



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:55 PM BST

PDB ID : 3ZW6
EMDB ID: : EMD-1940
Title : MODEL OF HEXAMERIC AAA DOMAIN ARRANGEMENT OF GREEN-
TYPE RUBISCO ACTIVASE FROM TOBACCO.
Authors : Stotz, M.; Mueller-Cajar, O.; Ciniawsky, S.; Wendler, P.; Hartl, F.U.; Bracher,
A.; Hayer-Hartl, M.
Deposited on : 2011-07-28
Resolution : 20.00 Å(reported)
Based on PDB ID : 3T15

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

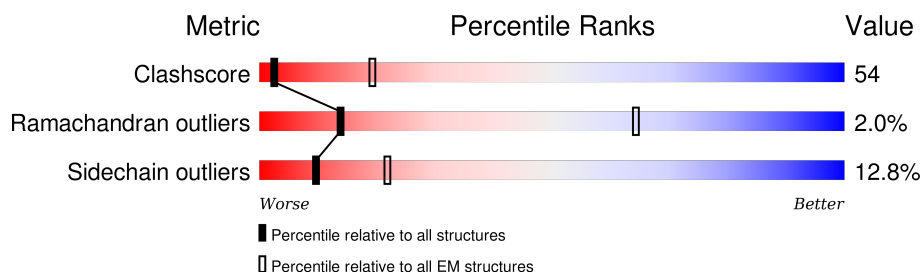
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	293	
1	B	293	
1	C	293	
1	D	293	
1	E	293	
1	F	293	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

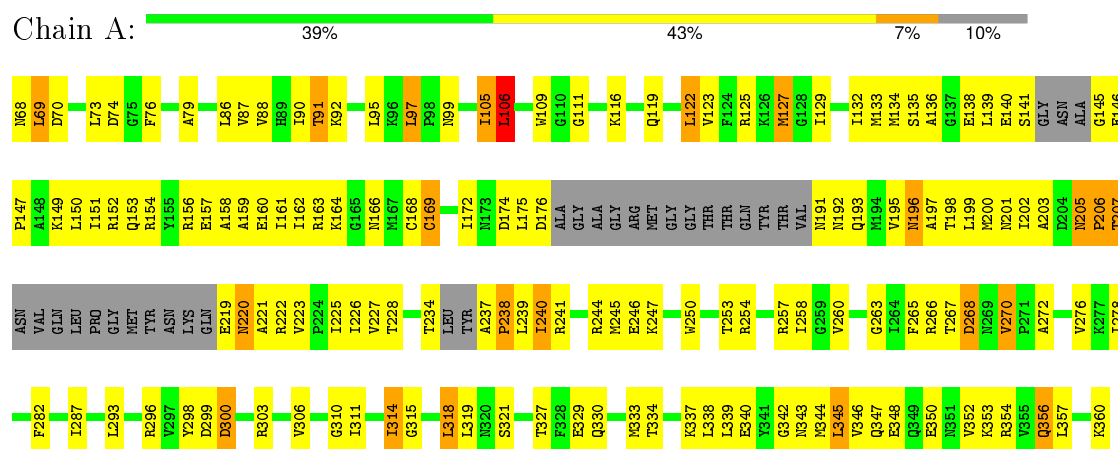
- Molecule 1 is a protein called RIBULOSE BISPSPHATE CARBOXYLASE/OXYGEN ASE ACTIVASE 1, CHLOROPLASTIC.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	B	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	C	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	D	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	E	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		
1	F	263	Total	C	N	O	S	0	0
			2082	1324	360	384	14		

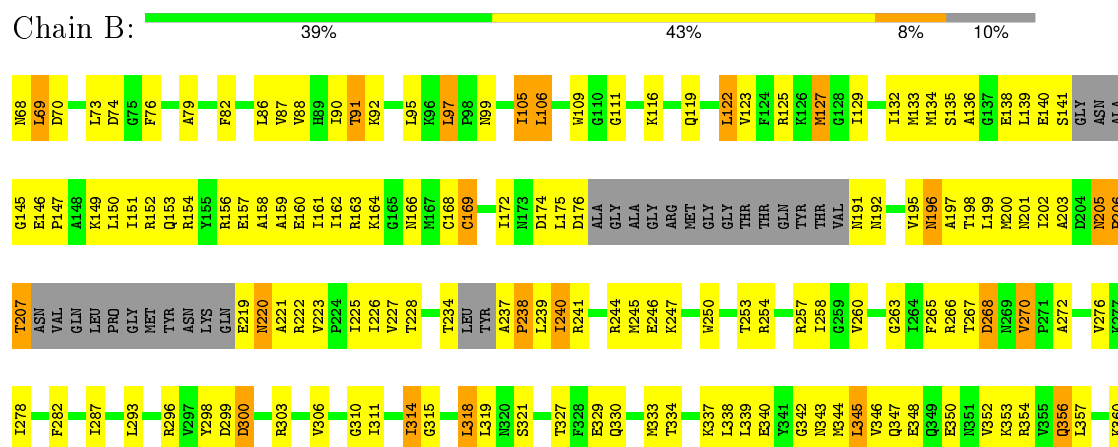
3 Residue-property plots

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

- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

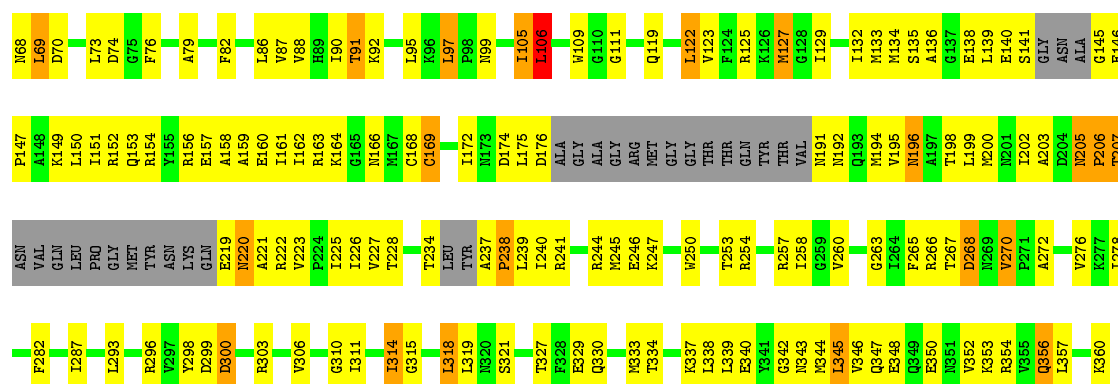


- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC



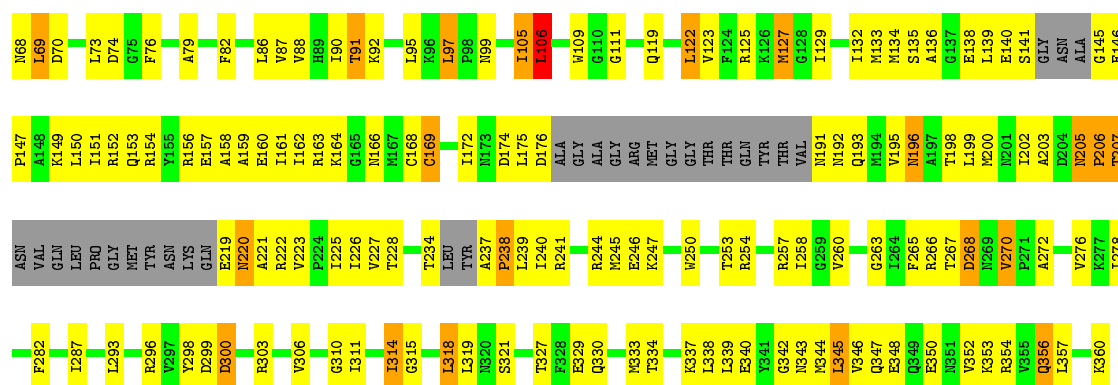
- Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC





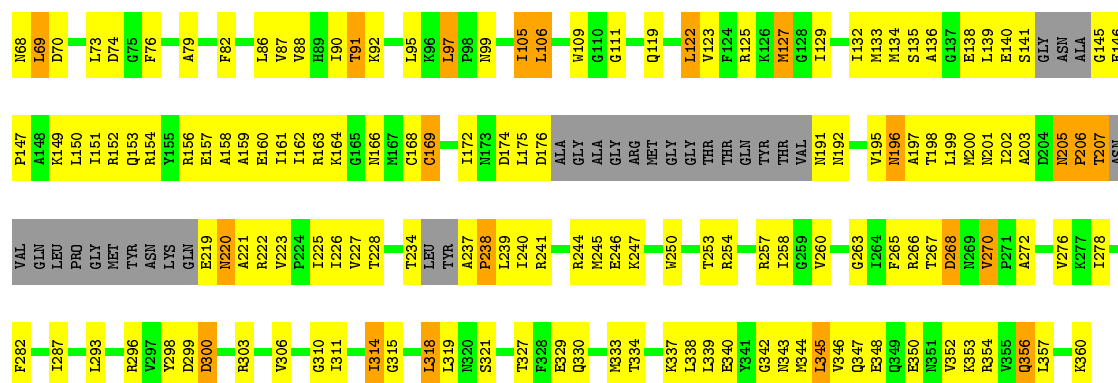
• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

Chain D: 40% 43% 7% 10%



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

Chain E: 39% 43% 7% 10%



• Molecule 1: RIBULOSE BISPHOSPHATE CARBOXYLASE/OXYGENASE ACTIVASE 1, CHLOROPLASTIC

Chain F: 39% 43% 7% 10%

N68	L69	D70	L73	D74	G75	F76	A79	F82	L86	V87	V88	H89	I90	T91	K92	L95	K96	L97	P98	N99	I105	L106	I109	G110	G111	K116	Q119	L122	V123	F124	R125	K126	M127	G128	I129	I132	M133	M134	S135	A136	G137	L138	M139	E140	S141	GLY	ASN	ALA											
G145	E146	P147	A148	K149	L150	I151	R152	Q153	R154	Y155	R156	E157	A158	A159	E160	I161	I162	R163	K164	G165	N166	M167	G168	G169	I172	N173	D174	L175	D176	ALA	GLY	ALA	GLY	ARG	MET	GLY	GLY	THR	THR	GLN	R125	TYR	THR	VAL	N191	N192	Q193	M194	V195	M196	A197	T198	L199	M200	N201	I202	A203	D204	N205
P206	T207	ASN	VAL	GLN	LEU	PRO	GLY	MET	TYR	ASN	LYS	GLN	E219	N220	A221	R222	V223	P224	I225	I226	V227	T228	T234	LEU	TYR	A237	P238	L239	T240	R241	R244	M245	E246	K247	N250	T253	R254	R257	I258	G259	V260	G263	T264	F265	R266	T267	D268	N269	V270	P271	A272	V276							
K277	I278	F282	I287	L293	R296	V297	Y298	D299	D300	R303	V306	G310	I311	I314	G315	L318	L319	N320	S321	T327	Q330	M333	T334	K337	L338	L339	E340	Y341	G342	N343	M344	V345	V346	Q347	E348	Q349	E350	N351	V352	K353	R354	V355	Q356	L357	K360														

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	PHASE FLIPPING, EACH PARTICLE	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	470	Depositor
Maximum defocus (nm)	950	Depositor
Magnification	Not provided	Depositor
Image detector	EAGLE 2K CCD	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	0.68	4/2116 (0.2%)	0.68	1/2847 (0.0%)
1	B	0.67	4/2116 (0.2%)	0.68	0/2847
1	C	0.68	4/2116 (0.2%)	0.68	1/2847 (0.0%)
1	D	0.68	4/2116 (0.2%)	0.68	1/2847 (0.0%)
1	E	0.67	4/2116 (0.2%)	0.68	0/2847
1	F	0.67	4/2116 (0.2%)	0.68	0/2847
All	All	0.68	24/12696 (0.2%)	0.68	3/17082 (0.0%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	207	THR	C-O	13.25	1.48	1.23
1	C	207	THR	C-O	13.21	1.48	1.23
1	B	207	THR	C-O	13.19	1.48	1.23
1	A	207	THR	C-O	13.16	1.48	1.23
1	E	207	THR	C-O	13.16	1.48	1.23
1	F	207	THR	C-O	13.12	1.48	1.23
1	B	157	GLU	CD-OE1	7.62	1.34	1.25
1	F	157	GLU	CD-OE1	7.59	1.34	1.25
1	D	157	GLU	CD-OE1	7.57	1.33	1.25
1	C	157	GLU	CD-OE1	7.55	1.33	1.25
1	A	157	GLU	CD-OE1	7.54	1.33	1.25
1	E	157	GLU	CD-OE1	7.51	1.33	1.25
1	A	157	GLU	CD-OE2	6.68	1.33	1.25
1	C	157	GLU	CD-OE2	6.67	1.32	1.25
1	B	157	GLU	CD-OE2	6.62	1.32	1.25
1	D	157	GLU	CD-OE2	6.58	1.32	1.25
1	E	157	GLU	CD-OE2	6.54	1.32	1.25
1	F	157	GLU	CD-OE2	6.49	1.32	1.25
1	F	219	GLU	N-CA	5.86	1.58	1.46
1	D	219	GLU	N-CA	5.85	1.58	1.46
1	C	219	GLU	N-CA	5.81	1.57	1.46
1	E	219	GLU	N-CA	5.77	1.57	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	GLU	N-CA	5.76	1.57	1.46
1	B	219	GLU	N-CA	5.72	1.57	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	LEU	CA-CB-CG	5.06	126.93	115.30
1	C	106	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	106	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2082	0	2097	233	0
1	B	2082	0	2097	231	0
1	C	2082	0	2097	236	0
1	D	2082	0	2097	231	0
1	E	2082	0	2097	226	0
1	F	2082	0	2097	234	0
All	All	12492	0	12582	1360	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

All (1360) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:GLU:HA	1:B:163:ARG:HG2	1.28	1.14
1:E:160:GLU:HA	1:E:163:ARG:HG2	1.28	1.13
1:A:109:TRP:HE1	1:A:247:LYS:HG2	1.09	1.13
1:F:160:GLU:HA	1:F:163:ARG:HG2	1.28	1.11

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:GLU:HA	1:F:163:ARG:CG	1.81	1.11
1:D:160:GLU:HA	1:D:163:ARG:CG	1.81	1.11
1:D:109:TRP:HE1	1:D:247:LYS:HG2	1.09	1.10
1:B:160:GLU:HA	1:B:163:ARG:CG	1.81	1.10
1:F:109:TRP:HE1	1:F:247:LYS:HG2	1.09	1.10
1:C:160:GLU:HA	1:C:163:ARG:HG2	1.28	1.09
1:D:160:GLU:HA	1:D:163:ARG:HG2	1.28	1.09
1:C:160:GLU:HA	1:C:163:ARG:CG	1.81	1.09
1:A:160:GLU:HA	1:A:163:ARG:CG	1.81	1.09
1:E:160:GLU:HA	1:E:163:ARG:CG	1.81	1.09
1:F:162:ILE:HD13	1:F:223:VAL:CG2	1.83	1.09
1:B:162:ILE:HD13	1:B:223:VAL:CG2	1.83	1.08
1:C:162:ILE:HD13	1:C:223:VAL:CG2	1.83	1.08
1:D:162:ILE:HD13	1:D:223:VAL:CG2	1.83	1.08
1:B:109:TRP:HE1	1:B:247:LYS:HG2	1.09	1.08
1:C:139:LEU:HD21	1:C:195:VAL:HG21	1.35	1.08
1:C:109:TRP:HE1	1:C:247:LYS:HG2	1.09	1.07
1:E:109:TRP:HE1	1:E:247:LYS:HG2	1.09	1.07
1:A:139:LEU:HD21	1:A:195:VAL:HG21	1.35	1.07
1:A:162:ILE:HD13	1:A:223:VAL:CG2	1.83	1.07
1:E:162:ILE:HD13	1:E:223:VAL:CG2	1.84	1.07
1:D:139:LEU:HD21	1:D:195:VAL:HG21	1.35	1.06
1:A:146:GLU:N	1:A:149:LYS:HE3	1.71	1.06
1:C:97:LEU:HD23	1:C:97:LEU:H	1.21	1.05
1:E:146:GLU:N	1:E:149:LYS:HE3	1.71	1.05
1:E:139:LEU:HD21	1:E:195:VAL:HG21	1.35	1.05
1:A:160:GLU:HA	1:A:163:ARG:HG2	1.28	1.05
1:B:97:LEU:HD23	1:B:97:LEU:H	1.21	1.05
1:D:146:GLU:N	1:D:149:LYS:HE3	1.71	1.05
1:F:146:GLU:N	1:F:149:LYS:HE3	1.71	1.04
1:B:146:GLU:N	1:B:149:LYS:HE3	1.71	1.04
1:C:146:GLU:N	1:C:149:LYS:HE3	1.71	1.03
1:F:139:LEU:HD21	1:F:195:VAL:HG21	1.35	1.03
1:B:139:LEU:HD21	1:B:195:VAL:HG21	1.35	1.03
1:E:97:LEU:H	1:E:97:LEU:HD23	1.21	1.03
1:F:350:GLU:CA	1:F:353:LYS:HE2	1.90	1.02
1:F:97:LEU:HD23	1:F:97:LEU:H	1.21	1.02
1:C:356:GLN:O	1:C:360:LYS:HG2	1.60	1.02
1:D:350:GLU:CA	1:D:353:LYS:HE2	1.90	1.02
1:B:350:GLU:CA	1:B:353:LYS:HE2	1.90	1.02
1:F:356:GLN:O	1:F:360:LYS:HG2	1.60	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLN:O	1:A:360:LYS:HG2	1.60	1.01
1:D:146:GLU:HA	1:D:149:LYS:HE3	1.43	1.01
1:E:356:GLN:O	1:E:360:LYS:HG2	1.60	1.01
1:E:350:GLU:CA	1:E:353:LYS:HE2	1.90	1.00
1:A:350:GLU:CA	1:A:353:LYS:HE2	1.90	1.00
1:A:109:TRP:NE1	1:A:247:LYS:HG2	1.77	1.00
1:F:109:TRP:NE1	1:F:247:LYS:HG2	1.77	1.00
1:B:146:GLU:HA	1:B:149:LYS:HE3	1.43	1.00
1:C:350:GLU:CA	1:C:353:LYS:HE2	1.90	1.00
1:D:97:LEU:H	1:D:97:LEU:HD23	1.21	1.00
1:D:356:GLN:O	1:D:360:LYS:HG2	1.60	1.00
1:A:97:LEU:HD23	1:A:97:LEU:H	1.21	1.00
1:D:109:TRP:NE1	1:D:247:LYS:HG2	1.77	1.00
1:A:193:GLN:HG2	1:F:140:GLU:CD	1.83	1.00
1:C:109:TRP:NE1	1:C:247:LYS:HG2	1.77	0.99
1:B:109:TRP:NE1	1:B:247:LYS:HG2	1.77	0.99
1:C:146:GLU:HA	1:C:149:LYS:HE3	1.43	0.99
1:E:109:TRP:NE1	1:E:247:LYS:HG2	1.77	0.99
1:A:146:GLU:HA	1:A:149:LYS:HE3	1.43	0.99
1:D:146:GLU:CA	1:D:149:LYS:HE3	1.93	0.99
1:B:356:GLN:O	1:B:360:LYS:HG2	1.60	0.99
1:A:146:GLU:CA	1:A:149:LYS:HE3	1.93	0.98
1:E:146:GLU:HA	1:E:149:LYS:HE3	1.43	0.98
1:E:73:LEU:HD21	1:E:125:ARG:CD	1.93	0.98
1:F:73:LEU:HD21	1:F:125:ARG:CD	1.93	0.98
1:C:140:GLU:CD	1:D:193:GLN:HG2	1.83	0.98
1:F:146:GLU:HA	1:F:149:LYS:HE3	1.43	0.98
1:F:146:GLU:CA	1:F:149:LYS:HE3	1.93	0.98
1:C:73:LEU:HD21	1:C:125:ARG:CD	1.93	0.98
1:D:73:LEU:HD21	1:D:125:ARG:CD	1.93	0.97
1:F:353:LYS:HE3	1:F:354:ARG:NH1	1.79	0.97
1:B:73:LEU:HD21	1:B:125:ARG:CD	1.93	0.97
1:C:353:LYS:HE3	1:C:354:ARG:NH1	1.79	0.97
1:A:73:LEU:HD21	1:A:125:ARG:CD	1.93	0.97
1:C:146:GLU:CA	1:C:149:LYS:HE3	1.93	0.97
1:D:162:ILE:HD13	1:D:223:VAL:HG23	1.46	0.97
1:A:162:ILE:HD13	1:A:223:VAL:HG23	1.46	0.97
1:B:146:GLU:CA	1:B:149:LYS:HE3	1.93	0.97
1:B:162:ILE:HD13	1:B:223:VAL:HG23	1.46	0.97
1:A:353:LYS:HE3	1:A:354:ARG:NH1	1.79	0.97
1:E:146:GLU:CA	1:E:149:LYS:HE3	1.93	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LYS:HE3	1:B:354:ARG:NH1	1.79	0.96
1:E:353:LYS:HE3	1:E:354:ARG:NH1	1.79	0.96
1:C:162:ILE:HD13	1:C:223:VAL:HG23	1.46	0.95
1:B:146:GLU:HA	1:B:149:LYS:CE	1.96	0.95
1:A:146:GLU:HA	1:A:149:LYS:CE	1.96	0.95
1:E:146:GLU:HA	1:E:149:LYS:CE	1.96	0.95
1:D:353:LYS:HE3	1:D:354:ARG:NH1	1.79	0.95
1:C:146:GLU:HA	1:C:149:LYS:CE	1.96	0.95
1:D:146:GLU:HA	1:D:149:LYS:CE	1.96	0.95
1:D:161:ILE:O	1:D:164:LYS:HG2	1.67	0.94
1:F:347:GLN:O	1:F:350:GLU:HG2	1.68	0.94
1:B:347:GLN:O	1:B:350:GLU:HG2	1.68	0.94
1:F:162:ILE:HD13	1:F:223:VAL:HG23	1.46	0.94
1:F:146:GLU:HA	1:F:149:LYS:CE	1.96	0.94
1:A:347:GLN:O	1:A:350:GLU:HG2	1.68	0.94
1:B:161:ILE:O	1:B:164:LYS:HG2	1.67	0.94
1:C:347:GLN:O	1:C:350:GLU:HG2	1.68	0.93
1:D:347:GLN:O	1:D:350:GLU:HG2	1.68	0.93
1:A:161:ILE:O	1:A:164:LYS:HG2	1.68	0.93
1:D:145:GLY:O	1:D:149:LYS:HG2	1.69	0.93
1:F:161:ILE:O	1:F:164:LYS:HG2	1.67	0.93
1:B:145:GLY:O	1:B:149:LYS:HG2	1.69	0.93
1:C:145:GLY:O	1:C:149:LYS:HG2	1.69	0.93
1:A:160:GLU:CA	1:A:163:ARG:HG2	1.99	0.92
1:E:161:ILE:O	1:E:164:LYS:HG2	1.67	0.92
1:E:347:GLN:O	1:E:350:GLU:HG2	1.68	0.92
1:E:162:ILE:HD13	1:E:223:VAL:HG23	1.47	0.92
1:F:145:GLY:O	1:F:149:LYS:HG2	1.69	0.92
1:C:161:ILE:O	1:C:164:LYS:HG2	1.68	0.92
1:E:160:GLU:CA	1:E:163:ARG:HG2	2.00	0.92
1:D:205:ASN:HB2	1:D:206:PRO:HD2	1.52	0.92
1:C:205:ASN:HB2	1:C:206:PRO:HD2	1.52	0.92
1:B:350:GLU:HA	1:B:353:LYS:HE2	1.52	0.92
1:F:205:ASN:HB2	1:F:206:PRO:HD2	1.52	0.92
1:C:160:GLU:CA	1:C:163:ARG:HG2	1.99	0.91
1:F:160:GLU:CA	1:F:163:ARG:HG2	1.99	0.91
1:B:205:ASN:HB2	1:B:206:PRO:HD2	1.52	0.91
1:E:205:ASN:HB2	1:E:206:PRO:HD2	1.52	0.91
1:C:350:GLU:HA	1:C:353:LYS:HE2	1.53	0.91
1:D:160:GLU:CA	1:D:163:ARG:HG2	2.00	0.91
1:A:145:GLY:O	1:A:149:LYS:HG2	1.69	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ILE:CD1	1:E:223:VAL:HG23	2.01	0.91
1:E:145:GLY:O	1:E:149:LYS:HG2	1.69	0.91
1:A:350:GLU:HA	1:A:353:LYS:HE2	1.53	0.91
1:C:162:ILE:CD1	1:C:223:VAL:HG23	2.00	0.91
1:D:350:GLU:HA	1:D:353:LYS:HE2	1.52	0.90
1:B:160:GLU:CA	1:B:163:ARG:HG2	1.99	0.90
1:B:162:ILE:CD1	1:B:223:VAL:HG23	2.01	0.90
1:A:162:ILE:CD1	1:A:223:VAL:HG23	2.01	0.90
1:F:350:GLU:O	1:F:353:LYS:HG2	1.71	0.90
1:D:350:GLU:O	1:D:353:LYS:HG2	1.71	0.90
1:D:162:ILE:CD1	1:D:223:VAL:HG23	2.01	0.90
1:E:350:GLU:HA	1:E:353:LYS:HE2	1.52	0.90
1:B:241:ARG:NH2	1:B:247:LYS:HD3	1.88	0.89
1:F:350:GLU:HA	1:F:353:LYS:HE2	1.52	0.89
1:A:241:ARG:NH2	1:A:247:LYS:HD3	1.87	0.89
1:A:205:ASN:HB2	1:A:206:PRO:HD2	1.52	0.89
1:A:350:GLU:O	1:A:353:LYS:HG2	1.71	0.89
1:F:162:ILE:CD1	1:F:223:VAL:HG23	2.00	0.89
1:C:241:ARG:NH2	1:C:247:LYS:HD3	1.88	0.88
1:C:350:GLU:O	1:C:353:LYS:HG2	1.71	0.88
1:B:350:GLU:O	1:B:353:LYS:HG2	1.71	0.88
1:E:241:ARG:NH2	1:E:247:LYS:HD3	1.87	0.88
1:E:350:GLU:O	1:E:353:LYS:HG2	1.71	0.88
1:C:109:TRP:NE1	1:C:247:LYS:CG	2.37	0.88
1:E:109:TRP:NE1	1:E:247:LYS:CG	2.37	0.88
1:D:241:ARG:NH2	1:D:247:LYS:HD3	1.88	0.87
1:F:241:ARG:NH2	1:F:247:LYS:HD3	1.88	0.87
1:A:109:TRP:NE1	1:A:247:LYS:CG	2.37	0.87
1:D:109:TRP:NE1	1:D:247:LYS:CG	2.37	0.87
1:F:350:GLU:CB	1:F:353:LYS:HE2	2.05	0.87
1:C:350:GLU:CB	1:C:353:LYS:HE2	2.04	0.87
1:F:109:TRP:NE1	1:F:247:LYS:CG	2.37	0.87
1:B:109:TRP:NE1	1:B:247:LYS:CG	2.37	0.87
1:D:350:GLU:CB	1:D:353:LYS:HE2	2.05	0.87
1:A:350:GLU:CB	1:A:353:LYS:HE2	2.05	0.86
1:E:350:GLU:CB	1:E:353:LYS:HE2	2.05	0.85
1:B:350:GLU:CB	1:B:353:LYS:HE2	2.05	0.85
1:D:139:LEU:HD21	1:D:195:VAL:CG2	2.07	0.85
1:B:139:LEU:HD21	1:B:195:VAL:CG2	2.07	0.84
1:F:353:LYS:CE	1:F:354:ARG:NH1	2.41	0.84
1:F:139:LEU:HD21	1:F:195:VAL:CG2	2.07	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD21	1:C:195:VAL:CG2	2.07	0.84
1:E:139:LEU:HD21	1:E:195:VAL:CG2	2.07	0.84
1:A:139:LEU:HD21	1:A:195:VAL:CG2	2.07	0.84
1:E:97:LEU:N	1:E:97:LEU:HD23	1.93	0.84
1:F:350:GLU:HB2	1:F:353:LYS:HE2	1.60	0.84
1:D:353:LYS:CE	1:D:354:ARG:NH1	2.40	0.83
1:E:353:LYS:CE	1:E:354:ARG:NH1	2.40	0.83
1:C:191:ASN:O	1:C:195:VAL:HG23	1.79	0.83
1:F:191:ASN:O	1:F:195:VAL:HG23	1.79	0.83
1:C:353:LYS:CE	1:C:354:ARG:NH1	2.40	0.83
1:D:350:GLU:HB2	1:D:353:LYS:HE2	1.60	0.83
1:D:191:ASN:O	1:D:195:VAL:HG23	1.79	0.83
1:B:97:LEU:HD23	1:B:97:LEU:N	1.93	0.83
1:B:353:LYS:CE	1:B:354:ARG:NH1	2.41	0.83
1:A:191:ASN:O	1:A:195:VAL:HG23	1.79	0.82
1:E:191:ASN:O	1:E:195:VAL:HG23	1.79	0.82
1:C:350:GLU:HB2	1:C:353:LYS:HE2	1.60	0.82
1:F:97:LEU:HD23	1:F:97:LEU:N	1.94	0.82
1:A:350:GLU:HB2	1:A:353:LYS:HE2	1.60	0.82
1:D:97:LEU:N	1:D:97:LEU:HD23	1.93	0.82
1:B:350:GLU:HB2	1:B:353:LYS:HE2	1.60	0.82
1:A:353:LYS:CE	1:A:354:ARG:NH1	2.41	0.82
1:A:97:LEU:HD23	1:A:97:LEU:N	1.93	0.82
1:E:340:GLU:OE2	1:E:344:MET:HE3	1.79	0.82
1:B:191:ASN:O	1:B:195:VAL:HG23	1.79	0.81
1:C:97:LEU:HD23	1:C:97:LEU:N	1.93	0.81
1:D:340:GLU:OE2	1:D:344:MET:HE3	1.81	0.81
1:B:340:GLU:OE2	1:B:344:MET:CE	2.29	0.81
1:E:350:GLU:HB2	1:E:353:LYS:HE2	1.60	0.81
1:A:340:GLU:OE2	1:A:344:MET:CE	2.29	0.81
1:B:90:ILE:HD12	1:B:127:MET:HE1	1.62	0.80
1:C:340:GLU:OE2	1:C:344:MET:CE	2.29	0.80
1:F:340:GLU:OE2	1:F:344:MET:CE	2.29	0.80
1:B:73:LEU:CD2	1:B:125:ARG:HD2	2.12	0.80
1:A:73:LEU:CD2	1:A:125:ARG:HD2	2.12	0.80
1:C:90:ILE:HD12	1:C:127:MET:HE1	1.64	0.80
1:E:162:ILE:HD13	1:E:223:VAL:HG22	1.64	0.80
1:C:73:LEU:CD2	1:C:125:ARG:HD2	2.12	0.80
1:F:163:ARG:HH21	1:F:221:ALA:HB3	1.47	0.80
1:E:150:LEU:HA	1:E:153:GLN:HG2	1.64	0.80
1:D:340:GLU:OE2	1:D:344:MET:CE	2.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:OE2	1:B:344:MET:HE3	1.80	0.80
1:E:73:LEU:CD2	1:E:125:ARG:HD2	2.12	0.80
1:F:150:LEU:HA	1:F:153:GLN:HG2	1.64	0.79
1:F:73:LEU:CD2	1:F:125:ARG:HD2	2.12	0.79
1:D:90:ILE:HD12	1:D:127:MET:HE1	1.62	0.79
1:E:73:LEU:HD21	1:E:125:ARG:HD2	1.64	0.79
1:F:73:LEU:HD21	1:F:125:ARG:HD2	1.64	0.79
1:F:342:GLY:O	1:F:346:VAL:HG23	1.83	0.79
1:A:342:GLY:O	1:A:346:VAL:HG23	1.83	0.79
1:B:163:ARG:HH21	1:B:221:ALA:HB3	1.47	0.79
1:D:73:LEU:CD2	1:D:125:ARG:HD2	2.12	0.79
1:A:162:ILE:HD13	1:A:223:VAL:HG22	1.64	0.79
1:C:73:LEU:HD21	1:C:125:ARG:HD2	1.64	0.79
1:C:342:GLY:O	1:C:346:VAL:HG23	1.83	0.79
1:A:340:GLU:OE2	1:A:344:MET:HE3	1.82	0.79
1:E:163:ARG:HH21	1:E:221:ALA:HB3	1.47	0.79
1:A:150:LEU:HA	1:A:153:GLN:HG2	1.64	0.79
1:B:344:MET:O	1:B:347:GLN:HG2	1.83	0.79
1:E:340:GLU:OE2	1:E:344:MET:CE	2.29	0.79
1:C:162:ILE:HD13	1:C:223:VAL:HG22	1.64	0.79
1:C:344:MET:O	1:C:347:GLN:HG2	1.83	0.79
1:F:350:GLU:O	1:F:353:LYS:CG	2.31	0.78
1:B:162:ILE:HD13	1:B:223:VAL:HG22	1.64	0.78
1:B:353:LYS:CE	1:B:354:ARG:HH12	1.96	0.78
1:E:342:GLY:O	1:E:346:VAL:HG23	1.83	0.78
1:C:150:LEU:HA	1:C:153:GLN:HG2	1.65	0.78
1:F:353:LYS:CE	1:F:354:ARG:HH12	1.96	0.78
1:B:350:GLU:O	1:B:353:LYS:CG	2.31	0.78
1:D:73:LEU:HD21	1:D:125:ARG:HD2	1.64	0.78
1:B:73:LEU:HD21	1:B:125:ARG:HD2	1.64	0.78
1:D:163:ARG:HH21	1:D:221:ALA:HB3	1.47	0.78
1:F:344:MET:O	1:F:347:GLN:HG2	1.83	0.78
1:A:73:LEU:HD21	1:A:125:ARG:HD2	1.64	0.78
1:E:344:MET:O	1:E:347:GLN:HG2	1.83	0.78
1:F:90:ILE:HD12	1:F:127:MET:HE1	1.66	0.78
1:F:340:GLU:OE2	1:F:344:MET:HE3	1.84	0.78
1:C:163:ARG:HH21	1:C:221:ALA:HB3	1.47	0.78
1:A:163:ARG:HH21	1:A:221:ALA:HB3	1.47	0.78
1:B:150:LEU:HA	1:B:153:GLN:HG2	1.65	0.78
1:E:350:GLU:O	1:E:353:LYS:CG	2.31	0.78
1:C:350:GLU:O	1:C:353:LYS:CG	2.31	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLY:O	1:B:346:VAL:HG23	1.83	0.78
1:D:350:GLU:O	1:D:353:LYS:CG	2.31	0.78
1:A:344:MET:O	1:A:347:GLN:HG2	1.83	0.78
1:E:90:ILE:HD12	1:E:127:MET:HE1	1.66	0.78
1:D:162:ILE:HD13	1:D:223:VAL:HG22	1.64	0.77
1:D:342:GLY:O	1:D:346:VAL:HG23	1.83	0.77
1:D:344:MET:O	1:D:347:GLN:HG2	1.83	0.77
1:F:162:ILE:HD13	1:F:223:VAL:HG22	1.64	0.77
1:D:150:LEU:HA	1:D:153:GLN:HG2	1.64	0.77
1:B:159:ALA:HA	1:B:162:ILE:HG12	1.67	0.77
1:E:244:ARG:HG2	1:E:244:ARG:O	1.85	0.77
1:D:244:ARG:O	1:D:244:ARG:HG2	1.85	0.77
1:D:159:ALA:HA	1:D:162:ILE:HG12	1.67	0.77
1:C:353:LYS:CE	1:C:354:ARG:HH12	1.96	0.77
1:A:146:GLU:HA	1:A:149:LYS:NZ	2.00	0.76
1:D:146:GLU:HA	1:D:149:LYS:NZ	2.00	0.76
1:E:146:GLU:HA	1:E:149:LYS:NZ	2.00	0.76
1:A:350:GLU:O	1:A:353:LYS:CG	2.31	0.76
1:A:244:ARG:O	1:A:244:ARG:HG2	1.85	0.76
1:F:244:ARG:HG2	1:F:244:ARG:O	1.85	0.76
1:B:234:THR:HA	1:B:238:PRO:HG2	1.67	0.76
1:D:234:THR:HA	1:D:238:PRO:HG2	1.67	0.76
1:E:159:ALA:HA	1:E:162:ILE:HG12	1.67	0.76
1:E:353:LYS:CE	1:E:354:ARG:HH12	1.96	0.76
1:A:353:LYS:CE	1:A:354:ARG:HH12	1.97	0.76
1:C:146:GLU:HA	1:C:149:LYS:NZ	2.00	0.76
1:D:353:LYS:CE	1:D:354:ARG:HH12	1.96	0.76
1:D:159:ALA:O	1:D:162:ILE:CG1	2.34	0.76
1:C:159:ALA:HA	1:C:162:ILE:HG12	1.67	0.76
1:F:73:LEU:HD21	1:F:125:ARG:CG	2.16	0.76
1:B:162:ILE:CD1	1:B:223:VAL:CG2	2.62	0.76
1:B:146:GLU:HA	1:B:149:LYS:NZ	2.00	0.76
1:B:73:LEU:HD21	1:B:125:ARG:CG	2.16	0.76
1:A:174:ASP:O	1:A:175:LEU:HG	1.86	0.76
1:C:234:THR:HA	1:C:238:PRO:HG2	1.67	0.76
1:A:162:ILE:CD1	1:A:223:VAL:CG2	2.62	0.75
1:B:174:ASP:O	1:B:175:LEU:HG	1.86	0.75
1:E:159:ALA:O	1:E:162:ILE:CG1	2.34	0.75
1:F:159:ALA:HA	1:F:162:ILE:HG12	1.67	0.75
1:D:73:LEU:HD21	1:D:125:ARG:CG	2.16	0.75
1:B:244:ARG:HG2	1:B:244:ARG:O	1.85	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:ASP:O	1:F:175:LEU:HG	1.87	0.75
1:A:159:ALA:HA	1:A:162:ILE:HG12	1.67	0.75
1:F:347:GLN:O	1:F:350:GLU:CG	2.34	0.75
1:C:347:GLN:O	1:C:350:GLU:CG	2.34	0.75
1:A:90:ILE:HD12	1:A:127:MET:HE1	1.67	0.75
1:D:174:ASP:O	1:D:175:LEU:HG	1.87	0.75
1:C:244:ARG:HG2	1:C:244:ARG:O	1.85	0.75
1:E:174:ASP:O	1:E:175:LEU:HG	1.86	0.75
1:C:162:ILE:CD1	1:C:223:VAL:CG2	2.62	0.75
1:A:159:ALA:O	1:A:162:ILE:CG1	2.34	0.75
1:C:73:LEU:HD21	1:C:125:ARG:CG	2.16	0.75
1:A:234:THR:HA	1:A:238:PRO:HG2	1.67	0.75
1:E:73:LEU:HD21	1:E:125:ARG:CG	2.16	0.75
1:E:234:THR:HA	1:E:238:PRO:HG2	1.67	0.75
1:B:159:ALA:O	1:B:162:ILE:CG1	2.34	0.75
1:F:159:ALA:O	1:F:162:ILE:CG1	2.34	0.75
1:F:134:MET:CE	1:F:150:LEU:CD2	2.65	0.74
1:D:134:MET:CE	1:D:150:LEU:CD2	2.65	0.74
1:C:340:GLU:OE2	1:C:344:MET:HE3	1.87	0.74
1:C:159:ALA:O	1:C:162:ILE:CG1	2.34	0.74
1:F:146:GLU:HA	1:F:149:LYS:NZ	2.00	0.74
1:B:347:GLN:O	1:B:350:GLU:CG	2.35	0.74
1:B:134:MET:CE	1:B:150:LEU:CD2	2.65	0.74
1:C:174:ASP:O	1:C:175:LEU:HG	1.87	0.74
1:F:234:THR:HA	1:F:238:PRO:HG2	1.67	0.74
1:D:347:GLN:O	1:D:350:GLU:CG	2.35	0.74
1:E:347:GLN:O	1:E:350:GLU:CG	2.35	0.74
1:A:347:GLN:O	1:A:350:GLU:CG	2.35	0.74
1:A:73:LEU:HD21	1:A:125:ARG:CG	2.16	0.74
1:F:162:ILE:CD1	1:F:223:VAL:CG2	2.62	0.74
1:E:134:MET:CE	1:E:150:LEU:CD2	2.65	0.74
1:D:73:LEU:HD21	1:D:125:ARG:HG3	1.70	0.74
1:C:134:MET:CE	1:C:150:LEU:CD2	2.65	0.73
1:F:73:LEU:HD21	1:F:125:ARG:HG3	1.70	0.73
1:A:134:MET:CE	1:A:150:LEU:CD2	2.65	0.73
1:C:140:GLU:CG	1:D:193:GLN:HG2	2.18	0.73
1:A:193:GLN:HG2	1:F:140:GLU:CG	2.18	0.73
1:E:138:GLU:O	1:E:146:GLU:CD	2.28	0.72
1:B:141:SER:HB2	1:C:194:MET:SD	2.29	0.72
1:B:109:TRP:HE1	1:B:247:LYS:CG	1.93	0.72
1:F:138:GLU:O	1:F:146:GLU:CD	2.28	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:SER:HB2	1:F:194:MET:SD	2.29	0.72
1:C:134:MET:HE3	1:C:150:LEU:CD2	2.20	0.72
1:B:138:GLU:O	1:B:146:GLU:CD	2.28	0.72
1:C:73:LEU:HD21	1:C:125:ARG:HG3	1.70	0.72
1:B:73:LEU:HD21	1:B:125:ARG:HG3	1.70	0.72
1:F:105:ILE:HD13	1:F:227:VAL:HG23	1.71	0.72
1:A:105:ILE:HD13	1:A:227:VAL:HG23	1.71	0.72
1:E:159:ALA:O	1:E:162:ILE:HG13	1.90	0.72
1:A:159:ALA:O	1:A:162:ILE:HG13	1.90	0.72
1:D:350:GLU:HA	1:D:353:LYS:CE	2.20	0.72
1:A:73:LEU:HD21	1:A:125:ARG:HG3	1.70	0.72
1:C:105:ILE:HD13	1:C:227:VAL:HG23	1.71	0.72
1:C:138:GLU:O	1:C:146:GLU:CD	2.28	0.71
1:A:150:LEU:HA	1:A:153:GLN:CG	2.20	0.71
1:F:350:GLU:HA	1:F:353:LYS:CE	2.20	0.71
1:E:105:ILE:HD13	1:E:227:VAL:HG23	1.71	0.71
1:A:138:GLU:O	1:A:146:GLU:CD	2.28	0.71
1:D:105:ILE:HD13	1:D:227:VAL:HG23	1.71	0.71
1:F:315:GLY:O	1:F:319:LEU:HB2	1.90	0.71
1:B:315:GLY:O	1:B:319:LEU:HB2	1.90	0.71
1:D:159:ALA:O	1:D:162:ILE:HG13	1.90	0.71
1:A:315:GLY:O	1:A:319:LEU:HB2	1.90	0.71
1:E:73:LEU:HD21	1:E:125:ARG:HG3	1.70	0.71
1:D:138:GLU:O	1:D:146:GLU:CD	2.28	0.71
1:E:150:LEU:HA	1:E:153:GLN:CG	2.20	0.71
1:E:350:GLU:HA	1:E:353:LYS:CE	2.20	0.71
1:B:150:LEU:HA	1:B:153:GLN:CG	2.21	0.71
1:A:193:GLN:CG	1:F:140:GLU:CD	2.58	0.71
1:C:159:ALA:O	1:C:162:ILE:HG13	1.90	0.71
1:C:315:GLY:O	1:C:319:LEU:HB2	1.90	0.71
1:D:150:LEU:HA	1:D:153:GLN:CG	2.20	0.71
1:F:150:LEU:HA	1:F:153:GLN:CG	2.20	0.71
1:B:105:ILE:HD13	1:B:227:VAL:HG23	1.71	0.71
1:B:159:ALA:O	1:B:162:ILE:HG13	1.90	0.71
1:B:350:GLU:HA	1:B:353:LYS:CE	2.20	0.71
1:C:150:LEU:HA	1:C:153:GLN:CG	2.20	0.70
1:C:350:GLU:HA	1:C:353:LYS:CE	2.20	0.70
1:C:162:ILE:HG23	1:C:168:CYS:HB3	1.73	0.70
1:F:159:ALA:O	1:F:162:ILE:HG13	1.90	0.70
1:C:97:LEU:H	1:C:97:LEU:CD2	2.03	0.70
1:D:315:GLY:O	1:D:319:LEU:HB2	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:GLY:O	1:E:319:LEU:HB2	1.90	0.70
1:D:162:ILE:HG23	1:D:168:CYS:HB3	1.73	0.70
1:B:162:ILE:HG23	1:B:168:CYS:HB3	1.73	0.70
1:A:350:GLU:HA	1:A:353:LYS:CE	2.20	0.70
1:A:73:LEU:CD2	1:A:125:ARG:CD	2.70	0.70
1:E:134:MET:HE2	1:E:150:LEU:CD2	2.21	0.70
1:E:162:ILE:HG23	1:E:168:CYS:HB3	1.73	0.69
1:F:97:LEU:CD2	1:F:97:LEU:H	2.03	0.69
1:E:139:LEU:O	1:E:139:LEU:HD23	1.93	0.69
1:F:162:ILE:HG23	1:F:168:CYS:HB3	1.73	0.69
1:C:139:LEU:O	1:C:139:LEU:HD23	1.93	0.69
1:A:139:LEU:O	1:A:139:LEU:HD23	1.93	0.69
1:C:160:GLU:HA	1:C:163:ARG:CD	2.23	0.69
1:F:139:LEU:HD23	1:F:139:LEU:O	1.93	0.68
1:D:97:LEU:H	1:D:97:LEU:CD2	2.03	0.68
1:D:139:LEU:HD23	1:D:139:LEU:O	1.93	0.68
1:B:73:LEU:CD2	1:B:125:ARG:CD	2.70	0.68
1:A:162:ILE:HG23	1:A:168:CYS:HB3	1.73	0.68
1:F:160:GLU:HA	1:F:163:ARG:CD	2.23	0.68
1:C:163:ARG:HH21	1:C:221:ALA:CB	2.07	0.68
1:B:163:ARG:HH21	1:B:221:ALA:CB	2.07	0.68
1:A:160:GLU:HA	1:A:163:ARG:CD	2.23	0.68
1:C:140:GLU:CD	1:D:193:GLN:CG	2.58	0.68
1:B:122:LEU:O	1:B:125:ARG:HG2	1.94	0.68
1:D:160:GLU:HA	1:D:163:ARG:CD	2.23	0.68
1:C:350:GLU:C	1:C:353:LYS:HG2	2.14	0.68
1:E:160:GLU:HA	1:E:163:ARG:CD	2.23	0.68
1:E:97:LEU:CD2	1:E:97:LEU:H	2.03	0.68
1:A:350:GLU:C	1:A:353:LYS:HG2	2.14	0.68
1:B:159:ALA:O	1:B:163:ARG:HG2	1.94	0.67
1:A:163:ARG:HH21	1:A:221:ALA:CB	2.07	0.67
1:B:134:MET:HE2	1:B:150:LEU:CD2	2.24	0.67
1:F:350:GLU:C	1:F:353:LYS:HG2	2.14	0.67
1:F:159:ALA:O	1:F:163:ARG:HG2	1.94	0.67
1:F:122:LEU:O	1:F:125:ARG:HG2	1.94	0.67
1:D:149:LYS:HG3	1:D:150:LEU:N	2.10	0.67
1:F:150:LEU:O	1:F:154:ARG:HG2	1.94	0.67
1:E:122:LEU:O	1:E:125:ARG:HG2	1.94	0.67
1:D:122:LEU:O	1:D:125:ARG:HG2	1.94	0.67
1:C:79:ALA:H	1:C:119:GLN:HE21	1.43	0.67
1:F:163:ARG:HH21	1:F:221:ALA:CB	2.07	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:ALA:O	1:D:163:ARG:HG2	1.93	0.67
1:A:122:LEU:O	1:A:125:ARG:HG2	1.94	0.67
1:F:79:ALA:H	1:F:119:GLN:HE21	1.42	0.67
1:B:300:ASP:HA	1:B:303:ARG:NH1	2.10	0.67
1:E:159:ALA:O	1:E:163:ARG:HG2	1.94	0.67
1:E:162:ILE:CD1	1:E:223:VAL:CG2	2.62	0.67
1:D:163:ARG:HH21	1:D:221:ALA:CB	2.07	0.67
1:C:159:ALA:O	1:C:163:ARG:HG2	1.94	0.67
1:A:145:GLY:C	1:A:149:LYS:HE3	2.15	0.67
1:E:149:LYS:HG3	1:E:150:LEU:N	2.10	0.67
1:A:265:PHE:HB3	1:A:270:VAL:HG21	1.77	0.67
1:D:150:LEU:O	1:D:154:ARG:HG2	1.95	0.67
1:E:134:MET:HE2	1:E:150:LEU:HD22	1.75	0.67
1:B:139:LEU:O	1:B:139:LEU:HD23	1.93	0.67
1:B:149:LYS:HG3	1:B:150:LEU:N	2.10	0.67
1:A:300:ASP:HA	1:A:303:ARG:NH1	2.10	0.67
1:B:265:PHE:HB3	1:B:270:VAL:HG21	1.77	0.67
1:B:79:ALA:H	1:B:119:GLN:HE21	1.43	0.67
1:A:159:ALA:O	1:A:163:ARG:HG2	1.94	0.67
1:D:350:GLU:C	1:D:353:LYS:HG2	2.14	0.67
1:B:160:GLU:HA	1:B:163:ARG:CD	2.23	0.67
1:E:145:GLY:C	1:E:149:LYS:HE3	2.15	0.67
1:F:145:GLY:C	1:F:149:LYS:HE3	2.15	0.67
1:B:350:GLU:C	1:B:353:LYS:HG2	2.14	0.67
1:D:300:ASP:HA	1:D:303:ARG:NH1	2.10	0.67
1:E:163:ARG:HH21	1:E:221:ALA:CB	2.07	0.66
1:D:162:ILE:CD1	1:D:223:VAL:CG2	2.62	0.66
1:A:150:LEU:O	1:A:154:ARG:HG2	1.94	0.66
1:F:265:PHE:HB3	1:F:270:VAL:HG21	1.77	0.66
1:E:350:GLU:C	1:E:353:LYS:HG2	2.14	0.66
1:D:79:ALA:H	1:D:119:GLN:HE21	1.43	0.66
1:A:149:LYS:HG3	1:A:150:LEU:N	2.10	0.66
1:A:97:LEU:CD2	1:A:97:LEU:N	2.59	0.66
1:C:300:ASP:HA	1:C:303:ARG:NH1	2.10	0.66
1:C:163:ARG:NH2	1:C:220:ASN:O	2.29	0.66
1:C:149:LYS:HG3	1:C:150:LEU:N	2.10	0.66
1:B:150:LEU:O	1:B:154:ARG:HG2	1.94	0.66
1:E:79:ALA:H	1:E:119:GLN:HE21	1.42	0.66
1:E:150:LEU:O	1:E:154:ARG:HG2	1.94	0.66
1:C:122:LEU:O	1:C:125:ARG:HG2	1.94	0.66
1:F:149:LYS:HG3	1:F:150:LEU:N	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:GLY:C	1:B:149:LYS:HE3	2.15	0.66
1:C:265:PHE:HB3	1:C:270:VAL:HG21	1.77	0.66
1:E:265:PHE:HB3	1:E:270:VAL:HG21	1.77	0.66
1:F:300:ASP:HA	1:F:303:ARG:NH1	2.10	0.66
1:E:97:LEU:CD2	1:E:97:LEU:N	2.59	0.66
1:C:73:LEU:CD2	1:C:125:ARG:CD	2.70	0.66
1:E:159:ALA:O	1:E:162:ILE:HG12	1.96	0.66
1:C:145:GLY:C	1:C:149:LYS:HE3	2.15	0.66
1:C:146:GLU:HA	1:C:149:LYS:HZ2	1.58	0.66
1:D:97:LEU:N	1:D:97:LEU:CD2	2.59	0.66
1:A:193:GLN:CB	1:F:140:GLU:OE1	2.44	0.66
1:E:163:ARG:NH2	1:E:220:ASN:O	2.29	0.65
1:C:139:LEU:HD11	1:C:195:VAL:HG13	1.78	0.65
1:F:163:ARG:NH2	1:F:220:ASN:O	2.29	0.65
1:A:134:MET:HE2	1:A:150:LEU:CD2	2.26	0.65
1:B:163:ARG:NH2	1:B:220:ASN:O	2.29	0.65
1:A:163:ARG:NH2	1:A:220:ASN:O	2.29	0.65
1:C:150:LEU:O	1:C:154:ARG:HG2	1.95	0.65
1:D:134:MET:HE1	1:D:150:LEU:CD2	2.26	0.65
1:E:139:LEU:HD11	1:E:195:VAL:HG13	1.78	0.65
1:B:134:MET:HE2	1:B:150:LEU:HD22	1.78	0.65
1:B:134:MET:CE	1:B:150:LEU:HD22	2.27	0.65
1:B:139:LEU:HD11	1:B:195:VAL:HG13	1.78	0.65
1:A:86:LEU:HD11	1:A:226:ILE:HG12	1.78	0.65
1:D:163:ARG:NH2	1:D:220:ASN:O	2.29	0.65
1:D:145:GLY:C	1:D:149:LYS:HE3	2.15	0.65
1:F:159:ALA:O	1:F:162:ILE:HG12	1.96	0.65
1:E:300:ASP:HA	1:E:303:ARG:NH1	2.10	0.65
1:D:265:PHE:HB3	1:D:270:VAL:HG21	1.77	0.65
1:C:140:GLU:OE1	1:D:193:GLN:CB	2.44	0.65
1:A:73:LEU:CD2	1:A:125:ARG:HG3	2.27	0.65
1:A:139:LEU:HD11	1:A:195:VAL:HG13	1.78	0.65
1:C:73:LEU:CD2	1:C:125:ARG:HG3	2.27	0.65
1:A:79:ALA:H	1:A:119:GLN:HE21	1.43	0.65
1:F:86:LEU:HD11	1:F:226:ILE:HG12	1.78	0.65
1:C:86:LEU:HD11	1:C:226:ILE:HG12	1.79	0.65
1:F:139:LEU:HD11	1:F:195:VAL:HG13	1.78	0.65
1:A:134:MET:CE	1:A:150:LEU:HD22	2.27	0.64
1:B:159:ALA:O	1:B:162:ILE:HG12	1.96	0.64
1:A:134:MET:HE2	1:A:150:LEU:HD22	1.80	0.64
1:F:134:MET:HE2	1:F:150:LEU:CD2	2.25	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:MET:CE	1:F:150:LEU:HD22	2.27	0.64
1:B:97:LEU:N	1:B:97:LEU:CD2	2.59	0.64
1:E:73:LEU:CD2	1:E:125:ARG:HG3	2.27	0.64
1:F:73:LEU:CD2	1:F:125:ARG:HG3	2.27	0.64
1:B:73:LEU:CD2	1:B:125:ARG:HG3	2.27	0.64
1:E:86:LEU:HD11	1:E:226:ILE:HG12	1.79	0.64
1:C:159:ALA:O	1:C:162:ILE:HG12	1.97	0.64
1:D:86:LEU:HD11	1:D:226:ILE:HG12	1.78	0.64
1:A:253:THR:HG22	1:A:254:ARG:N	2.13	0.64
1:A:159:ALA:O	1:A:162:ILE:HG12	1.96	0.64
1:D:139:LEU:HD11	1:D:195:VAL:HG13	1.79	0.64
1:D:159:ALA:O	1:D:162:ILE:HG12	1.97	0.64
1:E:141:SER:CB	1:F:194:MET:SD	2.86	0.64
1:D:253:THR:HG22	1:D:254:ARG:N	2.13	0.64
1:F:253:THR:HG22	1:F:254:ARG:N	2.13	0.64
1:D:134:MET:CE	1:D:150:LEU:HD22	2.27	0.64
1:E:253:THR:HG22	1:E:254:ARG:N	2.13	0.64
1:B:253:THR:HG22	1:B:254:ARG:N	2.13	0.63
1:A:306:VAL:HA	1:A:314:ILE:HD11	1.81	0.63
1:C:97:LEU:N	1:C:97:LEU:CD2	2.59	0.63
1:F:97:LEU:CD2	1:F:97:LEU:N	2.59	0.63
1:C:134:MET:CE	1:C:150:LEU:HD22	2.27	0.63
1:E:134:MET:CE	1:E:150:LEU:HD22	2.27	0.63
1:D:73:LEU:CD2	1:D:125:ARG:HG3	2.27	0.63
1:B:86:LEU:HD11	1:B:226:ILE:HG12	1.79	0.63
1:B:306:VAL:HA	1:B:314:ILE:HD11	1.81	0.63
1:F:134:MET:HE2	1:F:150:LEU:HD22	1.80	0.63
1:C:68:ASN:OD1	1:C:69:LEU:N	2.32	0.63
1:E:159:ALA:HA	1:E:162:ILE:CG1	2.29	0.63
1:E:205:ASN:ND2	1:E:207:THR:CG2	2.62	0.63
1:F:205:ASN:ND2	1:F:207:THR:CG2	2.62	0.63
1:A:159:ALA:HA	1:A:162:ILE:CG1	2.29	0.63
1:C:253:THR:HG22	1:C:254:ARG:N	2.13	0.63
1:F:159:ALA:HA	1:F:162:ILE:CG1	2.29	0.62
1:B:141:SER:CB	1:C:194:MET:SD	2.86	0.62
1:F:68:ASN:OD1	1:F:69:LEU:N	2.32	0.62
1:D:205:ASN:ND2	1:D:207:THR:CG2	2.62	0.62
1:C:306:VAL:HA	1:C:314:ILE:HD11	1.81	0.62
1:D:68:ASN:OD1	1:D:69:LEU:N	2.32	0.62
1:A:68:ASN:OD1	1:A:69:LEU:N	2.32	0.62
1:C:205:ASN:ND2	1:C:207:THR:CG2	2.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:ASN:OD1	1:F:192:ASN:N	2.31	0.62
1:D:306:VAL:HA	1:D:314:ILE:HD11	1.81	0.62
1:E:306:VAL:HA	1:E:314:ILE:HD11	1.81	0.62
1:B:205:ASN:ND2	1:B:207:THR:CG2	2.62	0.62
1:A:205:ASN:ND2	1:A:207:THR:CG2	2.62	0.62
1:C:340:GLU:OE2	1:C:344:MET:HE1	1.98	0.62
1:B:68:ASN:OD1	1:B:69:LEU:N	2.32	0.62
1:E:68:ASN:OD1	1:E:69:LEU:N	2.32	0.61
1:D:159:ALA:HA	1:D:162:ILE:CG1	2.29	0.61
1:B:159:ALA:HA	1:B:162:ILE:CG1	2.29	0.61
1:C:134:MET:HE3	1:C:150:LEU:HD23	1.82	0.61
1:F:152:ARG:O	1:F:156:ARG:HG2	2.01	0.61
1:F:340:GLU:OE2	1:F:344:MET:HE1	2.01	0.61
1:F:306:VAL:HA	1:F:314:ILE:HD11	1.81	0.61
1:B:152:ARG:O	1:B:156:ARG:HG2	2.00	0.61
1:E:146:GLU:HA	1:E:149:LYS:HZ2	1.64	0.61
1:C:159:ALA:HA	1:C:162:ILE:CG1	2.29	0.61
1:A:149:LYS:HG3	1:A:150:LEU:H	1.66	0.61
1:D:161:ILE:O	1:D:164:LYS:CG	2.47	0.61
1:E:152:ARG:O	1:E:156:ARG:HG2	2.01	0.61
1:F:105:ILE:HG13	1:F:245:MET:HG3	1.83	0.61
1:C:152:ARG:O	1:C:156:ARG:HG2	2.00	0.61
1:E:191:ASN:OD1	1:E:192:ASN:N	2.31	0.61
1:F:132:ILE:HG23	1:F:154:ARG:NH2	2.16	0.61
1:C:159:ALA:CA	1:C:162:ILE:HG12	2.31	0.60
1:A:159:ALA:HA	1:A:162:ILE:CD1	2.31	0.60
1:A:146:GLU:HA	1:A:149:LYS:HZ2	1.64	0.60
1:F:159:ALA:CA	1:F:162:ILE:HG12	2.31	0.60
1:C:132:ILE:HG23	1:C:154:ARG:NH2	2.16	0.60
1:D:149:LYS:HG3	1:D:150:LEU:H	1.66	0.60
1:F:146:GLU:HA	1:F:149:LYS:HZ2	1.67	0.60
1:B:149:LYS:HG3	1:B:150:LEU:H	1.66	0.60
1:D:152:ARG:O	1:D:156:ARG:HG2	2.01	0.60
1:B:159:ALA:CA	1:B:162:ILE:HG12	2.30	0.60
1:E:159:ALA:HA	1:E:162:ILE:CD1	2.32	0.60
1:F:159:ALA:HA	1:F:162:ILE:CD1	2.32	0.60
1:A:193:GLN:HG2	1:F:140:GLU:OE1	2.01	0.60
1:A:152:ARG:O	1:A:156:ARG:HG2	2.00	0.60
1:D:159:ALA:CA	1:D:162:ILE:HG12	2.31	0.60
1:A:132:ILE:HG23	1:A:154:ARG:NH2	2.16	0.60
1:E:159:ALA:CA	1:E:162:ILE:HG12	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ALA:CA	1:A:162:ILE:HG12	2.30	0.60
1:C:161:ILE:O	1:C:164:LYS:CG	2.47	0.60
1:D:73:LEU:O	1:D:76:PHE:HB2	2.02	0.60
1:A:73:LEU:O	1:A:76:PHE:HB2	2.02	0.60
1:B:159:ALA:HA	1:B:162:ILE:CD1	2.32	0.60
1:C:159:ALA:HA	1:C:162:ILE:CD1	2.31	0.60
1:E:149:LYS:HG3	1:E:150:LEU:H	1.66	0.60
1:B:105:ILE:HG13	1:B:245:MET:HG3	1.83	0.60
1:E:159:ALA:HB1	1:E:221:ALA:HB3	1.84	0.60
1:A:159:ALA:HB1	1:A:221:ALA:HB3	1.84	0.60
1:F:73:LEU:O	1:F:76:PHE:HB2	2.02	0.60
1:B:73:LEU:O	1:B:76:PHE:HB2	2.02	0.60
1:D:132:ILE:HG23	1:D:154:ARG:NH2	2.16	0.59
1:D:105:ILE:HG13	1:D:245:MET:HG3	1.83	0.59
1:D:159:ALA:HB1	1:D:221:ALA:HB3	1.84	0.59
1:B:109:TRP:CE2	1:B:247:LYS:HD2	2.38	0.59
1:E:132:ILE:HG23	1:E:154:ARG:NH2	2.16	0.59
1:B:132:ILE:HG23	1:B:154:ARG:NH2	2.16	0.59
1:D:159:ALA:HA	1:D:162:ILE:CD1	2.31	0.59
1:D:109:TRP:CE2	1:D:247:LYS:HD2	2.38	0.59
1:F:149:LYS:HG3	1:F:150:LEU:H	1.66	0.59
1:F:159:ALA:HB1	1:F:221:ALA:HB3	1.84	0.59
1:E:105:ILE:HG13	1:E:245:MET:HG3	1.84	0.59
1:C:150:LEU:HA	1:C:153:GLN:CD	2.23	0.59
1:C:105:ILE:HG13	1:C:245:MET:HG3	1.83	0.59
1:A:109:TRP:CE2	1:A:247:LYS:HD2	2.38	0.59
1:A:196:ASN:O	1:A:199:LEU:HB2	2.03	0.59
1:B:159:ALA:HB1	1:B:221:ALA:HB3	1.84	0.59
1:D:241:ARG:CZ	1:D:247:LYS:HD3	2.33	0.59
1:C:149:LYS:HG3	1:C:150:LEU:H	1.66	0.59
1:C:109:TRP:CE2	1:C:247:LYS:HD2	2.38	0.59
1:F:347:GLN:C	1:F:350:GLU:HG2	2.23	0.59
1:B:150:LEU:HA	1:B:153:GLN:CD	2.23	0.59
1:C:73:LEU:O	1:C:76:PHE:HB2	2.02	0.59
1:B:196:ASN:O	1:B:199:LEU:HB2	2.03	0.59
1:D:150:LEU:HA	1:D:153:GLN:CD	2.23	0.58
1:A:340:GLU:OE2	1:A:344:MET:HE1	2.02	0.58
1:C:140:GLU:OE1	1:D:193:GLN:HG2	2.01	0.58
1:B:105:ILE:CD1	1:B:227:VAL:HG23	2.33	0.58
1:B:161:ILE:O	1:B:164:LYS:CG	2.47	0.58
1:E:347:GLN:C	1:E:350:GLU:HG2	2.23	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:TRP:CE2	1:F:247:LYS:HD2	2.38	0.58
1:D:146:GLU:HA	1:D:149:LYS:HZ2	1.68	0.58
1:A:347:GLN:C	1:A:350:GLU:HG2	2.24	0.58
1:A:193:GLN:CG	1:F:140:GLU:OE1	2.52	0.58
1:E:73:LEU:O	1:E:76:PHE:HB2	2.02	0.58
1:F:334:THR:O	1:F:338:LEU:HD23	2.03	0.58
1:A:150:LEU:HA	1:A:153:GLN:CD	2.23	0.58
1:D:334:THR:O	1:D:338:LEU:HD23	2.03	0.58
1:B:334:THR:O	1:B:338:LEU:HD23	2.03	0.58
1:A:205:ASN:HB2	1:A:206:PRO:CD	2.31	0.58
1:B:241:ARG:CZ	1:B:247:LYS:HD3	2.33	0.58
1:B:347:GLN:C	1:B:350:GLU:HG2	2.23	0.58
1:A:105:ILE:HG13	1:A:245:MET:HG3	1.83	0.58
1:A:134:MET:HE3	1:A:150:LEU:CD2	2.33	0.58
1:C:159:ALA:HB1	1:C:221:ALA:HB3	1.84	0.58
1:E:109:TRP:CE2	1:E:247:LYS:HD2	2.38	0.58
1:E:105:ILE:CD1	1:E:227:VAL:HG23	2.33	0.58
1:F:196:ASN:O	1:F:199:LEU:HB2	2.03	0.58
1:F:134:MET:HE3	1:F:150:LEU:CD2	2.34	0.58
1:C:347:GLN:C	1:C:350:GLU:HG2	2.23	0.58
1:E:196:ASN:O	1:E:199:LEU:HB2	2.03	0.58
1:E:205:ASN:HB2	1:E:206:PRO:CD	2.31	0.58
1:F:241:ARG:CZ	1:F:247:LYS:HD3	2.33	0.57
1:D:134:MET:HE3	1:D:150:LEU:CD2	2.33	0.57
1:E:150:LEU:HA	1:E:153:GLN:CD	2.23	0.57
1:B:138:GLU:O	1:B:146:GLU:OE2	2.22	0.57
1:D:347:GLN:C	1:D:350:GLU:HG2	2.23	0.57
1:F:199:LEU:O	1:F:202:ILE:HG22	2.04	0.57
1:F:268:ASP:CG	1:F:333:MET:HG3	2.25	0.57
1:A:241:ARG:CZ	1:A:247:LYS:HD3	2.33	0.57
1:A:161:ILE:O	1:A:164:LYS:CG	2.47	0.57
1:F:150:LEU:HA	1:F:153:GLN:CD	2.23	0.57
1:C:105:ILE:CD1	1:C:227:VAL:HG23	2.33	0.57
1:C:138:GLU:O	1:C:146:GLU:OE2	2.23	0.57
1:A:191:ASN:OD1	1:A:192:ASN:N	2.31	0.57
1:E:268:ASP:CG	1:E:333:MET:HG3	2.25	0.57
1:C:241:ARG:CZ	1:C:247:LYS:HD3	2.33	0.57
1:E:241:ARG:CZ	1:E:247:LYS:HD3	2.33	0.57
1:B:199:LEU:O	1:B:202:ILE:HG22	2.04	0.57
1:C:199:LEU:O	1:C:202:ILE:HG22	2.04	0.57
1:D:196:ASN:O	1:D:199:LEU:HB2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ILE:O	1:F:164:LYS:CG	2.47	0.57
1:C:140:GLU:OE1	1:D:193:GLN:CG	2.52	0.57
1:C:196:ASN:O	1:C:199:LEU:HB2	2.03	0.57
1:A:199:LEU:O	1:A:202:ILE:HG22	2.04	0.57
1:D:199:LEU:O	1:D:202:ILE:HG22	2.04	0.57
1:E:334:THR:O	1:E:338:LEU:HD23	2.03	0.57
1:A:88:VAL:O	1:A:92:LYS:HB2	2.05	0.57
1:C:134:MET:HE3	1:C:150:LEU:HD22	1.85	0.57
1:D:340:GLU:OE2	1:D:344:MET:HE1	2.04	0.57
1:F:88:VAL:O	1:F:92:LYS:HB2	2.05	0.57
1:D:268:ASP:CG	1:D:333:MET:HG3	2.24	0.57
1:B:88:VAL:O	1:B:92:LYS:HB2	2.05	0.57
1:E:199:LEU:O	1:E:202:ILE:HG22	2.04	0.57
1:C:334:THR:O	1:C:338:LEU:HD23	2.03	0.57
1:D:162:ILE:HD11	1:D:223:VAL:HG23	1.86	0.57
1:B:132:ILE:HG23	1:B:154:ARG:CZ	2.35	0.57
1:C:140:GLU:HG3	1:D:193:GLN:HG2	1.86	0.57
1:A:334:THR:O	1:A:338:LEU:HD23	2.04	0.57
1:F:150:LEU:CA	1:F:153:GLN:HG2	2.34	0.57
1:F:73:LEU:CD2	1:F:125:ARG:CD	2.70	0.57
1:B:268:ASP:CG	1:B:333:MET:HG3	2.25	0.57
1:F:162:ILE:HD11	1:F:223:VAL:HG23	1.86	0.56
1:E:138:GLU:O	1:E:146:GLU:OE2	2.23	0.56
1:E:161:ILE:O	1:E:164:LYS:CG	2.47	0.56
1:B:150:LEU:CA	1:B:153:GLN:HG2	2.35	0.56
1:D:105:ILE:CD1	1:D:227:VAL:HG23	2.33	0.56
1:A:268:ASP:CG	1:A:333:MET:HG3	2.25	0.56
1:C:268:ASP:CG	1:C:333:MET:HG3	2.25	0.56
1:D:132:ILE:HG23	1:D:154:ARG:CZ	2.35	0.56
1:F:138:GLU:O	1:F:146:GLU:OE2	2.23	0.56
1:F:105:ILE:CD1	1:F:227:VAL:HG23	2.34	0.56
1:E:88:VAL:O	1:E:92:LYS:HB2	2.05	0.56
1:F:205:ASN:HB2	1:F:206:PRO:CD	2.31	0.56
1:C:150:LEU:CA	1:C:153:GLN:HG2	2.34	0.56
1:E:150:LEU:CA	1:E:153:GLN:HG2	2.34	0.56
1:D:88:VAL:O	1:D:92:LYS:HB2	2.05	0.56
1:A:132:ILE:HG23	1:A:154:ARG:CZ	2.36	0.56
1:C:88:VAL:O	1:C:92:LYS:HB2	2.05	0.56
1:B:272:ALA:O	1:B:276:VAL:HG23	2.06	0.56
1:C:73:LEU:HD23	1:C:125:ARG:HD2	1.88	0.56
1:B:73:LEU:HD23	1:B:125:ARG:HD2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HG23	1:C:154:ARG:CZ	2.36	0.56
1:D:138:GLU:O	1:D:146:GLU:OE2	2.23	0.56
1:F:132:ILE:HG23	1:F:154:ARG:CZ	2.35	0.56
1:A:105:ILE:CD1	1:A:227:VAL:HG23	2.33	0.56
1:D:105:ILE:CG1	1:D:245:MET:HG3	2.36	0.56
1:F:162:ILE:HG13	1:F:163:ARG:N	2.21	0.56
1:C:105:ILE:CG1	1:C:245:MET:HG3	2.36	0.56
1:E:272:ALA:O	1:E:276:VAL:HG23	2.06	0.56
1:A:138:GLU:O	1:A:146:GLU:OE2	2.23	0.56
1:E:340:GLU:OE2	1:E:344:MET:HE1	2.05	0.56
1:A:193:GLN:HG2	1:F:140:GLU:HG3	1.86	0.56
1:F:105:ILE:CG1	1:F:245:MET:HG3	2.36	0.56
1:B:162:ILE:HG13	1:B:163:ARG:N	2.21	0.56
1:B:162:ILE:HD11	1:B:223:VAL:HG23	1.86	0.56
1:C:205:ASN:HB2	1:C:206:PRO:CD	2.31	0.56
1:B:340:GLU:OE2	1:B:344:MET:HE1	2.04	0.56
1:A:105:ILE:CG1	1:A:245:MET:HG3	2.36	0.56
1:A:272:ALA:O	1:A:276:VAL:HG23	2.06	0.56
1:F:272:ALA:O	1:F:276:VAL:HG23	2.06	0.56
1:D:134:MET:HE1	1:D:150:LEU:HD23	1.87	0.55
1:B:162:ILE:CG2	1:B:168:CYS:HB3	2.36	0.55
1:E:162:ILE:HG13	1:E:163:ARG:N	2.21	0.55
1:E:132:ILE:HG23	1:E:154:ARG:CZ	2.35	0.55
1:F:161:ILE:HA	1:F:164:LYS:HE3	1.89	0.55
1:B:105:ILE:CG1	1:B:245:MET:HG3	2.36	0.55
1:C:191:ASN:OD1	1:C:192:ASN:N	2.31	0.55
1:E:205:ASN:ND2	1:E:207:THR:HG23	2.22	0.55
1:F:205:ASN:ND2	1:F:207:THR:HG23	2.22	0.55
1:C:162:ILE:HG13	1:C:163:ARG:N	2.21	0.55
1:C:272:ALA:O	1:C:276:VAL:HG23	2.06	0.55
1:D:162:ILE:HG13	1:D:163:ARG:N	2.21	0.55
1:A:205:ASN:ND2	1:A:207:THR:HG23	2.22	0.55
1:E:105:ILE:CG1	1:E:245:MET:HG3	2.36	0.55
1:A:162:ILE:HG13	1:A:163:ARG:N	2.21	0.55
1:D:161:ILE:HA	1:D:164:LYS:HE3	1.89	0.55
1:A:122:LEU:HD12	1:A:125:ARG:HD2	1.89	0.55
1:E:253:THR:O	1:E:257:ARG:HG3	2.06	0.55
1:D:272:ALA:O	1:D:276:VAL:HG23	2.06	0.55
1:E:162:ILE:HD11	1:E:223:VAL:HG23	1.86	0.55
1:C:162:ILE:HD11	1:C:223:VAL:HG23	1.86	0.55
1:A:253:THR:O	1:A:257: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:B:260:VAL:HG11	1:B:287:ILE:HG21	1.89	0.55
1:F:253:THR:O	1:F:257:ARG:HG3	2.07	0.55
1:C:162:ILE:CG2	1:C:168:CYS:HB3	2.36	0.55
1:C:161:ILE:HA	1:C:164:LYS:HE3	1.89	0.55
1:A:150:LEU:CA	1:A:153:GLN:HG2	2.34	0.55
1:D:134:MET:HE3	1:D:150:LEU:HD22	1.87	0.55
1:A:73:LEU:HD23	1:A:125:ARG:HD2	1.88	0.55
1:A:253:THR:HG22	1:A:254:ARG:H	1.71	0.55
1:D:253:THR:O	1:D:257:ARG:HG3	2.07	0.55
1:C:266:ARG:HG2	1:C:267:THR:H	1.72	0.55
1:A:267:THR:HG22	1:A:330:GLN:OE1	2.07	0.55
1:B:205:ASN:ND2	1:B:207:THR:HG23	2.22	0.54
1:E:267:THR:HG22	1:E:330:GLN:OE1	2.07	0.54
1:D:122:LEU:HD12	1:D:125:ARG:HD2	1.89	0.54
1:D:73:LEU:HD23	1:D:125:ARG:HD2	1.88	0.54
1:A:260:VAL:HG11	1:A:287:ILE:HG21	1.89	0.54
1:A:162:ILE:CG2	1:A:168:CYS:HB3	2.36	0.54
1:D:344:MET:O	1:D:347:GLN:CG	2.55	0.54
1:B:253:THR:O	1:B:257:ARG:HG3	2.07	0.54
1:C:267:THR:HG22	1:C:330:GLN:OE1	2.08	0.54
1:F:266:ARG:HG2	1:F:267:THR:H	1.72	0.54
1:D:205:ASN:ND2	1:D:207:THR:HG23	2.22	0.54
1:D:150:LEU:CA	1:D:153:GLN:HG2	2.34	0.54
1:B:134:MET:HE3	1:B:150:LEU:CD2	2.35	0.54
1:E:122:LEU:HD12	1:E:125:ARG:HD2	1.89	0.54
1:B:122:LEU:HD12	1:B:125:ARG:HD2	1.89	0.54
1:C:253:THR:HG22	1:C:254:ARG:H	1.72	0.54
1:D:162:ILE:CG2	1:D:168:CYS:HB3	2.36	0.54
1:A:161:ILE:HA	1:A:164:LYS:HE3	1.89	0.54
1:E:266:ARG:HG2	1:E:267:THR:H	1.72	0.54
1:F:162:ILE:CG2	1:F:168:CYS:HB3	2.36	0.54
1:E:260:VAL:HG11	1:E:287:ILE:HG21	1.89	0.54
1:F:344:MET:O	1:F:347:GLN:CG	2.56	0.54
1:F:350:GLU:HB2	1:F:353:LYS:CE	2.36	0.54
1:B:344:MET:O	1:B:347:GLN:CG	2.55	0.54
1:E:344:MET:O	1:E:347:GLN:CG	2.55	0.54
1:B:266:ARG:HG2	1:B:267:THR:H	1.72	0.54
1:D:253:THR:HG22	1:D:254:ARG:H	1.71	0.54
1:A:266:ARG:HG2	1:A:267:THR:H	1.72	0.54
1:D:267:THR:HG22	1:D:330:GLN:OE1	2.08	0.54
1:E:162:ILE:CG2	1:E:168:CYS:HB3	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD11	1:A:195:VAL:CG1	2.38	0.54
1:B:161:ILE:HA	1:B:164:LYS:HE3	1.89	0.54
1:B:191:ASN:OD1	1:B:192:ASN:N	2.30	0.54
1:E:73:LEU:HD23	1:E:125:ARG:HD2	1.88	0.54
1:D:266:ARG:HG2	1:D:267:THR:H	1.72	0.54
1:C:260:VAL:HG11	1:C:287:ILE:HG21	1.89	0.54
1:C:205:ASN:ND2	1:C:207:THR:HG23	2.22	0.54
1:F:260:VAL:HG11	1:F:287:ILE:HG21	1.89	0.54
1:B:129:ILE:HG23	1:B:168:CYS:HA	1.91	0.53
1:F:139:LEU:HD11	1:F:195:VAL:CG1	2.38	0.53
1:B:139:LEU:HD11	1:B:195:VAL:CG1	2.38	0.53
1:E:73:LEU:CD2	1:E:125:ARG:CG	2.85	0.53
1:C:122:LEU:HD12	1:C:125:ARG:HD2	1.89	0.53
1:D:260:VAL:HG11	1:D:287:ILE:HG21	1.89	0.53
1:A:129:ILE:HG23	1:A:168:CYS:HA	1.91	0.53
1:E:129:ILE:HG23	1:E:168:CYS:HA	1.91	0.53
1:E:161:ILE:HA	1:E:164:LYS:HE3	1.89	0.53
1:B:350:GLU:HA	1:B:353:LYS:CD	2.39	0.53
1:F:122:LEU:HD12	1:F:125:ARG:HD2	1.89	0.53
1:B:267:THR:HG22	1:B:330:GLN:OE1	2.07	0.53
1:C:253:THR:O	1:C:257:ARG:HG3	2.07	0.53
1:B:334:THR:O	1:B:338:LEU:CD2	2.57	0.53
1:F:129:ILE:HG23	1:F:168:CYS:HA	1.90	0.53
1:F:350:GLU:HA	1:F:353:LYS:CD	2.39	0.53
1:F:253:THR:HG22	1:F:254:ARG:H	1.72	0.53
1:E:253:THR:HG22	1:E:254:ARG:H	1.72	0.53
1:D:334:THR:O	1:D:338:LEU:CD2	2.57	0.53
1:E:334:THR:O	1:E:338:LEU:CD2	2.57	0.53
1:D:132:ILE:HD11	1:D:161:ILE:CD1	2.39	0.53
1:D:191:ASN:OD1	1:D:192:ASN:N	2.31	0.53
1:C:350:GLU:HA	1:C:353:LYS:CD	2.39	0.53
1:C:129:ILE:HG23	1:C:168:CYS:HA	1.91	0.53
1:B:253:THR:HG22	1:B:254:ARG:H	1.72	0.53
1:C:132:ILE:HD11	1:C:161:ILE:CD1	2.39	0.53
1:E:134:MET:HE3	1:E:150:LEU:CD2	2.38	0.53
1:D:73:LEU:CD2	1:D:125:ARG:CG	2.86	0.53
1:B:132:ILE:CG2	1:B:154:ARG:CZ	2.87	0.53
1:A:350:GLU:HA	1:A:353:LYS:CD	2.39	0.53
1:F:79:ALA:H	1:F:119:GLN:NE2	2.07	0.53
1:D:129:ILE:HG23	1:D:168:CYS:HA	1.91	0.53
1:B:353:LYS:HE3	1:B:354:ARG:HH12	1.60	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:LEU:CD2	1:E:125:ARG:CD	2.70	0.53
1:C:79:ALA:H	1:C:119:GLN:NE2	2.07	0.53
1:C:132:ILE:CG2	1:C:154:ARG:CZ	2.87	0.53
1:E:139:LEU:HD11	1:E:195:VAL:CG1	2.38	0.53
1:E:132:ILE:CG2	1:E:154:ARG:CZ	2.87	0.53
1:E:79:ALA:H	1:E:119:GLN:NE2	2.07	0.53
1:B:206:PRO:HB2	1:B:220:ASN:CB	2.39	0.52
1:C:139:LEU:HD11	1:C:195:VAL:CG1	2.38	0.52
1:A:132:ILE:HD11	1:A:161:ILE:CD1	2.39	0.52
1:A:132:ILE:CG2	1:A:154:ARG:CZ	2.87	0.52
1:C:344:MET:O	1:C:347:GLN:CG	2.55	0.52
1:D:303:ARG:HG2	1:E:68:ASN:HD21	1.75	0.52
1:D:139:LEU:HD11	1:D:195:VAL:CG1	2.38	0.52
1:C:347:GLN:HA	1:C:350:GLU:CD	2.30	0.52
1:F:73:LEU:HD23	1:F:125:ARG:HD2	1.88	0.52
1:B:79:ALA:H	1:B:119:GLN:NE2	2.07	0.52
1:F:267:THR:HG22	1:F:330:GLN:OE1	2.07	0.52
1:F:347:GLN:HA	1:F:350:GLU:CD	2.30	0.52
1:B:347:GLN:HA	1:B:350:GLU:CD	2.30	0.52
1:E:347:GLN:HA	1:E:350:GLU:CD	2.30	0.52
1:C:73:LEU:CD2	1:C:125:ARG:CG	2.86	0.52
1:F:206:PRO:HB2	1:F:220:ASN:CB	2.39	0.52
1:C:134:MET:HE2	1:C:150:LEU:CD2	2.40	0.52
1:A:139:LEU:HA	1:A:146:GLU:OE2	2.10	0.52
1:F:132:ILE:HD11	1:F:161:ILE:CD1	2.39	0.52
1:A:347:GLN:HA	1:A:350:GLU:CD	2.30	0.52
1:A:203:ALA:HB1	1:A:244:ARG:HD2	1.91	0.52
1:D:132:ILE:CG2	1:D:154:ARG:CZ	2.87	0.52
1:E:206:PRO:HB2	1:E:220:ASN:CB	2.39	0.52
1:A:206:PRO:HB2	1:A:220:ASN:CB	2.39	0.52
1:D:203:ALA:HB1	1:D:244:ARG:HD2	1.91	0.52
1:A:303:ARG:HG2	1:B:68:ASN:HD21	1.75	0.52
1:F:334:THR:O	1:F:338:LEU:CD2	2.57	0.52
1:C:334:THR:O	1:C:338:LEU:CD2	2.57	0.52
1:E:139:LEU:HA	1:E:146:GLU:OE2	2.10	0.52
1:C:206:PRO:HB2	1:C:220:ASN:CB	2.39	0.52
1:B:132:ILE:HD11	1:B:161:ILE:CD1	2.39	0.52
1:F:95:LEU:HB2	1:F:97:LEU:HD22	1.92	0.52
1:E:350:GLU:HA	1:E:353:LYS:CD	2.39	0.52
1:E:203:ALA:HB1	1:E:244:ARG:HD2	1.91	0.52
1:F:203:ALA:HB1	1:F:244:ARG:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:HG2	1:C:68:ASN:HD21	1.75	0.52
1:D:206:PRO:HB2	1:D:220:ASN:CB	2.39	0.52
1:A:68:ASN:HD21	1:F:303:ARG:HG2	1.75	0.52
1:A:334:THR:O	1:A:338:LEU:CD2	2.57	0.52
1:D:139:LEU:HA	1:D:146:GLU:OE2	2.10	0.51
1:E:132:ILE:HD11	1:E:161:ILE:CD1	2.39	0.51
1:D:347:GLN:HA	1:D:350:GLU:CD	2.30	0.51
1:D:350:GLU:HA	1:D:353:LYS:CD	2.39	0.51
1:C:350:GLU:HB2	1:C:353:LYS:CE	2.36	0.51
1:C:203:ALA:HB1	1:C:244:ARG:HD2	1.91	0.51
1:A:162:ILE:HD11	1:A:223:VAL:HG23	1.86	0.51
1:F:132:ILE:CG2	1:F:154:ARG:CZ	2.87	0.51
1:A:282:PHE:CZ	1:A:342:GLY:HA3	2.46	0.51
1:B:95:LEU:HB2	1:B:97:LEU:HD22	1.92	0.51
1:B:139:LEU:HA	1:B:146:GLU:OE2	2.10	0.51
1:E:95:LEU:HB2	1:E:97:LEU:HD22	1.92	0.51
1:F:350:GLU:HB2	1:F:354:ARG:HH12	1.76	0.51
1:A:350:GLU:HB2	1:A:353:LYS:CE	2.36	0.51
1:D:134:MET:CE	1:D:150:LEU:HD23	2.41	0.51
1:D:350:GLU:HB2	1:D:353:LYS:CE	2.36	0.51
1:D:353:LYS:HE2	1:D:354:ARG:NH1	2.25	0.51
1:A:353:LYS:HE2	1:A:354:ARG:NH1	2.25	0.51
1:F:73:LEU:CD2	1:F:125:ARG:CG	2.86	0.51
1:A:79:ALA:H	1:A:119:GLN:NE2	2.07	0.51
1:D:350:GLU:HB2	1:D:354:ARG:HH12	1.75	0.51
1:C:350:GLU:HB2	1:C:354:ARG:HH12	1.76	0.51
1:B:203:ALA:HB1	1:B:244:ARG:HD2	1.92	0.51
1:D:79:ALA:H	1:D:119:GLN:NE2	2.07	0.51
1:C:303:ARG:HG2	1:D:68:ASN:HD21	1.75	0.51
1:D:109:TRP:CZ2	1:D:247:LYS:HD2	2.46	0.51
1:C:139:LEU:HA	1:C:146:GLU:OE2	2.10	0.51
1:C:109:TRP:CZ2	1:C:247:LYS:HD2	2.46	0.51
1:B:350:GLU:HB2	1:B:354:ARG:HH12	1.76	0.51
1:C:347:GLN:HG3	1:C:348:GLU:N	2.26	0.51
1:F:282:PHE:CZ	1:F:342:GLY:HA3	2.46	0.51
1:B:314:ILE:O	1:B:318:LEU:HB2	2.11	0.51
1:E:347:GLN:HG3	1:E:348:GLU:N	2.26	0.51
1:A:350:GLU:HB2	1:A:354:ARG:HH12	1.76	0.51
1:A:95:LEU:HB2	1:A:97:LEU:HD22	1.92	0.51
1:D:73:LEU:CD2	1:D:125:ARG:CD	2.70	0.51
1:C:282:PHE:CZ	1:C:342:GLY:HA3	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:VAL:CG1	1:A:127:MET:HE2	2.40	0.51
1:E:159:ALA:C	1:E:162:ILE:HG12	2.32	0.51
1:D:134:MET:HE1	1:D:150:LEU:HD22	1.90	0.51
1:B:347:GLN:HG3	1:B:348:GLU:N	2.26	0.51
1:A:347:GLN:HG3	1:A:348:GLU:N	2.26	0.51
1:B:282:PHE:CZ	1:B:342:GLY:HA3	2.46	0.51
1:E:123:VAL:CG1	1:E:127:MET:HE2	2.41	0.51
1:E:163:ARG:NH2	1:E:221:ALA:CB	2.74	0.51
1:E:109:TRP:CZ2	1:E:247:LYS:HD2	2.46	0.51
1:F:353:LYS:HE2	1:F:354:ARG:NH1	2.25	0.51
1:F:206:PRO:HB2	1:F:220:ASN:HB3	1.92	0.51
1:A:206:PRO:HB2	1:A:220:ASN:HB3	1.92	0.51
1:A:134:MET:CE	1:A:150:LEU:HD23	2.41	0.51
1:C:95:LEU:HB2	1:C:97:LEU:HD22	1.92	0.51
1:F:139:LEU:HA	1:F:146:GLU:OE2	2.10	0.51
1:F:314:ILE:O	1:F:318:LEU:HB2	2.11	0.51
1:E:206:PRO:HB2	1:E:220:ASN:HB3	1.92	0.50
1:B:350:GLU:HB2	1:B:353:LYS:CE	2.36	0.50
1:C:353:LYS:HE3	1:C:354:ARG:HH12	1.59	0.50
1:D:314:ILE:O	1:D:318:LEU:HB2	2.11	0.50
1:B:134:MET:CE	1:B:150:LEU:HD23	2.41	0.50
1:B:73:LEU:CD2	1:B:125:ARG:CG	2.86	0.50
1:E:282:PHE:CZ	1:E:342:GLY:HA3	2.46	0.50
1:D:244:ARG:CG	1:D:244:ARG:O	2.57	0.50
1:F:105:ILE:HA	1:F:225:ILE:O	2.12	0.50
1:E:303:ARG:HG2	1:F:68:ASN:HD21	1.75	0.50
1:C:314:ILE:O	1:C:318:LEU:HB2	2.11	0.50
1:B:159:ALA:C	1:B:162:ILE:HG12	2.32	0.50
1:D:205:ASN:HB2	1:D:206:PRO:CD	2.31	0.50
1:A:163:ARG:CZ	1:A:220:ASN:O	2.60	0.50
1:B:109:TRP:CZ2	1:B:247:LYS:HD2	2.46	0.50
1:A:344:MET:O	1:A:347:GLN:CG	2.56	0.50
1:F:123:VAL:CG1	1:F:127:MET:HE2	2.41	0.50
1:D:282:PHE:CZ	1:D:342:GLY:HA3	2.46	0.50
1:D:347:GLN:HG3	1:D:348:GLU:N	2.26	0.50
1:D:95:LEU:HB2	1:D:97:LEU:HD22	1.93	0.50
1:F:163:ARG:CZ	1:F:220:ASN:O	2.60	0.50
1:F:347:GLN:HG3	1:F:348:GLU:N	2.26	0.50
1:C:357:LEU:HA	1:C:360:LYS:CG	2.42	0.50
1:E:357:LEU:HA	1:E:360:LYS:CG	2.42	0.50
1:E:353:LYS:HE2	1:E:354:ARG:NH1	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HB	1:C:225:ILE:HB	1.94	0.50
1:F:159:ALA:C	1:F:162:ILE:HG12	2.32	0.50
1:D:163:ARG:NH2	1:D:221:ALA:CB	2.74	0.50
1:A:105:ILE:HA	1:A:225:ILE:O	2.12	0.50
1:E:163:ARG:CZ	1:E:220:ASN:O	2.60	0.50
1:F:109:TRP:CZ2	1:F:247:LYS:HD2	2.46	0.50
1:D:133:MET:O	1:D:154:ARG:NH2	2.43	0.50
1:F:134:MET:HE3	1:F:150:LEU:HD23	1.94	0.50
1:D:105:ILE:HB	1:D:225:ILE:HB	1.94	0.50
1:D:163:ARG:CZ	1:D:220:ASN:O	2.60	0.50
1:A:357:LEU:HA	1:A:360:LYS:CG	2.41	0.50
1:A:105:ILE:HB	1:A:225:ILE:HB	1.94	0.50
1:E:105:ILE:HB	1:E:225:ILE:HB	1.94	0.50
1:A:314:ILE:O	1:A:318:LEU:HB2	2.11	0.50
1:D:159:ALA:C	1:D:162:ILE:HG12	2.32	0.49
1:C:206:PRO:HB2	1:C:220:ASN:HB3	1.93	0.49
1:C:134:MET:HE2	1:C:150:LEU:HD22	1.92	0.49
1:C:139:LEU:CD2	1:C:195:VAL:HG21	2.26	0.49
1:B:357:LEU:HA	1:B:360:LYS:CG	2.42	0.49
1:B:105:ILE:HB	1:B:225:ILE:HB	1.94	0.49
1:A:109:TRP:CZ2	1:A:247:LYS:HD2	2.46	0.49
1:D:206:PRO:HB2	1:D:220:ASN:HB3	1.93	0.49
1:F:357:LEU:HA	1:F:360:LYS:CG	2.42	0.49
1:E:350:GLU:HB2	1:E:354:ARG:HH12	1.76	0.49
1:D:357:LEU:HA	1:D:360:LYS:CG	2.42	0.49
1:B:163:ARG:CZ	1:B:220:ASN:O	2.60	0.49
1:C:159:ALA:C	1:C:162:ILE:HG12	2.32	0.49
1:B:146:GLU:HA	1:B:149:LYS:HZ2	1.76	0.49
1:F:163:ARG:NH2	1:F:221:ALA:CB	2.74	0.49
1:C:353:LYS:HE2	1:C:354:ARG:NH1	2.25	0.49
1:D:105:ILE:HA	1:D:225:ILE:O	2.11	0.49
1:C:163:ARG:NH2	1:C:221:ALA:CB	2.74	0.49
1:A:159:ALA:C	1:A:162:ILE:HG12	2.32	0.49
1:E:105:ILE:HA	1:E:225:ILE:O	2.12	0.49
1:C:105:ILE:HA	1:C:225:ILE:O	2.12	0.49
1:E:314:ILE:O	1:E:318:LEU:HB2	2.11	0.49
1:B:278:ILE:HG22	1:B:339:LEU:HD12	1.95	0.49
1:B:133:MET:O	1:B:154:ARG:NH2	2.43	0.49
1:B:105:ILE:HA	1:B:225:ILE:O	2.12	0.49
1:E:134:MET:CE	1:E:150:LEU:HD23	2.41	0.49
1:F:105:ILE:HB	1:F:225:ILE:HB	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:ILE:HG22	1:F:339:LEU:HD12	1.95	0.49
1:C:163:ARG:CZ	1:C:220:ASN:O	2.60	0.49
1:D:132:ILE:CG2	1:D:154:ARG:NH2	2.76	0.49
1:C:123:VAL:CG1	1:C:127:MET:HE2	2.42	0.49
1:C:172:ILE:HB	1:C:227:VAL:HG22	1.95	0.49
1:B:172:ILE:HB	1:B:227:VAL:HG22	1.95	0.49
1:B:206:PRO:HB2	1:B:220:ASN:HB3	1.92	0.48
1:B:132:ILE:CG2	1:B:154:ARG:NH2	2.76	0.48
1:A:350:GLU:HB2	1:A:354:ARG:NH1	2.28	0.48
1:A:73:LEU:CD2	1:A:125:ARG:CG	2.85	0.48
1:E:150:LEU:O	1:E:154:ARG:CG	2.61	0.48
1:E:350:GLU:HB2	1:E:353:LYS:CE	2.36	0.48
1:A:134:MET:HE3	1:A:150:LEU:HD23	1.94	0.48
1:A:132:ILE:CG2	1:A:154:ARG:NH2	2.76	0.48
1:B:347:GLN:CA	1:B:350:GLU:HG2	2.44	0.48
1:E:347:GLN:CA	1:E:350:GLU:HG2	2.43	0.48
1:C:347:GLN:CA	1:C:350:GLU:HG2	2.43	0.48
1:C:350:GLU:HB2	1:C:354:ARG:NH1	2.28	0.48
1:B:163:ARG:NH2	1:B:221:ALA:CB	2.74	0.48
1:F:347:GLN:CA	1:F:350:GLU:HG2	2.43	0.48
1:B:150:LEU:O	1:B:154:ARG:CG	2.61	0.48
1:D:350:GLU:HB2	1:D:354:ARG:NH1	2.28	0.48
1:C:133:MET:O	1:C:154:ARG:NH2	2.43	0.48
1:E:132:ILE:CG2	1:E:154:ARG:NH2	2.76	0.48
1:F:132:ILE:CG2	1:F:154:ARG:NH2	2.76	0.48
1:E:350:GLU:HB2	1:E:354:ARG:NH1	2.28	0.48
1:E:172:ILE:HB	1:E:227:VAL:HG22	1.95	0.48
1:B:258:ILE:HD13	1:B:276:VAL:HG22	1.96	0.48
1:C:132:ILE:CG2	1:C:154:ARG:NH2	2.76	0.48
1:D:347:GLN:CA	1:D:350:GLU:HG2	2.43	0.48
1:B:136:ALA:HB2	1:B:174:ASP:O	2.14	0.48
1:C:136:ALA:HB2	1:C:174:ASP:O	2.14	0.48
1:F:172:ILE:HB	1:F:227:VAL:HG22	1.95	0.48
1:E:258:ILE:HD13	1:E:276:VAL:HG22	1.96	0.48
1:B:350:GLU:HB2	1:B:354:ARG:NH1	2.29	0.48
1:A:347:GLN:CA	1:A:350:GLU:HG2	2.43	0.48
1:C:258:ILE:HD13	1:C:276:VAL:HG22	1.96	0.48
1:D:220:ASN:O	1:D:221:ALA:HB2	2.14	0.48
1:B:244:ARG:CG	1:B:244:ARG:O	2.57	0.48
1:E:278:ILE:HG22	1:E:339:LEU:HD12	1.95	0.48
1:F:136:ALA:HB2	1:F:174:ASP:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ALA:HB2	1:E:174:ASP:O	2.14	0.48
1:C:278:ILE:HG22	1:C:339:LEU:HD12	1.95	0.48
1:D:258:ILE:HD13	1:D:276:VAL:HG22	1.96	0.47
1:A:258:ILE:HD13	1:A:276:VAL:HG22	1.96	0.47
1:C:150:LEU:O	1:C:154:ARG:CG	2.61	0.47
1:D:172:ILE:HB	1:D:227:VAL:HG22	1.95	0.47
1:B:220:ASN:O	1:B:221:ALA:HB2	2.14	0.47
1:F:134:MET:CE	1:F:150:LEU:HD23	2.41	0.47
1:A:278:ILE:HG22	1:A:339:LEU:HD12	1.95	0.47
1:E:220:ASN:O	1:E:221:ALA:HB2	2.14	0.47
1:A:150:LEU:O	1:A:154:ARG:CG	2.61	0.47
1:B:134:MET:HE3	1:B:150:LEU:HD23	1.96	0.47
1:D:347:GLN:HA	1:D:350:GLU:HG2	1.97	0.47
1:E:347:GLN:HA	1:E:350:GLU:HG2	1.97	0.47
1:B:123:VAL:CG1	1:B:127:MET:HE2	2.45	0.47
1:A:136:ALA:HB2	1:A:174:ASP:O	2.14	0.47
1:D:278:ILE:HG22	1:D:339:LEU:HD12	1.95	0.47
1:F:150:LEU:O	1:F:154:ARG:CG	2.61	0.47
1:F:350:GLU:HB2	1:F:354:ARG:NH1	2.28	0.47
1:A:347:GLN:HA	1:A:350:GLU:HG2	1.97	0.47
1:A:172:ILE:HB	1:A:227:VAL:HG22	1.95	0.47
1:D:265:PHE:HB3	1:D:270:VAL:CG2	2.45	0.47
1:C:169:CYS:SG	1:C:226:ILE:HD13	2.55	0.47
1:D:169:CYS:SG	1:D:226:ILE:HD13	2.55	0.47
1:B:169:CYS:SG	1:B:226:ILE:HD13	2.55	0.47
1:C:220:ASN:O	1:C:221:ALA:HB2	2.14	0.47
1:A:163:ARG:NH2	1:A:221:ALA:CB	2.74	0.47
1:C:109:TRP:HZ2	1:C:247:LYS:HE3	1.80	0.47
1:A:133:MET:O	1:A:154:ARG:NH2	2.43	0.47
1:D:191:ASN:CG	1:D:192:ASN:H	2.17	0.47
1:C:347:GLN:HA	1:C:350:GLU:HG2	1.97	0.47
1:D:109:TRP:HZ2	1:D:247:LYS:HE3	1.80	0.47
1:A:220:ASN:O	1:A:221:ALA:HB2	2.14	0.47
1:D:136:ALA:HB2	1:D:174:ASP:O	2.14	0.47
1:F:111:GLY:HA3	1:F:250:TRP:CE3	2.50	0.47
1:F:220:ASN:O	1:F:221:ALA:HB2	2.14	0.47
1:D:149:LYS:CG	1:D:150:LEU:N	2.78	0.47
1:B:347:GLN:HA	1:B:350:GLU:HG2	1.97	0.47
1:D:111:GLY:HA3	1:D:250:TRP:CE3	2.50	0.47
1:B:109:TRP:HZ2	1:B:247:LYS:HE3	1.80	0.47
1:A:191:ASN:CG	1:A:192:ASN:H	2.17	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:VAL:CG1	1:D:127:MET:HE2	2.44	0.47
1:C:111:GLY:HA3	1:C:250:TRP:CE3	2.50	0.47
1:A:159:ALA:HA	1:A:162:ILE:HD11	1.97	0.46
1:F:169:CYS:SG	1:F:226:ILE:HD13	2.55	0.46
1:D:150:LEU:O	1:D:154:ARG:CG	2.61	0.46
1:C:350:GLU:C	1:C:353:LYS:HE2	2.35	0.46
1:F:258:ILE:HD13	1:F:276:VAL:HG22	1.96	0.46
1:C:159:ALA:HA	1:C:162:ILE:HD11	1.97	0.46
1:B:353:LYS:HE2	1:B:354:ARG:NH1	2.25	0.46
1:D:140:GLU:OE1	1:D:141:SER:HB2	2.15	0.46
1:A:140:GLU:OE1	1:A:141:SER:HB2	2.15	0.46
1:D:159:ALA:HA	1:D:162:ILE:HD11	1.97	0.46
1:E:149:LYS:CG	1:E:150:LEU:N	2.78	0.46
1:F:133:MET:O	1:F:154:ARG:NH2	2.43	0.46
1:D:350:GLU:C	1:D:353:LYS:HE2	2.36	0.46
1:A:109:TRP:HZ2	1:A:247:LYS:HE3	1.80	0.46
1:F:347:GLN:HA	1:F:350:GLU:HG2	1.97	0.46
1:E:265:PHE:HB3	1:E:270:VAL:CG2	2.45	0.46
1:E:169:CYS:SG	1:E:226:ILE:HD13	2.55	0.46
1:E:111:GLY:HA3	1:E:250:TRP:CE3	2.50	0.46
1:E:159:ALA:HA	1:E:162:ILE:HD11	1.97	0.46
1:F:159:ALA:HA	1:F:162:ILE:HD11	1.97	0.46
1:A:350:GLU:C	1:A:353:LYS:HE2	2.36	0.46
1:B:73:LEU:HD21	1:B:125:ARG:HD3	1.92	0.46
1:B:76:PHE:CE1	1:B:266:ARG:NH1	2.83	0.46
1:A:169:CYS:SG	1:A:226:ILE:HD13	2.55	0.46
1:F:109:TRP:HZ2	1:F:247:LYS:HE3	1.80	0.46
1:E:191:ASN:CG	1:E:192:ASN:H	2.17	0.46
1:E:140:GLU:OE1	1:E:141:SER:HB2	2.16	0.46
1:B:111:GLY:HA3	1:B:250:TRP:CE3	2.50	0.46
1:C:174:ASP:C	1:C:175:LEU:HG	2.36	0.46
1:B:140:GLU:OE1	1:B:141:SER:HB2	2.16	0.46
1:F:345:LEU:O	1:F:345:LEU:HD12	2.16	0.46
1:F:191:ASN:CG	1:F:192:ASN:H	2.17	0.45
1:C:345:LEU:HD12	1:C:345:LEU:O	2.16	0.45
1:B:149:LYS:CG	1:B:150:LEU:N	2.78	0.45
1:C:73:LEU:HD21	1:C:125:ARG:HD3	1.92	0.45
1:D:174:ASP:C	1:D:175:LEU:HG	2.36	0.45
1:A:111:GLY:HA3	1:A:250:TRP:CE3	2.50	0.45
1:E:350:GLU:C	1:E:353:LYS:HE2	2.35	0.45
1:F:265:PHE:HB3	1:F:270:VAL:CG2	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:LEU:O	1:E:345:LEU:HD12	2.16	0.45
1:A:160:GLU:HA	1:A:163:ARG:HD2	1.98	0.45
1:E:109:TRP:HZ2	1:E:247:LYS:HE3	1.80	0.45
1:B:191:ASN:CG	1:B:192:ASN:H	2.17	0.45
1:A:116:LYS:HB3	1:A:116:LYS:HE3	1.79	0.45
1:A:145:GLY:O	1:A:149:LYS:CG	2.54	0.45
1:A:139:LEU:CD2	1:A:195:VAL:HG21	2.26	0.45
1:F:350:GLU:C	1:F:353:LYS:HE2	2.35	0.45
1:C:265:PHE:HB3	1:C:270:VAL:CG2	2.45	0.45
1:B:345:LEU:O	1:B:345:LEU:HD12	2.16	0.45
1:F:174:ASP:C	1:F:175:LEU:HG	2.36	0.45
1:A:123:VAL:HG12	1:A:127:MET:HE2	1.98	0.45
1:B:350:GLU:C	1:B:353:LYS:HE2	2.35	0.45
1:A:253:THR:CG2	1:A:254:ARG:N	2.80	0.45
1:E:134:MET:HE3	1:E:150:LEU:HD23	1.99	0.45
1:C:149:LYS:CG	1:C:150:LEU:N	2.78	0.45
1:C:140:GLU:OE1	1:C:141:SER:HB2	2.15	0.45
1:A:174:ASP:C	1:A:175:LEU:HG	2.36	0.45
1:A:267:THR:HG21	1:B:99:ASN:CB	2.48	0.45
1:F:160:GLU:HA	1:F:163:ARG:HD2	1.98	0.44
1:E:76:PHE:CE1	1:E:266:ARG:NH1	2.83	0.44
1:F:73:LEU:HD21	1:F:125:ARG:HD3	1.92	0.44
1:F:123:VAL:HG12	1:F:127:MET:HE2	2.00	0.44
1:D:253:THR:CG2	1:D:254:ARG:N	2.80	0.44
1:A:99:ASN:CB	1:F:267:THR:HG21	2.47	0.44
1:D:298:TYR:O	1:D:299:ASP:C	2.56	0.44
1:B:159:ALA:HA	1:B:162:ILE:HD11	1.98	0.44
1:F:206:PRO:HG2	1:F:220:ASN:HD22	1.82	0.44
1:E:133:MET:O	1:E:154:ARG:NH2	2.43	0.44
1:F:200:MET:HG2	1:F:239:LEU:HD22	1.99	0.44
1:C:191:ASN:CG	1:C:192:ASN:H	2.17	0.44
1:E:158:ALA:HA	1:E:161:ILE:HD12	2.00	0.44
1:B:158:ALA:HA	1:B:161:ILE:HD12	2.00	0.44
1:F:140:GLU:OE1	1:F:141:SER:HB2	2.16	0.44
1:B:267:THR:HG21	1:C:99:ASN:CB	2.47	0.44
1:E:160:GLU:HA	1:E:163:ARG:HD2	1.98	0.44
1:C:158:ALA:HA	1:C:161:ILE:HD12	1.99	0.44
1:E:139:LEU:CD2	1:E:195:VAL:HG21	2.26	0.44
1:D:73:LEU:O	1:D:74:ASP:C	2.55	0.44
1:E:298:TYR:O	1:E:299:ASP:C	2.56	0.44
1:A:158:ALA:HA	1:A:161:ILE:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:ALA:HA	1:F:161:ILE:HD12	2.00	0.44
1:B:300:ASP:HB2	1:B:303:ARG:HH12	1.83	0.44
1:A:265:PHE:HB3	1:A:270:VAL:CG2	2.45	0.44
1:A:300:ASP:HB2	1:A:303:ARG:HH12	1.83	0.44
1:F:253:THR:CG2	1:F:254:ARG:N	2.81	0.44
1:F:150:LEU:O	1:F:150:LEU:HD23	2.18	0.44
1:C:73:LEU:O	1:C:74:ASP:C	2.55	0.44
1:C:253:THR:CG2	1:C:254:ARG:N	2.81	0.44
1:C:267:THR:HG21	1:D:99:ASN:CB	2.48	0.44
1:F:298:TYR:O	1:F:299:ASP:C	2.56	0.44
1:E:200:MET:HG2	1:E:239:LEU:HD22	1.99	0.44
1:A:345:LEU:HD12	1:A:345:LEU:O	2.16	0.44
1:D:345:LEU:HD12	1:D:345:LEU:O	2.16	0.44
1:E:73:LEU:O	1:E:74:ASP:C	2.55	0.44
1:B:73:LEU:O	1:B:74:ASP:C	2.55	0.44
1:B:174:ASP:C	1:B:175:LEU:HG	2.36	0.44
1:A:149:LYS:CG	1:A:150:LEU:N	2.78	0.44
1:F:149:LYS:CG	1:F:150:LEU:N	2.78	0.44
1:B:150:LEU:HD23	1:B:150:LEU:O	2.18	0.44
1:A:73:LEU:O	1:A:74:ASP:C	2.55	0.44
1:B:265:PHE:HB3	1:B:270:VAL:CG2	2.45	0.44
1:E:253:THR:CG2	1:E:254:ARG:N	2.81	0.44
1:A:298:TYR:O	1:A:299:ASP:C	2.56	0.44
1:B:206:PRO:HG2	1:B:220:ASN:HD22	1.82	0.44
1:C:150:LEU:O	1:C:150:LEU:HD23	2.18	0.44
1:D:150:LEU:HD23	1:D:150:LEU:O	2.18	0.44
1:C:200:MET:HG2	1:C:239:LEU:HD22	1.99	0.44
1:C:87:VAL:O	1:C:91:THR:HG22	2.18	0.44
1:E:150:LEU:O	1:E:150:LEU:HD23	2.18	0.43
1:E:174:ASP:C	1:E:175:LEU:HG	2.36	0.43
1:D:200:MET:HG2	1:D:239:LEU:HD22	1.99	0.43
1:A:200:MET:HG2	1:A:239:LEU:HD22	1.99	0.43
1:E:206:PRO:HG2	1:E:220:ASN:HD22	1.82	0.43
1:D:160:GLU:HA	1:D:163:ARG:HD2	1.98	0.43
1:F:300:ASP:HB2	1:F:303:ARG:HH12	1.83	0.43
1:D:267:THR:HG21	1:E:99:ASN:CB	2.48	0.43
1:F:87:VAL:O	1:F:91:THR:HG22	2.18	0.43
1:A:150:LEU:HD23	1:A:150:LEU:O	2.18	0.43
1:C:357:LEU:HA	1:C:360:LYS:HG2	2.00	0.43
1:A:357:LEU:HA	1:A:360:LYS:HG2	2.00	0.43
1:B:116:LYS:HB3	1:B:116:LYS:HE3	1.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:VAL:O	1:B:91:THR:HG22	2.18	0.43
1:E:344:MET:C	1:E:347:GLN:HG2	2.39	0.43
1:E:73:LEU:HD21	1:E:125:ARG:HD3	1.92	0.43
1:C:300:ASP:HB2	1:C:303:ARG:HH12	1.83	0.43
1:F:344:MET:C	1:F:347:GLN:HG2	2.39	0.43
1:B:200:MET:HG2	1:B:239:LEU:HD22	1.99	0.43
1:C:206:PRO:HG2	1:C:220:ASN:HD22	1.82	0.43
1:D:139:LEU:CD2	1:D:195:VAL:HG21	2.26	0.43
1:E:123:VAL:HG12	1:E:127:MET:HE2	2.00	0.43
1:E:87:VAL:O	1:E:91:THR:HG22	2.18	0.43
1:C:298:TYR:O	1:C:299:ASP:C	2.56	0.43
1:D:132:ILE:HD11	1:D:161:ILE:HD11	2.01	0.43
1:C:306:VAL:HG13	1:C:314:ILE:CD1	2.49	0.43
1:D:87:VAL:O	1:D:91:THR:HG22	2.18	0.43
1:C:134:MET:CE	1:C:150:LEU:HD23	2.41	0.43
1:A:347:GLN:HA	1:A:350:GLU:CG	2.49	0.43
1:F:265:PHE:CB	1:F:270:VAL:HG21	2.49	0.43
1:F:306:VAL:HG13	1:F:314:ILE:CD1	2.49	0.43
1:B:298:TYR:O	1:B:299:ASP:C	2.56	0.43
1:F:116:LYS:HE3	1:F:116:LYS:HB3	1.79	0.43
1:A:132:ILE:HD11	1:A:161:ILE:HD11	2.01	0.43
1:D:158:ALA:HA	1:D:161:ILE:HD12	2.00	0.43
1:D:357:LEU:HA	1:D:360:LYS:HG2	2.00	0.43
1:E:267:THR:HG21	1:F:99:ASN:CB	2.48	0.43
1:A:87:VAL:O	1:A:91:THR:HG22	2.18	0.43
1:D:206:PRO:HG2	1:D:220:ASN:HD22	1.82	0.42
1:A:134:MET:HE3	1:A:150:LEU:HD22	1.97	0.42
1:A:344:MET:C	1:A:347:GLN:HG2	2.39	0.42
1:C:347:GLN:HA	1:C:350:GLU:CG	2.49	0.42
1:F:73:LEU:O	1:F:74:ASP:C	2.55	0.42
1:F:278:ILE:HG22	1:F:339:LEU:CD1	2.49	0.42
1:B:205:ASN:HB2	1:B:206:PRO:CD	2.31	0.42
1:D:347:GLN:HA	1:D:350:GLU:CG	2.49	0.42
1:B:347:GLN:HA	1:B:350:GLU:CG	2.49	0.42
1:E:357:LEU:HA	1:E:360:LYS:HG2	2.00	0.42
1:F:122:LEU:O	1:F:125:ARG:CG	2.67	0.42
1:D:122:LEU:HD12	1:D:122:LEU:HA	1.90	0.42
1:D:73:LEU:HD21	1:D:125:ARG:HD3	1.92	0.42
1:A:206:PRO:HG2	1:A:220:ASN:HD22	1.82	0.42
1:C:132:ILE:HD11	1:C:161:ILE:HD11	2.01	0.42
1:B:132:ILE:HD11	1:B:161:ILE:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:MET:C	1:D:347:GLN:HG2	2.39	0.42
1:F:352:VAL:O	1:F:356:GLN:HB2	2.20	0.42
1:C:105:ILE:HG13	1:C:245:MET:CG	2.49	0.42
1:F:347:GLN:HA	1:F:350:GLU:CG	2.49	0.42
1:F:357:LEU:HA	1:F:360:LYS:HG2	2.00	0.42
1:E:122:LEU:O	1:E:125:ARG:CG	2.67	0.42
1:D:300:ASP:HB2	1:D:303:ARG:HH12	1.83	0.42
1:E:132:ILE:HD11	1:E:161:ILE:HD11	2.01	0.42
1:B:357:LEU:HA	1:B:360:LYS:HG2	2.01	0.42
1:C:149:LYS:CG	1:C:150:LEU:H	2.33	0.42
1:E:300:ASP:HB2	1:E:303:ARG:HH12	1.83	0.42
1:A:306:VAL:HG13	1:A:314:ILE:CD1	2.49	0.42
1:B:160:GLU:HA	1:B:163:ARG:HD2	1.98	0.42
1:D:191:ASN:CG	1:D:192:ASN:N	2.73	0.42
1:B:344:MET:C	1:B:347:GLN:HG2	2.39	0.42
1:E:306:VAL:HG13	1:E:314:ILE:CD1	2.49	0.42
1:C:123:VAL:HG12	1:C:127:MET:HE2	2.02	0.42
1:D:105:ILE:HG13	1:D:245:MET:CG	2.49	0.42
1:C:160:GLU:HA	1:C:163:ARG:HD2	1.98	0.42
1:B:300:ASP:HB2	1:B:303:ARG:NH1	2.35	0.42
1:E:278:ILE:HG22	1:E:339:LEU:CD1	2.50	0.42
1:D:151:ILE:HD12	1:D:198:THR:HG21	2.02	0.42
1:C:163:ARG:NH2	1:C:220:ASN:C	2.73	0.42
1:C:352:VAL:O	1:C:356:GLN:HB2	2.20	0.42
1:E:347:GLN:HA	1:E:350:GLU:CG	2.49	0.42
1:C:344:MET:C	1:C:347:GLN:HG2	2.39	0.42
1:C:172:ILE:O	1:C:227:VAL:HA	2.20	0.42
1:B:306:VAL:HG13	1:B:314:ILE:CD1	2.49	0.42
1:B:278:ILE:HG22	1:B:339:LEU:CD1	2.50	0.42
1:B:339:LEU:O	1:B:343:ASN:ND2	2.53	0.42
1:B:163:ARG:NH2	1:B:220:ASN:C	2.74	0.41
1:B:191:ASN:CG	1:B:192:ASN:N	2.73	0.41
1:D:352:VAL:O	1:D:356:GLN:HB2	2.20	0.41
1:B:352:VAL:O	1:B:356:GLN:HB2	2.20	0.41
1:D:172:ILE:O	1:D:227:VAL:HA	2.20	0.41
1:A:300:ASP:HB2	1:A:303:ARG:NH1	2.35	0.41
1:C:339:LEU:O	1:C:343:ASN:ND2	2.53	0.41
1:A:278:ILE:HG22	1:A:339:LEU:CD1	2.50	0.41
1:D:237:ALA:N	1:D:238:PRO:HD2	2.36	0.41
1:E:172:ILE:O	1:E:227:VAL:HA	2.20	0.41
1:B:172:ILE:O	1:B:227:VAL:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:O	1:A:343:ASN:ND2	2.53	0.41
1:E:163:ARG:NH2	1:E:220:ASN:C	2.73	0.41
1:C:191:ASN:CG	1:C:192:ASN:N	2.73	0.41
1:A:265:PHE:CB	1:A:270:VAL:HG21	2.48	0.41
1:F:339:LEU:O	1:F:343:ASN:ND2	2.53	0.41
1:D:278:ILE:HG22	1:D:339:LEU:CD1	2.50	0.41
1:A:163:ARG:NH2	1:A:220:ASN:C	2.73	0.41
1:F:344:MET:HE3	1:F:344:MET:HB2	2.00	0.41
1:E:352:VAL:O	1:E:356:GLN:HB2	2.20	0.41
1:C:265:PHE:CB	1:C:270:VAL:HG21	2.49	0.41
1:D:306:VAL:HG13	1:D:314:ILE:CD1	2.49	0.41
1:E:106:LEU:HD23	1:E:246:GLU:HB3	2.03	0.41
1:C:151:ILE:HD12	1:C:198:THR:HG21	2.02	0.41
1:C:106:LEU:HD23	1:C:246:GLU:HB3	2.03	0.41
1:D:163:ARG:NH2	1:D:220:ASN:C	2.73	0.41
1:A:191:ASN:CG	1:A:192:ASN:N	2.73	0.41
1:F:149:LYS:CG	1:F:150:LEU:H	2.33	0.41
1:B:237:ALA:N	1:B:238:PRO:HD2	2.35	0.41
1:D:300:ASP:HB2	1:D:303:ARG:NH1	2.35	0.41
1:F:300:ASP:HB2	1:F:303:ARG:NH1	2.35	0.41
1:E:146:GLU:HB3	1:E:147:PRO:HD3	2.03	0.41
1:A:193:GLN:HB2	1:F:140:GLU:OE1	2.21	0.41
1:F:172:ILE:O	1:F:227:VAL:HA	2.20	0.41
1:A:151:ILE:HD12	1:A:198:THR:HG21	2.02	0.41
1:F:159:ALA:O	1:F:163:ARG:N	2.47	0.41
1:E:191:ASN:CG	1:E:192:ASN:N	2.73	0.41
1:C:237:ALA:N	1:C:238:PRO:HD2	2.36	0.41
1:A:172:ILE:O	1:A:227:VAL:HA	2.20	0.41
1:B:82:PHE:CE1	1:B:119:GLN:HB3	2.56	0.41
1:E:300:ASP:HB2	1:E:303:ARG:NH1	2.35	0.41
1:D:263:GLY:O	1:D:266:ARG:HD3	2.21	0.41
1:B:106:LEU:HD23	1:B:246:GLU:HB3	2.03	0.41
1:A:106:LEU:HD23	1:A:246:GLU:HB3	2.02	0.41
1:B:146:GLU:HB3	1:B:147:PRO:HD3	2.03	0.41
1:B:149:LYS:CG	1:B:150:LEU:H	2.33	0.41
1:E:82:PHE:CE1	1:E:119:GLN:HB3	2.56	0.41
1:F:266:ARG:CG	1:F:267:THR:N	2.84	0.41
1:C:278:ILE:HG22	1:C:339:LEU:CD1	2.50	0.41
1:F:197:ALA:O	1:F:201:ASN:ND2	2.54	0.41
1:F:163:ARG:NH2	1:F:220:ASN:C	2.73	0.41
1:A:146:GLU:HB3	1:A:147:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:GLU:HB3	1:F:147:PRO:HD3	2.03	0.41
1:B:145:GLY:O	1:B:149:LYS:CG	2.54	0.41
1:A:352:VAL:O	1:A:356:GLN:HB2	2.20	0.41
1:A:237:ALA:N	1:A:238:PRO:HD2	2.36	0.41
1:C:82:PHE:CE1	1:C:119:GLN:HB3	2.56	0.41
1:F:82:PHE:CE1	1:F:119:GLN:HB3	2.56	0.41
1:A:300:ASP:CA	1:A:303:ARG:NH1	2.83	0.41
1:D:82:PHE:CE1	1:D:119:GLN:HB3	2.56	0.41
1:A:263:GLY:O	1:A:266:ARG:HD3	2.21	0.41
1:D:266:ARG:CG	1:D:267:THR:N	2.84	0.41
1:B:197:ALA:O	1:B:201:ASN:ND2	2.54	0.41
1:E:339:LEU:O	1:E:343:ASN:ND2	2.53	0.41
1:D:339:LEU:O	1:D:343:ASN:ND2	2.53	0.41
1:F:106:LEU:HD23	1:F:246:GLU:HB3	2.03	0.41
1:E:151:ILE:HD12	1:E:198:THR:HG21	2.02	0.41
1:C:344:MET:HE3	1:C:344:MET:HB2	1.98	0.40
1:C:300:ASP:HB2	1:C:303:ARG:NH1	2.35	0.40
1:C:263:GLY:O	1:C:266:ARG:HD3	2.21	0.40
1:A:266:ARG:CG	1:A:267:THR:N	2.84	0.40
1:C:146:GLU:HB3	1:C:147:PRO:HD3	2.03	0.40
1:E:344:MET:HB2	1:E:344:MET:HE3	2.03	0.40
1:B:263:GLY:O	1:B:266:ARG:HD3	2.21	0.40
1:E:237:ALA:N	1:E:238:PRO:HD2	2.36	0.40
1:E:197:ALA:O	1:E:201:ASN:ND2	2.54	0.40
1:B:134:MET:HE3	1:B:150:LEU:HD22	1.99	0.40
1:B:240:ILE:O	1:B:245:MET:N	2.55	0.40
1:B:300:ASP:CA	1:B:303:ARG:NH1	2.83	0.40
1:B:265:PHE:CB	1:B:270:VAL:HG21	2.49	0.40
1:B:151:ILE:HD12	1:B:198:THR:HG21	2.02	0.40
1:B:329:GLU:HG2	1:B:329:GLU:O	2.21	0.40
1:C:329:GLU:O	1:C:329:GLU:HG2	2.22	0.40
1:D:329:GLU:O	1:D:329:GLU:HG2	2.21	0.40
1:E:329:GLU:O	1:E:329:GLU:HG2	2.21	0.40
1:B:139:LEU:CD2	1:B:195:VAL:HG21	2.26	0.40
1:E:263:GLY:O	1:E:266:ARG:HD3	2.21	0.40
1:A:240:ILE:O	1:A:245:MET:N	2.55	0.40
1:F:263:GLY:O	1:F:266:ARG:HD3	2.21	0.40
1:F:151:ILE:HD12	1:F:198:THR:HG21	2.02	0.40
1:A:197:ALA:O	1:A:201:ASN:ND2	2.54	0.40
1:D:106:LEU:HD23	1:D:246:GLU:HB3	2.02	0.40
1:A:329:GLU:HG2	1:A:329:GLU:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:HB3	1:D:147:PRO:HD3	2.03	0.40
1:F:132:ILE:HD11	1:F:161:ILE:HD11	2.01	0.40
1:C:266:ARG:CG	1:C:267:THR:N	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9	51
1	B	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9	51
1	C	251/293 (86%)	218 (87%)	28 (11%)	5 (2%)	9	51
1	D	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9	51
1	E	251/293 (86%)	217 (86%)	29 (12%)	5 (2%)	9	51
1	F	251/293 (86%)	216 (86%)	30 (12%)	5 (2%)	9	51
All	All	1506/1758 (86%)	1299 (86%)	177 (12%)	30 (2%)	14	51

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	PRO
1	A	327	THR
1	B	206	PRO
1	B	327	THR
1	C	206	PRO
1	C	327	THR
1	D	206	PRO
1	D	327	THR
1	E	206	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	327	THR
1	F	206	PRO
1	F	327	THR
1	A	310	GLY
1	B	310	GLY
1	C	310	GLY
1	D	310	GLY
1	E	310	GLY
1	F	310	GLY
1	A	166	ASN
1	B	166	ASN
1	C	166	ASN
1	D	166	ASN
1	E	166	ASN
1	F	166	ASN
1	C	238	PRO
1	D	238	PRO
1	E	238	PRO
1	F	238	PRO
1	A	238	PRO
1	B	238	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	227/248 (92%)	198 (87%)	29 (13%)	5	29
1	B	227/248 (92%)	198 (87%)	29 (13%)	5	29
1	C	227/248 (92%)	198 (87%)	29 (13%)	5	29
1	D	227/248 (92%)	198 (87%)	29 (13%)	5	29
1	E	227/248 (92%)	198 (87%)	29 (13%)	5	29
1	F	227/248 (92%)	198 (87%)	29 (13%)	5	29
All	All	1362/1488 (92%)	1188 (87%)	174 (13%)	10	29

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	70	ASP
1	A	91	THR
1	A	97	LEU
1	A	105	ILE
1	A	106	LEU
1	A	122	LEU
1	A	127	MET
1	A	135	SER
1	A	169	CYS
1	A	176	ASP
1	A	196	ASN
1	A	205	ASN
1	A	220	ASN
1	A	222	ARG
1	A	228	THR
1	A	240	ILE
1	A	268	ASP
1	A	270	VAL
1	A	293	LEU
1	A	296	ARG
1	A	300	ASP
1	A	311	ILE
1	A	314	ILE
1	A	318	LEU
1	A	321	SER
1	A	337	LYS
1	A	345	LEU
1	A	356	GLN
1	B	69	LEU
1	B	70	ASP
1	B	91	THR
1	B	97	LEU
1	B	105	ILE
1	B	106	LEU
1	B	122	LEU
1	B	127	MET
1	B	135	SER
1	B	169	CYS
1	B	176	ASP
1	B	196	ASN
1	B	205	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	220	ASN
1	B	222	ARG
1	B	228	THR
1	B	240	ILE
1	B	268	ASP
1	B	270	VAL
1	B	293	LEU
1	B	296	ARG
1	B	300	ASP
1	B	311	ILE
1	B	314	ILE
1	B	318	LEU
1	B	321	SER
1	B	337	LYS
1	B	345	LEU
1	B	356	GLN
1	C	69	LEU
1	C	70	ASP
1	C	91	THR
1	C	97	LEU
1	C	105	ILE
1	C	106	LEU
1	C	122	LEU
1	C	127	MET
1	C	135	SER
1	C	169	CYS
1	C	176	ASP
1	C	196	ASN
1	C	205	ASN
1	C	220	ASN
1	C	222	ARG
1	C	228	THR
1	C	240	ILE
1	C	268	ASP
1	C	270	VAL
1	C	293	LEU
1	C	296	ARG
1	C	300	ASP
1	C	311	ILE
1	C	314	ILE
1	C	318	LEU
1	C	321	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	337	LYS
1	C	345	LEU
1	C	356	GLN
1	D	69	LEU
1	D	70	ASP
1	D	91	THR
1	D	97	LEU
1	D	105	ILE
1	D	106	LEU
1	D	122	LEU
1	D	127	MET
1	D	135	SER
1	D	169	CYS
1	D	176	ASP
1	D	196	ASN
1	D	205	ASN
1	D	220	ASN
1	D	222	ARG
1	D	228	THR
1	D	240	ILE
1	D	268	ASP
1	D	270	VAL
1	D	293	LEU
1	D	296	ARG
1	D	300	ASP
1	D	311	ILE
1	D	314	ILE
1	D	318	LEU
1	D	321	SER
1	D	337	LYS
1	D	345	LEU
1	D	356	GLN
1	E	69	LEU
1	E	70	ASP
1	E	91	THR
1	E	97	LEU
1	E	105	ILE
1	E	106	LEU
1	E	122	LEU
1	E	127	MET
1	E	135	SER
1	E	169	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	176	ASP
1	E	196	ASN
1	E	205	ASN
1	E	220	ASN
1	E	222	ARG
1	E	228	THR
1	E	240	ILE
1	E	268	ASP
1	E	270	VAL
1	E	293	LEU
1	E	296	ARG
1	E	300	ASP
1	E	311	ILE
1	E	314	ILE
1	E	318	LEU
1	E	321	SER
1	E	337	LYS
1	E	345	LEU
1	E	356	GLN
1	F	69	LEU
1	F	70	ASP
1	F	91	THR
1	F	97	LEU
1	F	105	ILE
1	F	106	LEU
1	F	122	LEU
1	F	127	MET
1	F	135	SER
1	F	169	CYS
1	F	176	ASP
1	F	196	ASN
1	F	205	ASN
1	F	220	ASN
1	F	222	ARG
1	F	228	THR
1	F	240	ILE
1	F	268	ASP
1	F	270	VAL
1	F	293	LEU
1	F	296	ARG
1	F	300	ASP
1	F	311	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	314	ILE
1	F	318	LEU
1	F	321	SER
1	F	337	LYS
1	F	345	LEU
1	F	356	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	119	GLN
1	A	166	ASN
1	A	196	ASN
1	A	205	ASN
1	A	269	ASN
1	A	343	ASN
1	B	93	ASN
1	B	119	GLN
1	B	166	ASN
1	B	196	ASN
1	B	205	ASN
1	B	269	ASN
1	B	343	ASN
1	C	93	ASN
1	C	119	GLN
1	C	166	ASN
1	C	196	ASN
1	C	205	ASN
1	C	269	ASN
1	C	343	ASN
1	D	93	ASN
1	D	119	GLN
1	D	166	ASN
1	D	196	ASN
1	D	205	ASN
1	D	269	ASN
1	D	343	ASN
1	E	93	ASN
1	E	119	GLN
1	E	166	ASN
1	E	196	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	205	ASN
1	E	269	ASN
1	E	343	ASN
1	F	93	ASN
1	F	119	GLN
1	F	166	ASN
1	F	196	ASN
1	F	205	ASN
1	F	269	ASN
1	F	343	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.