.55	0.42
1:D:80:LYS:HE3	1:D:80:LYS:HB3	1.93	0.42
2:F:167:GLN:HE22	2:F:219:LYS:HD2	1.84	0.42
2:G:113:VAL:C	2:G:115:ALA:H	2.22	0.42
2:G:168:LEU:HD12	2:G:219:LYS:CB	2.48	0.42
2:G:400:GLU:HG3	2:I:327:PRO:HB2	2.02	0.42
2:I:147:GLU:HG2	2:I:150:GLN:HE21	1.83	0.42
2:I:384:ASN:ND2	2:I:390:ILE:H	2.18	0.42
1:V:156:GLY:HA2	1:V:162:THR:HG22	2.02	0.42
1:Y:87:MET:O	1:Y:89:ARG:N	2.53	0.42
1:C:58:GLU:O	1:C:61:GLU:HB2	2.19	0.42
2:E:215:LYS:HG3	2:E:215:LYS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:240:LYS:HD3	2:E:240:LYS:C	2.40	0.42
2:E:392:ALA:HB3	3:E:450:ADP:C8	2.55	0.42
2:E:40:LEU:O	2:E:45:ARG:NH1	2.53	0.42
2:F:150:GLN:O	2:F:153:SER:OG	2.38	0.42
2:G:167:GLN:OE1	2:G:168:LEU:N	2.52	0.42
2:G:173:ILE:CD1	2:G:173:ILE:N	2.78	0.42
2:G:174:GLU:HB3	2:G:211:GLN:CB	2.49	0.42
2:I:393:ARG:HG2	2:I:393:ARG:NH1	2.33	0.42
2:G:349:ALA:HB1	2:I:44:LEU:HD23	2.02	0.42
1:V:134:ARG:HH11	1:V:134:ARG:HG2	1.84	0.42
1:X:105:ILE:HD12	1:X:122:ILE:CG2	2.50	0.42
1:B:6:VAL:HG12	1:B:7:ARG:H	1.82	0.42
1:C:123:GLY:O	1:C:126:GLY:N	2.43	0.42
1:C:71:LEU:HD13	1:C:71:LEU:C	2.40	0.42
1:D:68:GLN:O	1:D:70:HIS:N	2.53	0.42
2:F:148:GLN:HA	2:F:151:GLU:HG2	2.01	0.42
2:F:258:ILE:HD12	2:F:261:ILE:HD11	2.01	0.42
2:G:147:GLU:HG3	2:G:150:GLN:CD	2.40	0.42
2:G:358:LEU:HD22	2:I:36:ARG:CB	2.50	0.42
2:I:345:THR:HG23	2:I:373:ILE:HD13	2.02	0.42
2:I:344:LEU:HD11	2:I:395:LEU:HD22	2.01	0.42
1:V:90:LYS:NZ	1:X:83:ARG:O	2.49	0.42
1:Y:169:GLU:HA	1:Y:169:GLU:OE2	2.20	0.42
1:Y:7:ARG:NH2	1:Y:102:ALA:C	2.74	0.42
1:Z:71:LEU:O	1:Z:75:ALA:N	2.49	0.42
1:B:43:ILE:HG12	1:B:98:ALA:O	2.19	0.41
2:E:212:LYS:CD	2:E:216:LEU:HD21	2.29	0.41
2:E:42:GLU:HA	2:E:45:ARG:NH2	2.35	0.41
2:F:214:ARG:HE	2:F:216:LEU:HB3	1.85	0.41
2:G:103:LEU:O	2:G:107:ALA:HB2	2.20	0.41
2:G:442:ILE:HG22	2:G:442:ILE:O	2.20	0.41
1:Y:65:GLU:CG	2:I:143:TRP:CD1	3.02	0.41
1:V:56:LEU:HD11	1:V:91:LEU:HD13	2.01	0.41
1:X:3:ILE:HB	1:X:122:ILE:HG12	2.01	0.41
1:Y:18:GLY:HA2	1:Y:33:LYS:HE3	2.01	0.41
1:Z:103:SER:O	1:Z:104:LEU:HB3	2.20	0.41
1:A:17:ASP:O	1:A:33:LYS:HD2	2.20	0.41
1:C:46:PHE:HA	1:C:94:LEU:O	2.20	0.41
2:E:117:GLU:OE2	2:E:120:ARG:NH1	2.53	0.41
2:E:33:ASN:ND2	2:E:36:ARG:HD2	2.35	0.41
2:E:89:VAL:CG1	2:E:93:GLY:HA3	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:114:GLN:HA	2:F:117:GLU:HG2	2.01	0.41
2:F:147:GLU:HA	2:F:150:GLN:HB3	2.01	0.41
2:F:282:LEU:HA	2:F:282:LEU:HD12	1.84	0.41
2:G:217:LYS:CG	2:G:219:LYS:HZ3	2.32	0.41
1:X:42:VAL:HG13	1:X:98:ALA:O	2.20	0.41
2:E:160:ARG:HH12	2:E:164:ARG:HH22	1.68	0.41
2:E:168:LEU:HA	2:E:219:LYS:HB3	2.01	0.41
2:E:231:ALA:C	2:E:233:LEU:N	2.74	0.41
2:E:43:GLU:O	2:E:45:ARG:N	2.53	0.41
2:G:92:VAL:HG23	2:G:92:VAL:O	2.20	0.41
2:I:135:LEU:HD13	2:I:159:PHE:HB3	2.01	0.41
1:V:134:ARG:HG2	1:V:134:ARG:NH1	2.35	0.41
1:Y:159:CYS:HB3	1:Y:162:THR:HB	2.02	0.41
1:Y:18:GLY:C	1:Y:163:ASN:HD21	2.23	0.41
1:B:139:ASN:HD22	1:Z:136:LEU:HD11	1.85	0.41
1:C:50:THR:HG22	1:C:50:THR:O	2.20	0.41
2:E:312:ILE:CG1	2:E:313:ALA:N	2.81	0.41
2:E:402:LEU:HD12	2:E:428:HIS:HB2	2.03	0.41
2:F:269:GLY:N	2:F:270:PRO:CD	2.84	0.41
2:F:355:TYR:CE1	2:F:403:MET:HE3	2.55	0.41
2:G:145:GLN:O	2:G:147:GLU:N	2.54	0.41
2:G:384:ASN:HD21	2:G:390:ILE:HG12	1.86	0.41
2:G:27:VAL:CG1	2:G:70:LEU:HG	2.50	0.41
1:Y:65:GLU:HB3	2:I:143:TRP:HA	2.01	0.41
2:I:17:ILE:HD11	2:I:69:ARG:HG3	2.02	0.41
2:I:86:PHE:HB2	2:I:277:VAL:HG13	2.02	0.41
1:V:10:GLY:HA3	1:V:174:LYS:HA	2.01	0.41
1:V:20:ALA:HB2	1:V:31:VAL:HG21	2.02	0.41
1:X:84:THR:O	1:X:89:ARG:NH1	2.54	0.41
2:E:160:ARG:HG2	2:E:160:ARG:HH11	1.86	0.41
2:E:173:ILE:N	2:E:173:ILE:CD1	2.78	0.41
2:E:432:LEU:N	2:E:432:LEU:CD1	2.81	0.41
2:G:112:ARG:O	2:G:115:ALA:HB3	2.21	0.41
1:X:160:ILE:HD13	1:X:160:ILE:HA	1.87	0.41
1:X:7:ARG:O	1:X:8:ARG:HB2	2.20	0.41
1:A:104:LEU:HD12	1:A:104:LEU:O	2.20	0.41
2:F:403:MET:SD	2:F:420:ILE:HD13	2.61	0.41
2:F:47:GLU:OE1	2:F:47:GLU:HA	2.20	0.41
2:G:212:LYS:O	2:G:214:ARG:N	2.54	0.41
1:V:30:ASN:N	1:V:30:ASN:ND2	2.57	0.41
2:E:134:VAL:HG11	2:E:171:LYS:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:167:GLN:NE2	2:F:219:LYS:HD2	2.35	0.41
2:F:91:TYR:O	2:F:92:VAL:CG1	2.60	0.41
2:G:123:ALA:O	2:G:127:ALA:HB2	2.21	0.41
2:I:130:ARG:HD2	2:I:225:LEU:CD1	2.51	0.41
2:I:345:THR:HG21	2:I:373:ILE:HD13	1.98	0.41
1:V:11:HIS:CE1	1:V:172:SER:OG	2.73	0.41
1:V:86:ARG:O	1:V:90:LYS:HG2	2.21	0.41
1:X:43:ILE:N	1:X:43:ILE:HD13	2.28	0.41
1:A:149:GLU:OE2	1:A:166:HIS:CD2	2.74	0.41
1:A:173:TYR:O	1:A:174:LYS:C	2.58	0.41
1:B:131:ALA:HA	1:Z:154:ILE:HG21	2.03	0.41
1:B:63:LYS:HD3	1:B:63:LYS:HA	1.90	0.41
1:C:100:GLU:OE2	1:C:173:TYR:HD1	2.04	0.41
1:C:17:ASP:OD1	1:C:33:LYS:NZ	2.50	0.41
2:E:151:GLU:CB	2:E:152:PRO:HD3	2.50	0.41
2:E:173:ILE:O	2:E:212:LYS:HD2	2.21	0.41
2:F:216:LEU:HD11	2:F:221:ALA:HA	2.03	0.41
2:F:45:ARG:HH11	2:F:45:ARG:HG3	1.86	0.41
2:G:312:ILE:CG1	2:G:313:ALA:N	2.83	0.41
2:G:5:THR:O	2:G:6:PRO:C	2.59	0.41
2:I:145:GLN:HE21	2:I:145:GLN:HA	1.85	0.41
1:V:35:ARG:HB2	1:V:36:ARG:H	1.69	0.41
1:X:8:ARG:NH2	1:X:137:LEU:HD12	2.35	0.41
1:A:20:ALA:HB2	1:A:31:VAL:HG21	2.03	0.41
2:F:171:LYS:O	2:F:172:GLU:HB3	2.21	0.41
2:G:142:ASN:HB2	2:G:149:GLN:HE22	1.83	0.41
2:G:402:LEU:HD11	2:G:425:VAL:HA	2.03	0.41
2:G:91:TYR:CE1	2:I:91:TYR:CE2	3.09	0.41
1:V:123:GLY:O	1:V:126:GLY:N	2.43	0.41
1:Y:38:TYR:HB2	1:Y:64:LEU:CD1	2.51	0.41
1:D:6:VAL:HG21	1:D:147:ILE:CG2	2.49	0.41
2:E:159:PHE:O	2:E:163:LEU:HB2	2.21	0.41
2:E:165:GLU:HG2	2:E:166:GLY:H	1.86	0.41
2:E:255:ILE:HD13	2:E:281:LEU:CD2	2.51	0.41
2:F:108:VAL:HG23	2:F:243:ALA:CB	2.51	0.41
2:G:145:GLN:C	2:G:147:GLU:N	2.73	0.41
2:G:158:ALA:O	2:G:162:LYS:HG3	2.21	0.41
2:G:171:LYS:HB2	2:G:218:ILE:CG1	2.47	0.41
2:I:257:GLU:HB2	2:I:260:LYS:CG	2.48	0.41
1:X:80:LYS:HE3	1:X:80:LYS:HB3	1.94	0.41
1:Y:3:ILE:O	1:Y:121:ALA:HA	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ILE:HG23	1:C:171:LEU:HD13	2.03	0.41
2:E:362:GLU:HG2	2:E:410:ALA:HB1	2.02	0.41
2:G:174:GLU:HG3	2:G:213:ALA:CA	2.51	0.41
2:G:119:ASN:OD1	2:G:234:VAL:HG22	2.21	0.41
2:G:358:LEU:CD2	2:I:36:ARG:CB	2.99	0.41
2:G:89:VAL:HA	2:G:93:GLY:HA3	2.03	0.41
2:G:86:PHE:HA	2:G:89:VAL:HG13	2.03	0.41
1:V:97:VAL:HB	1:V:104:LEU:CD1	2.50	0.41
1:A:149:GLU:CG	1:A:168:ILE:HD11	2.52	0.40
1:A:6:VAL:HG21	1:A:147:ILE:CG2	2.50	0.40
1:B:104:LEU:N	1:B:104:LEU:HD23	2.35	0.40
1:C:86:ARG:CA	1:C:89:ARG:HH12	2.29	0.40
2:E:171:LYS:HB3	2:E:172:GLU:H	1.63	0.40
2:E:34:ARG:NH2	2:E:250:HIS:HA	2.36	0.40
2:F:135:LEU:HD22	2:F:159:PHE:HE2	1.83	0.40
2:F:219:LYS:O	2:F:223:LYS:HD3	2.21	0.40
2:I:244:ILE:HD11	2:I:294:HIS:O	2.21	0.40
1:V:67:HIS:O	1:V:68:GLN:C	2.58	0.40
1:Y:101:THR:HG22	1:Y:102:ALA:N	2.35	0.40
1:Z:88:LEU:N	1:Z:88:LEU:CD1	2.82	0.40
1:B:14:ILE:HD12	1:B:44:ALA:HA	2.03	0.40
1:C:28:LYS:CE	1:C:30:ASN:HD21	2.34	0.40
2:F:150:GLN:C	2:F:153:SER:OG	2.59	0.40
2:F:134:VAL:HG13	2:F:171:LYS:HD2	2.03	0.40
2:G:362:GLU:OE2	2:I:32:ARG:NH2	2.34	0.40
2:I:344:LEU:HA	2:I:344:LEU:HD12	1.84	0.40
1:V:99:ASP:OD1	1:V:99:ASP:N	2.55	0.40
1:Z:173:TYR:O	1:Z:174:LYS:C	2.59	0.40
1:C:71:LEU:HD11	1:C:104:LEU:HD11	2.04	0.40
1:D:64:LEU:CB	1:D:69:GLY:HA2	2.52	0.40
1:A:62:ARG:HD2	2:E:141:ASN:HD21	1.86	0.40
2:E:226:ILE:O	2:E:230:ALA:HB2	2.22	0.40
2:E:54:LEU:HB3	2:E:329:ARG:HD3	2.03	0.40
2:G:388:GLU:O	2:G:394:ARG:NH2	2.52	0.40
2:G:413:LEU:O	2:G:416:GLN:HG3	2.21	0.40
2:I:236:PRO:C	2:I:238:GLU:H	2.21	0.40
1:Y:11:HIS:HA	1:Y:171:LEU:O	2.22	0.40
1:A:139:ASN:ND2	1:Y:136:LEU:HD11	2.36	0.40
1:Z:10:GLY:HA3	1:Z:174:LYS:N	2.37	0.40
1:B:66:MET:O	1:B:67:HIS:ND1	2.54	0.40
2:E:169:ASP:O	2:E:218:ILE:CG1	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:GLY:O	2:F:24:LYS:HE3	2.21	0.40
2:F:41:ASN:HD21	2:F:44:LEU:H	1.69	0.40
2:F:443:LEU:HD23	2:F:443:LEU:HA	1.91	0.40
2:F:74:ALA:O	2:F:75:ASN:C	2.60	0.40
2:G:21:ASP:HA	2:G:24:LYS:HD2	2.02	0.40
2:G:96:VAL:HG12	2:G:284:LEU:HD11	2.02	0.40
1:Y:65:GLU:OE1	2:I:143:TRP:CE2	2.74	0.40
1:V:21:THR:HG22	1:V:22:LEU:N	2.36	0.40
2:E:111:VAL:HG21	2:E:243:ALA:HB2	2.04	0.40
2:E:121:TYR:C	2:E:123:ALA:H	2.24	0.40
2:E:164:ARG:NH1	2:E:164:ARG:HG2	2.36	0.40
2:E:248:GLU:HG2	2:E:297:VAL:HG13	2.04	0.40
2:E:351:ILE:HD13	2:E:396:HIS:ND1	2.37	0.40
2:F:289:THR:CG2	2:F:296:MET:HG3	2.51	0.40
2:G:270:PRO:O	2:G:271:ASP:C	2.60	0.40
2:I:125:GLU:HB3	2:I:126:LEU:H	1.73	0.40
2:I:147:GLU:HA	2:I:150:GLN:HB3	2.04	0.40
2:I:172:GLU:O	2:I:173:ILE:HG23	2.22	0.40
2:I:174:GLU:C	2:I:212:LYS:HB3	2.42	0.40
2:I:218:ILE:HA	2:I:221:ALA:HB3	2.04	0.40
2:I:96:VAL:CG1	2:I:281:LEU:HD12	2.50	0.40
2:I:61:VAL:C	3:I:3450:ADP:N7	2.75	0.40
1:V:11:HIS:HE1	1:V:172:SER:OG	2.04	0.40
1:C:160:ILE:HG21	1:V:160:ILE:HG23	2.01	0.40
1:X:114:GLN:HA	1:X:115:PRO:HD2	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:7:ARG:NH2	2:F:409:ASP:OD2[2_665]	2.06	0.14

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	172/175 (98%)	151 (88%)	17 (10%)	4 (2%)	8 26
1	B	172/175 (98%)	138 (80%)	27 (16%)	7 (4%)	3 11
1	C	172/175 (98%)	140 (81%)	27 (16%)	5 (3%)	6 19
1	D	172/175 (98%)	146 (85%)	23 (13%)	3 (2%)	11 36
1	V	172/175 (98%)	144 (84%)	25 (14%)	3 (2%)	11 36
1	X	172/175 (98%)	148 (86%)	20 (12%)	4 (2%)	8 26
1	Y	172/175 (98%)	136 (79%)	26 (15%)	10 (6%)	2 5
1	Z	172/175 (98%)	150 (87%)	18 (10%)	4 (2%)	8 26
2	E	404/449 (90%)	349 (86%)	46 (11%)	9 (2%)	8 28
2	F	404/449 (90%)	343 (85%)	45 (11%)	16 (4%)	4 12
2	G	404/449 (90%)	344 (85%)	45 (11%)	15 (4%)	4 14
2	I	404/449 (90%)	347 (86%)	43 (11%)	14 (4%)	4 15
All	All	2992/3196 (94%)	2536 (85%)	362 (12%)	94 (3%)	5 17

All (94) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	116	GLU
1	V	116	GLU
1	Y	54	PHE
1	Y	68	GLN
1	Y	71	LEU
1	Y	72	VAL
2	E	92	VAL
2	E	144	GLY
2	E	153	SER
2	F	92	VAL
2	F	153	SER
2	F	165	GLU
2	F	212	LYS
2	F	236	PRO
2	G	92	VAL
2	G	153	SER
2	I	92	VAL
2	I	153	SER
2	I	165	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	212	LYS
2	I	236	PRO
2	I	237	GLU
1	C	40	ASP
1	C	68	GLN
1	C	69	GLY
1	V	68	GLN
1	V	69	GLY
1	X	69	GLY
1	X	116	GLU
1	A	9	ASN
1	B	54	PHE
1	B	69	GLY
1	B	70	HIS
1	B	116	GLU
1	Z	71	LEU
1	Y	69	GLY
1	Y	116	GLU
2	E	44	LEU
2	E	165	GLU
2	E	212	LYS
2	F	143	TRP
2	F	230	ALA
2	G	141	ASN
2	G	144	GLY
2	G	165	GLU
2	G	170	ASP
2	G	212	LYS
2	G	213	ALA
2	I	230	ALA
1	C	113	VAL
1	D	115	PRO
1	X	115	PRO
1	A	71	LEU
1	Z	9	ASN
1	Y	70	HIS
1	Y	88	LEU
2	E	146	THR
2	F	154	ALA
2	F	237	GLU
2	F	300	ASP
2	G	44	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	146	THR
2	G	154	ALA
2	G	410	ALA
2	I	138	PRO
2	I	143	TRP
2	I	146	THR
1	A	115	PRO
1	B	68	GLN
1	B	88	LEU
2	E	213	ALA
2	F	137	PRO
2	F	138	PRO
2	F	293	LYS
2	G	232	LYS
2	I	137	PRO
1	D	116	GLU
1	X	8	ARG
1	Z	115	PRO
1	Y	38	TYR
1	Y	86	ARG
2	E	141	ASN
2	F	140	LYS
2	G	271	ASP
2	I	42	GLU
2	I	144	GLY
1	D	69	GLY
1	Z	72	VAL
1	B	72	VAL
2	F	144	GLY
1	A	72	VAL
2	G	235	ASN
2	I	173	ILE
2	F	173	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	136/136 (100%)	129 (95%)	7 (5%)	29 63
1	B	136/136 (100%)	125 (92%)	11 (8%)	15 39
1	C	136/136 (100%)	121 (89%)	15 (11%)	8 23
1	D	136/136 (100%)	124 (91%)	12 (9%)	12 35
1	V	136/136 (100%)	119 (88%)	17 (12%)	6 17
1	X	136/136 (100%)	124 (91%)	12 (9%)	12 35
1	Y	136/136 (100%)	127 (93%)	9 (7%)	21 51
1	Z	136/136 (100%)	128 (94%)	8 (6%)	24 57
2	E	350/383 (91%)	308 (88%)	42 (12%)	6 19
2	F	350/383 (91%)	301 (86%)	49 (14%)	4 13
2	G	350/383 (91%)	307 (88%)	43 (12%)	6 18
2	I	350/383 (91%)	301 (86%)	49 (14%)	4 13
All	All	2488/2620 (95%)	2214 (89%)	274 (11%)	8 23

All (274) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1	THR
1	C	4	VAL
1	C	30	ASN
1	C	37	LEU
1	C	40	ASP
1	C	54	PHE
1	C	80	LYS
1	C	83	ARG
1	C	91	LEU
1	C	104	LEU
1	C	116	GLU
1	C	136	LEU
1	C	149	GLU
1	C	152	LEU
1	C	173	TYR
1	D	1	THR
1	D	30	ASN
1	D	37	LEU
1	D	43	ILE
1	D	54	PHE
1	D	71	LEU
1	D	73	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	118	ASP
1	D	136	LEU
1	D	152	LEU
1	D	160	ILE
1	D	174	LYS
1	V	1	THR
1	V	30	ASN
1	V	37	LEU
1	V	54	PHE
1	V	73	LYS
1	V	77	GLU
1	V	83	ARG
1	V	104	LEU
1	V	111	ASP
1	V	114	GLN
1	V	136	LEU
1	V	139	ASN
1	V	152	LEU
1	V	154	ILE
1	V	160	ILE
1	V	168	ILE
1	V	173	TYR
1	X	1	THR
1	X	30	ASN
1	X	37	LEU
1	X	40	ASP
1	X	43	ILE
1	X	54	PHE
1	X	58	GLU
1	X	71	LEU
1	X	73	LYS
1	X	118	ASP
1	X	152	LEU
1	X	174	LYS
1	A	1	THR
1	A	9	ASN
1	A	30	ASN
1	A	71	LEU
1	A	97	VAL
1	A	136	LEU
1	A	152	LEU
1	B	1	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	30	ASN
1	B	35	ARG
1	B	54	PHE
1	B	104	LEU
1	B	112	VAL
1	B	116	GLU
1	B	136	LEU
1	B	152	LEU
1	B	160	ILE
1	B	174	LYS
1	Z	1	THR
1	Z	9	ASN
1	Z	30	ASN
1	Z	58	GLU
1	Z	71	LEU
1	Z	107	THR
1	Z	136	LEU
1	Z	152	LEU
1	Y	1	THR
1	Y	30	ASN
1	Y	54	PHE
1	Y	72	VAL
1	Y	116	GLU
1	Y	136	LEU
1	Y	152	LEU
1	Y	160	ILE
1	Y	174	LYS
2	E	11	SER
2	E	13	LEU
2	E	27	VAL
2	E	31	LEU
2	E	37	ARG
2	E	49	THR
2	E	59	THR
2	E	70	LEU
2	E	92	VAL
2	E	94	LYS
2	E	117	GLU
2	E	130	ARG
2	E	140	LYS
2	E	148	GLN
2	E	153	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	165	GLU
2	E	169	ASP
2	E	171	LYS
2	E	173	ILE
2	E	216	LEU
2	E	220	ASP
2	E	238	GLU
2	E	240	LYS
2	E	241	GLN
2	E	266	GLU
2	E	281	LEU
2	E	296	MET
2	E	300	ASP
2	E	311	GLN
2	E	312	ILE
2	E	318	LEU
2	E	326	LEU
2	E	337	THR
2	E	344	LEU
2	E	352	THR
2	E	353	VAL
2	E	355	TYR
2	E	375	ARG
2	E	385	GLU
2	E	389	ASN
2	E	412	ASP
2	E	413	LEU
2	F	13	LEU
2	F	27	VAL
2	F	31	LEU
2	F	37	ARG
2	F	41	ASN
2	F	59	THR
2	F	68	ARG
2	F	70	LEU
2	F	87	THR
2	F	94	LYS
2	F	103	LEU
2	F	104	THR
2	F	108	VAL
2	F	121	TYR
2	F	130	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	140	LYS
2	F	141	ASN
2	F	145	GLN
2	F	148	GLN
2	F	150	GLN
2	F	152	PRO
2	F	153	SER
2	F	173	ILE
2	F	210	LYS
2	F	211	GLN
2	F	214	ARG
2	F	217	LYS
2	F	219	LYS
2	F	220	ASP
2	F	232	LYS
2	F	266	GLU
2	F	281	LEU
2	F	296	MET
2	F	312	ILE
2	F	318	LEU
2	F	326	LEU
2	F	331	GLU
2	F	337	THR
2	F	344	LEU
2	F	351	ILE
2	F	352	THR
2	F	355	TYR
2	F	375	ARG
2	F	382	GLN
2	F	385	GLU
2	F	389	ASN
2	F	404	GLU
2	F	423	ASP
2	F	438	LEU
2	G	11	SER
2	G	13	LEU
2	G	27	VAL
2	G	31	LEU
2	G	37	ARG
2	G	59	THR
2	G	70	LEU
2	G	94	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	103	LEU
2	G	117	GLU
2	G	130	ARG
2	G	140	LYS
2	G	148	GLN
2	G	152	PRO
2	G	153	SER
2	G	165	GLU
2	G	168	LEU
2	G	169	ASP
2	G	171	LYS
2	G	173	ILE
2	G	216	LEU
2	G	238	GLU
2	G	240	LYS
2	G	241	GLN
2	G	266	GLU
2	G	296	MET
2	G	300	ASP
2	G	311	GLN
2	G	312	ILE
2	G	318	LEU
2	G	326	LEU
2	G	337	THR
2	G	344	LEU
2	G	352	THR
2	G	353	VAL
2	G	355	TYR
2	G	375	ARG
2	G	385	GLU
2	G	386	SER
2	G	389	ASN
2	G	419	THR
2	G	423	ASP
2	G	438	LEU
2	I	11	SER
2	I	13	LEU
2	I	27	VAL
2	I	31	LEU
2	I	37	ARG
2	I	41	ASN
2	I	49	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	59	THR
2	I	68	ARG
2	I	70	LEU
2	I	87	THR
2	I	94	LYS
2	I	103	LEU
2	I	104	THR
2	I	121	TYR
2	I	130	ARG
2	I	140	LYS
2	I	141	ASN
2	I	145	GLN
2	I	148	GLN
2	I	150	GLN
2	I	152	PRO
2	I	173	ILE
2	I	210	LYS
2	I	211	GLN
2	I	214	ARG
2	I	217	LYS
2	I	220	ASP
2	I	232	LYS
2	I	266	GLU
2	I	296	MET
2	I	300	ASP
2	I	311	GLN
2	I	312	ILE
2	I	318	LEU
2	I	326	LEU
2	I	337	THR
2	I	344	LEU
2	I	351	ILE
2	I	352	THR
2	I	355	TYR
2	I	375	ARG
2	I	382	GLN
2	I	385	GLU
2	I	389	ASN
2	I	404	GLU
2	I	413	LEU
2	I	438	LEU
2	I	442	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	9	ASN
1	C	30	ASN
1	C	114	GLN
1	D	9	ASN
1	D	30	ASN
1	D	139	ASN
1	V	9	ASN
1	V	11	HIS
1	V	30	ASN
1	V	114	GLN
1	X	9	ASN
1	X	30	ASN
1	X	114	GLN
1	X	139	ASN
1	A	30	ASN
1	A	39	ASN
1	A	68	GLN
1	A	109	ASN
1	A	139	ASN
1	B	11	HIS
1	B	30	ASN
1	B	109	ASN
1	B	114	GLN
1	Z	30	ASN
1	Z	39	ASN
1	Z	109	ASN
1	Y	11	HIS
1	Y	30	ASN
1	Y	109	ASN
1	Y	114	GLN
1	Y	130	GLN
2	E	22	ASN
2	E	33	ASN
2	E	75	ASN
2	E	114	GLN
2	E	141	ASN
2	E	145	GLN
2	E	149	GLN
2	E	150	GLN
2	E	241	GLN
2	E	311	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	348	ASN
2	E	382	GLN
2	E	384	ASN
2	E	389	ASN
2	E	416	GLN
2	E	428	HIS
2	F	22	ASN
2	F	33	ASN
2	F	41	ASN
2	F	114	GLN
2	F	141	ASN
2	F	142	ASN
2	F	145	GLN
2	F	149	GLN
2	F	150	GLN
2	F	157	GLN
2	F	211	GLN
2	F	348	ASN
2	F	365	ASN
2	F	384	ASN
2	F	389	ASN
2	F	416	GLN
2	F	417	ASN
2	G	22	ASN
2	G	33	ASN
2	G	75	ASN
2	G	114	GLN
2	G	149	GLN
2	G	150	GLN
2	G	241	GLN
2	G	311	GLN
2	G	348	ASN
2	G	382	GLN
2	G	384	ASN
2	G	389	ASN
2	G	416	GLN
2	G	428	HIS
2	I	22	ASN
2	I	41	ASN
2	I	75	ASN
2	I	114	GLN
2	I	142	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	I	145	GLN
2	I	149	GLN
2	I	150	GLN
2	I	211	GLN
2	I	311	GLN
2	I	348	ASN
2	I	384	ASN
2	I	389	ASN
2	I	416	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
3	ADP	E	450	-	24,29,29	1.51	7 (29%)	23,45,45	1.98	3 (13%)
3	ADP	F	1450	-	24,29,29	1.48	5 (20%)	23,45,45	2.00	3 (13%)
3	ADP	G	2450	-	24,29,29	1.53	7 (29%)	23,45,45	2.05	4 (17%)
3	ADP	I	3450	-	24,29,29	1.46	5 (20%)	23,45,45	2.02	3 (13%)

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
3	ADP	E	450	-	-	0/12/32/32	0/3/3/3
3	ADP	F	1450	-	-	0/12/32/32	0/3/3/3
3	ADP	G	2450	-	-	0/12/32/32	0/3/3/3
3	ADP	I	3450	-	-	0/12/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2450	ADP	C8-N7	-3.88	1.27	1.34
3	E	450	ADP	C8-N7	-3.82	1.27	1.34
3	F	1450	ADP	C8-N7	-3.81	1.27	1.34
3	I	3450	ADP	C8-N7	-3.73	1.27	1.34
3	E	450	ADP	PA-O1A	-2.25	1.43	1.51
3	E	450	ADP	PA-O2A	-2.19	1.45	1.55
3	I	3450	ADP	PA-O2A	-2.17	1.45	1.55
3	G	2450	ADP	PB-O3B	-2.17	1.47	1.54
3	G	2450	ADP	PA-O2A	-2.15	1.45	1.55
3	G	2450	ADP	PA-O1A	-2.15	1.43	1.51
3	E	450	ADP	PB-O3B	-2.14	1.47	1.54
3	F	1450	ADP	PB-O3B	-2.11	1.47	1.54
3	F	1450	ADP	PA-O2A	-2.08	1.46	1.55
3	I	3450	ADP	PA-O1A	-2.08	1.43	1.51
3	E	450	ADP	C2'-C1'	2.07	1.56	1.53
3	G	2450	ADP	C2-N3	2.10	1.35	1.32
3	E	450	ADP	C2-N3	2.18	1.36	1.32
3	E	450	ADP	C4-N3	2.27	1.38	1.35
3	I	3450	ADP	C2-N3	2.29	1.36	1.32
3	G	2450	ADP	C2'-C1'	2.31	1.57	1.53
3	G	2450	ADP	C4-N3	2.33	1.39	1.35
3	F	1450	ADP	C2-N3	2.41	1.36	1.32
3	I	3450	ADP	C4-N3	2.64	1.39	1.35
3	F	1450	ADP	C4-N3	2.73	1.39	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1450	ADP	N3-C2-N1	-5.09	124.87	128.87
3	G	2450	ADP	N3-C2-N1	-5.03	124.92	128.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	3450	ADP	N3-C2-N1	-4.90	125.02	128.87
3	E	450	ADP	N3-C2-N1	-4.66	125.21	128.87
3	G	2450	ADP	C2'-C1'-N9	-2.13	107.76	113.47
3	F	1450	ADP	C2'-C3'-C4'	2.90	108.58	102.64
3	I	3450	ADP	C2'-C3'-C4'	2.92	108.61	102.64
3	E	450	ADP	C2'-C3'-C4'	2.95	108.67	102.64
3	G	2450	ADP	C2'-C3'-C4'	2.99	108.75	102.64
3	F	1450	ADP	C4'-O4'-C1'	6.53	116.56	109.64
3	E	450	ADP	C4'-O4'-C1'	6.55	116.58	109.64
3	G	2450	ADP	C4'-O4'-C1'	6.66	116.70	109.64
3	I	3450	ADP	C4'-O4'-C1'	6.77	116.82	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	450	ADP	3	0
3	F	1450	ADP	3	0
3	G	2450	ADP	3	0
3	I	3450	ADP	4	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	174/175 (99%)	0.45	3 (1%) 73 63	30, 54, 89, 98	0
1	B	174/175 (99%)	0.56	12 (6%) 20 11	36, 68, 101, 102	0
1	C	174/175 (99%)	0.58	14 (8%) 15 7	54, 81, 100, 102	0
1	D	174/175 (99%)	0.45	7 (4%) 42 30	49, 71, 97, 100	0
1	V	174/175 (99%)	0.53	12 (6%) 20 11	54, 80, 98, 102	0
1	X	174/175 (99%)	0.39	3 (1%) 73 63	51, 70, 98, 101	0
1	Y	174/175 (99%)	0.50	4 (2%) 64 52	36, 68, 100, 102	0
1	Z	174/175 (99%)	0.44	3 (1%) 73 63	30, 55, 90, 97	0
2	E	408/449 (90%)	0.59	37 (9%) 11 6	32, 59, 102, 102	0
2	F	408/449 (90%)	0.85	54 (13%) 4 2	33, 61, 102, 102	0
2	G	408/449 (90%)	0.62	34 (8%) 14 7	32, 59, 102, 102	0
2	I	408/449 (90%)	0.82	53 (12%) 5 2	32, 60, 102, 102	0
All	All	3024/3196 (94%)	0.61	236 (7%) 16 8	30, 63, 102, 102	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	90	GLY	9.0
2	G	144	GLY	8.7
2	F	90	GLY	8.1
2	I	141	ASN	7.5
2	F	141	ASN	7.2
2	I	145	GLN	7.1
2	F	144	GLY	6.9
2	I	143	TRP	6.2
2	E	140	LYS	6.1
2	F	146	THR	6.0
2	E	89	VAL	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	154	ALA	5.9
2	F	165	GLU	5.8
2	F	123	ALA	5.8
2	I	132	LEU	5.6
2	F	267	SER	5.5
2	E	148	GLN	5.5
2	F	134	VAL	5.5
2	F	226	ILE	5.4
2	I	226	ILE	5.4
2	G	214	ARG	5.2
2	G	267	SER	5.1
2	F	153	SER	5.1
2	I	134	VAL	5.1
2	G	89	VAL	5.0
2	I	131	ILE	4.9
2	I	140	LYS	4.8
2	F	170	ASP	4.8
2	G	265	GLY	4.7
2	F	173	ILE	4.6
2	F	117	GLU	4.6
2	F	151	GLU	4.5
2	I	165	GLU	4.5
2	E	145	GLN	4.5
2	I	219	LYS	4.5
2	E	215	LYS	4.5
2	I	152	PRO	4.5
2	E	143	TRP	4.4
2	G	148	GLN	4.3
2	I	91	TYR	4.3
2	I	92	VAL	4.3
2	G	146	THR	4.2
2	F	133	ASP	4.2
2	I	173	ILE	4.2
2	G	171	LYS	4.2
2	I	222	MET	4.2
2	G	140	LYS	4.2
2	F	138	PRO	4.2
1	Y	60	PHE	4.1
2	F	91	TYR	4.1
2	I	117	GLU	4.1
2	F	222	MET	4.1
2	I	123	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	170	ASP	4.0
2	G	210	LYS	4.0
2	F	140	LYS	4.0
2	I	89	VAL	4.0
2	I	211	GLN	3.9
1	B	60	PHE	3.9
2	I	144	GLY	3.9
2	G	134	VAL	3.9
2	G	143	TRP	3.9
2	F	266	GLU	3.8
2	F	169	ASP	3.8
2	F	264	ARG	3.8
2	E	173	ILE	3.7
2	F	89	VAL	3.7
1	V	34	VAL	3.7
2	I	139	ALA	3.7
2	F	219	LYS	3.6
2	G	153	SER	3.6
2	F	124	GLU	3.6
2	I	221	ALA	3.6
1	X	91	LEU	3.6
2	G	91	TYR	3.5
2	G	117	GLU	3.5
1	V	93	ALA	3.4
2	F	152	PRO	3.4
2	F	211	GLN	3.4
2	G	141	ASN	3.4
2	F	227	GLU	3.4
2	I	266	GLU	3.4
1	V	94	LEU	3.3
2	E	91	TYR	3.3
2	I	168	LEU	3.3
2	I	113	VAL	3.3
2	E	267	SER	3.2
1	D	93	ALA	3.2
2	I	146	THR	3.2
2	E	92	VAL	3.1
2	G	264	ARG	3.1
2	E	270	PRO	3.1
1	X	93	ALA	3.1
2	F	234	VAL	3.1
2	I	137	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	212	LYS	3.1
2	F	129	GLU	3.1
2	F	112	ARG	3.0
2	I	216	LEU	3.0
2	E	134	VAL	3.0
2	E	266	GLU	3.0
2	I	90	GLY	3.0
1	Z	83	ARG	3.0
2	E	141	ASN	3.0
2	E	221	ALA	2.9
1	V	174	LYS	2.9
2	G	234	VAL	2.9
2	I	213	ALA	2.9
2	I	223	LYS	2.9
2	I	151	GLU	2.9
2	F	139	ALA	2.9
1	C	42	VAL	2.9
2	I	217	LYS	2.9
1	X	90	LYS	2.8
2	E	212	LYS	2.8
1	B	86	ARG	2.8
2	E	239	LEU	2.8
2	I	138	PRO	2.8
2	I	264	ARG	2.8
2	E	144	GLY	2.8
1	B	78	LEU	2.8
2	F	119	ASN	2.7
1	Y	57	PHE	2.7
1	V	42	VAL	2.7
2	I	224	LEU	2.7
2	E	151	GLU	2.7
2	I	128	GLU	2.7
1	B	42	VAL	2.7
2	F	154	ALA	2.7
1	C	93	ALA	2.7
1	C	67	HIS	2.6
2	G	215	LYS	2.6
2	I	83	ALA	2.6
1	B	95	LEU	2.6
1	A	83	ARG	2.6
2	F	233	LEU	2.6
1	V	35	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	214	ARG	2.6
2	E	214	ARG	2.6
2	I	136	ILE	2.6
2	F	224	LEU	2.6
2	G	227	GLU	2.6
2	E	147	GLU	2.5
2	I	153	SER	2.5
2	I	148	GLN	2.5
2	I	133	ASP	2.5
2	I	169	ASP	2.5
2	F	168	LEU	2.5
2	E	170	ASP	2.5
2	E	153	SER	2.5
2	F	143	TRP	2.5
1	V	44	ALA	2.5
2	F	130	ARG	2.5
2	I	267	SER	2.5
1	V	173	TYR	2.5
2	I	116	ILE	2.5
1	B	46	PHE	2.4
2	G	266	GLU	2.4
2	G	83	ALA	2.4
1	C	112	VAL	2.4
1	A	46	PHE	2.4
2	I	234	VAL	2.4
2	G	222	MET	2.4
1	V	43	ILE	2.4
2	F	113	VAL	2.4
2	E	210	LYS	2.4
2	G	151	GLU	2.4
1	D	89	ARG	2.4
2	E	219	LYS	2.4
2	F	244	ILE	2.4
2	F	128	GLU	2.3
2	F	137	PRO	2.3
2	I	172	GLU	2.3
2	E	149	GLN	2.3
2	F	215	LYS	2.3
2	E	117	GLU	2.3
1	C	53	ALA	2.3
1	C	98	ALA	2.3
2	G	35	TRP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	82	TRP	2.3
2	F	83	ALA	2.3
2	F	115	ALA	2.3
2	G	173	ILE	2.3
2	F	156	ARG	2.3
1	D	70	HIS	2.3
2	E	90	GLY	2.3
1	C	174	LYS	2.3
2	E	224	LEU	2.3
2	G	211	GLN	2.2
1	Y	97	VAL	2.2
1	A	73	LYS	2.2
1	C	60	PHE	2.2
1	Z	60	PHE	2.2
2	I	156	ARG	2.2
1	V	90	LYS	2.2
2	E	171	LYS	2.2
1	Z	44	ALA	2.2
2	F	220	ASP	2.2
2	G	147	GLU	2.2
1	C	43	ILE	2.2
2	F	210	LYS	2.2
1	V	51	ALA	2.2
2	F	217	LYS	2.2
2	E	6	PRO	2.2
2	E	225	LEU	2.2
2	F	223	LYS	2.2
1	V	60	PHE	2.1
1	B	87	MET	2.1
1	B	116	GLU	2.1
1	C	38	TYR	2.1
2	G	216	LEU	2.1
2	G	123	ALA	2.1
2	I	129	GLU	2.1
1	D	91	LEU	2.1
2	E	284	LEU	2.1
2	E	172	GLU	2.1
1	C	55	THR	2.1
2	G	170	ASP	2.1
1	D	113	VAL	2.1
1	B	69	GLY	2.1
2	F	355	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	418	ILE	2.1
1	Y	37	LEU	2.1
2	E	234	VAL	2.1
2	E	264	ARG	2.1
1	B	112	VAL	2.1
2	E	119	ASN	2.1
2	I	233	LEU	2.1
2	F	92	VAL	2.0
1	C	89	ARG	2.0
1	D	103	SER	2.0
1	D	108	GLY	2.0
1	B	57	PHE	2.0
1	C	94	LEU	2.0
1	C	109	ASN	2.0
2	I	112	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	ADP	G	2450	27/27	0.96	0.26	0.90	38,46,58,59	0
3	ADP	F	1450	27/27	0.95	0.26	0.85	47,51,56,58	0
3	ADP	E	450	27/27	0.96	0.25	0.65	40,46,58,58	0
3	ADP	I	3450	27/27	0.96	0.23	0.26	45,49,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.