Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 08:58 am BST

PDB ID	:	2EWO
Title	:	X-ray structure of putative agmatine deiminase Q8DW17, Northeast Structural Genomics target SmR6.
Authors	:	Kuzin, A.P.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on	:	2005-11-04
Resolution	:	2.90 Å(reported)

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

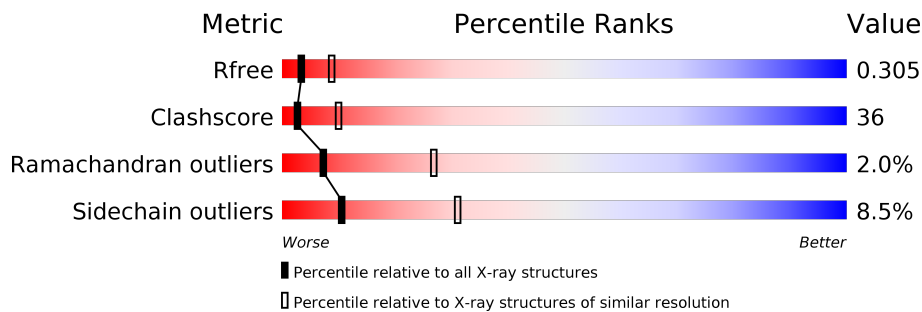|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
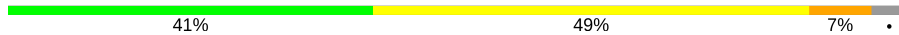
Metric	Percentile Ranks	Value
Rfree		0.305
Clashscore		36
Ramachandran outliers		2.0%
Sidechain outliers		8.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	377	40% 50% 6% •
1	B	377	41% 49% 6% •
1	C	377	41% 49% 6% •
1	D	377	40% 49% 7% •
1	E	377	40% 50% 6% •
1	F	377	41% 49% 7% •
1	G	377	41% 49% 6% •

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	377	44% 45% 9%
1	I	377	41% 48% 7%
1	J	377	41% 48% 7%
1	K	377	41% 49% 7%
1	L	377	40% 49% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34934 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 Putative agmatine deiminase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	C	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	D	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	E	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	F	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	G	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	H	369	Total	C	N	O	S	Se	0	0	0
			2942	1868	496	561	10	7			
1	I	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	J	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	K	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			
1	L	362	Total	C	N	O	S	Se	0	0	0
			2888	1836	486	549	10	7			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8DW17
A	17	MSE	MET	modified residue	UNP Q8DW17
A	29	MSE	MET	modified residue	UNP Q8DW17
A	91	MSE	MET	modified residue	UNP Q8DW17
A	178	MSE	MET	modified residue	UNP Q8DW17

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	MSE	MET	modified residue	UNP Q8DW17
A	303	MSE	MET	modified residue	UNP Q8DW17
A	338	MSE	MET	modified residue	UNP Q8DW17
A	370	LEU	-	cloning artifact	UNP Q8DW17
A	371	GLU	-	cloning artifact	UNP Q8DW17
A	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
A	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	1	MSE	MET	modified residue	UNP Q8DW17
B	17	MSE	MET	modified residue	UNP Q8DW17
B	29	MSE	MET	modified residue	UNP Q8DW17
B	91	MSE	MET	modified residue	UNP Q8DW17
B	178	MSE	MET	modified residue	UNP Q8DW17
B	274	MSE	MET	modified residue	UNP Q8DW17
B	303	MSE	MET	modified residue	UNP Q8DW17
B	338	MSE	MET	modified residue	UNP Q8DW17
B	370	LEU	-	cloning artifact	UNP Q8DW17
B	371	GLU	-	cloning artifact	UNP Q8DW17
B	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
B	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	1	MSE	MET	modified residue	UNP Q8DW17
C	17	MSE	MET	modified residue	UNP Q8DW17
C	29	MSE	MET	modified residue	UNP Q8DW17
C	91	MSE	MET	modified residue	UNP Q8DW17
C	178	MSE	MET	modified residue	UNP Q8DW17
C	274	MSE	MET	modified residue	UNP Q8DW17
C	303	MSE	MET	modified residue	UNP Q8DW17
C	338	MSE	MET	modified residue	UNP Q8DW17
C	370	LEU	-	cloning artifact	UNP Q8DW17
C	371	GLU	-	cloning artifact	UNP Q8DW17
C	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
C	376	HIS	-	EXPRESSION TAG	UNP Q8DW17

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	1	MSE	MET	modified residue	UNP Q8DW17
D	17	MSE	MET	modified residue	UNP Q8DW17
D	29	MSE	MET	modified residue	UNP Q8DW17
D	91	MSE	MET	modified residue	UNP Q8DW17
D	178	MSE	MET	modified residue	UNP Q8DW17
D	274	MSE	MET	modified residue	UNP Q8DW17
D	303	MSE	MET	modified residue	UNP Q8DW17
D	338	MSE	MET	modified residue	UNP Q8DW17
D	370	LEU	-	cloning artifact	UNP Q8DW17
D	371	GLU	-	cloning artifact	UNP Q8DW17
D	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
D	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	1	MSE	MET	modified residue	UNP Q8DW17
E	17	MSE	MET	modified residue	UNP Q8DW17
E	29	MSE	MET	modified residue	UNP Q8DW17
E	91	MSE	MET	modified residue	UNP Q8DW17
E	178	MSE	MET	modified residue	UNP Q8DW17
E	274	MSE	MET	modified residue	UNP Q8DW17
E	303	MSE	MET	modified residue	UNP Q8DW17
E	338	MSE	MET	modified residue	UNP Q8DW17
E	370	LEU	-	cloning artifact	UNP Q8DW17
E	371	GLU	-	cloning artifact	UNP Q8DW17
E	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
E	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	1	MSE	MET	modified residue	UNP Q8DW17
F	17	MSE	MET	modified residue	UNP Q8DW17
F	29	MSE	MET	modified residue	UNP Q8DW17
F	91	MSE	MET	modified residue	UNP Q8DW17
F	178	MSE	MET	modified residue	UNP Q8DW17
F	274	MSE	MET	modified residue	UNP Q8DW17
F	303	MSE	MET	modified residue	UNP Q8DW17
F	338	MSE	MET	modified residue	UNP Q8DW17
F	370	LEU	-	cloning artifact	UNP Q8DW17

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	371	GLU	-	cloning artifact	UNP Q8DW17
F	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
F	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	1	MSE	MET	modified residue	UNP Q8DW17
G	17	MSE	MET	modified residue	UNP Q8DW17
G	29	MSE	MET	modified residue	UNP Q8DW17
G	91	MSE	MET	modified residue	UNP Q8DW17
G	178	MSE	MET	modified residue	UNP Q8DW17
G	274	MSE	MET	modified residue	UNP Q8DW17
G	303	MSE	MET	modified residue	UNP Q8DW17
G	338	MSE	MET	modified residue	UNP Q8DW17
G	370	LEU	-	cloning artifact	UNP Q8DW17
G	371	GLU	-	cloning artifact	UNP Q8DW17
G	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
G	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	1	MSE	MET	modified residue	UNP Q8DW17
H	17	MSE	MET	modified residue	UNP Q8DW17
H	29	MSE	MET	modified residue	UNP Q8DW17
H	91	MSE	MET	modified residue	UNP Q8DW17
H	178	MSE	MET	modified residue	UNP Q8DW17
H	274	MSE	MET	modified residue	UNP Q8DW17
H	303	MSE	MET	modified residue	UNP Q8DW17
H	338	MSE	MET	modified residue	UNP Q8DW17
H	370	LEU	-	cloning artifact	UNP Q8DW17
H	371	GLU	-	cloning artifact	UNP Q8DW17
H	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
H	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	1	MSE	MET	modified residue	UNP Q8DW17
I	17	MSE	MET	modified residue	UNP Q8DW17
I	29	MSE	MET	modified residue	UNP Q8DW17

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	91	MSE	MET	modified residue	UNP Q8DW17
I	178	MSE	MET	modified residue	UNP Q8DW17
I	274	MSE	MET	modified residue	UNP Q8DW17
I	303	MSE	MET	modified residue	UNP Q8DW17
I	338	MSE	MET	modified residue	UNP Q8DW17
I	370	LEU	-	cloning artifact	UNP Q8DW17
I	371	GLU	-	cloning artifact	UNP Q8DW17
I	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
I	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	1	MSE	MET	modified residue	UNP Q8DW17
J	17	MSE	MET	modified residue	UNP Q8DW17
J	29	MSE	MET	modified residue	UNP Q8DW17
J	91	MSE	MET	modified residue	UNP Q8DW17
J	178	MSE	MET	modified residue	UNP Q8DW17
J	274	MSE	MET	modified residue	UNP Q8DW17
J	303	MSE	MET	modified residue	UNP Q8DW17
J	338	MSE	MET	modified residue	UNP Q8DW17
J	370	LEU	-	cloning artifact	UNP Q8DW17
J	371	GLU	-	cloning artifact	UNP Q8DW17
J	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
J	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	1	MSE	MET	modified residue	UNP Q8DW17
K	17	MSE	MET	modified residue	UNP Q8DW17
K	29	MSE	MET	modified residue	UNP Q8DW17
K	91	MSE	MET	modified residue	UNP Q8DW17
K	178	MSE	MET	modified residue	UNP Q8DW17
K	274	MSE	MET	modified residue	UNP Q8DW17
K	303	MSE	MET	modified residue	UNP Q8DW17
K	338	MSE	MET	modified residue	UNP Q8DW17
K	370	LEU	-	cloning artifact	UNP Q8DW17
K	371	GLU	-	cloning artifact	UNP Q8DW17
K	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	374	HIS	-	EXPRESSION TAG	UNP Q8DW17

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
K	377	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	1	MSE	MET	modified residue	UNP Q8DW17
L	17	MSE	MET	modified residue	UNP Q8DW17
L	29	MSE	MET	modified residue	UNP Q8DW17
L	91	MSE	MET	modified residue	UNP Q8DW17
L	178	MSE	MET	modified residue	UNP Q8DW17
L	274	MSE	MET	modified residue	UNP Q8DW17
L	303	MSE	MET	modified residue	UNP Q8DW17
L	338	MSE	MET	modified residue	UNP Q8DW17
L	370	LEU	-	cloning artifact	UNP Q8DW17
L	371	GLU	-	cloning artifact	UNP Q8DW17
L	372	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	373	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	374	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	375	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	376	HIS	-	EXPRESSION TAG	UNP Q8DW17
L	377	HIS	-	EXPRESSION TAG	UNP Q8DW17

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total 26	O 26	0	0
2	B	22	Total 22	O 22	0	0
2	C	18	Total 18	O 18	0	0
2	D	20	Total 20	O 20	0	0
2	E	15	Total 15	O 15	0	0
2	F	19	Total 19	O 19	0	0
2	G	27	Total 27	O 27	0	0
2	H	23	Total 23	O 23	0	0
2	I	13	Total 13	O 13	0	0
2	J	11	Total 11	O 11	0	0

Continued on next page...

Continued from previous page...

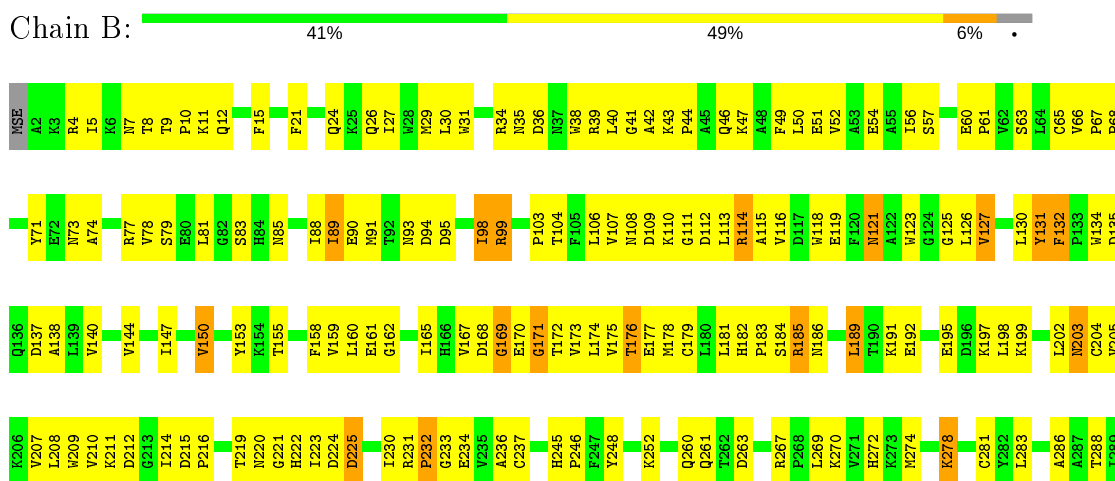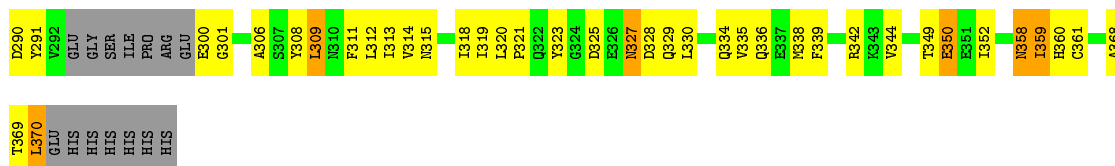| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	17	Total 17	O 17	0	0
2	L	13	Total 13	O 13	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

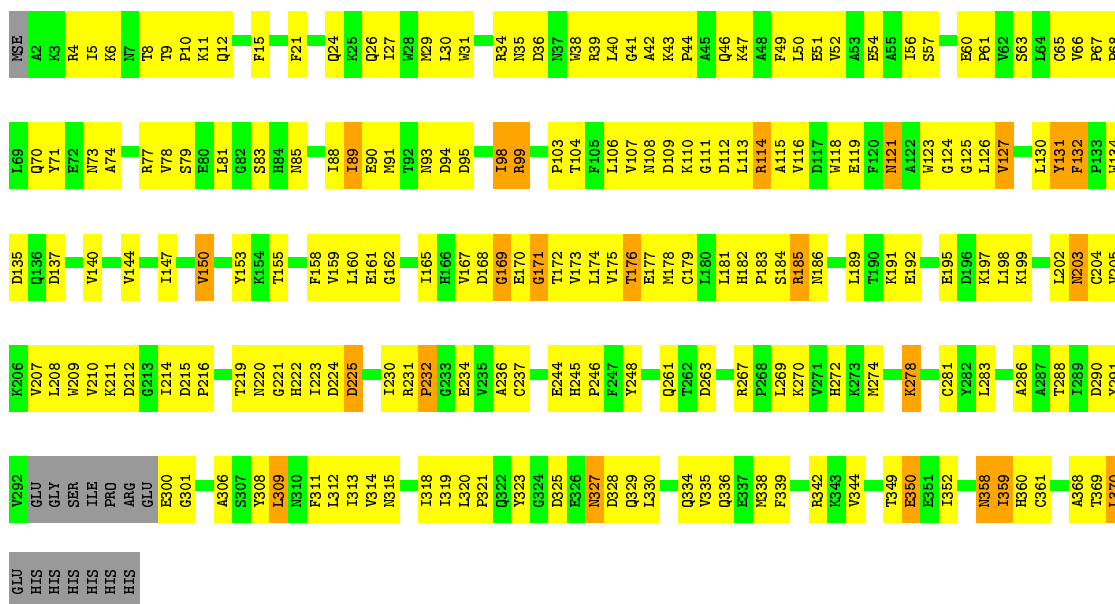- Molecule 1: Putative agmatine deiminase
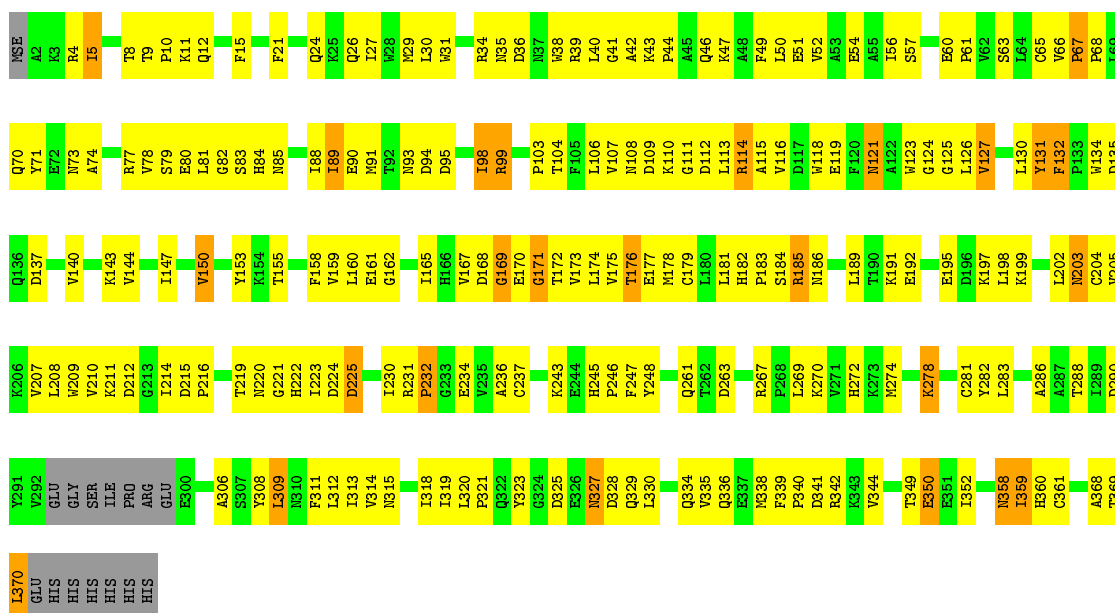

- Molecule 1: Putative agmatine deiminase

D290 Y291 V292 GLU GLY SER ILE PRO ARG GLU E300 G301 A306 S307 Y308 L309 N310 F311 L312 I313 V314 N315 I318 I319 L320 P321 Q322 Y323 G324 D325 E326 N327 D328 Q329 L330 Q334 V335 Q336 E337 M338 F339 R342 K343 V344 T349 E350 E351 I352 N358 I359 H360 C361 A368

T369 L370 GLU HIS HIS HIS HIS HIS

• Molecule 1: Putative agmatine deiminase

Chain C:

41%   49%   6%   •

MSE A2 K3 R4 I5 K6 N7 T8 T9 P10 K11 Q12 F15 F21 Q24 K25 Q26 I27 W28 M29 L30 W31 R34 N35 D36 M37 W38 R39 L40 G41 A42 K43 P44 A45 Q46 K47 A48 F49 L50 E51 V52 A53 E54 A55 I56 S57 E60 P61 V62 S63 L64 C65 V66 P67 P68

L69 Q70 Y71 E72 N73 A74 R77 V78 S79 E80 L81 G82 S83 H84 N85 I88 I89 E90 M91 T92 N93 D94 D95 I98 R99 P103 T104 F105 L106 V107 N108 D109 K110 G111 D112 L113 R114 A115 V116 D117 W118 E119 F120 N121 A122 W123 G124 G125 L126 V127 L130 Y131 F132 P133 W134

D135 Q136 D137 V140 V144 I147 V150 Y153 K154 T155 F158 V159 L160 E161 G162 I165 H166 V167 D168 G169 E170 T171 T172 V173 L174 V175 T176 E177 M178 C179 L180 L181 H182 P183 S184 R185 N186 L189 T190 K191 E192 E195 D196 K197 L198 K199 L202 N203 C204 V205

K206 V207 L208 W209 V210 K211 D212 G213 I214 D215 P216 T219 N220 G221 H222 I223 D224 D225 I230 R231 P232 G233 E234 V235 A236 C237 E244 H245 P246 F247 Y248 Q261 T262 D263 R267 P268 L269 K270 V271 H272 K273 M274 K278 C281 Y282 L283 A286 A287 T288 I289 D290 Y291

V292 GLU GLY SER ILE PRO ARG GLU E300 G301 A306 S307 Y308 L309 N310 F311 I312 I313 V314 N315 I318 I319 L320 P321 Q322 Y323 G324 D325 E326 N327 D328 Q329 L330 Q334 V335 Q336 E337 M338 F339 R342 K343 V344 T349 E350 E351 I352 N358 I359 H360 C361 A368 T369 L370

GLU HIS HIS HIS HIS HIS

• Molecule 1: Putative agmatine deiminase

Chain D:

40%   49%   7%   •

MSE A2 K3 R4 I5 T8 T9 P10 K11 Q12 F15 F21 Q24 K25 Q26 I27 M28 L30 W31 R34 N35 D36 M37 W38 R39 L40 G41 A42 K43 P44 A45 Q46 K47 A48 F49 L50 E51 V52 A53 E54 A55 I56 S57 E60 P61 V62 S63 L64 C65 V66 P67 P68 L69

Q70 Y71 E72 N73 A74 R77 V78 S79 E80 L81 G82 S83 H84 N85 I88 I89 E90 M91 T92 N93 D94 D95 I98 R99 P103 T104 F105 L106 V107 N108 D109 K110 G111 D112 L113 R114 A115 V116 D117 W118 E119 F120 N121 A122 W123 G124 G125 L126 V127 L130 Y131 F132 P133 W134 D135

Q136 D137 V140 K143 V144 I147 V150 Y153 K154 T155 F158 V159 L160 E161 G162 I165 H166 V167 D168 G169 E170 T171 T172 V173 L174 V175 T176 E177 M178 C179 L180 L181 H182 P183 S184 R185 N186 L189 T190 K191 E192 E195 D196 K197 L198 K199 L202 N203 C204 V205

K206 V207 L208 W209 V210 K211 D212 G213 I214 D215 P216 T219 N220 G221 H222 I223 D224 D225 I230 R231 P232 G233 E234 V235 A236 C237 K243 E244 H245 P246 F247 Y248 Q261 T262 D263 R267 P268 L269 K270 V271 H272 K273 M274 K278 C281 Y282 L283 A286 A287 T288 I289 D290

Y291 V292 GLU GLY SER ILE PRO ARG GLU E300 A306 S307 Y308 L309 N310 F311 I312 I313 V314 N315 I318 I319 L320 P321 Q322 Y323 G324 D325 E326 N327 D328 Q329 L330 Q334 V335 Q336 E337 M338 F339 P340 D341 R342 K343 V344 T349 E350 E351 I352 N358 I359 H360 C361 A368 T369

L370 GLU HIS HIS HIS HIS HIS

• Molecule 1: Putative agmatine deiminase

Chain E:

• Molecule 1: Putative agmatine deiminase

Chain F:

• Molecule 1: Putative agmatine deiminase
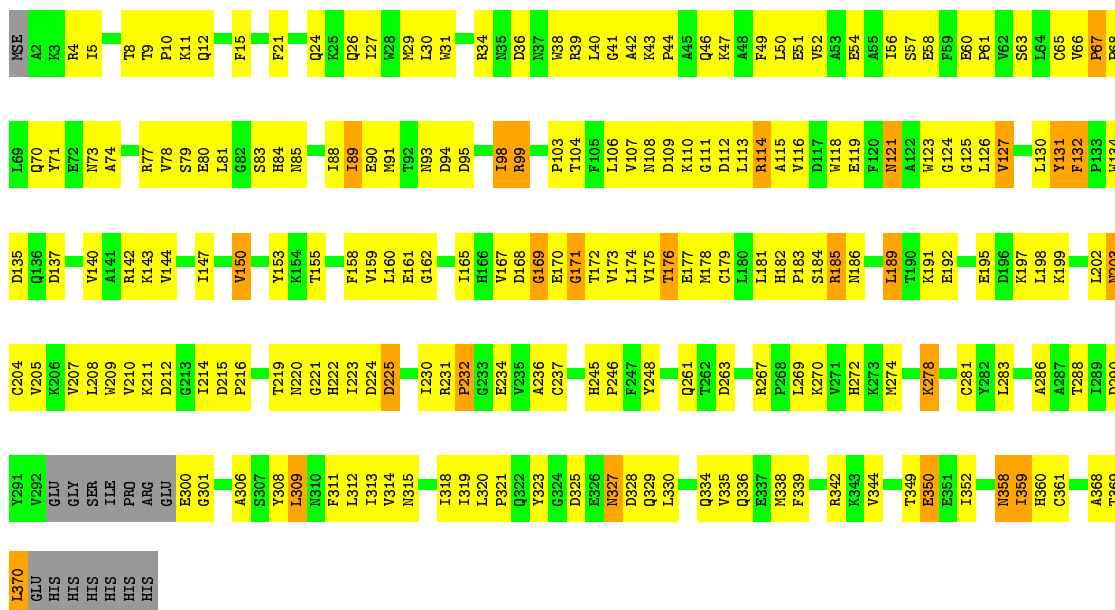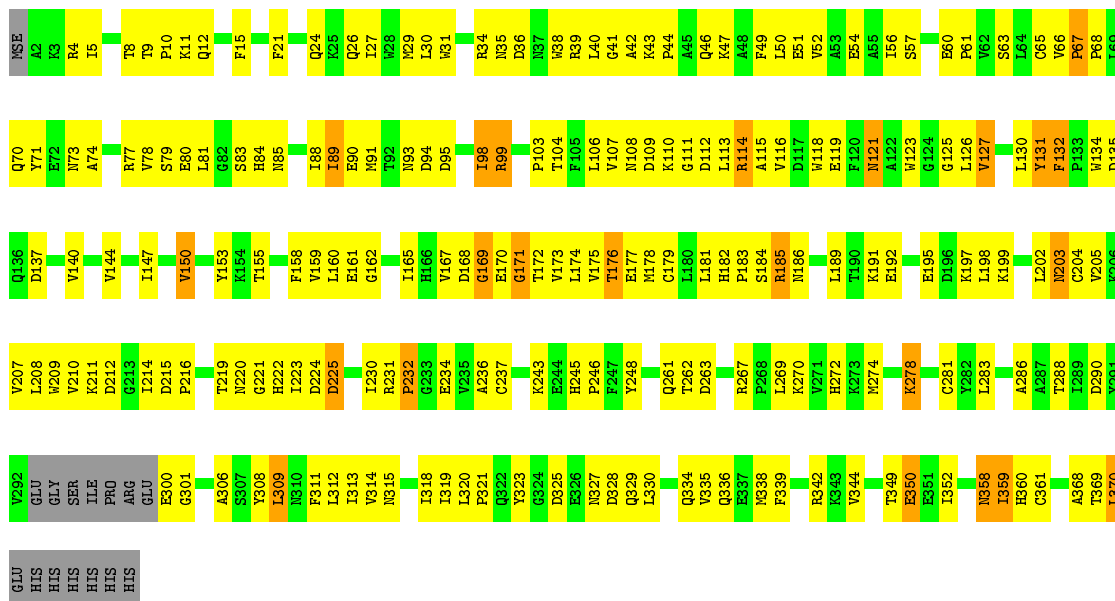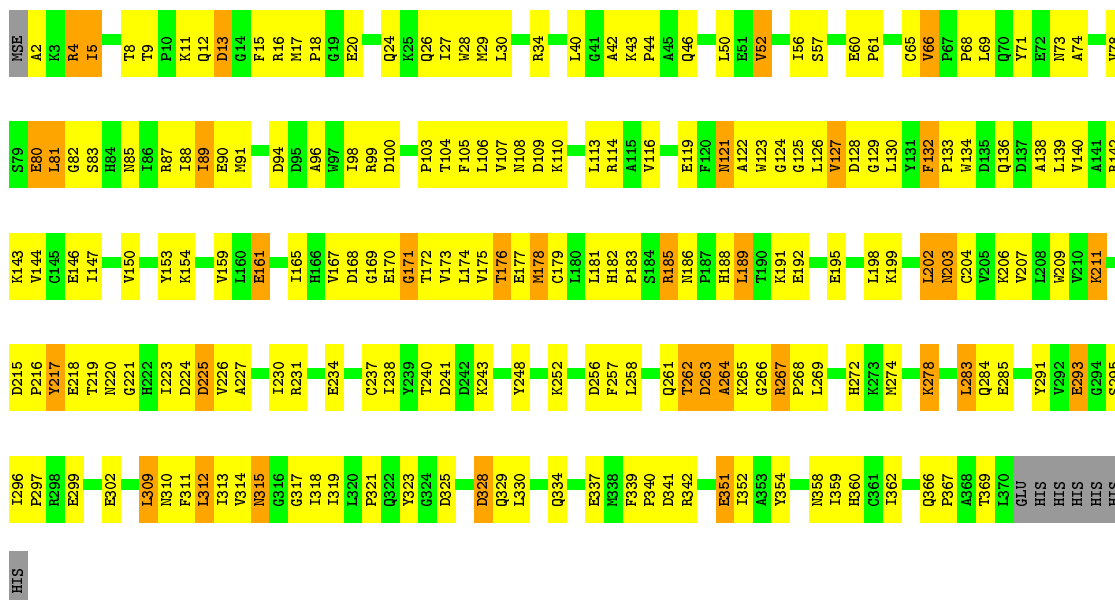
Chain G:

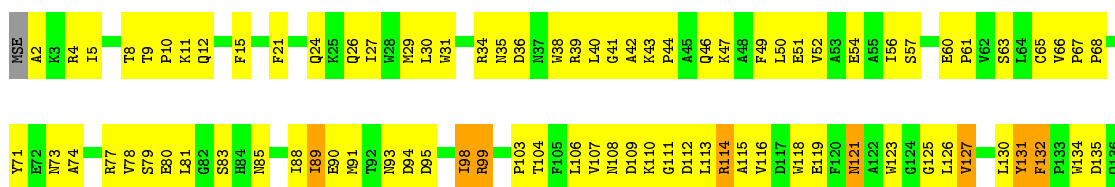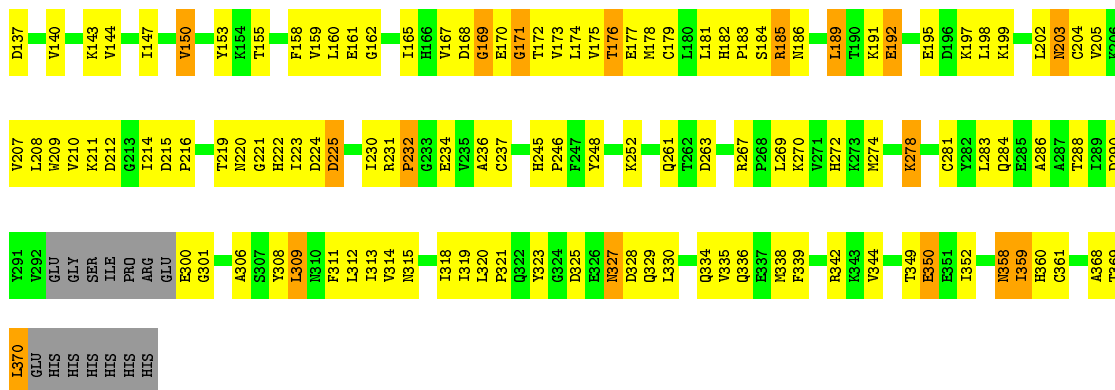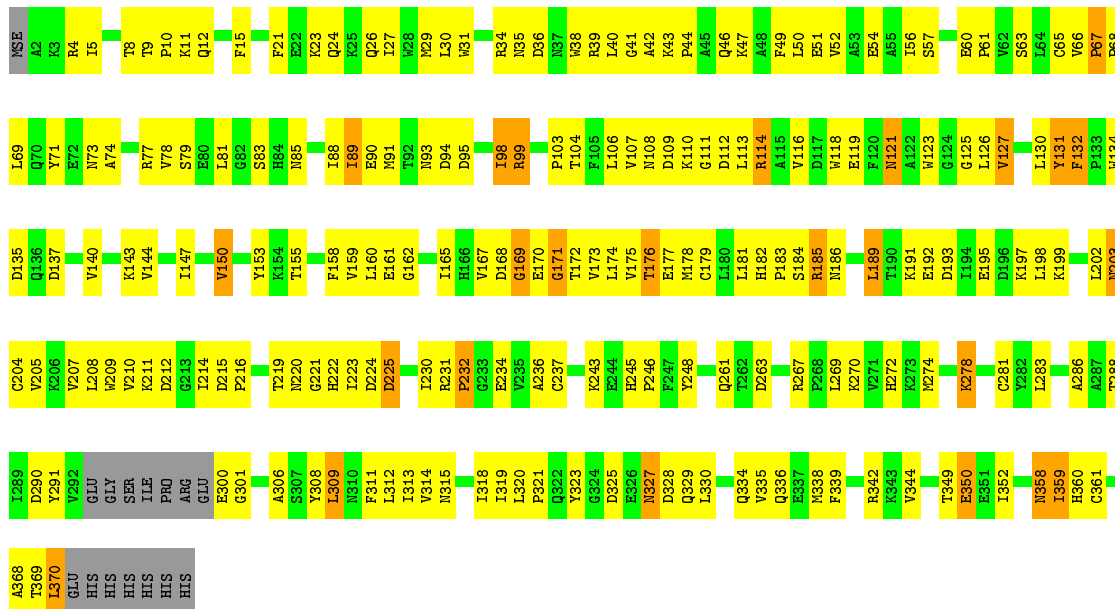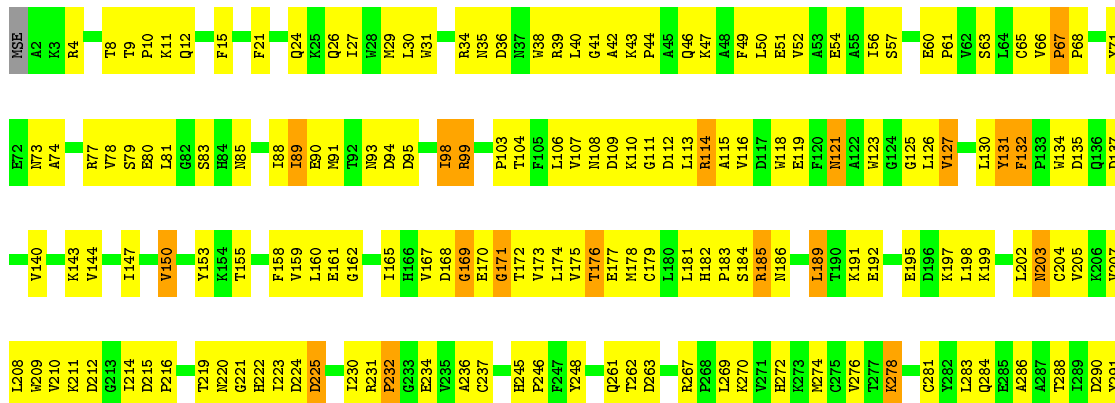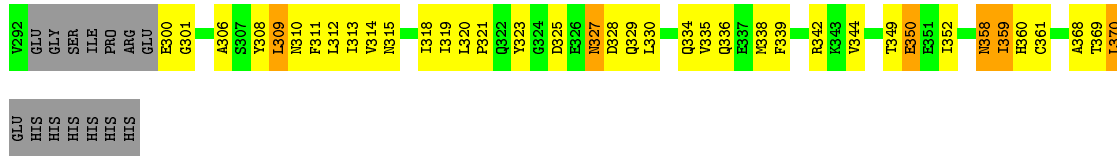• Molecule 1: Putative agmatine deiminase

Chain H:

• Molecule 1: Putative agmatine deiminase

Chain I:

• Molecule 1: Putative agmatine deiminase

Chain J:

• Molecule 1: Putative agmatine deiminase

Chain K:

V292 GLU GLY SER ILE PRO ARG GLU E300 G301 A306 S307 Y308 L309 N310 F311 L312 I313 V314 N315 I318 I319 L320 P321 Q322 Y323 G324 D325 E326 N327 D328 Q329 L330 Q334 V335 Q336 E337 M338 F339 R342 K343 V344 T349 E350 E351 I352 N358 I359 H360 C361 A368 T369 L370

GLU HIS HIS HIS HIS HIS

- **Molecule 1: Putative agmatine deiminase**

Chain L:

40%	49%	6%

MSE A2 K3 R4 I5 T8 T9 P10 K11 Q12 F15 F21 Q24 K25 Q26 I27 W28 M29 L30 W31 R34 N35 D36 N37 W38 R39 L40 G41 A42 K43 P44 A45 Q46 K47 A48 F49 L50 E51 V52 A53 E54 A55 I56 S57 E60 P61 V62 S63 L64 C65 V66 P67 P68

Y71 E72 N73 A74 L75 A76 R77 V78 S79 E80 L81 G82 S83 H84 N85 I88 I89 E90 M91 T92 N93 D94 D95 I98 R99 P103 T104 F105 L106 V107 N108 D109 K110 G111 D112 L113 R114 A115 V116 D117 W118 E119 F120 N121 A122 W123 G124 G125 L126 V127 L130 Y131 F132 P133 W134 D135

Q136 D137 V140 K143 V144 I147 V150 Y153 K154 T155 F158 V159 L160 E161 G162 I165 H166 V167 D168 G169 E170 G171 T172 V173 L174 V175 T176 E177 M178 C179 L180 L181 H182 P183 S184 R185 N186 P187 H188 L189 T190 K191 E192 E195 D196 K197 L198 K199 L202 N203 C204

V205 K206 V207 L208 W209 V210 K211 D212 G213 I214 D215 P216 T219 N220 G221 H222 I223 D224 D225 I230 R231 P232 G233 E234 V235 A236 C237 H245 P246 V247 Y248 K252 Q261 T262 D263 R267 P268 L269 K270 V271 H272 K273 M274 K278 C281 Y282 L283 A286 A287 T288 I289

D290 Y291 V292 GLU GLY SER ILE PRO ARG GLU E300 G301 A306 S307 Y308 L309 N310 F311 L312 I313 V314 N315 I318 I319 L320 P321 Q322 Y323 G324 D325 E326 N327 D328 Q329 L330 Q334 V335 Q336 E337 M338 F339 R342 K343 V344 T349 E350 E351 I352 N358 I359 H360 C361 Q365

A368 T369 L370 GLU HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.52Å 203.69Å 139.54Å 90.00° 104.72° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 29.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	83.8 (19.99-2.90) 98.5 (29.95-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.269 0.282 , 0.305	Depositor DCC
R_{free} test set	10723 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 20.2	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	34934	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

---

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

5 Model quality (i)

5.1 Standard geometry (i)

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	0.48	0/2950	0.65	0/3992
1	B	0.48	0/2950	0.65	0/3992
1	C	0.48	0/2950	0.65	0/3992
1	D	0.48	0/2950	0.65	0/3992
1	E	0.48	0/2950	0.65	0/3992
1	F	0.48	0/2950	0.65	0/3992
1	G	0.48	0/2950	0.65	0/3992
1	H	0.48	0/3006	0.68	1/4069 (0.0%)
1	I	0.48	0/2950	0.65	0/3992
1	J	0.48	0/2950	0.65	0/3992
1	K	0.48	0/2950	0.65	0/3992
1	L	0.48	0/2950	0.65	0/3992
All	All	0.48	0/35456	0.65	1/47981 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	267	ARG	NE-CZ-NH2	6.56	123.58	120.30

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	2888	0	2800	236	8
1	B	2888	0	2800	207	11
1	C	2888	0	2800	205	2
1	D	2888	0	2800	258	6
1	E	2888	0	2800	207	19
1	F	2888	0	2800	227	2
1	G	2888	0	2800	213	5
1	H	2942	0	2852	212	2
1	I	2888	0	2800	211	3
1	J	2888	0	2800	211	8
1	K	2888	0	2800	210	3
1	L	2888	0	2800	210	1
2	A	26	0	0	10	0
2	B	22	0	0	5	0
2	C	18	0	0	5	0
2	D	20	0	0	9	0
2	E	15	0	0	5	0
2	F	19	0	0	6	0
2	G	27	0	0	13	0
2	H	23	0	0	6	0
2	I	13	0	0	3	0
2	J	11	0	0	5	0
2	K	17	0	0	4	0
2	L	13	0	0	4	0
All	All	34934	0	33652	2456	35

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 36.

All (2456) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ASN:ND2	1:D:84:HIS:CE1	1.86	1.40
1:A:7:ASN:ND2	1:D:84:HIS:HE1	1.16	1.36
1:A:7:ASN:CG	1:D:84:HIS:CE1	2.06	1.28
1:A:7:ASN:CB	1:D:84:HIS:CE1	2.23	1.21
1:G:211:LYS:HG2	1:G:211:LYS:O	1.41	1.16
1:J:211:LYS:HG2	1:J:211:LYS:O	1.41	1.16
1:D:341:ASP:C	1:F:84:HIS:NE2	2.00	1.15
1:B:211:LYS:O	1:B:211:LYS:HG2	1.41	1.14
1:F:211:LYS:HG2	1:F:211:LYS:O	1.41	1.14
1:D:211:LYS:O	1:D:211:LYS:HG2	1.41	1.10

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:LYS:O	1:I:211:LYS:HG2	1.41	1.10
1:E:211:LYS:HG2	1:E:211:LYS:O	1.41	1.10
1:K:211:LYS:HG2	1:K:211:LYS:O	1.42	1.09
1:C:211:LYS:O	1:C:211:LYS:HG2	1.41	1.09
1:L:211:LYS:O	1:L:211:LYS:HG2	1.41	1.07
1:A:12:GLN:NE2	1:D:82:GLY:HA3	1.68	1.06
1:A:211:LYS:O	1:A:211:LYS:HG2	1.41	1.06
1:C:369:THR:HG23	1:C:370:LEU:N	1.71	1.06
1:I:369:THR:HG23	1:I:370:LEU:N	1.71	1.06
1:A:7:ASN:CB	1:D:84:HIS:ND1	2.18	1.06
1:J:369:THR:HG23	1:J:370:LEU:N	1.71	1.05
1:J:185:ARG:HB2	1:J:185:ARG:HH11	1.22	1.05
1:D:167:VAL:HB	2:D:391:HOH:O	1.56	1.05
1:A:185:ARG:HB2	1:A:185:ARG:HH11	1.22	1.05
1:A:369:THR:HG23	1:A:370:LEU:N	1.71	1.04
1:K:369:THR:HG23	1:K:370:LEU:N	1.71	1.04
1:D:185:ARG:HH11	1:D:185:ARG:HB2	1.22	1.03
1:J:167:VAL:HB	2:J:387:HOH:O	1.55	1.03
1:I:185:ARG:HH11	1:I:185:ARG:HB2	1.22	1.03
1:E:185:ARG:HB2	1:E:185:ARG:HH11	1.22	1.03
1:D:369:THR:HG23	1:D:370:LEU:N	1.71	1.03
1:B:369:THR:HG23	1:B:370:LEU:N	1.71	1.03
1:G:369:THR:HG23	1:G:370:LEU:N	1.71	1.03
1:F:185:ARG:HH11	1:F:185:ARG:HB2	1.22	1.02
1:L:185:ARG:HB2	1:L:185:ARG:HH11	1.22	1.02
1:G:185:ARG:HB2	1:G:185:ARG:HH11	1.22	1.02
1:F:369:THR:HG23	1:F:370:LEU:N	1.71	1.02
1:K:185:ARG:HH11	1:K:185:ARG:HB2	1.22	1.02
1:B:185:ARG:HH11	1:B:185:ARG:HB2	1.22	1.02
1:L:369:THR:HG23	1:L:370:LEU:N	1.71	1.02
1:E:369:THR:HG23	1:E:370:LEU:N	1.71	1.01
1:D:341:ASP:OD2	1:F:58:GLU:CB	2.08	1.01
1:D:342:ARG:N	1:F:84:HIS:NE2	2.08	1.01
1:C:185:ARG:HB2	1:C:185:ARG:HH11	1.22	1.00
1:D:341:ASP:OD2	1:F:58:GLU:CA	2.09	1.00
1:A:7:ASN:HD22	1:D:84:HIS:CE1	1.71	1.00
1:I:2:ALA:HB2	2:I:384:HOH:O	1.61	1.00
1:A:7:ASN:HB3	1:D:84:HIS:ND1	1.77	1.00
1:D:341:ASP:HA	1:F:84:HIS:CD2	1.98	0.98
1:B:369:THR:HG23	1:B:370:LEU:H	1.26	0.98
1:C:70:GLN:HB3	2:C:382:HOH:O	1.62	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:LYS:HE3	2:G:389:HOH:O	1.61	0.98
1:H:358:ASN:HD22	1:H:359:ILE:H	1.12	0.98
1:A:7:ASN:HB2	1:D:84:HIS:CE1	1.95	0.97
1:E:369:THR:O	1:E:370:LEU:HB2	1.64	0.97
1:C:369:THR:HG23	1:C:370:LEU:H	1.26	0.97
1:D:369:THR:HG23	1:D:370:LEU:H	1.26	0.96
1:F:369:THR:HG23	1:F:370:LEU:H	1.26	0.96
1:D:341:ASP:HB3	1:F:58:GLU:HA	1.43	0.96
1:G:369:THR:O	1:G:370:LEU:HB2	1.64	0.96
1:I:369:THR:O	1:I:370:LEU:HB2	1.64	0.96
1:L:369:THR:HG23	1:L:370:LEU:H	1.26	0.96
1:A:369:THR:O	1:A:370:LEU:HB2	1.64	0.96
1:E:70:GLN:HB3	2:E:383:HOH:O	1.65	0.95
1:B:369:THR:O	1:B:370:LEU:HB2	1.64	0.95
1:K:369:THR:O	1:K:370:LEU:HB2	1.64	0.95
1:L:369:THR:O	1:L:370:LEU:HB2	1.64	0.95
1:F:369:THR:O	1:F:370:LEU:HB2	1.64	0.95
1:G:369:THR:HG23	1:G:370:LEU:H	1.26	0.94
1:D:89:ILE:HG22	1:I:147:ILE:HG22	1.49	0.94
1:D:341:ASP:OD2	1:F:58:GLU:HA	1.65	0.94
1:E:369:THR:CG2	1:E:370:LEU:H	1.81	0.94
1:B:369:THR:CG2	1:B:370:LEU:H	1.81	0.94
1:K:369:THR:CG2	1:K:370:LEU:H	1.81	0.94
1:A:369:THR:CG2	1:A:370:LEU:H	1.81	0.94
1:F:369:THR:CG2	1:F:370:LEU:H	1.81	0.93
1:L:369:THR:CG2	1:L:370:LEU:H	1.81	0.93
1:G:79:SER:HA	1:G:83:SER:HB2	1.51	0.93
1:J:369:THR:O	1:J:370:LEU:HB2	1.64	0.93
1:D:369:THR:O	1:D:370:LEU:HB2	1.64	0.93
1:C:369:THR:O	1:C:370:LEU:HB2	1.64	0.93
1:D:369:THR:CG2	1:D:370:LEU:H	1.81	0.93
1:I:369:THR:CG2	1:I:370:LEU:H	1.81	0.93
1:G:369:THR:CG2	1:G:370:LEU:H	1.81	0.93
1:J:369:THR:CG2	1:J:370:LEU:H	1.80	0.93
1:D:147:ILE:HG22	1:I:89:ILE:HG22	1.50	0.92
1:D:79:SER:HA	1:D:83:SER:HB2	1.51	0.92
1:B:79:SER:HA	1:B:83:SER:HB2	1.51	0.92
1:J:79:SER:HA	1:J:83:SER:HB2	1.51	0.92
1:K:79:SER:HA	1:K:83:SER:HB2	1.51	0.92
1:C:369:THR:CG2	1:C:370:LEU:H	1.81	0.92
1:J:369:THR:HG23	1:J:370:LEU:H	1.26	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:369:THR:HG23	1:I:370:LEU:H	1.26	0.92
1:E:147:ILE:HG22	1:K:89:ILE:HG22	1.50	0.91
1:A:369:THR:HG23	1:A:370:LEU:H	1.26	0.91
1:E:89:ILE:HG22	1:K:147:ILE:HG22	1.51	0.91
1:D:341:ASP:CA	1:F:84:HIS:CD2	2.52	0.91
1:L:79:SER:HA	1:L:83:SER:HB2	1.51	0.91
1:F:79:SER:HA	1:F:83:SER:HB2	1.51	0.90
1:L:47:LYS:HB3	2:L:388:HOH:O	1.70	0.90
1:C:79:SER:HA	1:C:83:SER:HB2	1.51	0.90
1:E:79:SER:HA	1:E:83:SER:HB2	1.51	0.90
1:K:369:THR:HG23	1:K:370:LEU:H	1.26	0.90
1:C:89:ILE:HG22	1:J:147:ILE:HG22	1.53	0.90
1:A:12:GLN:NE2	1:D:82:GLY:CA	2.34	0.90
1:E:369:THR:HG23	1:E:370:LEU:H	1.26	0.90
1:I:99:ARG:HD2	1:I:360:HIS:O	1.72	0.89
1:I:79:SER:HA	1:I:83:SER:HB2	1.51	0.89
1:E:99:ARG:HD2	1:E:360:HIS:O	1.72	0.89
1:B:99:ARG:HD2	1:B:360:HIS:O	1.72	0.89
1:A:99:ARG:HD2	1:A:360:HIS:O	1.72	0.89
1:A:79:SER:HA	1:A:83:SER:HB2	1.51	0.89
1:H:358:ASN:ND2	1:H:359:ILE:H	1.71	0.88
1:L:89:ILE:H	1:L:89:ILE:HD13	1.38	0.88
1:K:99:ARG:HD2	1:K:360:HIS:O	1.72	0.88
1:D:99:ARG:HD2	1:D:360:HIS:O	1.72	0.88
1:F:99:ARG:HD2	1:F:360:HIS:O	1.72	0.88
1:A:89:ILE:H	1:A:89:ILE:HD13	1.38	0.88
1:A:89:ILE:HG22	1:F:147:ILE:HG22	1.56	0.88
1:I:89:ILE:H	1:I:89:ILE:HD13	1.38	0.88
1:C:369:THR:CG2	1:C:370:LEU:N	2.37	0.88
1:G:99:ARG:HD2	1:G:360:HIS:O	1.72	0.88
1:J:89:ILE:H	1:J:89:ILE:HD13	1.39	0.88
1:J:99:ARG:HD2	1:J:360:HIS:O	1.72	0.88
1:A:211:LYS:O	1:A:211:LYS:CG	2.22	0.87
1:C:89:ILE:H	1:C:89:ILE:HD13	1.38	0.87
1:D:341:ASP:CB	1:F:58:GLU:HA	2.03	0.87
1:L:99:ARG:HD2	1:L:360:HIS:O	1.72	0.87
1:C:99:ARG:HD2	1:C:360:HIS:O	1.72	0.87
1:B:89:ILE:H	1:B:89:ILE:HD13	1.38	0.87
1:I:211:LYS:O	1:I:211:LYS:CG	2.22	0.87
1:E:89:ILE:H	1:E:89:ILE:HD13	1.38	0.87
1:G:89:ILE:H	1:G:89:ILE:HD13	1.38	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:LYS:NZ	1:H:192:GLU:HG3	1.90	0.86
1:D:89:ILE:H	1:D:89:ILE:HD13	1.38	0.86
1:H:61:PRO:HA	1:H:85:ASN:HD22	1.38	0.86
1:K:165:ILE:HG22	1:K:175:VAL:HG12	1.58	0.86
1:K:369:THR:CG2	1:K:370:LEU:N	2.37	0.86
1:D:247:PHE:HE2	2:D:390:HOH:O	1.59	0.86
1:E:165:ILE:HG22	1:E:175:VAL:HG12	1.58	0.86
1:D:341:ASP:CA	1:F:84:HIS:NE2	2.38	0.86
1:A:165:ILE:HG22	1:A:175:VAL:HG12	1.58	0.86
1:D:165:ILE:HG22	1:D:175:VAL:HG12	1.58	0.86
1:J:193:ASP:HA	2:J:381:HOH:O	1.75	0.86
1:B:90:GLU:OE2	1:G:90:GLU:OE2	1.94	0.85
1:C:211:LYS:O	1:C:211:LYS:CG	2.22	0.85
1:F:165:ILE:HG22	1:F:175:VAL:HG12	1.58	0.85
1:A:369:THR:CG2	1:A:370:LEU:N	2.37	0.85
1:K:89:ILE:HD13	1:K:89:ILE:H	1.39	0.85
1:I:165:ILE:HG22	1:I:175:VAL:HG12	1.58	0.85
1:G:165:ILE:HG22	1:G:175:VAL:HG12	1.58	0.85
1:B:165:ILE:HG22	1:B:175:VAL:HG12	1.58	0.85
1:C:165:ILE:HG22	1:C:175:VAL:HG12	1.58	0.85
1:D:211:LYS:O	1:D:211:LYS:CG	2.22	0.85
1:I:369:THR:CG2	1:I:370:LEU:N	2.37	0.85
1:J:165:ILE:HG22	1:J:175:VAL:HG12	1.58	0.85
1:F:369:THR:CG2	1:F:370:LEU:N	2.37	0.85
1:F:89:ILE:HD13	1:F:89:ILE:H	1.38	0.85
1:H:113:LEU:HB2	1:H:369:THR:HG21	1.57	0.85
1:K:41:GLY:HA3	1:L:41:GLY:HA3	1.59	0.84
1:L:211:LYS:CG	1:L:211:LYS:O	2.22	0.84
1:D:341:ASP:C	1:F:84:HIS:CD2	2.49	0.84
1:D:5:ILE:HD12	2:D:384:HOH:O	1.76	0.84
1:L:165:ILE:HG22	1:L:175:VAL:HG12	1.58	0.84
1:B:111:GLY:O	1:B:369:THR:OG1	1.96	0.84
1:C:147:ILE:HG22	1:J:89:ILE:HG22	1.58	0.84
1:D:90:GLU:OE2	1:I:90:GLU:OE2	1.95	0.84
1:D:341:ASP:HA	1:F:84:HIS:NE2	1.92	0.83
1:C:111:GLY:O	1:C:369:THR:OG1	1.96	0.83
1:A:147:ILE:HG22	1:F:89:ILE:HG22	1.61	0.83
1:E:111:GLY:O	1:E:369:THR:OG1	1.96	0.83
1:B:185:ARG:NH1	1:B:185:ARG:HB2	1.94	0.82
1:H:43:LYS:HB2	1:H:44:PRO:HD3	1.61	0.82
1:H:65:CYS:SG	1:H:89:ILE:HD11	2.19	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:185:ARG:NH1	1:K:185:ARG:HB2	1.94	0.82
1:F:185:ARG:NH1	1:F:185:ARG:HB2	1.94	0.82
1:H:147:ILE:HG22	1:L:89:ILE:HG22	1.58	0.82
1:D:111:GLY:O	1:D:369:THR:OG1	1.96	0.82
1:I:111:GLY:O	1:I:369:THR:OG1	1.96	0.82
1:J:111:GLY:O	1:J:369:THR:OG1	1.96	0.82
1:E:185:ARG:HB2	1:E:185:ARG:NH1	1.94	0.82
1:F:111:GLY:O	1:F:369:THR:OG1	1.96	0.82
1:K:111:GLY:O	1:K:369:THR:OG1	1.96	0.82
1:D:185:ARG:NH1	1:D:185:ARG:HB2	1.94	0.81
1:I:185:ARG:NH1	1:I:185:ARG:HB2	1.94	0.81
1:L:111:GLY:O	1:L:369:THR:OG1	1.96	0.81
1:J:185:ARG:HB2	1:J:185:ARG:NH1	1.94	0.81
1:C:185:ARG:HB2	1:C:185:ARG:NH1	1.94	0.81
1:H:42:ALA:O	1:H:46:GLN:HG3	1.79	0.81
1:J:211:LYS:CG	1:J:211:LYS:O	2.22	0.81
1:G:185:ARG:HB2	1:G:185:ARG:NH1	1.94	0.81
1:L:185:ARG:HB2	1:L:185:ARG:NH1	1.94	0.81
1:A:111:GLY:O	1:A:369:THR:OG1	1.96	0.81
1:A:185:ARG:HB2	1:A:185:ARG:NH1	1.94	0.81
1:G:111:GLY:O	1:G:369:THR:OG1	1.96	0.80
1:G:211:LYS:CG	1:G:211:LYS:O	2.22	0.80
1:E:90:GLU:OE2	1:K:90:GLU:OE2	1.99	0.80
1:E:127:VAL:HG11	2:E:386:HOH:O	1.80	0.80
1:C:90:GLU:OE2	1:J:90:GLU:OE2	2.00	0.79
1:H:165:ILE:HD13	1:H:202:LEU:HD21	1.64	0.79
1:A:90:GLU:OE2	1:F:90:GLU:OE2	2.00	0.79
1:D:126:LEU:HD12	1:J:126:LEU:HD12	1.64	0.79
1:D:341:ASP:OD2	1:F:58:GLU:HB2	1.83	0.79
1:E:211:LYS:CG	1:E:211:LYS:O	2.22	0.79
1:K:211:LYS:O	1:K:211:LYS:CG	2.22	0.79
1:G:70:GLN:HG3	2:G:383:HOH:O	1.83	0.78
1:B:107:VAL:HG22	1:B:109:ASP:H	1.49	0.78
1:L:107:VAL:HG22	1:L:109:ASP:H	1.49	0.78
1:D:67:PRO:HD3	2:D:385:HOH:O	1.83	0.77
1:D:70:GLN:HB3	2:D:387:HOH:O	1.84	0.77
1:C:171:GLY:HA2	1:C:204:CYS:HA	1.67	0.77
1:D:171:GLY:HA2	1:D:204:CYS:HA	1.67	0.77
1:E:107:VAL:HG22	1:E:109:ASP:H	1.49	0.77
1:F:171:GLY:HA2	1:F:204:CYS:HA	1.67	0.77
1:G:107:VAL:HG22	1:G:109:ASP:H	1.49	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:ARG:HH11	1:H:185:ARG:HB2	1.47	0.77
1:J:171:GLY:HA2	1:J:204:CYS:HA	1.67	0.77
1:A:171:GLY:HA2	1:A:204:CYS:HA	1.67	0.77
1:E:171:GLY:HA2	1:E:204:CYS:HA	1.67	0.77
1:G:199:LYS:HD2	2:G:399:HOH:O	1.85	0.77
1:I:171:GLY:HA2	1:I:204:CYS:HA	1.67	0.77
1:K:107:VAL:HG22	1:K:109:ASP:H	1.49	0.77
1:H:132:PHE:HB3	1:H:133:PRO:HD3	1.64	0.76
1:A:41:GLY:HA3	1:G:41:GLY:HA3	1.67	0.76
1:C:315:ASN:HB3	2:C:390:HOH:O	1.85	0.76
1:H:24:GLN:H	1:H:315:ASN:ND2	1.84	0.76
1:J:369:THR:CG2	1:J:370:LEU:N	2.37	0.76
1:F:26:GLN:HB3	1:F:61:PRO:HG2	1.68	0.76
1:A:107:VAL:HG22	1:A:109:ASP:H	1.49	0.76
1:B:274:MSE:HE1	1:B:335:VAL:HG12	1.68	0.76
1:I:274:MSE:HE1	1:I:335:VAL:HG12	1.68	0.76
1:J:107:VAL:HG22	1:J:109:ASP:H	1.49	0.76
1:A:274:MSE:HE1	1:A:335:VAL:HG12	1.68	0.76
1:E:274:MSE:HE1	1:E:335:VAL:HG12	1.68	0.76
1:G:274:MSE:HE1	1:G:335:VAL:HG12	1.68	0.76
1:I:26:GLN:HB3	1:I:61:PRO:HG2	1.68	0.76
1:J:274:MSE:HE1	1:J:335:VAL:HG12	1.68	0.76
1:G:121:ASN:HD22	1:G:121:ASN:H	1.34	0.76
1:K:274:MSE:HE1	1:K:335:VAL:HG12	1.68	0.76
1:F:107:VAL:HG22	1:F:109:ASP:H	1.49	0.75
1:L:171:GLY:HA2	1:L:204:CYS:HA	1.67	0.75
1:D:274:MSE:HE1	1:D:335:VAL:HG12	1.68	0.75
1:A:7:ASN:CG	1:D:84:HIS:HE1	1.62	0.75
1:L:274:MSE:HE1	1:L:335:VAL:HG12	1.68	0.75
1:B:171:GLY:HA2	1:B:204:CYS:HA	1.67	0.75
1:G:171:GLY:HA2	1:G:204:CYS:HA	1.67	0.75
1:C:107:VAL:HG22	1:C:109:ASP:H	1.49	0.75
1:B:41:GLY:HA3	1:F:41:GLY:HA3	1.69	0.75
1:D:107:VAL:HG22	1:D:109:ASP:H	1.49	0.75
1:I:107:VAL:HG22	1:I:109:ASP:H	1.49	0.75
1:F:126:LEU:HD12	1:G:126:LEU:HD12	1.67	0.75
1:F:274:MSE:HE1	1:F:335:VAL:HG12	1.68	0.75
1:D:341:ASP:CG	1:F:58:GLU:HA	2.07	0.75
1:L:26:GLN:HB3	1:L:61:PRO:HG2	1.68	0.75
1:A:70:GLN:HB3	2:A:380:HOH:O	1.86	0.74
1:K:171:GLY:HA2	1:K:204:CYS:HA	1.67	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLN:HE21	1:D:82:GLY:HA3	1.52	0.74
1:A:26:GLN:HB3	1:A:61:PRO:HG2	1.68	0.74
1:B:26:GLN:HB3	1:B:61:PRO:HG2	1.68	0.74
1:E:121:ASN:H	1:E:121:ASN:HD22	1.34	0.74
1:E:127:VAL:CG1	2:E:386:HOH:O	2.33	0.74
1:E:26:GLN:HB3	1:E:61:PRO:HG2	1.68	0.74
1:C:26:GLN:HB3	1:C:61:PRO:HG2	1.68	0.74
1:G:26:GLN:HB3	1:G:61:PRO:HG2	1.68	0.74
1:B:369:THR:CG2	1:B:370:LEU:N	2.37	0.74
1:C:274:MSE:HE1	1:C:335:VAL:HG12	1.68	0.74
1:F:121:ASN:H	1:F:121:ASN:HD22	1.34	0.74
1:K:26:GLN:HB3	1:K:61:PRO:HG2	1.68	0.74
1:K:121:ASN:H	1:K:121:ASN:HD22	1.34	0.74
1:D:26:GLN:HB3	1:D:61:PRO:HG2	1.68	0.74
1:H:188:HIS:ND1	1:H:189:LEU:HD13	2.03	0.74
1:L:121:ASN:H	1:L:121:ASN:HD22	1.34	0.74
1:C:121:ASN:HD22	1:C:121:ASN:H	1.34	0.73
1:I:234:GLU:HG2	1:I:270:LYS:HB3	1.70	0.73
1:J:26:GLN:HB3	1:J:61:PRO:HG2	1.68	0.73
1:K:234:GLU:HG2	1:K:270:LYS:HB3	1.70	0.73
1:B:211:LYS:CG	1:B:211:LYS:O	2.22	0.73
1:D:135:ASP:HB3	1:J:132:PHE:CE2	2.23	0.73
1:A:234:GLU:HG2	1:A:270:LYS:HB3	1.70	0.73
1:G:336:GLN:HG2	2:G:404:HOH:O	1.87	0.73
1:D:234:GLU:HG2	1:D:270:LYS:HB3	1.70	0.73
1:B:89:ILE:HG22	1:G:147:ILE:HG22	1.69	0.73
1:A:168:ASP:OD1	1:A:172:THR:HB	1.89	0.73
1:F:211:LYS:O	1:F:211:LYS:CG	2.22	0.73
1:I:41:GLY:HA3	1:J:41:GLY:HA3	1.70	0.73
1:H:123:TRP:CE3	1:H:130:LEU:HD22	2.24	0.73
1:H:89:ILE:H	1:H:89:ILE:HD13	1.53	0.73
1:L:168:ASP:OD1	1:L:172:THR:HB	1.89	0.73
1:E:234:GLU:HG2	1:E:270:LYS:HB3	1.70	0.73
1:F:168:ASP:OD1	1:F:172:THR:HB	1.89	0.73
1:G:234:GLU:HG2	1:G:270:LYS:HB3	1.70	0.73
1:J:121:ASN:H	1:J:121:ASN:HD22	1.34	0.73
1:A:121:ASN:HD22	1:A:121:ASN:H	1.34	0.72
1:B:121:ASN:H	1:B:121:ASN:HD22	1.34	0.72
1:D:121:ASN:HD22	1:D:121:ASN:H	1.34	0.72
1:G:369:THR:CG2	1:G:370:LEU:N	2.37	0.72
1:I:168:ASP:OD1	1:I:172:THR:HB	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLU:HG2	1:C:270:LYS:HB3	1.70	0.72
1:H:165:ILE:HG22	1:H:175:VAL:HG12	1.69	0.72
1:H:89:ILE:HG22	1:L:147:ILE:HG22	1.70	0.72
1:B:234:GLU:HG2	1:B:270:LYS:HB3	1.70	0.72
1:B:290:ASP:HB3	1:F:73:ASN:ND2	2.05	0.72
1:C:168:ASP:OD1	1:C:172:THR:HB	1.89	0.72
1:E:126:LEU:HD12	1:L:126:LEU:HD12	1.71	0.72
1:D:168:ASP:OD1	1:D:172:THR:HB	1.89	0.72
1:D:243:LYS:HZ1	1:H:192:GLU:HG3	1.53	0.72
1:B:168:ASP:OD1	1:B:172:THR:HB	1.89	0.72
1:I:121:ASN:H	1:I:121:ASN:HD22	1.34	0.72
1:K:73:ASN:ND2	1:L:290:ASP:HB3	2.03	0.72
1:L:234:GLU:HG2	1:L:270:LYS:HB3	1.70	0.72
1:F:234:GLU:HG2	1:F:270:LYS:HB3	1.70	0.72
1:G:168:ASP:OD1	1:G:172:THR:HB	1.89	0.72
1:H:318:ILE:HD13	1:H:342:ARG:HD3	1.72	0.71
1:J:168:ASP:OD1	1:J:172:THR:HB	1.89	0.71
1:A:45:ALA:HB2	2:A:395:HOH:O	1.89	0.71
1:H:99:ARG:HD2	1:H:360:HIS:O	1.89	0.71
1:E:168:ASP:OD1	1:E:172:THR:HB	1.89	0.71
1:D:93:ASN:ND2	2:D:385:HOH:O	2.21	0.71
1:F:349:THR:HG21	1:F:359:ILE:HG12	1.73	0.71
1:K:168:ASP:OD1	1:K:172:THR:HB	1.89	0.71
1:L:349:THR:HG21	1:L:359:ILE:HG12	1.73	0.71
1:E:24:GLN:H	1:E:315:ASN:HD22	1.39	0.71
1:H:159:VAL:H	1:H:186:ASN:HD21	1.37	0.71
1:E:349:THR:HG21	1:E:359:ILE:HG12	1.73	0.71
1:G:349:THR:HG21	1:G:359:ILE:HG12	1.73	0.71
1:J:234:GLU:HG2	1:J:270:LYS:HB3	1.70	0.71
1:K:24:GLN:H	1:K:315:ASN:HD22	1.39	0.71
1:B:147:ILE:HG22	1:G:89:ILE:HG22	1.72	0.70
1:D:24:GLN:H	1:D:315:ASN:HD22	1.39	0.70
1:B:24:GLN:H	1:B:315:ASN:HD22	1.39	0.70
1:A:349:THR:HG21	1:A:359:ILE:HG12	1.73	0.70
1:H:274:MSE:HE3	1:H:309:LEU:HD22	1.72	0.70
1:H:24:GLN:H	1:H:315:ASN:HD22	1.38	0.70
1:D:159:VAL:H	1:D:186:ASN:HD21	1.40	0.70
1:H:121:ASN:HD22	1:H:121:ASN:H	1.38	0.70
1:A:24:GLN:H	1:A:315:ASN:HD22	1.39	0.70
1:B:349:THR:HG21	1:B:359:ILE:HG12	1.73	0.70
1:C:24:GLN:H	1:C:315:ASN:HD22	1.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:349:THR:HG21	1:K:359:ILE:HG12	1.72	0.70
1:H:178:MSE:HG2	2:H:398:HOH:O	1.92	0.69
1:J:349:THR:HG21	1:J:359:ILE:HG12	1.73	0.69
1:I:349:THR:HG21	1:I:359:ILE:HG12	1.73	0.69
1:J:24:GLN:H	1:J:315:ASN:HD22	1.39	0.69
1:L:283:LEU:HD12	1:L:286:ALA:HB2	1.75	0.69
1:A:135:ASP:HB3	1:B:132:PHE:CE2	2.27	0.69
1:H:43:LYS:NZ	1:H:46:GLN:HE22	1.89	0.69
1:B:159:VAL:H	1:B:186:ASN:HD21	1.40	0.69
1:D:349:THR:HG21	1:D:359:ILE:HG12	1.73	0.69
1:F:159:VAL:H	1:F:186:ASN:HD21	1.40	0.69
1:L:24:GLN:H	1:L:315:ASN:HD22	1.39	0.69
1:C:349:THR:HG21	1:C:359:ILE:HG12	1.73	0.69
1:K:283:LEU:HD12	1:K:286:ALA:HB2	1.74	0.69
1:I:159:VAL:H	1:I:186:ASN:HD21	1.40	0.69
1:K:159:VAL:H	1:K:186:ASN:HD21	1.40	0.69
1:C:283:LEU:HD12	1:C:286:ALA:HB2	1.75	0.69
1:D:283:LEU:HD12	1:D:286:ALA:HB2	1.75	0.69
1:L:159:VAL:H	1:L:186:ASN:HD21	1.40	0.69
1:C:135:ASP:HB3	1:I:132:PHE:CE2	2.28	0.68
1:G:27:ILE:HD12	1:G:56:ILE:HG21	1.76	0.68
1:K:27:ILE:HD12	1:K:56:ILE:HG21	1.75	0.68
1:A:283:LEU:HD12	1:A:286:ALA:HB2	1.75	0.68
1:D:247:PHE:CE2	2:D:390:HOH:O	2.38	0.68
1:F:24:GLN:H	1:F:315:ASN:HD22	1.39	0.68
1:E:24:GLN:HG3	1:E:60:GLU:OE1	1.94	0.68
1:I:24:GLN:HG3	1:I:60:GLU:OE1	1.94	0.68
1:J:159:VAL:H	1:J:186:ASN:HD21	1.40	0.68
1:K:290:ASP:HB3	1:L:73:ASN:ND2	2.09	0.68
1:C:159:VAL:H	1:C:186:ASN:HD21	1.40	0.68
1:D:24:GLN:HG3	1:D:60:GLU:OE1	1.94	0.68
1:G:24:GLN:H	1:G:315:ASN:HD22	1.39	0.68
1:H:123:TRP:HB2	1:H:130:LEU:HD13	1.73	0.68
1:I:27:ILE:HD12	1:I:56:ILE:HG21	1.76	0.68
1:A:27:ILE:HD12	1:A:56:ILE:HG21	1.75	0.68
1:E:135:ASP:HB3	1:L:132:PHE:CE2	2.28	0.68
1:A:24:GLN:HG3	1:A:60:GLU:OE1	1.94	0.68
1:B:27:ILE:HD12	1:B:56:ILE:HG21	1.76	0.68
1:A:159:VAL:H	1:A:186:ASN:HD21	1.40	0.68
1:E:283:LEU:HD12	1:E:286:ALA:HB2	1.75	0.68
1:F:24:GLN:HG3	1:F:60:GLU:OE1	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:LEU:HD12	1:G:286:ALA:HB2	1.75	0.68
1:B:283:LEU:HD12	1:B:286:ALA:HB2	1.74	0.68
1:E:27:ILE:HD12	1:E:56:ILE:HG21	1.75	0.68
1:G:261:GLN:NE2	2:G:392:HOH:O	2.26	0.68
1:I:283:LEU:HD12	1:I:286:ALA:HB2	1.75	0.68
1:I:24:GLN:HA	1:I:368:ALA:H	1.59	0.68
1:C:24:GLN:HG3	1:C:60:GLU:OE1	1.94	0.68
1:E:24:GLN:HA	1:E:368:ALA:H	1.59	0.68
1:F:283:LEU:HD12	1:F:286:ALA:HB2	1.75	0.68
1:H:43:LYS:HZ1	1:H:46:GLN:HE22	1.41	0.68
1:B:24:GLN:HG3	1:B:60:GLU:OE1	1.94	0.67
1:E:159:VAL:H	1:E:186:ASN:HD21	1.40	0.67
1:D:24:GLN:HA	1:D:368:ALA:H	1.59	0.67
1:I:24:GLN:H	1:I:315:ASN:HD22	1.39	0.67
1:J:283:LEU:HD12	1:J:286:ALA:HB2	1.75	0.67
1:K:24:GLN:HG3	1:K:60:GLU:OE1	1.94	0.67
1:A:24:GLN:HA	1:A:368:ALA:H	1.59	0.67
1:D:27:ILE:HD12	1:D:56:ILE:HG21	1.76	0.67
1:F:24:GLN:HA	1:F:368:ALA:H	1.59	0.67
1:G:24:GLN:HA	1:G:368:ALA:H	1.59	0.67
1:J:24:GLN:HG3	1:J:60:GLU:OE1	1.94	0.67
1:L:24:GLN:HG3	1:L:60:GLU:OE1	1.94	0.67
1:F:27:ILE:HD12	1:F:56:ILE:HG21	1.76	0.67
1:J:27:ILE:HD12	1:J:56:ILE:HG21	1.75	0.67
1:A:290:ASP:HB3	1:G:73:ASN:ND2	2.09	0.67
1:C:24:GLN:HA	1:C:368:ALA:H	1.59	0.67
1:C:41:GLY:HA3	1:D:41:GLY:HA3	1.76	0.67
1:G:159:VAL:H	1:G:186:ASN:HD21	1.40	0.67
1:G:361:CYS:SG	2:G:393:HOH:O	2.53	0.67
1:K:24:GLN:HA	1:K:368:ALA:H	1.59	0.67
1:G:24:GLN:HG3	1:G:60:GLU:OE1	1.94	0.67
1:B:24:GLN:HA	1:B:368:ALA:H	1.60	0.66
1:C:27:ILE:HD12	1:C:56:ILE:HG21	1.76	0.66
1:I:73:ASN:ND2	1:J:290:ASP:HB3	2.10	0.66
1:A:132:PHE:CE2	1:B:135:ASP:HB3	2.29	0.66
1:J:24:GLN:HA	1:J:368:ALA:H	1.59	0.66
1:L:27:ILE:HD12	1:L:56:ILE:HG21	1.75	0.66
1:K:276:VAL:HG13	2:K:394:HOH:O	1.96	0.65
1:F:121:ASN:ND2	2:F:389:HOH:O	2.28	0.65
1:H:177:GLU:HB3	1:H:209:TRP:HE3	1.62	0.65
1:L:24:GLN:HA	1:L:368:ALA:H	1.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLN:CD	1:D:82:GLY:HA2	2.16	0.65
1:A:315:ASN:HB3	2:A:379:HOH:O	1.97	0.65
1:H:198:LEU:HD22	1:H:202:LEU:HD22	1.78	0.65
1:A:121:ASN:ND2	2:A:392:HOH:O	2.30	0.64
1:A:133:PRO:HG2	2:A:390:HOH:O	1.96	0.64
1:C:290:ASP:HB3	1:D:73:ASN:ND2	2.11	0.64
1:D:29:MSE:HA	1:D:98:ILE:HG21	1.80	0.64
1:E:80:GLU:CD	1:H:291:TYR:OH	2.36	0.64
1:L:29:MSE:HA	1:L:98:ILE:HG21	1.80	0.64
1:E:29:MSE:HA	1:E:98:ILE:HG21	1.80	0.64
1:G:262:THR:HG22	2:G:392:HOH:O	1.95	0.64
1:A:135:ASP:HB3	1:B:132:PHE:CD2	2.33	0.64
1:B:29:MSE:HA	1:B:98:ILE:HG21	1.80	0.64
1:F:29:MSE:HA	1:F:98:ILE:HG21	1.80	0.64
1:J:71:TYR:N	2:J:386:HOH:O	2.31	0.63
1:D:191:LYS:O	1:D:195:GLU:HG3	1.99	0.63
1:I:27:ILE:HD11	1:I:314:VAL:HG12	1.81	0.63
1:K:29:MSE:HA	1:K:98:ILE:HG21	1.80	0.63
1:L:27:ILE:HD11	1:L:314:VAL:HG12	1.81	0.63
1:A:132:PHE:CD2	1:B:135:ASP:HB3	2.34	0.63
1:F:27:ILE:HD11	1:F:314:VAL:HG12	1.81	0.63
1:G:215:ASP:CG	2:G:401:HOH:O	2.37	0.63
1:I:191:LYS:O	1:I:195:GLU:HG3	1.99	0.63
1:E:27:ILE:HD11	1:E:314:VAL:HG12	1.81	0.63
1:F:185:ARG:HH22	1:F:220:ASN:HD22	1.47	0.63
1:K:191:LYS:O	1:K:195:GLU:HG3	1.99	0.63
1:A:73:ASN:ND2	1:G:290:ASP:HB3	2.14	0.63
1:J:29:MSE:HA	1:J:98:ILE:HG21	1.80	0.63
1:K:185:ARG:HH22	1:K:220:ASN:HD22	1.47	0.63
1:B:191:LYS:O	1:B:195:GLU:HG3	1.99	0.63
1:I:29:MSE:HA	1:I:98:ILE:HG21	1.80	0.63
1:J:103:PRO:HD3	1:J:144:VAL:HG11	1.81	0.63
1:C:29:MSE:HA	1:C:98:ILE:HG21	1.80	0.63
1:J:27:ILE:HD11	1:J:314:VAL:HG12	1.80	0.63
1:A:29:MSE:HA	1:A:98:ILE:HG21	1.80	0.63
1:H:312:LEU:HD22	1:H:313:ILE:N	2.13	0.63
1:I:103:PRO:HD3	1:I:144:VAL:HG11	1.81	0.63
1:A:185:ARG:HH22	1:A:220:ASN:HD22	1.47	0.62
1:D:185:ARG:HG2	2:D:396:HOH:O	1.99	0.62
1:G:191:LYS:O	1:G:195:GLU:HG3	1.99	0.62
1:L:103:PRO:HD3	1:L:144:VAL:HG11	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PRO:HD3	1:A:144:VAL:HG11	1.81	0.62
1:D:27:ILE:HD11	1:D:314:VAL:HG12	1.81	0.62
1:E:185:ARG:HH22	1:E:220:ASN:HD22	1.47	0.62
1:F:191:LYS:O	1:F:195:GLU:HG3	1.99	0.62
1:H:100:ASP:HB3	1:H:161:GLU:HB2	1.80	0.62
1:C:126:LEU:HD12	1:I:126:LEU:HD12	1.79	0.62
1:H:352:ILE:HD13	1:H:362:ILE:HD13	1.82	0.62
1:J:159:VAL:HG22	1:J:185:ARG:HD2	1.82	0.62
1:L:170:GLU:HA	2:L:389:HOH:O	1.99	0.62
1:F:159:VAL:HG22	1:F:185:ARG:HD2	1.82	0.62
1:G:103:PRO:HD3	1:G:144:VAL:HG11	1.81	0.62
1:C:15:PHE:CE2	1:C:114:ARG:HD3	2.35	0.62
1:C:191:LYS:O	1:C:195:GLU:HG3	1.99	0.62
1:E:80:GLU:CD	1:H:291:TYR:HH	2.03	0.62
1:K:103:PRO:HD3	1:K:144:VAL:HG11	1.81	0.62
1:G:15:PHE:CE2	1:G:114:ARG:HD3	2.35	0.62
1:J:15:PHE:CE2	1:J:114:ARG:HD3	2.35	0.62
1:A:159:VAL:HG22	1:A:185:ARG:HD2	1.82	0.62
1:C:27:ILE:HD11	1:C:314:VAL:HG12	1.81	0.62
1:D:159:VAL:HG22	1:D:185:ARG:HD2	1.82	0.62
1:I:15:PHE:CE2	1:I:114:ARG:HD3	2.35	0.62
1:A:15:PHE:CE2	1:A:114:ARG:HD3	2.35	0.62
1:E:103:PRO:HD3	1:E:144:VAL:HG11	1.81	0.62
1:F:15:PHE:CE2	1:F:114:ARG:HD3	2.35	0.62
1:G:159:VAL:HG22	1:G:185:ARG:HD2	1.82	0.62
1:G:29:MSE:HA	1:G:98:ILE:HG21	1.80	0.62
1:I:290:ASP:HB3	1:J:73:ASN:ND2	2.15	0.62
1:L:15:PHE:CE2	1:L:114:ARG:HD3	2.35	0.62
1:E:191:LYS:O	1:E:195:GLU:HG3	1.99	0.61
1:A:191:LYS:O	1:A:195:GLU:HG3	1.99	0.61
1:A:27:ILE:HD11	1:A:314:VAL:HG12	1.81	0.61
1:H:139:LEU:HB3	1:H:143:LYS:HE3	1.82	0.61
1:J:191:LYS:O	1:J:195:GLU:HG3	1.99	0.61
1:L:191:LYS:O	1:L:195:GLU:HG3	1.99	0.61
1:E:159:VAL:HG22	1:E:185:ARG:HD2	1.82	0.61
1:G:185:ARG:HH22	1:G:220:ASN:HD22	1.47	0.61
1:I:159:VAL:HG22	1:I:185:ARG:HD2	1.82	0.61
1:K:159:VAL:HG22	1:K:185:ARG:HD2	1.82	0.61
1:B:103:PRO:HD3	1:B:144:VAL:HG11	1.81	0.61
1:B:15:PHE:CE2	1:B:114:ARG:HD3	2.35	0.61
1:B:27:ILE:HD11	1:B:314:VAL:HG12	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HH22	1:C:220:ASN:HD22	1.47	0.61
1:J:278:LYS:HA	1:J:278:LYS:HE2	1.83	0.61
1:C:103:PRO:HD3	1:C:144:VAL:HG11	1.81	0.61
1:H:91:MSE:SE	1:H:140:VAL:HG13	2.49	0.61
1:I:185:ARG:HH22	1:I:220:ASN:HD22	1.47	0.61
1:K:27:ILE:HD11	1:K:314:VAL:HG12	1.81	0.61
1:D:185:ARG:HH22	1:D:220:ASN:HD22	1.47	0.61
1:H:18:PRO:HD3	1:H:107:VAL:HG12	1.83	0.61
1:J:185:ARG:HH22	1:J:220:ASN:HD22	1.47	0.61
1:B:159:VAL:HG22	1:B:185:ARG:HD2	1.82	0.61
1:B:278:LYS:HA	1:B:278:LYS:HE2	1.83	0.61
1:C:278:LYS:HE2	1:C:278:LYS:HA	1.83	0.61
1:D:103:PRO:HD3	1:D:144:VAL:HG11	1.81	0.61
1:D:15:PHE:CE2	1:D:114:ARG:HD3	2.35	0.61
1:K:15:PHE:CE2	1:K:114:ARG:HD3	2.35	0.61
1:B:185:ARG:HH22	1:B:220:ASN:HD22	1.47	0.61
1:E:15:PHE:CE2	1:E:114:ARG:HD3	2.35	0.61
1:G:278:LYS:HE2	1:G:278:LYS:HA	1.83	0.61
1:F:103:PRO:HD3	1:F:144:VAL:HG11	1.81	0.61
1:G:27:ILE:HD11	1:G:314:VAL:HG12	1.81	0.61
1:H:284:GLN:O	1:H:285:GLU:HB2	1.99	0.61
1:E:179:CYS:HB2	1:E:220:ASN:O	2.01	0.60
1:F:89:ILE:HD13	1:F:89:ILE:N	2.14	0.60
1:L:185:ARG:HH22	1:L:220:ASN:HD22	1.47	0.60
1:H:104:THR:HB	1:H:116:VAL:HG13	1.83	0.60
1:G:214:ILE:HG13	2:G:401:HOH:O	2.00	0.60
1:H:358:ASN:HD22	1:H:359:ILE:N	1.93	0.60
1:K:278:LYS:HA	1:K:278:LYS:HE2	1.83	0.60
1:F:15:PHE:CE2	1:F:114:ARG:HB2	2.37	0.60
1:A:278:LYS:HA	1:A:278:LYS:HE2	1.83	0.60
1:C:159:VAL:HG22	1:C:185:ARG:HD2	1.82	0.60
1:G:15:PHE:CE2	1:G:114:ARG:HB2	2.37	0.60
1:L:159:VAL:HG22	1:L:185:ARG:HD2	1.82	0.60
1:A:15:PHE:CE2	1:A:114:ARG:HB2	2.37	0.60
1:A:179:CYS:HB2	1:A:220:ASN:O	2.01	0.60
1:G:179:CYS:HB2	1:G:220:ASN:O	2.01	0.60
1:H:4:ARG:HH22	1:H:154:LYS:HD3	1.66	0.60
1:I:278:LYS:HA	1:I:278:LYS:HE2	1.83	0.60
1:C:198:LEU:O	1:C:202:LEU:HB2	2.02	0.60
1:C:9:THR:HG22	1:C:12:GLN:CD	2.23	0.60
1:I:198:LEU:O	1:I:202:LEU:HB2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:198:LEU:O	1:L:202:LEU:HB2	2.02	0.60
1:E:198:LEU:O	1:E:202:LEU:HB2	2.02	0.60
1:E:278:LYS:HE2	1:E:278:LYS:HA	1.83	0.60
1:F:198:LEU:O	1:F:202:LEU:HB2	2.02	0.60
1:H:24:GLN:HA	1:H:367:PRO:HA	1.83	0.60
1:I:15:PHE:CE2	1:I:114:ARG:HB2	2.37	0.60
1:A:9:THR:HG22	1:A:12:GLN:CD	2.23	0.59
1:C:104:THR:HB	1:C:116:VAL:HG13	1.84	0.59
1:E:9:THR:HG22	1:E:12:GLN:CD	2.22	0.59
1:J:9:THR:HG22	1:J:12:GLN:CD	2.23	0.59
1:C:15:PHE:CE2	1:C:114:ARG:HB2	2.37	0.59
1:C:179:CYS:HB2	1:C:220:ASN:O	2.01	0.59
1:J:198:LEU:O	1:J:202:LEU:HB2	2.02	0.59
1:K:89:ILE:N	1:K:89:ILE:HD13	2.14	0.59
1:B:179:CYS:HB2	1:B:220:ASN:O	2.02	0.59
1:I:179:CYS:HB2	1:I:220:ASN:O	2.02	0.59
1:J:104:THR:HB	1:J:116:VAL:HG13	1.84	0.59
1:I:77:ARG:NH2	1:J:290:ASP:OD1	2.30	0.59
1:D:179:CYS:HB2	1:D:220:ASN:O	2.01	0.59
1:G:104:THR:HB	1:G:116:VAL:HG13	1.84	0.59
1:F:132:PHE:CE2	1:G:135:ASP:HB3	2.36	0.59
1:H:230:ILE:HD11	1:H:272:HIS:CD2	2.37	0.59
1:H:80:GLU:OE1	1:H:81:LEU:HD23	2.03	0.59
1:J:89:ILE:HD13	1:J:89:ILE:N	2.15	0.59
1:K:15:PHE:CE2	1:K:114:ARG:HB2	2.37	0.59
1:L:15:PHE:CE2	1:L:114:ARG:HB2	2.37	0.59
1:A:198:LEU:O	1:A:202:LEU:HB2	2.02	0.59
1:B:15:PHE:CE2	1:B:114:ARG:HB2	2.37	0.59
1:C:132:PHE:CE2	1:I:135:ASP:HB3	2.38	0.59
1:D:104:THR:HB	1:D:116:VAL:HG13	1.84	0.59
1:D:15:PHE:CE2	1:D:114:ARG:HB2	2.37	0.59
1:D:278:LYS:HE2	1:D:278:LYS:HA	1.83	0.59
1:E:15:PHE:CE2	1:E:114:ARG:HB2	2.37	0.59
1:E:369:THR:CG2	1:E:370:LEU:N	2.37	0.59
1:D:198:LEU:O	1:D:202:LEU:HB2	2.02	0.59
1:K:179:CYS:HB2	1:K:220:ASN:O	2.02	0.59
1:L:9:THR:HG22	1:L:12:GLN:CD	2.23	0.59
1:D:9:THR:HG22	1:D:12:GLN:CD	2.23	0.59
1:F:278:LYS:HA	1:F:278:LYS:HE2	1.83	0.59
1:I:9:THR:HG22	1:I:12:GLN:CD	2.23	0.59
1:K:9:THR:HG22	1:K:12:GLN:CD	2.23	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:CYS:HB2	1:L:220:ASN:O	2.01	0.59
1:J:15:PHE:CE2	1:J:114:ARG:HB2	2.37	0.59
1:D:89:ILE:HG22	1:I:147:ILE:CG2	2.29	0.59
1:F:104:THR:HB	1:F:116:VAL:HG13	1.84	0.59
1:H:318:ILE:CD1	1:H:342:ARG:HD3	2.32	0.59
1:J:179:CYS:HB2	1:J:220:ASN:O	2.01	0.59
1:E:147:ILE:CG2	1:K:89:ILE:HG22	2.29	0.59
1:H:142:ARG:CZ	1:L:75:LEU:HD21	2.33	0.59
1:B:9:THR:HG22	1:B:12:GLN:CD	2.23	0.59
1:L:278:LYS:HE2	1:L:278:LYS:HA	1.83	0.59
1:F:9:THR:HG22	1:F:12:GLN:CD	2.23	0.58
1:J:199:LYS:HG2	1:J:204:CYS:O	2.03	0.58
1:B:89:ILE:N	1:B:89:ILE:HD13	2.14	0.58
1:D:199:LYS:HG2	1:D:204:CYS:O	2.03	0.58
1:G:198:LEU:O	1:G:202:LEU:HB2	2.02	0.58
1:I:263:ASP:OD2	1:I:267:ARG:NH1	2.37	0.58
1:J:263:ASP:OD2	1:J:267:ARG:NH1	2.36	0.58
1:B:198:LEU:O	1:B:202:LEU:HB2	2.02	0.58
1:C:171:GLY:HA3	1:C:205:VAL:HG22	1.85	0.58
1:C:263:ASP:OD2	1:C:267:ARG:NH1	2.37	0.58
1:D:185:ARG:CG	2:D:396:HOH:O	2.50	0.58
1:F:179:CYS:HB2	1:F:220:ASN:O	2.01	0.58
1:I:104:THR:HB	1:I:116:VAL:HG13	1.84	0.58
1:L:121:ASN:N	1:L:121:ASN:HD22	1.96	0.58
1:A:104:THR:HB	1:A:116:VAL:HG13	1.84	0.58
1:A:199:LYS:HG2	1:A:204:CYS:O	2.03	0.58
1:A:263:ASP:OD2	1:A:267:ARG:NH1	2.36	0.58
1:B:263:ASP:OD2	1:B:267:ARG:NH1	2.37	0.58
1:E:89:ILE:N	1:E:89:ILE:HD13	2.14	0.58
1:F:199:LYS:HG2	1:F:204:CYS:O	2.03	0.58
1:G:9:THR:HG22	1:G:12:GLN:CD	2.23	0.58
1:I:171:GLY:HA3	1:I:205:VAL:HG22	1.86	0.58
1:I:31:TRP:HB2	1:I:66:VAL:HG12	1.86	0.58
1:J:171:GLY:HA3	1:J:205:VAL:HG22	1.85	0.58
1:K:198:LEU:O	1:K:202:LEU:HB2	2.02	0.58
1:K:263:ASP:OD2	1:K:267:ARG:NH1	2.37	0.58
1:L:263:ASP:OD2	1:L:267:ARG:NH1	2.37	0.58
1:D:121:ASN:N	1:D:121:ASN:HD22	1.96	0.58
1:D:263:ASP:OD2	1:D:267:ARG:NH1	2.37	0.58
1:E:199:LYS:HG2	1:E:204:CYS:O	2.03	0.58
1:F:171:GLY:HA3	1:F:205:VAL:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:ARG:HG2	1:G:153:TYR:HE1	1.69	0.58
1:G:114:ARG:HG2	1:G:153:TYR:CE1	2.39	0.58
1:G:171:GLY:HA3	1:G:205:VAL:HG22	1.86	0.58
1:I:199:LYS:HG2	1:I:204:CYS:O	2.03	0.58
1:K:171:GLY:HA3	1:K:205:VAL:HG22	1.85	0.58
1:L:104:THR:HB	1:L:116:VAL:HG13	1.84	0.58
1:A:114:ARG:HG2	1:A:153:TYR:CE1	2.39	0.58
1:B:199:LYS:HG2	1:B:204:CYS:O	2.03	0.58
1:B:171:GLY:HA3	1:B:205:VAL:HG22	1.85	0.58
1:D:114:ARG:HG2	1:D:153:TYR:HE1	1.69	0.58
1:G:199:LYS:HG2	1:G:204:CYS:O	2.03	0.58
1:I:114:ARG:HG2	1:I:153:TYR:CE1	2.39	0.58
1:J:69:LEU:HG	2:J:380:HOH:O	2.02	0.58
1:L:114:ARG:HG2	1:L:153:TYR:HE1	1.69	0.58
1:B:104:THR:HB	1:B:116:VAL:HG13	1.84	0.58
1:C:199:LYS:HG2	1:C:204:CYS:O	2.03	0.58
1:E:159:VAL:HG12	1:E:186:ASN:ND2	2.19	0.58
1:E:263:ASP:OD2	1:E:267:ARG:NH1	2.37	0.58
1:D:147:ILE:CG2	1:I:89:ILE:HG22	2.30	0.58
1:A:114:ARG:HG2	1:A:153:TYR:HE1	1.69	0.58
1:D:27:ILE:HD12	1:D:56:ILE:CG2	2.34	0.58
1:D:31:TRP:HB2	1:D:66:VAL:HG12	1.86	0.58
1:E:114:ARG:HG2	1:E:153:TYR:HE1	1.69	0.58
1:F:27:ILE:HD12	1:F:56:ILE:CG2	2.34	0.58
1:G:177:GLU:HB3	1:G:209:TRP:CE3	2.39	0.58
1:H:105:PHE:O	1:H:106:LEU:HD23	2.03	0.58
1:H:108:ASN:ND2	1:H:110:LYS:HB2	2.18	0.58
1:H:231:ARG:HD2	1:H:234:GLU:OE2	2.04	0.58
1:J:114:ARG:HG2	1:J:153:TYR:HE1	1.69	0.58
1:K:27:ILE:HD12	1:K:56:ILE:CG2	2.34	0.58
1:K:31:TRP:HB2	1:K:66:VAL:HG12	1.86	0.58
1:A:312:LEU:HD13	1:A:313:ILE:N	2.19	0.58
1:C:114:ARG:HG2	1:C:153:TYR:HE1	1.69	0.58
1:G:170:GLU:O	1:G:172:THR:N	2.37	0.58
1:G:167:VAL:HG22	1:G:173:VAL:HG23	1.86	0.58
1:G:89:ILE:HD13	1:G:89:ILE:N	2.14	0.58
1:H:321:PRO:HB3	1:H:358:ASN:ND2	2.19	0.58
1:I:170:GLU:O	1:I:172:THR:N	2.37	0.58
1:I:159:VAL:HG12	1:I:186:ASN:ND2	2.19	0.58
1:J:31:TRP:HB2	1:J:66:VAL:HG12	1.86	0.58
1:K:114:ARG:HG2	1:K:153:TYR:CE1	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:VAL:HG12	1:K:186:ASN:ND2	2.19	0.58
1:C:312:LEU:HD13	1:C:313:ILE:N	2.19	0.58
1:C:89:ILE:HD13	1:C:89:ILE:N	2.14	0.58
1:D:114:ARG:HG2	1:D:153:TYR:CE1	2.39	0.58
1:D:177:GLU:HB3	1:D:209:TRP:CE3	2.39	0.58
1:D:312:LEU:HD13	1:D:313:ILE:N	2.19	0.58
1:E:114:ARG:HG2	1:E:153:TYR:CE1	2.39	0.58
1:H:142:ARG:NH1	1:H:146:GLU:HG2	2.19	0.58
1:H:88:ILE:HD12	1:H:88:ILE:N	2.19	0.58
1:K:114:ARG:HG2	1:K:153:TYR:HE1	1.69	0.58
1:K:312:LEU:HD13	1:K:313:ILE:N	2.19	0.58
1:K:34:ARG:HD2	1:K:94:ASP:O	2.04	0.58
1:A:31:TRP:HB2	1:A:66:VAL:HG12	1.86	0.57
1:B:177:GLU:HB3	1:B:209:TRP:CE3	2.39	0.57
1:B:312:LEU:HD13	1:B:313:ILE:N	2.19	0.57
1:C:167:VAL:HG22	1:C:173:VAL:HG23	1.86	0.57
1:C:34:ARG:HD2	1:C:94:ASP:O	2.04	0.57
1:D:170:GLU:O	1:D:172:THR:N	2.37	0.57
1:D:89:ILE:N	1:D:89:ILE:HD13	2.14	0.57
1:E:177:GLU:HB3	1:E:209:TRP:CE3	2.39	0.57
1:F:170:GLU:O	1:F:172:THR:N	2.37	0.57
1:I:27:ILE:HD12	1:I:56:ILE:CG2	2.34	0.57
1:I:312:LEU:HD13	1:I:313:ILE:N	2.19	0.57
1:J:170:GLU:O	1:J:172:THR:N	2.37	0.57
1:J:312:LEU:HD13	1:J:313:ILE:N	2.19	0.57
1:K:199:LYS:HG2	1:K:204:CYS:O	2.03	0.57
1:L:89:ILE:N	1:L:89:ILE:HD13	2.14	0.57
1:C:170:GLU:O	1:C:172:THR:N	2.37	0.57
1:D:121:ASN:ND2	1:D:159:VAL:HG21	2.19	0.57
1:E:104:THR:HB	1:E:116:VAL:HG13	1.84	0.57
1:F:114:ARG:HG2	1:F:153:TYR:HE1	1.69	0.57
1:G:159:VAL:HG12	1:G:186:ASN:ND2	2.19	0.57
1:H:167:VAL:HG13	1:H:172:THR:O	2.02	0.57
1:K:104:THR:HB	1:K:116:VAL:HG13	1.84	0.57
1:K:170:GLU:O	1:K:172:THR:N	2.37	0.57
1:L:177:GLU:HB3	1:L:209:TRP:CE3	2.39	0.57
1:L:34:ARG:HD2	1:L:94:ASP:O	2.04	0.57
1:A:170:GLU:O	1:A:172:THR:N	2.37	0.57
1:A:27:ILE:HD12	1:A:56:ILE:CG2	2.34	0.57
1:F:263:ASP:OD2	1:F:267:ARG:NH1	2.37	0.57
1:H:224:ASP:HB2	1:H:360:HIS:CD2	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:ILE:N	1:I:89:ILE:HD13	2.14	0.57
1:L:159:VAL:HG12	1:L:186:ASN:ND2	2.19	0.57
1:A:159:VAL:HG12	1:A:186:ASN:ND2	2.19	0.57
1:C:159:VAL:HG12	1:C:186:ASN:ND2	2.19	0.57
1:C:121:ASN:ND2	1:C:159:VAL:HG21	2.20	0.57
1:C:31:TRP:HB2	1:C:66:VAL:HG12	1.86	0.57
1:D:159:VAL:HG12	1:D:186:ASN:ND2	2.19	0.57
1:E:312:LEU:HD13	1:E:313:ILE:N	2.19	0.57
1:F:159:VAL:HG12	1:F:186:ASN:ND2	2.19	0.57
1:F:312:LEU:HD13	1:F:313:ILE:N	2.19	0.57
1:H:90:GLU:OE2	1:L:90:GLU:OE2	2.22	0.57
1:I:114:ARG:HG2	1:I:153:TYR:HE1	1.69	0.57
1:L:114:ARG:HG2	1:L:153:TYR:CE1	2.39	0.57
1:L:199:LYS:HG2	1:L:204:CYS:O	2.03	0.57
1:L:312:LEU:HD13	1:L:313:ILE:N	2.19	0.57
1:B:114:ARG:HG2	1:B:153:TYR:HE1	1.69	0.57
1:B:34:ARG:HD2	1:B:94:ASP:O	2.04	0.57
1:C:177:GLU:HB3	1:C:209:TRP:CE3	2.39	0.57
1:F:167:VAL:HG22	1:F:173:VAL:HG23	1.86	0.57
1:A:177:GLU:HB3	1:A:209:TRP:CE3	2.39	0.57
1:C:27:ILE:HD12	1:C:56:ILE:CG2	2.34	0.57
1:E:121:ASN:N	1:E:121:ASN:HD22	1.96	0.57
1:E:171:GLY:HA3	1:E:205:VAL:HG22	1.86	0.57
1:E:27:ILE:HD12	1:E:56:ILE:CG2	2.34	0.57
1:G:263:ASP:OD2	1:G:267:ARG:NH1	2.37	0.57
1:G:27:ILE:HD12	1:G:56:ILE:CG2	2.34	0.57
1:H:319:ILE:HG22	1:H:359:ILE:HD13	1.85	0.57
1:H:61:PRO:CA	1:H:85:ASN:HD22	2.13	0.57
1:J:114:ARG:HG2	1:J:153:TYR:CE1	2.39	0.57
1:K:167:VAL:HG22	1:K:173:VAL:HG23	1.86	0.57
1:L:170:GLU:O	1:L:172:THR:N	2.37	0.57
1:L:27:ILE:HD12	1:L:56:ILE:CG2	2.34	0.57
1:B:170:GLU:O	1:B:172:THR:N	2.37	0.57
1:G:34:ARG:HD2	1:G:94:ASP:O	2.04	0.57
1:I:121:ASN:ND2	1:I:159:VAL:HG21	2.20	0.57
1:J:159:VAL:HG12	1:J:186:ASN:ND2	2.19	0.57
1:C:135:ASP:HB3	1:I:132:PHE:CD2	2.40	0.57
1:C:114:ARG:HG2	1:C:153:TYR:CE1	2.39	0.57
1:D:171:GLY:HA3	1:D:205:VAL:HG22	1.85	0.57
1:I:177:GLU:HB3	1:I:209:TRP:CE3	2.39	0.57
1:A:121:ASN:ND2	1:A:159:VAL:HG21	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLY:HA3	1:A:205:VAL:HG22	1.86	0.57
1:A:34:ARG:HD2	1:A:94:ASP:O	2.04	0.57
1:E:31:TRP:HB2	1:E:66:VAL:HG12	1.86	0.57
1:G:121:ASN:ND2	1:G:159:VAL:HG21	2.19	0.57
1:J:177:GLU:HB3	1:J:209:TRP:CE3	2.39	0.57
1:K:121:ASN:ND2	1:K:159:VAL:HG21	2.20	0.57
1:L:171:GLY:HA3	1:L:205:VAL:HG22	1.85	0.57
1:B:77:ARG:O	1:B:81:LEU:HG	2.05	0.57
1:F:114:ARG:HG2	1:F:153:TYR:CE1	2.39	0.57
1:G:312:LEU:HD13	1:G:313:ILE:N	2.19	0.57
1:E:290:ASP:HB3	1:H:73:ASN:ND2	2.20	0.57
1:J:77:ARG:O	1:J:81:LEU:HG	2.05	0.57
1:L:31:TRP:HB2	1:L:66:VAL:HG12	1.86	0.57
1:L:77:ARG:O	1:L:81:LEU:HG	2.05	0.57
1:B:114:ARG:HG2	1:B:153:TYR:CE1	2.39	0.56
1:D:167:VAL:HG22	1:D:173:VAL:HG23	1.86	0.56
1:E:167:VAL:HG22	1:E:173:VAL:HG23	1.86	0.56
1:F:177:GLU:HB3	1:F:209:TRP:CE3	2.39	0.56
1:I:34:ARG:HD2	1:I:94:ASP:O	2.04	0.56
1:J:121:ASN:ND2	1:J:159:VAL:HG21	2.20	0.56
1:L:121:ASN:ND2	1:L:159:VAL:HG21	2.19	0.56
1:B:27:ILE:HD12	1:B:56:ILE:CG2	2.34	0.56
1:C:6:LYS:HB2	2:C:393:HOH:O	2.05	0.56
1:D:342:ARG:N	1:F:84:HIS:CE1	2.72	0.56
1:E:170:GLU:O	1:E:172:THR:N	2.37	0.56
1:F:121:ASN:ND2	1:F:159:VAL:HG21	2.19	0.56
1:F:34:ARG:HD2	1:F:94:ASP:O	2.04	0.56
1:F:31:TRP:HB2	1:F:66:VAL:HG12	1.86	0.56
1:H:330:LEU:O	1:H:334:GLN:HG3	2.05	0.56
1:H:87:ARG:HG3	1:H:87:ARG:O	2.04	0.56
1:K:77:ARG:O	1:K:81:LEU:HG	2.05	0.56
1:A:77:ARG:O	1:A:81:LEU:HG	2.05	0.56
1:B:159:VAL:HG12	1:B:186:ASN:ND2	2.19	0.56
1:B:31:TRP:HB2	1:B:66:VAL:HG12	1.86	0.56
1:E:121:ASN:ND2	1:E:159:VAL:HG21	2.19	0.56
1:G:31:TRP:HB2	1:G:66:VAL:HG12	1.86	0.56
1:J:34:ARG:HD2	1:J:94:ASP:O	2.04	0.56
1:K:106:LEU:O	1:K:113:LEU:HD12	2.06	0.56
1:L:167:VAL:HG22	1:L:173:VAL:HG23	1.86	0.56
1:A:167:VAL:HG22	1:A:173:VAL:HG23	1.86	0.56
1:C:106:LEU:O	1:C:113:LEU:HD12	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ARG:O	1:D:81:LEU:HG	2.05	0.56
1:B:9:THR:HG22	1:B:12:GLN:OE1	2.06	0.56
1:H:159:VAL:HG22	1:H:185:ARG:HD2	1.86	0.56
1:J:27:ILE:HD12	1:J:56:ILE:CG2	2.34	0.56
1:A:106:LEU:O	1:A:113:LEU:HD12	2.06	0.56
1:B:121:ASN:ND2	1:B:159:VAL:HG21	2.20	0.56
1:D:106:LEU:O	1:D:113:LEU:HD12	2.06	0.56
1:D:34:ARG:HD2	1:D:94:ASP:O	2.04	0.56
1:E:106:LEU:O	1:E:113:LEU:HD12	2.06	0.56
1:E:9:THR:HG22	1:E:12:GLN:OE1	2.06	0.56
1:H:283:LEU:HD12	1:H:302:GLU:HG2	1.87	0.56
1:I:106:LEU:O	1:I:113:LEU:HD12	2.06	0.56
1:K:174:LEU:HB3	1:K:223:ILE:HD13	1.88	0.56
1:B:174:LEU:HB3	1:B:223:ILE:HD13	1.88	0.56
1:E:34:ARG:HD2	1:E:94:ASP:O	2.04	0.56
1:F:135:ASP:HB3	1:G:132:PHE:CE2	2.40	0.56
1:L:174:LEU:HB3	1:L:223:ILE:HD13	1.88	0.56
1:A:9:THR:HG22	1:A:12:GLN:OE1	2.06	0.56
1:B:106:LEU:O	1:B:113:LEU:HD12	2.06	0.56
1:H:2:ALA:HB1	1:H:146:GLU:OE2	2.05	0.56
1:I:167:VAL:HG22	1:I:173:VAL:HG23	1.86	0.56
1:I:9:THR:HG22	1:I:12:GLN:OE1	2.06	0.56
1:K:177:GLU:HB3	1:K:209:TRP:CE3	2.39	0.56
1:B:127:VAL:HG13	1:B:184:SER:HB2	1.88	0.56
1:C:77:ARG:O	1:C:81:LEU:HG	2.05	0.56
1:J:167:VAL:HG22	1:J:173:VAL:HG23	1.86	0.56
1:J:195:GLU:O	1:J:199:LYS:HG3	2.06	0.56
1:K:127:VAL:HG13	1:K:184:SER:HB2	1.88	0.56
1:A:127:VAL:HG13	1:A:184:SER:HB2	1.88	0.56
1:A:89:ILE:N	1:A:89:ILE:HD13	2.14	0.56
1:C:43:LYS:NZ	1:C:46:GLN:HE22	2.04	0.56
1:F:127:VAL:HG13	1:F:184:SER:HB2	1.88	0.56
1:F:174:LEU:HB3	1:F:223:ILE:HD13	1.88	0.56
1:F:43:LYS:NZ	1:F:46:GLN:HE22	2.04	0.56
1:H:337:GLU:O	1:H:340:PRO:HD3	2.06	0.56
1:I:65:CYS:SG	1:I:89:ILE:HD11	2.46	0.56
1:J:106:LEU:O	1:J:113:LEU:HD12	2.06	0.56
1:J:174:LEU:HB3	1:J:223:ILE:HD13	1.88	0.56
1:J:65:CYS:SG	1:J:89:ILE:HD11	2.46	0.56
1:L:65:CYS:SG	1:L:89:ILE:HD11	2.46	0.56
1:C:349:THR:HG21	1:C:359:ILE:CG1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:GLU:O	1:D:199:LYS:HG3	2.06	0.56
1:D:340:PRO:HG2	1:F:58:GLU:O	2.06	0.56
1:E:77:ARG:O	1:E:81:LEU:HG	2.05	0.56
1:G:77:ARG:O	1:G:81:LEU:HG	2.05	0.56
1:G:9:THR:HG22	1:G:12:GLN:OE1	2.06	0.56
1:H:165:ILE:HG22	1:H:175:VAL:CG1	2.36	0.56
1:I:127:VAL:HG13	1:I:184:SER:HB2	1.88	0.56
1:J:127:VAL:HG13	1:J:184:SER:HB2	1.88	0.56
1:K:195:GLU:O	1:K:199:LYS:HG3	2.06	0.56
1:L:43:LYS:NZ	1:L:46:GLN:HE22	2.04	0.56
1:A:65:CYS:SG	1:A:89:ILE:HD11	2.47	0.55
1:C:9:THR:HG22	1:C:12:GLN:OE1	2.06	0.55
1:C:195:GLU:O	1:C:199:LYS:HG3	2.06	0.55
1:I:195:GLU:O	1:I:199:LYS:HG3	2.06	0.55
1:K:43:LYS:NZ	1:K:46:GLN:HE22	2.04	0.55
1:L:195:GLU:O	1:L:199:LYS:HG3	2.06	0.55
1:A:195:GLU:O	1:A:199:LYS:HG3	2.06	0.55
1:B:167:VAL:HG22	1:B:173:VAL:HG23	1.86	0.55
1:B:65:CYS:SG	1:B:89:ILE:HD11	2.46	0.55
1:D:127:VAL:HG13	1:D:184:SER:HB2	1.88	0.55
1:G:106:LEU:O	1:G:113:LEU:HD12	2.06	0.55
1:I:174:LEU:HB3	1:I:223:ILE:HD13	1.88	0.55
1:K:9:THR:HG22	1:K:12:GLN:OE1	2.06	0.55
1:A:43:LYS:NZ	1:A:46:GLN:HE22	2.04	0.55
1:G:127:VAL:HG13	1:G:184:SER:HB2	1.88	0.55
1:G:174:LEU:HB3	1:G:223:ILE:HD13	1.88	0.55
1:I:252:LYS:HD3	2:I:387:HOH:O	2.06	0.55
1:I:43:LYS:NZ	1:I:46:GLN:HE22	2.04	0.55
1:L:127:VAL:HG13	1:L:184:SER:HB2	1.88	0.55
1:B:349:THR:HG21	1:B:359:ILE:CG1	2.36	0.55
1:C:174:LEU:HB3	1:C:223:ILE:HD13	1.88	0.55
1:E:65:CYS:SG	1:E:89:ILE:HD11	2.46	0.55
1:F:77:ARG:O	1:F:81:LEU:HG	2.05	0.55
1:G:43:LYS:NZ	1:G:46:GLN:HE22	2.04	0.55
1:G:65:CYS:SG	1:G:89:ILE:HD11	2.46	0.55
1:I:77:ARG:O	1:I:81:LEU:HG	2.05	0.55
1:K:283:LEU:CD1	1:K:286:ALA:HB2	2.37	0.55
1:K:349:THR:HG21	1:K:359:ILE:CG1	2.36	0.55
1:A:318:ILE:HB	1:A:344:VAL:HG22	1.89	0.55
1:D:65:CYS:SG	1:D:89:ILE:HD11	2.46	0.55
1:H:65:CYS:HB3	1:H:91:MSE:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:318:ILE:HB	1:I:344:VAL:HG22	1.89	0.55
1:A:349:THR:HG21	1:A:359:ILE:CG1	2.36	0.55
1:C:127:VAL:HG13	1:C:184:SER:HB2	1.88	0.55
1:D:281:CYS:SG	1:D:306:ALA:HB2	2.47	0.55
1:D:43:LYS:NZ	1:D:46:GLN:HE22	2.04	0.55
1:E:174:LEU:HB3	1:E:223:ILE:HD13	1.88	0.55
1:G:195:GLU:O	1:G:199:LYS:HG3	2.06	0.55
1:E:40:LEU:HD12	1:H:40:LEU:HD12	1.89	0.55
1:J:349:THR:HG21	1:J:359:ILE:CG1	2.36	0.55
1:K:65:CYS:SG	1:K:89:ILE:HD11	2.46	0.55
1:E:281:CYS:SG	1:E:306:ALA:HB2	2.47	0.55
1:E:318:ILE:HB	1:E:344:VAL:HG22	1.89	0.55
1:F:195:GLU:O	1:F:199:LYS:HG3	2.06	0.55
1:F:9:THR:HG22	1:F:12:GLN:OE1	2.06	0.55
1:H:30:LEU:HG	1:H:98:ILE:HB	1.89	0.55
1:J:121:ASN:N	1:J:121:ASN:HD22	1.96	0.55
1:K:281:CYS:SG	1:K:306:ALA:HB2	2.47	0.55
1:A:174:LEU:HB3	1:A:223:ILE:HD13	1.88	0.55
1:B:281:CYS:SG	1:B:306:ALA:HB2	2.47	0.55
1:B:283:LEU:CD1	1:B:286:ALA:HB2	2.36	0.55
1:I:349:THR:HG21	1:I:359:ILE:CG1	2.36	0.55
1:L:106:LEU:O	1:L:113:LEU:HD12	2.06	0.55
1:L:281:CYS:SG	1:L:306:ALA:HB2	2.47	0.55
1:L:9:THR:HG22	1:L:12:GLN:OE1	2.06	0.55
1:E:195:GLU:O	1:E:199:LYS:HG3	2.06	0.55
1:F:349:THR:HG21	1:F:359:ILE:CG1	2.36	0.55
1:L:349:THR:HG21	1:L:359:ILE:CG1	2.37	0.55
1:A:12:GLN:CD	1:D:82:GLY:CA	2.75	0.55
1:A:283:LEU:CD1	1:A:286:ALA:HB2	2.37	0.55
1:A:281:CYS:SG	1:A:306:ALA:HB2	2.47	0.55
1:B:195:GLU:O	1:B:199:LYS:HG3	2.06	0.55
1:B:73:ASN:ND2	1:F:290:ASP:HB3	2.22	0.55
1:D:135:ASP:HB3	1:J:132:PHE:HE2	1.70	0.55
1:F:106:LEU:O	1:F:113:LEU:HD12	2.06	0.55
1:F:65:CYS:SG	1:F:89:ILE:HD11	2.46	0.55
2:C:392:HOH:O	1:J:147:ILE:C	2.44	0.55
1:J:281:CYS:SG	1:J:306:ALA:HB2	2.47	0.55
1:L:283:LEU:CD1	1:L:286:ALA:HB2	2.37	0.55
1:A:74:ALA:O	1:A:78:VAL:HG23	2.07	0.54
1:B:43:LYS:NZ	1:B:46:GLN:HE22	2.04	0.54
1:D:174:LEU:HB3	1:D:223:ILE:HD13	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:CYS:SG	1:G:306:ALA:HB2	2.47	0.54
1:H:122:ALA:O	1:H:129:GLY:HA2	2.07	0.54
1:H:252:LYS:HG2	1:H:256:ASP:OD2	2.07	0.54
1:I:321:PRO:HD3	1:I:359:ILE:HD12	1.89	0.54
1:J:283:LEU:CD1	1:J:286:ALA:HB2	2.37	0.54
1:L:9:THR:HG22	1:L:12:GLN:HG3	1.89	0.54
1:B:74:ALA:O	1:B:78:VAL:HG23	2.08	0.54
1:C:283:LEU:CD1	1:C:286:ALA:HB2	2.37	0.54
1:D:318:ILE:HB	1:D:344:VAL:HG22	1.89	0.54
1:E:349:THR:HG21	1:E:359:ILE:CG1	2.36	0.54
1:G:318:ILE:HB	1:G:344:VAL:HG22	1.89	0.54
1:C:65:CYS:SG	1:C:89:ILE:HD11	2.46	0.54
1:D:9:THR:HG22	1:D:12:GLN:HG3	1.89	0.54
1:E:309:LEU:O	1:E:309:LEU:HD13	2.08	0.54
1:E:43:LYS:NZ	1:E:46:GLN:HE22	2.04	0.54
1:F:74:ALA:O	1:F:78:VAL:HG23	2.08	0.54
1:I:281:CYS:SG	1:I:306:ALA:HB2	2.47	0.54
1:J:321:PRO:HD3	1:J:359:ILE:HD12	1.90	0.54
1:J:43:LYS:NZ	1:J:46:GLN:HE22	2.04	0.54
1:J:74:ALA:O	1:J:78:VAL:HG23	2.07	0.54
1:J:9:THR:HG22	1:J:12:GLN:OE1	2.06	0.54
1:L:318:ILE:HB	1:L:344:VAL:HG22	1.89	0.54
1:C:281:CYS:SG	1:C:306:ALA:HB2	2.47	0.54
1:H:262:THR:HG23	2:H:395:HOH:O	2.07	0.54
1:I:74:ALA:O	1:I:78:VAL:HG23	2.07	0.54
1:L:74:ALA:O	1:L:78:VAL:HG23	2.07	0.54
1:C:309:LEU:O	1:C:309:LEU:HD13	2.08	0.54
1:E:127:VAL:HG13	1:E:184:SER:HB2	1.88	0.54
1:F:283:LEU:CD1	1:F:286:ALA:HB2	2.37	0.54
1:G:309:LEU:O	1:G:309:LEU:HD13	2.08	0.54
1:H:107:VAL:HG22	1:H:109:ASP:H	1.73	0.54
1:I:9:THR:HG22	1:I:12:GLN:HG3	1.89	0.54
1:L:309:LEU:HD13	1:L:309:LEU:O	2.08	0.54
1:A:320:LEU:HD13	1:A:335:VAL:HG11	1.90	0.54
1:A:321:PRO:HD3	1:A:359:ILE:HD12	1.90	0.54
1:B:318:ILE:HB	1:B:344:VAL:HG22	1.89	0.54
1:C:74:ALA:O	1:C:78:VAL:HG23	2.07	0.54
1:D:309:LEU:O	1:D:309:LEU:HD13	2.08	0.54
1:G:283:LEU:CD1	1:G:286:ALA:HB2	2.37	0.54
1:H:257:PHE:O	1:H:261:GLN:HG2	2.08	0.54
1:H:170:GLU:HG3	1:H:267:ARG:HH22	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:PRO:HD3	1:C:359:ILE:HD12	1.90	0.54
1:D:9:THR:HG22	1:D:12:GLN:OE1	2.06	0.54
1:E:9:THR:HG22	1:E:12:GLN:HG3	1.90	0.54
1:K:320:LEU:HD13	1:K:335:VAL:HG11	1.90	0.54
1:K:318:ILE:HB	1:K:344:VAL:HG22	1.89	0.54
1:F:318:ILE:HB	1:F:344:VAL:HG22	1.89	0.54
1:G:321:PRO:HD3	1:G:359:ILE:HD12	1.90	0.54
1:J:309:LEU:HD13	1:J:309:LEU:O	2.08	0.54
1:J:88:ILE:N	1:J:88:ILE:HD12	2.23	0.54
1:K:321:PRO:HD3	1:K:359:ILE:HD12	1.90	0.54
1:B:121:ASN:HD22	1:B:121:ASN:N	1.96	0.54
1:C:88:ILE:HD12	1:C:88:ILE:N	2.23	0.54
2:C:385:HOH:O	1:D:70:GLN:HG3	2.08	0.54
1:E:321:PRO:HD3	1:E:359:ILE:HD12	1.90	0.54
1:F:9:THR:HG22	1:F:12:GLN:HG3	1.89	0.54
1:F:281:CYS:SG	1:F:306:ALA:HB2	2.47	0.54
1:H:43:LYS:NZ	1:H:46:GLN:NE2	2.55	0.54
1:A:121:ASN:N	1:A:121:ASN:HD22	1.96	0.54
1:A:9:THR:HG22	1:A:12:GLN:HG3	1.90	0.54
1:B:321:PRO:HD3	1:B:359:ILE:HD12	1.90	0.54
1:B:88:ILE:N	1:B:88:ILE:HD12	2.23	0.54
1:C:15:PHE:CD2	1:C:114:ARG:HB2	2.43	0.54
1:C:89:ILE:HG22	1:J:147:ILE:CG2	2.32	0.54
1:D:74:ALA:O	1:D:78:VAL:HG23	2.07	0.54
1:F:309:LEU:O	1:F:309:LEU:HD13	2.08	0.54
1:G:320:LEU:HD13	1:G:335:VAL:HG11	1.90	0.54
1:J:318:ILE:HB	1:J:344:VAL:HG22	1.89	0.54
1:K:9:THR:HG22	1:K:12:GLN:HG3	1.89	0.54
1:B:369:THR:O	1:B:370:LEU:CB	2.47	0.53
1:C:318:ILE:HB	1:C:344:VAL:HG22	1.89	0.53
1:D:283:LEU:CD1	1:D:286:ALA:HB2	2.37	0.53
1:D:88:ILE:HD12	1:D:88:ILE:N	2.23	0.53
1:E:320:LEU:HD13	1:E:335:VAL:HG11	1.90	0.53
1:F:121:ASN:N	1:F:121:ASN:HD22	1.96	0.53
1:F:88:ILE:HD12	1:F:88:ILE:N	2.23	0.53
1:G:88:ILE:N	1:G:88:ILE:HD12	2.23	0.53
1:H:176:THR:HG21	1:H:221:GLY:O	2.07	0.53
1:H:27:ILE:HD12	1:H:56:ILE:HD12	1.90	0.53
1:L:321:PRO:HD3	1:L:359:ILE:HD12	1.90	0.53
1:G:9:THR:HG22	1:G:12:GLN:HG3	1.89	0.53
1:H:124:GLY:HA3	1:H:128:ASP:C	2.28	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:66:VAL:CG2	1:H:71:TYR:HA	2.38	0.53
1:J:15:PHE:CD2	1:J:114:ARG:HB2	2.43	0.53
1:K:309:LEU:O	1:K:309:LEU:HD13	2.08	0.53
1:L:320:LEU:HD13	1:L:335:VAL:HG11	1.90	0.53
1:B:320:LEU:HD13	1:B:335:VAL:HG11	1.90	0.53
1:D:349:THR:HG21	1:D:359:ILE:CG1	2.36	0.53
1:B:291:TYR:OH	1:F:80:GLU:HB2	2.08	0.53
1:G:349:THR:HG21	1:G:359:ILE:CG1	2.36	0.53
1:G:74:ALA:O	1:G:78:VAL:HG23	2.08	0.53
1:A:309:LEU:HD13	1:A:309:LEU:O	2.08	0.53
1:B:9:THR:HG22	1:B:12:GLN:HG3	1.89	0.53
1:D:15:PHE:CD2	1:D:114:ARG:HB2	2.43	0.53
1:E:132:PHE:CE2	1:L:135:ASP:HB3	2.43	0.53
1:G:15:PHE:CD2	1:G:114:ARG:HB2	2.44	0.53
1:K:15:PHE:CZ	1:K:114:ARG:HD3	2.44	0.53
1:L:88:ILE:N	1:L:88:ILE:HD12	2.23	0.53
1:B:312:LEU:HD12	1:B:314:VAL:CG1	2.39	0.53
1:D:320:LEU:HD13	1:D:335:VAL:HG11	1.90	0.53
1:H:185:ARG:HH22	1:H:220:ASN:HD22	1.57	0.53
1:I:15:PHE:CZ	1:I:114:ARG:HD3	2.44	0.53
1:I:43:LYS:NZ	1:J:35:ASN:HD22	2.06	0.53
1:J:9:THR:HG22	1:J:12:GLN:HG3	1.89	0.53
1:K:121:ASN:N	1:K:121:ASN:HD22	1.96	0.53
1:A:7:ASN:HB2	1:D:84:HIS:NE2	2.22	0.53
1:D:312:LEU:HD12	1:D:314:VAL:CG1	2.39	0.53
1:I:15:PHE:CD2	1:I:114:ARG:HB2	2.44	0.53
1:I:283:LEU:CD1	1:I:286:ALA:HB2	2.37	0.53
1:I:312:LEU:HD12	1:I:314:VAL:CG1	2.39	0.53
1:K:15:PHE:CD2	1:K:114:ARG:HB2	2.43	0.53
1:L:15:PHE:CZ	1:L:114:ARG:HD3	2.44	0.53
1:A:15:PHE:CZ	1:A:114:ARG:HD3	2.44	0.53
1:A:312:LEU:HD12	1:A:314:VAL:CG1	2.39	0.53
1:C:121:ASN:N	1:C:121:ASN:HD22	1.96	0.53
1:C:320:LEU:HD13	1:C:335:VAL:HG11	1.90	0.53
1:E:74:ALA:O	1:E:78:VAL:HG23	2.08	0.53
1:F:15:PHE:CZ	1:F:114:ARG:HD3	2.44	0.53
1:K:74:ALA:O	1:K:78:VAL:HG23	2.07	0.53
1:L:15:PHE:CD2	1:L:114:ARG:HB2	2.43	0.53
1:E:135:ASP:HB3	1:L:132:PHE:CD2	2.44	0.53
1:F:15:PHE:CD2	1:F:114:ARG:HB2	2.43	0.53
1:F:312:LEU:HD12	1:F:314:VAL:CG1	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:LEU:HD12	1:K:314:VAL:CG1	2.39	0.53
1:B:15:PHE:CD2	1:B:114:ARG:HB2	2.44	0.53
1:B:309:LEU:O	1:B:309:LEU:HD13	2.08	0.53
1:C:9:THR:HG22	1:C:12:GLN:HG3	1.89	0.53
1:F:321:PRO:HD3	1:F:359:ILE:HD12	1.90	0.53
1:G:210:VAL:HG12	1:G:211:LYS:N	2.24	0.53
1:D:243:LYS:HZ3	1:H:192:GLU:HG3	1.73	0.53
1:H:174:LEU:HD22	1:H:223:ILE:HD11	1.91	0.53
1:J:15:PHE:CZ	1:J:114:ARG:HD3	2.44	0.53
1:A:15:PHE:CD2	1:A:114:ARG:HB2	2.44	0.53
1:C:15:PHE:CZ	1:C:114:ARG:HD3	2.44	0.53
1:D:11:LYS:HG3	1:D:203:ASN:HD21	1.74	0.53
1:F:11:LYS:HG3	1:F:203:ASN:HD21	1.74	0.53
1:F:320:LEU:HD13	1:F:335:VAL:HG11	1.90	0.53
1:G:121:ASN:HD22	1:G:121:ASN:N	1.96	0.53
1:G:15:PHE:CZ	1:G:114:ARG:HD3	2.44	0.53
1:H:124:GLY:O	1:H:128:ASP:N	2.39	0.53
1:K:88:ILE:HD12	1:K:88:ILE:N	2.23	0.53
1:L:312:LEU:HD12	1:L:314:VAL:CG1	2.39	0.53
1:D:321:PRO:HD3	1:D:359:ILE:HD12	1.90	0.52
1:E:283:LEU:CD1	1:E:286:ALA:HB2	2.37	0.52
1:I:121:ASN:ND2	1:I:121:ASN:H	2.06	0.52
1:I:309:LEU:HD13	1:I:309:LEU:O	2.08	0.52
1:J:11:LYS:HG3	1:J:203:ASN:HD21	1.74	0.52
1:J:320:LEU:HD13	1:J:335:VAL:HG11	1.90	0.52
1:B:15:PHE:CZ	1:B:114:ARG:HD3	2.44	0.52
1:C:261:GLN:O	1:C:269:LEU:HD13	2.10	0.52
1:E:312:LEU:HD12	1:E:314:VAL:CG1	2.39	0.52
1:E:88:ILE:HD12	1:E:88:ILE:N	2.23	0.52
1:A:77:ARG:NH2	1:G:290:ASP:OD1	2.37	0.52
1:A:312:LEU:HD12	1:A:314:VAL:HG12	1.92	0.52
1:A:88:ILE:HD12	1:A:88:ILE:N	2.23	0.52
1:B:261:GLN:O	1:B:269:LEU:HD13	2.10	0.52
1:B:290:ASP:CB	1:F:73:ASN:ND2	2.72	0.52
1:C:121:ASN:ND2	1:C:121:ASN:H	2.07	0.52
1:E:15:PHE:CD2	1:E:114:ARG:HB2	2.43	0.52
1:G:11:LYS:CE	2:G:389:HOH:O	2.34	0.52
1:G:312:LEU:HD12	1:G:314:VAL:CG1	2.39	0.52
1:H:26:GLN:HG2	1:H:366:GLN:HE21	1.75	0.52
1:J:312:LEU:HD12	1:J:314:VAL:CG1	2.39	0.52
1:K:210:VAL:HG12	1:K:211:LYS:N	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:TRP:HB2	1:L:130:LEU:HD13	1.92	0.52
1:L:210:VAL:HG12	1:L:211:LYS:N	2.24	0.52
1:B:121:ASN:H	1:B:121:ASN:ND2	2.07	0.52
1:E:15:PHE:CZ	1:E:114:ARG:HD3	2.44	0.52
1:E:214:ILE:C	1:E:216:PRO:HD3	2.30	0.52
1:E:89:ILE:HG22	1:K:147:ILE:CG2	2.31	0.52
1:I:11:LYS:HG3	1:I:203:ASN:HD21	1.74	0.52
1:I:121:ASN:N	1:I:121:ASN:HD22	1.96	0.52
1:K:261:GLN:O	1:K:269:LEU:HD13	2.10	0.52
1:L:11:LYS:HG3	1:L:203:ASN:HD21	1.74	0.52
1:D:123:TRP:HB2	1:D:130:LEU:HD13	1.92	0.52
1:D:214:ILE:C	1:D:216:PRO:HD3	2.30	0.52
1:I:210:VAL:HG12	1:I:211:LYS:N	2.24	0.52
1:I:320:LEU:HD13	1:I:335:VAL:HG11	1.90	0.52
1:I:88:ILE:HD12	1:I:88:ILE:N	2.23	0.52
1:C:312:LEU:HD12	1:C:314:VAL:CG1	2.39	0.52
1:D:312:LEU:HD12	1:D:314:VAL:HG12	1.92	0.52
1:F:210:VAL:HG12	1:F:211:LYS:N	2.24	0.52
1:H:168:ASP:OD2	1:H:170:GLU:HG2	2.09	0.52
1:J:336:GLN:HG2	2:J:382:HOH:O	2.10	0.52
1:A:11:LYS:HG3	1:A:203:ASN:HD21	1.74	0.52
1:D:15:PHE:CZ	1:D:114:ARG:HD3	2.44	0.52
1:D:210:VAL:HG12	1:D:211:LYS:N	2.24	0.52
1:F:219:THR:HG21	2:F:396:HOH:O	2.09	0.52
1:I:312:LEU:HD12	1:I:314:VAL:HG12	1.92	0.52
1:C:214:ILE:C	1:C:216:PRO:HD3	2.30	0.52
1:D:135:ASP:HB3	1:J:132:PHE:CD2	2.44	0.52
1:D:311:PHE:HB3	1:D:320:LEU:HD12	1.92	0.52
1:G:214:ILE:C	1:G:216:PRO:HD3	2.30	0.52
1:I:214:ILE:C	1:I:216:PRO:HD3	2.30	0.52
1:J:312:LEU:HD12	1:J:314:VAL:HG12	1.92	0.52
1:K:11:LYS:HG3	1:K:203:ASN:HD21	1.74	0.52
1:F:137:ASP:HA	1:F:140:VAL:HG23	1.92	0.52
1:G:261:GLN:O	1:G:269:LEU:HD13	2.10	0.52
1:G:311:PHE:HB3	1:G:320:LEU:HD12	1.92	0.52
1:H:71:TYR:CZ	1:L:143:LYS:HG2	2.45	0.52
1:J:123:TRP:HB2	1:J:130:LEU:HD13	1.92	0.52
1:J:214:ILE:C	1:J:216:PRO:HD3	2.30	0.52
1:K:281:CYS:HA	2:K:391:HOH:O	2.10	0.52
1:K:312:LEU:HD12	1:K:314:VAL:HG12	1.92	0.52
1:A:214:ILE:C	1:A:216:PRO:HD3	2.30	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:HB2	1:A:44:PRO:HD3	1.93	0.51
1:C:9:THR:OG1	1:C:10:PRO:HD2	2.11	0.51
1:H:215:ASP:HB3	1:H:218:GLU:HB3	1.91	0.51
1:K:123:TRP:HB2	1:K:130:LEU:HD13	1.92	0.51
1:L:214:ILE:C	1:L:216:PRO:HD3	2.30	0.51
1:L:43:LYS:HB2	1:L:44:PRO:HD3	1.93	0.51
1:A:210:VAL:HG12	1:A:211:LYS:N	2.24	0.51
1:B:9:THR:OG1	1:B:10:PRO:HD2	2.10	0.51
1:C:159:VAL:HG12	1:C:186:ASN:HD21	1.76	0.51
1:F:312:LEU:HD12	1:F:314:VAL:HG12	1.92	0.51
1:G:49:PHE:O	1:G:52:VAL:HG12	2.10	0.51
1:I:261:GLN:O	1:I:269:LEU:HD13	2.10	0.51
1:J:210:VAL:HG12	1:J:211:LYS:N	2.24	0.51
1:A:311:PHE:HB3	1:A:320:LEU:HD12	1.92	0.51
1:D:49:PHE:O	1:D:52:VAL:HG12	2.10	0.51
1:E:261:GLN:O	1:E:269:LEU:HD13	2.10	0.51
1:E:49:PHE:O	1:E:52:VAL:HG12	2.10	0.51
1:E:9:THR:OG1	1:E:10:PRO:HD2	2.11	0.51
1:F:159:VAL:HG12	1:F:186:ASN:HD21	1.76	0.51
1:G:11:LYS:HG3	1:G:203:ASN:HD21	1.74	0.51
1:G:43:LYS:HB2	1:G:44:PRO:HD3	1.92	0.51
1:H:174:LEU:HD21	1:H:258:LEU:HD21	1.93	0.51
1:H:274:MSE:HE1	1:H:311:PHE:HE2	1.75	0.51
1:J:261:GLN:O	1:J:269:LEU:HD13	2.10	0.51
1:J:49:PHE:O	1:J:52:VAL:HG12	2.10	0.51
1:A:261:GLN:O	1:A:269:LEU:HD13	2.09	0.51
1:B:11:LYS:HG3	1:B:203:ASN:HD21	1.74	0.51
1:B:311:PHE:HB3	1:B:320:LEU:HD12	1.92	0.51
1:C:311:PHE:HB3	1:C:320:LEU:HD12	1.92	0.51
1:E:11:LYS:HG3	1:E:203:ASN:HD21	1.74	0.51
1:F:123:TRP:HB2	1:F:130:LEU:HD13	1.92	0.51
1:G:123:TRP:HB2	1:G:130:LEU:HD13	1.92	0.51
1:H:26:GLN:HG2	1:H:366:GLN:NE2	2.25	0.51
1:I:43:LYS:HB2	1:I:44:PRO:HD3	1.93	0.51
1:J:159:VAL:HG12	1:J:186:ASN:HD21	1.76	0.51
1:K:49:PHE:O	1:K:52:VAL:HG12	2.10	0.51
1:L:137:ASP:HA	1:L:140:VAL:HG23	1.92	0.51
1:A:123:TRP:HB2	1:A:130:LEU:HD13	1.92	0.51
1:A:137:ASP:HA	1:A:140:VAL:HG23	1.92	0.51
1:B:49:PHE:O	1:B:52:VAL:HG12	2.10	0.51
1:C:49:PHE:O	1:C:52:VAL:HG12	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:LYS:HB2	1:F:44:PRO:HD3	1.92	0.51
1:F:9:THR:OG1	1:F:10:PRO:HD2	2.11	0.51
1:I:123:TRP:HB2	1:I:130:LEU:HD13	1.92	0.51
1:I:9:THR:OG1	1:I:10:PRO:HD2	2.11	0.51
1:L:261:GLN:O	1:L:269:LEU:HD13	2.10	0.51
1:L:9:THR:OG1	1:L:10:PRO:HD2	2.11	0.51
1:C:123:TRP:HB2	1:C:130:LEU:HD13	1.92	0.51
1:C:210:VAL:HG12	1:C:211:LYS:N	2.24	0.51
1:C:369:THR:O	1:C:370:LEU:CB	2.47	0.51
1:E:43:LYS:HB2	1:E:44:PRO:HD3	1.92	0.51
1:H:321:PRO:HB3	1:H:358:ASN:HD21	1.73	0.51
1:J:137:ASP:HA	1:J:140:VAL:HG23	1.92	0.51
1:L:311:PHE:HB3	1:L:320:LEU:HD12	1.92	0.51
1:D:121:ASN:ND2	1:D:121:ASN:H	2.07	0.51
1:D:261:GLN:O	1:D:269:LEU:HD13	2.10	0.51
1:E:159:VAL:HG12	1:E:186:ASN:HD21	1.76	0.51
1:F:261:GLN:O	1:F:269:LEU:HD13	2.10	0.51
1:A:49:PHE:O	1:A:52:VAL:HG12	2.10	0.51
1:C:68:PRO:HG3	1:C:90:GLU:OE2	2.11	0.51
1:D:137:ASP:HA	1:D:140:VAL:HG23	1.92	0.51
1:G:9:THR:OG1	1:G:10:PRO:HD2	2.11	0.51
1:H:167:VAL:HG22	1:H:173:VAL:HG23	1.93	0.51
1:H:317:GLY:O	1:H:318:ILE:HD12	2.11	0.51
1:I:68:PRO:HG3	1:I:90:GLU:OE2	2.11	0.51
1:J:43:LYS:HB2	1:J:44:PRO:HD3	1.93	0.51
1:K:174:LEU:O	1:K:223:ILE:HD13	2.11	0.51
1:A:315:ASN:CA	2:A:379:HOH:O	2.58	0.51
1:A:9:THR:OG1	1:A:10:PRO:HD2	2.11	0.51
1:B:214:ILE:C	1:B:216:PRO:HD3	2.30	0.51
1:F:49:PHE:O	1:F:52:VAL:HG12	2.10	0.51
1:G:137:ASP:HA	1:G:140:VAL:HG23	1.92	0.51
1:G:312:LEU:HD12	1:G:314:VAL:HG12	1.92	0.51
1:K:177:GLU:HB3	1:K:209:TRP:HE3	1.76	0.51
1:K:214:ILE:C	1:K:216:PRO:HD3	2.30	0.51
1:L:312:LEU:HD12	1:L:314:VAL:HG12	1.92	0.51
1:A:159:VAL:HG12	1:A:186:ASN:HD21	1.76	0.51
1:D:43:LYS:HB2	1:D:44:PRO:HD3	1.93	0.51
1:D:68:PRO:HG3	1:D:90:GLU:OE2	2.11	0.51
1:E:132:PHE:O	1:E:134:TRP:CE3	2.64	0.51
1:I:49:PHE:O	1:I:52:VAL:HG12	2.10	0.51
1:J:174:LEU:O	1:J:223:ILE:HD13	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:68:PRO:HG3	1:L:90:GLU:OE2	2.11	0.51
1:B:137:ASP:HA	1:B:140:VAL:HG23	1.92	0.50
1:B:210:VAL:HG12	1:B:211:LYS:N	2.24	0.50
1:C:137:ASP:HA	1:C:140:VAL:HG23	1.92	0.50
1:C:11:LYS:HG3	1:C:203:ASN:HD21	1.74	0.50
1:C:290:ASP:OD1	1:D:77:ARG:NH2	2.36	0.50
1:D:140:VAL:O	1:D:144:VAL:HG12	2.12	0.50
1:D:9:THR:OG1	1:D:10:PRO:HD2	2.11	0.50
1:E:140:VAL:O	1:E:144:VAL:HG12	2.12	0.50
1:E:210:VAL:HG12	1:E:211:LYS:N	2.24	0.50
1:I:137:ASP:HA	1:I:140:VAL:HG23	1.92	0.50
1:I:177:GLU:HB3	1:I:209:TRP:HE3	1.76	0.50
1:K:137:ASP:HA	1:K:140:VAL:HG23	1.92	0.50
1:B:123:TRP:HB2	1:B:130:LEU:HD13	1.92	0.50
1:B:159:VAL:HG12	1:B:186:ASN:HD21	1.76	0.50
1:B:312:LEU:HD12	1:B:314:VAL:HG12	1.92	0.50
1:C:174:LEU:O	1:C:223:ILE:HD13	2.11	0.50
1:E:312:LEU:HD12	1:E:314:VAL:HG12	1.92	0.50
1:F:174:LEU:O	1:F:223:ILE:HD13	2.11	0.50
1:I:159:VAL:HG12	1:I:186:ASN:HD21	1.76	0.50
1:I:174:LEU:O	1:I:223:ILE:HD13	2.11	0.50
1:J:132:PHE:O	1:J:134:TRP:CE3	2.64	0.50
1:K:311:PHE:HB3	1:K:320:LEU:HD12	1.92	0.50
1:D:158:PHE:HE1	1:D:160:LEU:HB2	1.76	0.50
1:D:174:LEU:O	1:D:223:ILE:HD13	2.11	0.50
1:F:177:GLU:HB3	1:F:209:TRP:HE3	1.76	0.50
1:G:132:PHE:O	1:G:134:TRP:CE3	2.64	0.50
1:H:43:LYS:HZ1	1:H:46:GLN:NE2	2.08	0.50
1:K:43:LYS:HZ2	1:K:46:GLN:HE22	1.57	0.50
1:B:158:PHE:HE1	1:B:160:LEU:HB2	1.76	0.50
1:E:123:TRP:HB2	1:E:130:LEU:HD13	1.92	0.50
1:E:311:PHE:HB3	1:E:320:LEU:HD12	1.92	0.50
1:E:41:GLY:O	1:E:42:ALA:HB3	2.12	0.50
1:F:132:PHE:CD2	1:G:135:ASP:HB3	2.47	0.50
1:F:132:PHE:O	1:F:134:TRP:CE3	2.64	0.50
1:H:311:PHE:HE1	1:H:313:ILE:HD11	1.75	0.50
1:I:140:VAL:O	1:I:144:VAL:HG12	2.12	0.50
1:K:158:PHE:HE1	1:K:160:LEU:HB2	1.76	0.50
1:A:41:GLY:O	1:A:42:ALA:HB3	2.12	0.50
1:A:7:ASN:CG	1:D:84:HIS:ND1	2.53	0.50
1:B:41:GLY:O	1:B:42:ALA:HB3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:LYS:HB2	1:B:44:PRO:HD3	1.92	0.50
1:C:158:PHE:HE1	1:C:160:LEU:HB2	1.77	0.50
1:C:177:GLU:HB3	1:C:209:TRP:HE3	1.76	0.50
1:C:41:GLY:O	1:C:42:ALA:HB3	2.12	0.50
1:D:177:GLU:HB3	1:D:209:TRP:HE3	1.76	0.50
1:F:214:ILE:C	1:F:216:PRO:HD3	2.30	0.50
1:H:27:ILE:CD1	1:H:312:LEU:HD11	2.41	0.50
1:J:68:PRO:HG3	1:J:90:GLU:OE2	2.11	0.50
1:K:9:THR:OG1	1:K:10:PRO:HD2	2.11	0.50
1:L:132:PHE:O	1:L:134:TRP:CE3	2.64	0.50
1:L:365:GLN:NE2	2:L:383:HOH:O	2.42	0.50
1:A:140:VAL:O	1:A:144:VAL:HG12	2.12	0.50
1:A:7:ASN:CB	1:D:84:HIS:CG	2.92	0.50
1:B:68:PRO:HG3	1:B:90:GLU:OE2	2.11	0.50
1:D:132:PHE:O	1:D:134:TRP:CE3	2.64	0.50
1:E:68:PRO:HG3	1:E:90:GLU:OE2	2.11	0.50
1:F:311:PHE:HB3	1:F:320:LEU:HD12	1.92	0.50
1:H:219:THR:O	1:H:220:ASN:HB2	2.10	0.50
1:H:52:VAL:O	1:H:56:ILE:HG12	2.12	0.50
1:I:311:PHE:HB3	1:I:320:LEU:HD12	1.93	0.50
1:J:41:GLY:O	1:J:42:ALA:HB3	2.12	0.50
1:L:174:LEU:O	1:L:223:ILE:HD13	2.11	0.50
1:L:49:PHE:O	1:L:52:VAL:HG12	2.10	0.50
1:A:132:PHE:O	1:A:134:TRP:CE3	2.64	0.50
1:B:121:ASN:ND2	2:B:387:HOH:O	2.44	0.50
1:D:41:GLY:O	1:D:42:ALA:HB3	2.12	0.50
1:E:137:ASP:HA	1:E:140:VAL:HG23	1.92	0.50
1:F:140:VAL:O	1:F:144:VAL:HG12	2.12	0.50
1:G:158:PHE:HE1	1:G:160:LEU:HB2	1.76	0.50
1:I:121:ASN:N	1:I:121:ASN:ND2	2.60	0.50
1:I:132:PHE:O	1:I:134:TRP:CE3	2.64	0.50
1:A:68:PRO:HG3	1:A:90:GLU:OE2	2.11	0.50
1:B:8:THR:HB	1:B:12:GLN:NE2	2.27	0.50
1:B:358:ASN:O	1:B:361:CYS:N	2.45	0.50
1:C:43:LYS:HB2	1:C:44:PRO:HD3	1.93	0.50
1:D:358:ASN:O	1:D:361:CYS:N	2.45	0.50
1:F:8:THR:HB	1:F:12:GLN:NE2	2.27	0.50
1:F:68:PRO:HG3	1:F:90:GLU:OE2	2.11	0.50
1:G:174:LEU:O	1:G:223:ILE:HD13	2.11	0.50
1:G:41:GLY:O	1:G:42:ALA:HB3	2.12	0.50
1:H:296:ILE:N	1:H:297:PRO:HD3	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:358:ASN:O	1:I:361:CYS:N	2.45	0.50
1:J:9:THR:OG1	1:J:10:PRO:HD2	2.10	0.50
1:J:121:ASN:N	1:J:121:ASN:ND2	2.60	0.50
1:L:159:VAL:HG12	1:L:186:ASN:HD21	1.76	0.50
1:L:8:THR:HB	1:L:12:GLN:NE2	2.27	0.50
1:A:358:ASN:O	1:A:361:CYS:N	2.45	0.50
1:A:8:THR:HB	1:A:12:GLN:NE2	2.27	0.50
1:E:158:PHE:HE1	1:E:160:LEU:HB2	1.76	0.50
1:F:70:GLN:HB3	2:F:387:HOH:O	2.11	0.50
1:G:68:PRO:HG3	1:G:90:GLU:OE2	2.11	0.50
1:J:311:PHE:HB3	1:J:320:LEU:HD12	1.92	0.50
1:K:43:LYS:HB2	1:K:44:PRO:HD3	1.93	0.50
1:B:174:LEU:O	1:B:223:ILE:HD13	2.11	0.49
1:D:159:VAL:HG12	1:D:186:ASN:HD21	1.76	0.49
1:E:174:LEU:O	1:E:223:ILE:HD13	2.11	0.49
1:J:177:GLU:HB3	1:J:209:TRP:HE3	1.76	0.49
1:H:126:LEU:CD1	1:K:126:LEU:HD12	2.41	0.49
1:K:132:PHE:O	1:K:134:TRP:CE3	2.64	0.49
1:K:41:GLY:O	1:K:42:ALA:HB3	2.12	0.49
1:C:132:PHE:O	1:C:134:TRP:CE3	2.64	0.49
1:E:8:THR:HB	1:E:12:GLN:NE2	2.27	0.49
1:F:158:PHE:HE1	1:F:160:LEU:HB2	1.76	0.49
1:F:26:GLN:NE2	1:F:63:SER:OG	2.45	0.49
1:I:26:GLN:NE2	1:I:63:SER:OG	2.45	0.49
1:K:8:THR:HB	1:K:12:GLN:NE2	2.27	0.49
1:L:41:GLY:O	1:L:42:ALA:HB3	2.12	0.49
1:A:26:GLN:NE2	1:A:63:SER:OG	2.45	0.49
1:C:312:LEU:HD12	1:C:314:VAL:HG12	1.92	0.49
1:G:159:VAL:HG12	1:G:186:ASN:HD21	1.76	0.49
1:H:167:VAL:HG12	1:H:168:ASP:O	2.11	0.49
1:H:206:LYS:HB3	1:H:264:ALA:HB2	1.93	0.49
1:J:8:THR:HB	1:J:12:GLN:NE2	2.27	0.49
1:K:43:LYS:NZ	1:L:35:ASN:HD22	2.10	0.49
1:K:68:PRO:HG3	1:K:90:GLU:OE2	2.11	0.49
1:L:108:ASN:ND2	1:L:110:LYS:HB2	2.28	0.49
1:K:290:ASP:CB	1:L:73:ASN:ND2	2.76	0.49
1:A:121:ASN:N	1:A:121:ASN:ND2	2.60	0.49
1:A:174:LEU:O	1:A:223:ILE:HD13	2.11	0.49
1:B:108:ASN:ND2	1:B:110:LYS:HB2	2.28	0.49
1:B:132:PHE:O	1:B:134:TRP:CE3	2.64	0.49
1:B:26:GLN:NE2	1:B:63:SER:OG	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:THR:HB	1:D:12:GLN:NE2	2.27	0.49
1:E:26:GLN:NE2	1:E:63:SER:OG	2.45	0.49
1:F:113:LEU:O	1:F:150:VAL:HG23	2.13	0.49
1:G:108:ASN:ND2	1:G:110:LYS:HB2	2.28	0.49
1:H:296:ILE:HG12	1:H:296:ILE:O	2.12	0.49
1:I:108:ASN:ND2	1:I:110:LYS:HB2	2.28	0.49
1:J:113:LEU:O	1:J:150:VAL:HG23	2.13	0.49
1:K:262:THR:HG22	2:K:387:HOH:O	2.12	0.49
1:A:177:GLU:HB3	1:A:209:TRP:HE3	1.76	0.49
1:B:231:ARG:HG2	2:B:389:HOH:O	2.12	0.49
1:C:321:PRO:HB3	1:C:358:ASN:HD22	1.78	0.49
1:G:113:LEU:O	1:G:150:VAL:HG23	2.13	0.49
1:G:230:ILE:HG22	1:G:339:PHE:CE1	2.48	0.49
1:H:185:ARG:NH1	1:H:185:ARG:HB2	2.23	0.49
1:I:41:GLY:O	1:I:42:ALA:HB3	2.12	0.49
1:I:8:THR:HB	1:I:12:GLN:NE2	2.27	0.49
1:C:147:ILE:CG2	1:J:89:ILE:HG22	2.37	0.49
1:L:358:ASN:O	1:L:361:CYS:N	2.45	0.49
1:L:26:GLN:NE2	1:L:63:SER:OG	2.45	0.49
1:A:158:PHE:HE1	1:A:160:LEU:HB2	1.76	0.49
1:A:315:ASN:HA	2:A:379:HOH:O	2.11	0.49
1:B:230:ILE:HG22	1:B:339:PHE:CE1	2.48	0.49
1:C:108:ASN:ND2	1:C:110:LYS:HB2	2.28	0.49
1:C:113:LEU:O	1:C:150:VAL:HG23	2.13	0.49
1:C:26:GLN:NE2	1:C:63:SER:OG	2.45	0.49
1:D:113:LEU:O	1:D:150:VAL:HG23	2.13	0.49
1:D:321:PRO:HB3	1:D:358:ASN:HD22	1.78	0.49
1:D:369:THR:O	1:D:370:LEU:CB	2.47	0.49
1:E:230:ILE:HG22	1:E:339:PHE:CE1	2.48	0.49
1:F:41:GLY:O	1:F:42:ALA:HB3	2.12	0.49
1:G:140:VAL:O	1:G:144:VAL:HG12	2.12	0.49
1:G:321:PRO:HB3	1:G:358:ASN:HD22	1.78	0.49
1:H:132:PHE:O	1:H:134:TRP:CE3	2.65	0.49
1:H:182:HIS:CG	1:H:183:PRO:HD2	2.48	0.49
1:K:159:VAL:HG12	1:K:186:ASN:HD21	1.76	0.49
1:K:26:GLN:NE2	1:K:63:SER:OG	2.45	0.49
1:L:140:VAL:O	1:L:144:VAL:HG12	2.12	0.49
1:L:230:ILE:HG22	1:L:339:PHE:CE1	2.48	0.49
1:A:43:LYS:NZ	1:G:35:ASN:HD22	2.11	0.49
1:C:358:ASN:O	1:C:361:CYS:N	2.45	0.49
1:G:358:ASN:O	1:G:361:CYS:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:GLN:NE2	1:G:63:SER:OG	2.45	0.49
1:H:132:PHE:CD2	1:K:135:ASP:HB3	2.46	0.49
1:K:80:GLU:HB2	1:L:291:TYR:OH	2.13	0.49
1:A:230:ILE:HG22	1:A:339:PHE:CE1	2.48	0.49
1:B:321:PRO:HB3	1:B:358:ASN:HD22	1.78	0.49
1:C:140:VAL:O	1:C:144:VAL:HG12	2.12	0.49
1:C:230:ILE:HG22	1:C:339:PHE:CE1	2.48	0.49
1:H:15:PHE:CZ	1:H:114:ARG:HD3	2.48	0.49
1:I:230:ILE:HG22	1:I:339:PHE:CE1	2.48	0.49
1:I:231:ARG:HG3	1:I:232:PRO:HD2	1.95	0.49
1:J:358:ASN:O	1:J:361:CYS:N	2.45	0.49
1:K:358:ASN:O	1:K:361:CYS:N	2.45	0.49
1:B:140:VAL:O	1:B:144:VAL:HG12	2.11	0.49
1:C:8:THR:HB	1:C:12:GLN:NE2	2.27	0.49
1:D:231:ARG:HG3	1:D:232:PRO:HD2	1.95	0.49
1:D:71:TYR:CZ	1:I:143:LYS:HG2	2.48	0.49
1:E:113:LEU:O	1:E:150:VAL:HG23	2.13	0.49
1:F:358:ASN:O	1:F:361:CYS:N	2.45	0.49
1:I:158:PHE:HE1	1:I:160:LEU:HB2	1.76	0.49
1:J:158:PHE:HE1	1:J:160:LEU:HB2	1.76	0.49
1:D:108:ASN:ND2	1:D:110:LYS:HB2	2.28	0.49
1:D:121:ASN:N	1:D:121:ASN:ND2	2.60	0.49
1:D:26:GLN:NE2	1:D:63:SER:OG	2.45	0.49
1:E:321:PRO:HB3	1:E:358:ASN:HD22	1.78	0.49
1:G:177:GLU:HB3	1:G:209:TRP:HE3	1.76	0.49
1:H:176:THR:HG23	1:H:179:CYS:HB3	1.95	0.49
1:H:195:GLU:HG2	1:H:207:VAL:HG11	1.94	0.49
1:H:27:ILE:HD11	1:H:314:VAL:HG12	1.93	0.49
1:H:28:TRP:CH2	1:H:144:VAL:HG23	2.48	0.49
1:H:50:LEU:HD11	1:H:78:VAL:HG22	1.95	0.49
1:J:108:ASN:ND2	1:J:110:LYS:HB2	2.27	0.49
1:J:140:VAL:O	1:J:144:VAL:HG12	2.12	0.49
1:J:26:GLN:NE2	1:J:63:SER:OG	2.45	0.49
1:A:108:ASN:ND2	1:A:110:LYS:HB2	2.28	0.48
1:A:113:LEU:O	1:A:150:VAL:HG23	2.13	0.48
1:C:320:LEU:HD12	1:C:321:PRO:HD2	1.95	0.48
1:F:230:ILE:HG22	1:F:339:PHE:CE1	2.48	0.48
1:G:8:THR:HB	1:G:12:GLN:NE2	2.27	0.48
1:I:320:LEU:HD12	1:I:321:PRO:HD2	1.95	0.48
1:K:321:PRO:HB3	1:K:358:ASN:HD22	1.78	0.48
1:L:113:LEU:O	1:L:150:VAL:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:HG3	1:A:232:PRO:HD2	1.95	0.48
1:B:113:LEU:O	1:B:150:VAL:HG23	2.13	0.48
1:B:121:ASN:ND2	1:B:121:ASN:N	2.60	0.48
1:C:73:ASN:ND2	1:D:290:ASP:HB3	2.28	0.48
1:E:177:GLU:O	1:E:181:LEU:HB2	2.13	0.48
1:E:358:ASN:O	1:E:361:CYS:N	2.45	0.48
1:H:104:THR:HB	1:H:116:VAL:CG1	2.43	0.48
1:H:237:CYS:SG	1:H:238:ILE:N	2.87	0.48
1:H:278:LYS:N	1:H:325:ASP:OD2	2.43	0.48
1:H:30:LEU:HB2	1:H:96:ALA:HB1	1.95	0.48
1:I:369:THR:O	1:I:370:LEU:CB	2.47	0.48
1:L:158:PHE:HE1	1:L:160:LEU:HB2	1.76	0.48
1:C:272:HIS:ND1	1:C:338:MSE:HG2	2.29	0.48
1:D:272:HIS:ND1	1:D:338:MSE:HG2	2.29	0.48
1:F:108:ASN:ND2	1:F:110:LYS:HB2	2.28	0.48
1:G:177:GLU:O	1:G:181:LEU:HB2	2.13	0.48
1:G:181:LEU:C	2:G:397:HOH:O	2.51	0.48
1:G:231:ARG:HG3	1:G:232:PRO:HD2	1.95	0.48
1:A:291:TYR:OH	1:G:80:GLU:HB2	2.12	0.48
1:I:321:PRO:HB3	1:I:358:ASN:HD22	1.78	0.48
1:J:272:HIS:ND1	1:J:338:MSE:HG2	2.29	0.48
1:K:140:VAL:O	1:K:144:VAL:HG12	2.12	0.48
1:A:9:THR:HG22	1:A:12:GLN:CG	2.44	0.48
1:B:272:HIS:ND1	1:B:338:MSE:HG2	2.29	0.48
1:C:177:GLU:O	1:C:181:LEU:HB2	2.13	0.48
1:D:369:THR:CG2	1:D:370:LEU:N	2.37	0.48
1:E:231:ARG:HG3	1:E:232:PRO:HD2	1.95	0.48
1:F:231:ARG:HG3	1:F:232:PRO:HD2	1.95	0.48
1:H:161:GLU:CD	1:H:161:GLU:H	2.16	0.48
1:H:169:GLY:HA3	2:H:393:HOH:O	2.13	0.48
1:H:30:LEU:HB2	1:H:96:ALA:CB	2.44	0.48
1:I:177:GLU:O	1:I:181:LEU:HB2	2.13	0.48
1:J:231:ARG:HG3	1:J:232:PRO:HD2	1.95	0.48
1:J:60:GLU:HB2	1:J:61:PRO:HD2	1.96	0.48
1:K:108:ASN:ND2	1:K:110:LYS:HB2	2.28	0.48
1:L:177:GLU:HB3	1:L:209:TRP:HE3	1.76	0.48
1:C:231:ARG:HG3	1:C:232:PRO:HD2	1.95	0.48
1:D:230:ILE:HG22	1:D:339:PHE:CE1	2.48	0.48
1:E:108:ASN:ND2	1:E:110:LYS:HB2	2.28	0.48
1:H:293:GLU:C	1:H:295:SER:H	2.16	0.48
1:J:121:ASN:H	1:J:121:ASN:ND2	2.07	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:230:ILE:HG22	1:J:339:PHE:CE1	2.48	0.48
1:J:56:ILE:HD13	1:J:319:ILE:HG13	1.96	0.48
1:K:177:GLU:O	1:K:181:LEU:HB2	2.13	0.48
1:A:290:ASP:CB	1:G:73:ASN:ND2	2.75	0.48
1:A:60:GLU:HB2	1:A:61:PRO:HD2	1.96	0.48
1:E:60:GLU:HB2	1:E:61:PRO:HD2	1.96	0.48
1:F:320:LEU:HD12	1:F:321:PRO:HD2	1.95	0.48
1:G:56:ILE:HD13	1:G:319:ILE:HG13	1.96	0.48
1:G:60:GLU:HB2	1:G:61:PRO:HD2	1.96	0.48
1:K:230:ILE:HG22	1:K:339:PHE:CE1	2.48	0.48
1:A:272:HIS:ND1	1:A:338:MSE:HG2	2.29	0.48
1:E:308:TYR:OH	1:E:325:ASP:HB3	2.14	0.48
1:E:71:TYR:CZ	1:K:143:LYS:HG2	2.49	0.48
1:F:321:PRO:HB3	1:F:358:ASN:HD22	1.78	0.48
1:F:60:GLU:HB2	1:F:61:PRO:HD2	1.96	0.48
1:H:103:PRO:HD3	1:H:144:VAL:HG11	1.94	0.48
1:H:9:THR:HG22	1:H:12:GLN:CD	2.33	0.48
1:I:113:LEU:O	1:I:150:VAL:HG23	2.13	0.48
1:K:121:ASN:H	1:K:121:ASN:ND2	2.07	0.48
1:K:320:LEU:HD12	1:K:321:PRO:HD2	1.95	0.48
1:L:121:ASN:H	1:L:121:ASN:ND2	2.07	0.48
1:L:272:HIS:ND1	1:L:338:MSE:HG2	2.29	0.48
1:A:369:THR:O	1:A:370:LEU:CB	2.47	0.48
1:B:177:GLU:O	1:B:181:LEU:HB2	2.13	0.48
1:E:177:GLU:HB3	1:E:209:TRP:HE3	1.76	0.48
1:E:210:VAL:CG1	1:E:211:LYS:N	2.77	0.48
1:D:341:ASP:HB3	1:F:57:SER:O	2.14	0.48
1:G:320:LEU:HD12	1:G:321:PRO:HD2	1.95	0.48
1:H:177:GLU:HG2	1:H:211:LYS:HA	1.96	0.48
1:H:224:ASP:OD2	1:H:360:HIS:HD2	1.96	0.48
1:K:9:THR:HG22	1:K:12:GLN:CG	2.44	0.48
1:A:177:GLU:O	1:A:181:LEU:HB2	2.13	0.48
1:C:56:ILE:HD13	1:C:319:ILE:HG13	1.96	0.48
1:C:9:THR:HG22	1:C:12:GLN:CG	2.44	0.48
1:D:177:GLU:O	1:D:181:LEU:HB2	2.13	0.48
1:F:210:VAL:CG1	1:F:211:LYS:N	2.77	0.48
1:G:272:HIS:ND1	1:G:338:MSE:HG2	2.29	0.48
1:J:308:TYR:OH	1:J:325:ASP:HB3	2.14	0.48
1:E:143:LYS:HG2	1:K:71:TYR:CZ	2.49	0.48
1:L:308:TYR:OH	1:L:325:ASP:HB3	2.14	0.48
1:B:231:ARG:HG3	1:B:232:PRO:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:VAL:CG1	1:D:211:LYS:N	2.77	0.48
1:D:340:PRO:CG	1:F:58:GLU:O	2.61	0.48
1:D:60:GLU:HB2	1:D:61:PRO:HD2	1.96	0.48
1:E:320:LEU:HD12	1:E:321:PRO:HD2	1.95	0.48
1:F:177:GLU:O	1:F:181:LEU:HB2	2.13	0.48
1:F:47:LYS:O	1:F:51:GLU:HG3	2.14	0.48
1:H:207:VAL:HG22	1:H:209:TRP:NE1	2.28	0.48
1:I:272:HIS:ND1	1:I:338:MSE:HG2	2.29	0.48
1:J:321:PRO:HB3	1:J:358:ASN:HD22	1.78	0.48
1:L:203:ASN:HD22	1:L:203:ASN:HA	1.50	0.48
1:A:210:VAL:CG1	1:A:211:LYS:N	2.77	0.47
1:A:320:LEU:HD12	1:A:321:PRO:HD2	1.95	0.47
1:A:56:ILE:HD13	1:A:319:ILE:HG13	1.96	0.47
1:B:9:THR:HG22	1:B:12:GLN:CG	2.44	0.47
1:C:121:ASN:ND2	1:C:121:ASN:N	2.60	0.47
1:C:308:TYR:OH	1:C:325:ASP:HB3	2.14	0.47
1:C:61:PRO:HA	1:C:85:ASN:ND2	2.29	0.47
1:D:47:LYS:O	1:D:51:GLU:HG3	2.14	0.47
1:E:272:HIS:ND1	1:E:338:MSE:HG2	2.29	0.47
1:F:231:ARG:CG	1:F:232:PRO:HD2	2.44	0.47
1:F:308:TYR:OH	1:F:325:ASP:HB3	2.14	0.47
1:G:210:VAL:CG1	1:G:211:LYS:N	2.77	0.47
1:G:176:THR:HG21	1:G:221:GLY:O	2.14	0.47
1:G:308:TYR:OH	1:G:325:ASP:HB3	2.14	0.47
1:H:29:MSE:HE1	1:H:52:VAL:CG2	2.44	0.47
1:H:27:ILE:HG13	1:H:60:GLU:OE2	2.13	0.47
1:I:210:VAL:CG1	1:I:211:LYS:N	2.77	0.47
1:J:231:ARG:CG	1:J:232:PRO:HD2	2.44	0.47
1:K:56:ILE:HD13	1:K:319:ILE:HG13	1.96	0.47
1:K:308:TYR:OH	1:K:325:ASP:HB3	2.14	0.47
1:K:60:GLU:HB2	1:K:61:PRO:HD2	1.96	0.47
1:L:320:LEU:HD12	1:L:321:PRO:HD2	1.95	0.47
1:L:47:LYS:HD3	2:L:388:HOH:O	2.13	0.47
1:A:176:THR:HG21	1:A:221:GLY:O	2.14	0.47
1:D:21:PHE:CZ	1:D:232:PRO:HD3	2.50	0.47
1:D:341:ASP:CA	1:F:84:HIS:HD2	2.19	0.47
1:E:61:PRO:HA	1:E:85:ASN:ND2	2.29	0.47
1:F:176:THR:HG21	1:F:221:GLY:O	2.14	0.47
1:F:272:HIS:ND1	1:F:338:MSE:HG2	2.29	0.47
1:H:119:GLU:O	1:H:159:VAL:HG23	2.14	0.47
1:H:181:LEU:HD21	1:H:191:LYS:HG3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:267:ARG:C	1:H:268:PRO:O	2.50	0.47
1:I:9:THR:HG22	1:I:12:GLN:CG	2.44	0.47
1:I:56:ILE:HD13	1:I:319:ILE:HG13	1.96	0.47
1:J:210:VAL:CG1	1:J:211:LYS:N	2.77	0.47
1:J:47:LYS:O	1:J:51:GLU:HG3	2.14	0.47
1:J:9:THR:HG22	1:J:12:GLN:CG	2.44	0.47
1:K:231:ARG:HG3	1:K:232:PRO:HD2	1.95	0.47
1:K:272:HIS:ND1	1:K:338:MSE:HG2	2.29	0.47
1:L:61:PRO:HA	1:L:85:ASN:ND2	2.29	0.47
1:L:9:THR:HG22	1:L:12:GLN:CG	2.44	0.47
1:A:321:PRO:HB3	1:A:358:ASN:HD22	1.78	0.47
1:A:7:ASN:HB2	1:D:84:HIS:CG	2.49	0.47
1:C:176:THR:HG21	1:C:221:GLY:O	2.14	0.47
1:C:47:LYS:O	1:C:51:GLU:HG3	2.14	0.47
1:D:39:ARG:HG3	1:D:40:LEU:HD23	1.97	0.47
1:D:56:ILE:HD13	1:D:319:ILE:HG13	1.96	0.47
1:E:121:ASN:ND2	1:E:121:ASN:N	2.60	0.47
1:E:323:TYR:HA	1:E:350:GLU:HB3	1.97	0.47
1:G:336:GLN:CG	2:G:404:HOH:O	2.54	0.47
1:G:39:ARG:HG3	1:G:40:LEU:HD23	1.97	0.47
1:H:27:ILE:HD11	1:H:312:LEU:HD11	1.97	0.47
1:L:21:PHE:CZ	1:L:232:PRO:HD3	2.50	0.47
1:L:60:GLU:HB2	1:L:61:PRO:HD2	1.96	0.47
1:A:308:TYR:OH	1:A:325:ASP:HB3	2.14	0.47
1:A:61:PRO:HA	1:A:85:ASN:ND2	2.29	0.47
1:B:21:PHE:CZ	1:B:232:PRO:HD3	2.50	0.47
1:B:308:TYR:OH	1:B:325:ASP:HB3	2.14	0.47
1:C:231:ARG:CG	1:C:232:PRO:HD2	2.44	0.47
1:D:171:GLY:CA	1:D:204:CYS:HA	2.43	0.47
1:D:231:ARG:CG	1:D:232:PRO:HD2	2.44	0.47
1:G:339:PHE:HB3	2:G:391:HOH:O	2.15	0.47
1:H:68:PRO:HD2	2:H:386:HOH:O	2.14	0.47
1:I:47:LYS:O	1:I:51:GLU:HG3	2.14	0.47
1:J:61:PRO:HA	1:J:85:ASN:ND2	2.29	0.47
1:L:321:PRO:HB3	1:L:358:ASN:HD22	1.78	0.47
1:L:47:LYS:O	1:L:51:GLU:HG3	2.14	0.47
1:A:126:LEU:HD12	1:B:126:LEU:HD12	1.96	0.47
1:A:21:PHE:CZ	1:A:232:PRO:HD3	2.50	0.47
1:B:60:GLU:HB2	1:B:61:PRO:HD2	1.96	0.47
1:E:21:PHE:CZ	1:E:232:PRO:HD3	2.50	0.47
1:E:39:ARG:HG3	1:E:40:LEU:HD23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ILE:HD13	1:F:319:ILE:HG13	1.96	0.47
1:I:231:ARG:CG	1:I:232:PRO:HD2	2.44	0.47
1:I:66:VAL:CG2	1:I:71:TYR:HA	2.45	0.47
1:J:177:GLU:O	1:J:181:LEU:HB2	2.13	0.47
1:J:323:TYR:HA	1:J:350:GLU:HB3	1.97	0.47
1:J:39:ARG:HG3	1:J:40:LEU:HD23	1.97	0.47
1:K:176:THR:HG21	1:K:221:GLY:O	2.14	0.47
1:L:56:ILE:HD13	1:L:319:ILE:HG13	1.96	0.47
1:D:143:LYS:HG2	1:I:71:TYR:CZ	2.50	0.47
1:D:308:TYR:OH	1:D:325:ASP:HB3	2.14	0.47
1:E:176:THR:HG21	1:E:221:GLY:O	2.14	0.47
1:F:309:LEU:HD22	1:F:311:PHE:HE2	1.80	0.47
1:F:66:VAL:CG2	1:F:71:TYR:HA	2.45	0.47
1:G:9:THR:HG22	1:G:12:GLN:CG	2.44	0.47
1:H:266:GLY:O	1:H:267:ARG:C	2.53	0.47
1:H:358:ASN:ND2	1:H:359:ILE:HG13	2.29	0.47
1:I:176:THR:HG21	1:I:221:GLY:O	2.14	0.47
1:I:60:GLU:HB2	1:I:61:PRO:HD2	1.96	0.47
1:J:176:THR:HG21	1:J:221:GLY:O	2.14	0.47
1:J:21:PHE:CZ	1:J:232:PRO:HD3	2.50	0.47
1:K:231:ARG:CG	1:K:232:PRO:HD2	2.44	0.47
1:K:61:PRO:HA	1:K:85:ASN:ND2	2.29	0.47
1:L:210:VAL:CG1	1:L:211:LYS:N	2.77	0.47
1:L:231:ARG:CG	1:L:232:PRO:HD2	2.44	0.47
1:L:231:ARG:HG3	1:L:232:PRO:HD2	1.95	0.47
1:L:323:TYR:HA	1:L:350:GLU:HB3	1.97	0.47
1:A:168:ASP:O	1:A:169:GLY:C	2.53	0.47
1:A:39:ARG:HG3	1:A:40:LEU:HD23	1.97	0.47
1:A:66:VAL:CG2	1:A:71:TYR:HA	2.45	0.47
1:B:54:GLU:O	1:B:57:SER:HB2	2.15	0.47
1:C:21:PHE:CZ	1:C:232:PRO:HD3	2.50	0.47
1:C:39:ARG:HG3	1:C:40:LEU:HD23	1.97	0.47
1:D:320:LEU:HD12	1:D:321:PRO:HD2	1.95	0.47
1:D:9:THR:HG22	1:D:12:GLN:CG	2.44	0.47
1:E:318:ILE:HD11	1:E:339:PHE:CD1	2.50	0.47
1:E:9:THR:HG22	1:E:12:GLN:CG	2.44	0.47
1:F:61:PRO:HA	1:F:85:ASN:ND2	2.29	0.47
1:G:318:ILE:HD11	1:G:339:PHE:CD1	2.50	0.47
1:H:69:LEU:HG	2:H:386:HOH:O	2.15	0.47
1:L:176:THR:HG21	1:L:221:GLY:O	2.14	0.47
1:L:54:GLU:O	1:L:57:SER:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ILE:HD11	1:A:339:PHE:CD1	2.50	0.47
1:B:177:GLU:HB3	1:B:209:TRP:HE3	1.76	0.47
1:B:231:ARG:CG	1:B:232:PRO:HD2	2.45	0.47
1:C:323:TYR:HA	1:C:350:GLU:HB3	1.97	0.47
1:D:61:PRO:HA	1:D:85:ASN:ND2	2.29	0.47
1:F:9:THR:HG22	1:F:12:GLN:CG	2.44	0.47
1:G:118:TRP:CZ3	1:G:155:THR:HG21	2.50	0.47
1:G:21:PHE:CZ	1:G:232:PRO:HD3	2.50	0.47
1:H:108:ASN:HD21	1:H:110:LYS:HB2	1.80	0.47
1:H:188:HIS:CE1	1:H:189:LEU:HD13	2.49	0.47
1:H:181:LEU:HD21	1:H:191:LYS:CG	2.45	0.47
1:K:54:GLU:O	1:K:57:SER:HB2	2.15	0.47
1:L:177:GLU:O	1:L:181:LEU:HB2	2.13	0.47
1:L:318:ILE:HD11	1:L:339:PHE:CD1	2.50	0.47
1:L:39:ARG:HG3	1:L:40:LEU:HD23	1.97	0.47
1:A:65:CYS:HB3	1:A:91:MSE:HB3	1.97	0.47
1:B:118:TRP:CZ3	1:B:155:THR:HG21	2.50	0.47
1:B:320:LEU:HD12	1:B:321:PRO:HD2	1.95	0.47
1:B:39:ARG:HG3	1:B:40:LEU:HD23	1.97	0.47
1:B:47:LYS:O	1:B:51:GLU:HG3	2.14	0.47
1:C:168:ASP:O	1:C:169:GLY:C	2.53	0.47
1:C:171:GLY:CA	1:C:204:CYS:HA	2.43	0.47
1:F:65:CYS:HB3	1:F:91:MSE:HB3	1.97	0.47
1:G:121:ASN:H	1:G:121:ASN:ND2	2.07	0.47
1:G:47:LYS:O	1:G:51:GLU:HG3	2.15	0.47
1:H:159:VAL:O	1:H:159:VAL:HG13	2.15	0.47
1:I:54:GLU:O	1:I:57:SER:HB2	2.15	0.47
1:I:61:PRO:HA	1:I:85:ASN:ND2	2.29	0.47
1:K:113:LEU:O	1:K:150:VAL:HG23	2.13	0.47
1:K:323:TYR:HA	1:K:350:GLU:HB3	1.97	0.47
1:L:168:ASP:O	1:L:169:GLY:C	2.53	0.47
1:L:65:CYS:HB3	1:L:91:MSE:HB3	1.97	0.47
1:L:66:VAL:CG2	1:L:71:TYR:HA	2.45	0.47
1:B:309:LEU:HD22	1:B:311:PHE:HE2	1.80	0.47
1:C:174:LEU:O	1:C:223:ILE:HG21	2.15	0.47
1:C:210:VAL:CG1	1:C:211:LYS:N	2.77	0.47
1:C:43:LYS:HZ2	1:C:46:GLN:HE22	1.63	0.47
1:C:54:GLU:O	1:C:57:SER:HB2	2.15	0.47
1:C:60:GLU:HB2	1:C:61:PRO:HD2	1.96	0.47
1:D:224:ASP:HB2	1:D:360:HIS:HD2	1.80	0.47
1:D:66:VAL:CG2	1:D:71:TYR:HA	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:O	1:E:223:ILE:HG21	2.15	0.47
1:E:47:LYS:O	1:E:51:GLU:HG3	2.14	0.47
1:F:318:ILE:HD11	1:F:339:PHE:CD1	2.50	0.47
1:G:66:VAL:CG2	1:G:71:TYR:HA	2.45	0.47
1:H:124:GLY:O	1:H:127:VAL:HG13	2.15	0.47
1:J:54:GLU:O	1:J:57:SER:HB2	2.15	0.47
1:K:224:ASP:HB2	1:K:360:HIS:HD2	1.80	0.47
1:K:66:VAL:CG2	1:K:71:TYR:HA	2.45	0.47
1:B:176:THR:HG21	1:B:221:GLY:O	2.14	0.47
1:B:56:ILE:HD13	1:B:319:ILE:HG13	1.96	0.47
1:C:68:PRO:HG3	1:C:90:GLU:CD	2.36	0.47
1:D:318:ILE:HD11	1:D:339:PHE:CD1	2.50	0.47
1:E:224:ASP:HB2	1:E:360:HIS:HD2	1.80	0.47
1:F:21:PHE:CZ	1:F:232:PRO:HD3	2.50	0.47
1:G:231:ARG:CG	1:G:232:PRO:HD2	2.44	0.47
1:G:323:TYR:HA	1:G:350:GLU:HB3	1.97	0.47
1:I:323:TYR:HA	1:I:350:GLU:HB3	1.97	0.47
1:J:118:TRP:CZ3	1:J:155:THR:HG21	2.50	0.47
1:J:168:ASP:O	1:J:169:GLY:C	2.53	0.47
1:J:318:ILE:HD11	1:J:339:PHE:CD1	2.50	0.47
1:J:65:CYS:HB3	1:J:91:MSE:HB3	1.97	0.47
1:K:309:LEU:HD22	1:K:311:PHE:HE2	1.80	0.47
1:A:231:ARG:CG	1:A:232:PRO:HD2	2.44	0.46
1:A:224:ASP:HB2	1:A:360:HIS:HD2	1.80	0.46
1:B:174:LEU:O	1:B:223:ILE:HG21	2.15	0.46
1:B:318:ILE:HD11	1:B:339:PHE:CD1	2.50	0.46
1:B:66:VAL:CG2	1:B:71:TYR:HA	2.45	0.46
1:C:29:MSE:HE1	1:C:52:VAL:HG13	1.97	0.46
1:D:174:LEU:O	1:D:223:ILE:HG21	2.15	0.46
1:E:168:ASP:O	1:E:169:GLY:C	2.53	0.46
1:E:309:LEU:HD22	1:E:311:PHE:HE2	1.80	0.46
1:E:56:ILE:HD13	1:E:319:ILE:HG13	1.96	0.46
1:F:68:PRO:HG3	1:F:90:GLU:CD	2.36	0.46
1:G:168:ASP:O	1:G:169:GLY:C	2.53	0.46
1:G:245:HIS:ND1	1:G:246:PRO:HD2	2.30	0.46
1:G:61:PRO:HA	1:G:85:ASN:ND2	2.29	0.46
1:H:27:ILE:HD11	1:H:314:VAL:CG1	2.45	0.46
1:I:118:TRP:CZ3	1:I:155:THR:HG21	2.50	0.46
1:I:21:PHE:CZ	1:I:232:PRO:HD3	2.50	0.46
1:I:245:HIS:ND1	1:I:246:PRO:HD2	2.30	0.46
1:I:308:TYR:OH	1:I:325:ASP:HB3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:318:ILE:HD11	1:I:339:PHE:CD1	2.50	0.46
1:I:68:PRO:HG3	1:I:90:GLU:CD	2.36	0.46
1:J:320:LEU:HD12	1:J:321:PRO:HD2	1.95	0.46
1:K:210:VAL:CG1	1:K:211:LYS:N	2.77	0.46
1:K:47:LYS:O	1:K:51:GLU:HG3	2.14	0.46
1:L:174:LEU:O	1:L:223:ILE:HG21	2.15	0.46
1:A:11:LYS:HG3	1:A:203:ASN:ND2	2.31	0.46
1:A:171:GLY:CA	1:A:204:CYS:HA	2.43	0.46
1:A:47:LYS:O	1:A:51:GLU:HG3	2.14	0.46
1:A:54:GLU:O	1:A:57:SER:HB2	2.15	0.46
1:C:11:LYS:HG3	1:C:203:ASN:ND2	2.31	0.46
1:C:318:ILE:HD11	1:C:339:PHE:CD1	2.50	0.46
1:D:309:LEU:HD22	1:D:311:PHE:HE2	1.80	0.46
1:D:323:TYR:HA	1:D:350:GLU:HB3	1.97	0.46
1:F:224:ASP:HB2	1:F:360:HIS:HD2	1.80	0.46
1:F:369:THR:O	1:F:370:LEU:CB	2.47	0.46
1:G:174:LEU:O	1:G:223:ILE:HG21	2.15	0.46
1:G:29:MSE:HE1	1:G:52:VAL:HG13	1.97	0.46
1:I:171:GLY:CA	1:I:204:CYS:HA	2.43	0.46
1:I:224:ASP:HB2	1:I:360:HIS:HD2	1.80	0.46
1:J:68:PRO:HG3	1:J:90:GLU:CD	2.36	0.46
1:L:245:HIS:ND1	1:L:246:PRO:HD2	2.30	0.46
1:L:224:ASP:HB2	1:L:360:HIS:HD2	1.80	0.46
1:A:118:TRP:CZ3	1:A:155:THR:HG21	2.50	0.46
1:B:311:PHE:CE1	1:B:313:ILE:HD11	2.51	0.46
1:B:336:GLN:HA	1:B:336:GLN:OE1	2.15	0.46
1:B:224:ASP:HB2	1:B:360:HIS:HD2	1.80	0.46
1:C:311:PHE:CE1	1:C:313:ILE:HD11	2.51	0.46
1:E:121:ASN:H	1:E:121:ASN:ND2	2.07	0.46
1:E:65:CYS:HB3	1:E:91:MSE:HB3	1.97	0.46
1:E:66:VAL:CG2	1:E:71:TYR:HA	2.45	0.46
1:F:245:HIS:ND1	1:F:246:PRO:HD2	2.30	0.46
1:F:39:ARG:HH11	1:F:40:LEU:HD23	1.81	0.46
1:G:67:PRO:HA	1:G:68:PRO:HD3	1.80	0.46
1:G:68:PRO:HG3	1:G:90:GLU:CD	2.36	0.46
1:H:16:ARG:HH12	1:H:109:ASP:CG	2.19	0.46
1:H:29:MSE:HA	1:H:98:ILE:HG21	1.96	0.46
1:I:65:CYS:HB3	1:I:91:MSE:HB3	1.97	0.46
1:J:39:ARG:HH11	1:J:40:LEU:HD23	1.81	0.46
1:K:318:ILE:HD11	1:K:339:PHE:CD1	2.50	0.46
1:K:77:ARG:NH2	1:L:290:ASP:OD1	2.38	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:311:PHE:CE1	1:L:313:ILE:HD11	2.51	0.46
1:L:68:PRO:HG3	1:L:90:GLU:CD	2.36	0.46
1:A:89:ILE:HG22	1:F:147:ILE:CG2	2.36	0.46
1:B:168:ASP:O	1:B:169:GLY:C	2.53	0.46
1:B:210:VAL:CG1	1:B:211:LYS:N	2.77	0.46
1:C:65:CYS:HB3	1:C:91:MSE:HB3	1.97	0.46
1:F:171:GLY:CA	1:F:204:CYS:HA	2.43	0.46
1:F:174:LEU:O	1:F:223:ILE:HG21	2.15	0.46
1:F:54:GLU:O	1:F:57:SER:HB2	2.15	0.46
1:I:311:PHE:CE1	1:I:313:ILE:HD11	2.51	0.46
1:J:215:ASP:HB2	1:J:221:GLY:HA2	1.98	0.46
1:K:11:LYS:HG3	1:K:203:ASN:ND2	2.31	0.46
1:K:203:ASN:HD22	1:K:203:ASN:HA	1.50	0.46
1:K:21:PHE:CZ	1:K:232:PRO:HD3	2.50	0.46
1:K:245:HIS:ND1	1:K:246:PRO:HD2	2.31	0.46
1:K:68:PRO:HG3	1:K:90:GLU:CD	2.36	0.46
1:A:311:PHE:CE1	1:A:313:ILE:HD11	2.51	0.46
1:A:68:PRO:HG3	1:A:90:GLU:CD	2.36	0.46
1:D:118:TRP:CZ3	1:D:155:THR:HG21	2.50	0.46
1:D:168:ASP:O	1:D:169:GLY:C	2.53	0.46
1:D:215:ASP:HB2	1:D:221:GLY:HA2	1.98	0.46
1:D:176:THR:HG21	1:D:221:GLY:O	2.14	0.46
1:D:39:ARG:HH11	1:D:40:LEU:HD23	1.81	0.46
1:C:35:ASN:HD22	1:D:43:LYS:NZ	2.14	0.46
1:I:168:ASP:O	1:I:169:GLY:C	2.53	0.46
1:J:158:PHE:CE1	1:J:160:LEU:HB2	2.51	0.46
1:K:174:LEU:O	1:K:223:ILE:HG21	2.15	0.46
1:L:309:LEU:HD22	1:L:311:PHE:HE2	1.80	0.46
1:B:323:TYR:HA	1:B:350:GLU:HB3	1.97	0.46
1:B:68:PRO:HG3	1:B:90:GLU:CD	2.36	0.46
1:C:215:ASP:HB2	1:C:221:GLY:HA2	1.98	0.46
1:C:66:VAL:CG2	1:C:71:TYR:HA	2.45	0.46
1:D:29:MSE:HE1	1:D:52:VAL:HG13	1.97	0.46
1:D:68:PRO:HG3	1:D:90:GLU:CD	2.36	0.46
1:E:118:TRP:CZ3	1:E:155:THR:HG21	2.50	0.46
1:E:231:ARG:CG	1:E:232:PRO:HD2	2.44	0.46
1:E:311:PHE:CE1	1:E:313:ILE:HD11	2.51	0.46
1:F:168:ASP:O	1:F:169:GLY:C	2.53	0.46
1:G:39:ARG:HH11	1:G:40:LEU:HD23	1.80	0.46
1:H:330:LEU:O	1:H:330:LEU:HD12	2.16	0.46
1:J:11:LYS:HG3	1:J:203:ASN:ND2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:245:HIS:ND1	1:J:246:PRO:HD2	2.31	0.46
1:J:309:LEU:HD22	1:J:311:PHE:HE2	1.80	0.46
1:J:311:PHE:CE1	1:J:313:ILE:HD11	2.51	0.46
1:K:158:PHE:CE1	1:K:160:LEU:HB2	2.51	0.46
1:K:311:PHE:CE1	1:K:313:ILE:HD11	2.51	0.46
1:K:65:CYS:HB3	1:K:91:MSE:HB3	1.97	0.46
1:L:29:MSE:HE1	1:L:52:VAL:HG13	1.98	0.46
1:A:71:TYR:CZ	1:F:143:LYS:HG2	2.50	0.46
1:B:215:ASP:HB2	1:B:221:GLY:HA2	1.98	0.46
1:B:61:PRO:HA	1:B:85:ASN:ND2	2.29	0.46
1:C:309:LEU:HD22	1:C:311:PHE:HE2	1.80	0.46
1:C:336:GLN:OE1	1:C:336:GLN:HA	2.15	0.46
1:C:39:ARG:HH11	1:C:40:LEU:HD23	1.81	0.46
1:D:245:HIS:ND1	1:D:246:PRO:HD2	2.31	0.46
1:E:11:LYS:HG3	1:E:203:ASN:ND2	2.31	0.46
1:F:158:PHE:CE1	1:F:160:LEU:HB2	2.51	0.46
1:F:29:MSE:HE1	1:F:52:VAL:HG13	1.98	0.46
1:F:135:ASP:HB3	1:G:132:PHE:CD2	2.51	0.46
1:G:311:PHE:CE1	1:G:313:ILE:HD11	2.51	0.46
1:H:195:GLU:O	1:H:199:LYS:HG3	2.16	0.46
1:H:243:LYS:HA	1:H:248:TYR:CG	2.50	0.46
1:J:224:ASP:HB2	1:J:360:HIS:HD2	1.80	0.46
1:A:29:MSE:HE1	1:A:52:VAL:HG13	1.98	0.46
1:C:245:HIS:ND1	1:C:246:PRO:HD2	2.30	0.46
1:D:311:PHE:CE1	1:D:313:ILE:HD11	2.51	0.46
1:E:77:ARG:NH1	1:H:291:TYR:HE1	2.13	0.46
1:E:50:LEU:HG	1:E:81:LEU:HD11	1.98	0.46
1:F:118:TRP:CZ3	1:F:155:THR:HG21	2.50	0.46
1:F:215:ASP:HB2	1:F:221:GLY:HA2	1.98	0.46
1:F:336:GLN:HA	1:F:336:GLN:OE1	2.15	0.46
1:G:11:LYS:HG3	1:G:203:ASN:ND2	2.31	0.46
1:G:215:ASP:HB2	1:G:221:GLY:HA2	1.98	0.46
1:H:113:LEU:O	1:H:114:ARG:HG3	2.15	0.46
1:I:158:PHE:CE1	1:I:160:LEU:HB2	2.51	0.46
1:I:39:ARG:HG3	1:I:40:LEU:HD23	1.97	0.46
1:J:336:GLN:OE1	1:J:336:GLN:HA	2.15	0.46
1:J:29:MSE:HE1	1:J:52:VAL:HG13	1.97	0.46
1:L:49:PHE:HA	1:L:52:VAL:HG12	1.98	0.46
1:B:245:HIS:ND1	1:B:246:PRO:HD2	2.31	0.46
1:B:50:LEU:HG	1:B:81:LEU:HD11	1.98	0.46
1:D:158:PHE:CE1	1:D:160:LEU:HB2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:PHE:HA	1:D:52:VAL:HG12	1.98	0.46
1:D:65:CYS:HB3	1:D:91:MSE:HB3	1.97	0.46
1:E:245:HIS:ND1	1:E:246:PRO:HD2	2.30	0.46
1:E:46:GLN:NE2	2:E:379:HOH:O	2.48	0.46
1:E:49:PHE:HA	1:E:52:VAL:HG12	1.98	0.46
1:E:68:PRO:HG3	1:E:90:GLU:CD	2.36	0.46
1:F:121:ASN:CG	1:F:159:VAL:HG21	2.37	0.46
1:F:311:PHE:CE1	1:F:313:ILE:HD11	2.51	0.46
1:G:50:LEU:HG	1:G:81:LEU:HD11	1.98	0.46
1:H:132:PHE:CB	1:H:133:PRO:HD3	2.40	0.46
1:I:11:LYS:HG3	1:I:203:ASN:ND2	2.31	0.46
1:I:29:MSE:HE1	1:I:52:VAL:HG13	1.98	0.46
1:J:174:LEU:O	1:J:223:ILE:HG21	2.15	0.46
1:K:118:TRP:CZ3	1:K:155:THR:HG21	2.50	0.46
1:K:39:ARG:HG3	1:K:40:LEU:HD23	1.97	0.46
1:K:39:ARG:HH11	1:K:40:LEU:HD23	1.80	0.46
1:A:158:PHE:CE1	1:A:160:LEU:HB2	2.51	0.46
1:B:11:LYS:HG3	1:B:203:ASN:ND2	2.30	0.46
1:C:118:TRP:CZ3	1:C:155:THR:HG21	2.50	0.46
1:E:158:PHE:CE1	1:E:160:LEU:HB2	2.51	0.46
1:H:4:ARG:NH2	1:H:154:LYS:HD3	2.31	0.46
1:I:336:GLN:HA	1:I:336:GLN:OE1	2.15	0.46
1:J:121:ASN:CG	1:J:159:VAL:HG21	2.37	0.46
1:J:94:ASP:HB2	1:J:137:ASP:OD2	2.16	0.46
1:J:171:GLY:CA	1:J:204:CYS:HA	2.43	0.46
1:J:49:PHE:HA	1:J:52:VAL:HG12	1.98	0.46
1:A:323:TYR:HA	1:A:350:GLU:HB3	1.97	0.45
1:A:38:TRP:HZ3	1:A:352:ILE:HA	1.81	0.45
1:A:49:PHE:HA	1:A:52:VAL:HG12	1.98	0.45
1:B:39:ARG:HH11	1:B:40:LEU:HD23	1.81	0.45
1:C:158:PHE:CE1	1:C:160:LEU:HB2	2.51	0.45
1:C:224:ASP:HB2	1:C:360:HIS:HD2	1.80	0.45
1:E:203:ASN:HD22	1:E:203:ASN:HA	1.50	0.45
1:F:39:ARG:HG3	1:F:40:LEU:HD23	1.97	0.45
1:G:54:GLU:O	1:G:57:SER:HB2	2.15	0.45
1:H:159:VAL:HG12	1:H:186:ASN:ND2	2.31	0.45
1:J:38:TRP:HZ3	1:J:352:ILE:HA	1.81	0.45
1:L:118:TRP:CZ3	1:L:155:THR:HG21	2.50	0.45
1:L:94:ASP:HB2	1:L:137:ASP:OD2	2.16	0.45
1:K:291:TYR:OH	1:L:80:GLU:HB2	2.15	0.45
1:A:161:GLU:HG3	1:A:222:HIS:CE1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ASN:CG	1:B:159:VAL:HG21	2.37	0.45
1:B:65:CYS:HB3	1:B:91:MSE:HB3	1.97	0.45
1:D:11:LYS:HG3	1:D:203:ASN:ND2	2.31	0.45
1:E:29:MSE:HE1	1:E:52:VAL:HG13	1.97	0.45
1:F:323:TYR:HA	1:F:350:GLU:HB3	1.97	0.45
1:F:38:TRP:HZ3	1:F:352:ILE:HA	1.81	0.45
1:G:224:ASP:HB2	1:G:360:HIS:HD2	1.80	0.45
1:H:351:GLU:HA	1:H:354:TYR:HD2	1.82	0.45
1:I:49:PHE:HA	1:I:52:VAL:HG12	1.98	0.45
1:L:11:LYS:HG3	1:L:203:ASN:ND2	2.30	0.45
1:D:54:GLU:O	1:D:57:SER:HB2	2.15	0.45
1:E:121:ASN:CG	1:E:159:VAL:HG21	2.37	0.45
1:E:38:TRP:HZ3	1:E:352:ILE:HA	1.81	0.45
1:F:94:ASP:HB2	1:F:137:ASP:OD2	2.16	0.45
1:G:161:GLU:HG3	1:G:222:HIS:CE1	2.52	0.45
1:G:336:GLN:HA	1:G:336:GLN:OE1	2.15	0.45
1:H:34:ARG:HD2	1:H:94:ASP:O	2.17	0.45
1:I:174:LEU:O	1:I:223:ILE:HG21	2.15	0.45
1:I:309:LEU:HD22	1:I:311:PHE:HE2	1.80	0.45
1:I:39:ARG:HH11	1:I:40:LEU:HD23	1.81	0.45
1:I:50:LEU:HG	1:I:81:LEU:HD11	1.98	0.45
1:I:94:ASP:HB2	1:I:137:ASP:OD2	2.16	0.45
1:J:66:VAL:CG2	1:J:71:TYR:HA	2.45	0.45
1:J:50:LEU:HG	1:J:81:LEU:HD11	1.98	0.45
1:K:29:MSE:HE1	1:K:52:VAL:HG13	1.98	0.45
1:L:121:ASN:CG	1:L:159:VAL:HG21	2.37	0.45
1:L:158:PHE:CE1	1:L:160:LEU:HB2	2.51	0.45
1:A:174:LEU:O	1:A:223:ILE:HG21	2.15	0.45
1:B:29:MSE:HE1	1:B:52:VAL:HG13	1.98	0.45
1:C:121:ASN:CG	1:C:159:VAL:HG21	2.37	0.45
1:C:49:PHE:HA	1:C:52:VAL:HG12	1.98	0.45
1:D:341:ASP:OD2	1:F:58:GLU:HB3	2.09	0.45
1:E:94:ASP:HB2	1:E:137:ASP:OD2	2.16	0.45
1:F:121:ASN:H	1:F:121:ASN:ND2	2.07	0.45
1:G:309:LEU:HD22	1:G:311:PHE:HE2	1.80	0.45
1:I:161:GLU:HG3	1:I:222:HIS:CE1	2.52	0.45
1:J:161:GLU:HG3	1:J:222:HIS:CE1	2.52	0.45
1:L:38:TRP:HZ3	1:L:352:ILE:HA	1.82	0.45
1:A:50:LEU:HG	1:A:81:LEU:HD11	1.98	0.45
1:A:7:ASN:HB3	1:D:84:HIS:CG	2.50	0.45
1:B:99:ARG:O	1:B:162:GLY:HA3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:GLU:HG3	1:D:222:HIS:CE1	2.52	0.45
1:D:38:TRP:HZ3	1:D:352:ILE:HA	1.81	0.45
1:E:336:GLN:HA	1:E:336:GLN:OE1	2.15	0.45
1:E:339:PHE:HD2	2:E:391:HOH:O	1.99	0.45
1:F:11:LYS:HG3	1:F:203:ASN:ND2	2.31	0.45
1:G:121:ASN:CG	1:G:159:VAL:HG21	2.37	0.45
1:G:65:CYS:HB3	1:G:91:MSE:HB3	1.97	0.45
1:H:231:ARG:CB	1:H:231:ARG:NH1	2.79	0.45
1:J:99:ARG:O	1:J:162:GLY:HA3	2.17	0.45
1:K:168:ASP:O	1:K:169:GLY:C	2.53	0.45
1:L:215:ASP:HB2	1:L:221:GLY:HA2	1.98	0.45
1:L:336:GLN:OE1	1:L:336:GLN:HA	2.15	0.45
1:A:309:LEU:HD22	1:A:311:PHE:HE2	1.80	0.45
1:A:336:GLN:OE1	1:A:336:GLN:HA	2.16	0.45
1:B:49:PHE:HA	1:B:52:VAL:HG12	1.98	0.45
1:C:99:ARG:O	1:C:162:GLY:HA3	2.17	0.45
1:C:339:PHE:HB3	1:C:342:ARG:HB2	1.99	0.45
1:C:38:TRP:HZ3	1:C:352:ILE:HA	1.81	0.45
1:D:234:GLU:OE1	1:D:270:LYS:HD3	2.17	0.45
1:E:215:ASP:HB2	1:E:221:GLY:HA2	1.98	0.45
1:E:339:PHE:HB3	1:E:342:ARG:HB2	1.99	0.45
1:E:54:GLU:O	1:E:57:SER:HB2	2.15	0.45
1:F:234:GLU:OE1	1:F:270:LYS:HD3	2.17	0.45
1:G:158:PHE:CE1	1:G:160:LEU:HB2	2.51	0.45
1:G:49:PHE:HA	1:G:52:VAL:HG12	1.98	0.45
1:G:99:ARG:O	1:G:162:GLY:HA3	2.17	0.45
1:H:5:ILE:HG23	1:H:5:ILE:O	2.15	0.45
1:I:203:ASN:HA	1:I:203:ASN:HD22	1.50	0.45
1:A:121:ASN:CG	1:A:159:VAL:HG21	2.37	0.45
1:A:174:LEU:HD23	1:A:208:LEU:HB2	1.99	0.45
1:A:234:GLU:OE1	1:A:270:LYS:HD3	2.17	0.45
1:D:121:ASN:CG	1:D:159:VAL:HG21	2.37	0.45
1:E:39:ARG:HH11	1:E:40:LEU:HD23	1.81	0.45
1:F:161:GLU:HG3	1:F:222:HIS:CE1	2.52	0.45
1:F:49:PHE:HA	1:F:52:VAL:HG12	1.98	0.45
1:H:223:ILE:C	1:H:225:ASP:H	2.19	0.45
1:I:99:ARG:O	1:I:162:GLY:HA3	2.17	0.45
1:I:219:THR:O	1:I:220:ASN:HB2	2.17	0.45
1:K:234:GLU:OE1	1:K:270:LYS:HD3	2.17	0.45
1:K:49:PHE:HA	1:K:52:VAL:HG12	1.98	0.45
1:K:80:GLU:HB2	1:L:291:TYR:HH	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:39:ARG:HH11	1:L:40:LEU:HD23	1.81	0.45
1:A:245:HIS:ND1	1:A:246:PRO:HD2	2.30	0.45
1:C:234:GLU:OE1	1:C:270:LYS:HD3	2.17	0.45
1:D:43:LYS:HZ2	1:D:46:GLN:HE22	1.63	0.45
1:H:104:THR:O	1:H:104:THR:HG22	2.17	0.45
1:H:191:LYS:HD2	2:H:397:HOH:O	2.17	0.45
1:H:339:PHE:HB3	1:H:342:ARG:HG3	1.99	0.45
1:I:174:LEU:HD23	1:I:208:LEU:HB2	1.99	0.45
1:K:195:GLU:HG2	1:K:207:VAL:HG11	1.99	0.45
1:K:215:ASP:HB2	1:K:221:GLY:HA2	1.98	0.45
1:A:215:ASP:HB2	1:A:221:GLY:HA2	1.98	0.45
1:A:39:ARG:HH11	1:A:40:LEU:HD23	1.81	0.45
1:B:339:PHE:HB3	1:B:342:ARG:HB2	1.99	0.45
1:C:219:THR:O	1:C:220:ASN:HB2	2.17	0.45
1:C:50:LEU:HG	1:C:81:LEU:HD11	1.98	0.45
1:F:99:ARG:O	1:F:162:GLY:HA3	2.17	0.45
1:F:167:VAL:HG12	1:F:168:ASP:N	2.32	0.45
1:G:339:PHE:HB3	1:G:342:ARG:HB2	1.99	0.45
1:H:142:ARG:HH12	1:H:146:GLU:HG2	1.81	0.45
1:H:231:ARG:HB2	1:H:231:ARG:CZ	2.47	0.45
1:H:329:GLN:H	1:H:329:GLN:CD	2.21	0.45
1:I:121:ASN:CG	1:I:159:VAL:HG21	2.37	0.45
1:J:219:THR:O	1:J:220:ASN:HB2	2.17	0.45
1:J:330:LEU:O	1:J:334:GLN:HG3	2.17	0.45
1:J:67:PRO:HA	1:J:68:PRO:HD3	1.80	0.45
1:K:310:ASN:ND2	2:K:389:HOH:O	2.49	0.45
1:K:38:TRP:HZ3	1:K:352:ILE:HA	1.82	0.45
1:K:50:LEU:HG	1:K:81:LEU:HD11	1.98	0.45
1:L:223:ILE:C	1:L:225:ASP:H	2.21	0.45
1:L:234:GLU:OE1	1:L:270:LYS:HD3	2.17	0.45
1:A:219:THR:O	1:A:220:ASN:HB2	2.17	0.45
1:B:158:PHE:CE1	1:B:160:LEU:HB2	2.51	0.45
1:C:195:GLU:HG2	1:C:207:VAL:HG11	1.99	0.45
1:D:327:ASN:HD22	1:D:327:ASN:HA	1.63	0.45
1:D:339:PHE:HB3	1:D:342:ARG:HB2	1.99	0.45
1:E:167:VAL:HG12	1:E:168:ASP:N	2.33	0.45
1:F:327:ASN:HA	1:F:327:ASN:HD22	1.63	0.45
1:G:38:TRP:HZ3	1:G:352:ILE:HA	1.82	0.45
1:I:38:TRP:HZ3	1:I:352:ILE:HA	1.82	0.45
1:K:223:ILE:C	1:K:225:ASP:H	2.21	0.45
1:C:94:ASP:HB2	1:C:137:ASP:OD2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:LEU:HD23	1:C:208:LEU:HB2	1.99	0.44
1:E:369:THR:O	1:E:370:LEU:CB	2.47	0.44
1:G:219:THR:O	1:G:220:ASN:HB2	2.17	0.44
1:G:43:LYS:HZ2	1:G:46:GLN:HE22	1.64	0.44
1:H:177:GLU:HB3	1:H:209:TRP:CE3	2.46	0.44
1:H:181:LEU:HD13	1:H:209:TRP:HZ3	1.81	0.44
1:I:290:ASP:CB	1:J:73:ASN:ND2	2.80	0.44
1:K:121:ASN:CG	1:K:159:VAL:HG21	2.37	0.44
1:K:336:GLN:OE1	1:K:336:GLN:HA	2.15	0.44
1:K:40:LEU:HD12	1:L:40:LEU:HB3	1.97	0.44
1:L:195:GLU:HG2	1:L:207:VAL:HG11	1.99	0.44
1:L:219:THR:O	1:L:220:ASN:HB2	2.17	0.44
1:L:161:GLU:HG3	1:L:222:HIS:CE1	2.52	0.44
1:L:99:ARG:O	1:L:162:GLY:HA3	2.17	0.44
1:A:98:ILE:HG22	2:A:393:HOH:O	2.16	0.44
1:B:223:ILE:C	1:B:225:ASP:H	2.21	0.44
1:B:234:GLU:OE1	1:B:270:LYS:HD3	2.17	0.44
1:C:161:GLU:HG3	1:C:222:HIS:CE1	2.52	0.44
1:C:223:ILE:C	1:C:225:ASP:H	2.21	0.44
1:D:336:GLN:OE1	1:D:336:GLN:HA	2.16	0.44
1:D:50:LEU:HG	1:D:81:LEU:HD11	1.98	0.44
1:E:234:GLU:OE1	1:E:270:LYS:HD3	2.17	0.44
1:F:339:PHE:HB3	1:F:342:ARG:HB2	1.99	0.44
1:G:223:ILE:C	1:G:225:ASP:H	2.21	0.44
1:I:2:ALA:CB	2:I:384:HOH:O	2.40	0.44
1:I:327:ASN:HD22	1:I:327:ASN:HA	1.63	0.44
1:I:91:MSE:SE	1:I:140:VAL:HG13	2.67	0.44
1:K:94:ASP:HB2	1:K:137:ASP:OD2	2.17	0.44
1:K:99:ARG:O	1:K:162:GLY:HA3	2.17	0.44
1:K:161:GLU:HG3	1:K:222:HIS:CE1	2.52	0.44
1:A:223:ILE:C	1:A:225:ASP:H	2.21	0.44
1:A:94:ASP:HB2	1:A:137:ASP:OD2	2.17	0.44
1:B:94:ASP:HB2	1:B:137:ASP:OD2	2.17	0.44
1:B:167:VAL:HG12	1:B:168:ASP:N	2.32	0.44
1:B:219:THR:O	1:B:220:ASN:HB2	2.17	0.44
1:B:330:LEU:O	1:B:334:GLN:HG3	2.17	0.44
1:C:91:MSE:SE	1:C:140:VAL:HG13	2.68	0.44
1:D:167:VAL:HG12	1:D:168:ASP:N	2.32	0.44
1:D:330:LEU:O	1:D:334:GLN:HG3	2.17	0.44
1:D:91:MSE:SE	1:D:140:VAL:HG13	2.67	0.44
1:F:50:LEU:HG	1:F:81:LEU:HD11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:PRO:HA	1:F:68:PRO:HD3	1.80	0.44
1:G:94:ASP:HB2	1:G:137:ASP:OD2	2.17	0.44
1:H:61:PRO:HA	1:H:85:ASN:ND2	2.18	0.44
1:I:234:GLU:OE1	1:I:270:LYS:HD3	2.17	0.44
1:I:330:LEU:O	1:I:334:GLN:HG3	2.17	0.44
1:J:195:GLU:HG2	1:J:207:VAL:HG11	1.99	0.44
1:J:234:GLU:OE1	1:J:270:LYS:HD3	2.17	0.44
1:K:121:ASN:N	1:K:121:ASN:ND2	2.60	0.44
1:L:339:PHE:HB3	1:L:342:ARG:HB2	1.99	0.44
1:A:167:VAL:HG12	1:A:168:ASP:N	2.32	0.44
1:A:195:GLU:HG2	1:A:207:VAL:HG11	1.99	0.44
1:A:99:ARG:O	1:A:162:GLY:HA3	2.17	0.44
1:B:161:GLU:HG3	1:B:222:HIS:CE1	2.52	0.44
1:C:119:GLU:HB2	1:C:159:VAL:HA	2.00	0.44
1:D:94:ASP:HB2	1:D:137:ASP:OD2	2.17	0.44
1:D:30:LEU:HD22	1:D:93:ASN:HD22	1.83	0.44
1:D:99:ARG:O	1:D:162:GLY:HA3	2.17	0.44
1:E:99:ARG:O	1:E:162:GLY:HA3	2.17	0.44
1:G:119:GLU:HB2	1:G:159:VAL:HA	2.00	0.44
1:G:30:LEU:HD22	1:G:93:ASN:HD22	1.83	0.44
1:G:91:MSE:SE	1:G:140:VAL:HG13	2.68	0.44
1:H:57:SER:HA	1:H:85:ASN:HD21	1.82	0.44
1:J:43:LYS:HZ2	1:J:46:GLN:HE22	1.66	0.44
1:K:30:LEU:HD22	1:K:93:ASN:HD22	1.83	0.44
1:K:73:ASN:ND2	1:L:290:ASP:CB	2.76	0.44
1:L:50:LEU:HG	1:L:81:LEU:HD11	1.98	0.44
1:B:91:MSE:SE	1:B:140:VAL:HG13	2.68	0.44
1:D:223:ILE:C	1:D:225:ASP:H	2.21	0.44
1:H:119:GLU:HB2	1:H:159:VAL:HA	2.00	0.44
1:I:161:GLU:HG3	1:I:222:HIS:NE2	2.33	0.44
1:I:30:LEU:HD22	1:I:93:ASN:HD22	1.83	0.44
1:J:167:VAL:HG12	1:J:168:ASP:N	2.32	0.44
1:J:369:THR:O	1:J:370:LEU:CB	2.47	0.44
1:K:219:THR:O	1:K:220:ASN:HB2	2.17	0.44
1:A:108:ASN:OD1	1:A:112:ASP:HB2	2.18	0.44
1:A:161:GLU:HG3	1:A:222:HIS:NE2	2.33	0.44
1:A:339:PHE:HB3	1:A:342:ARG:HB2	1.99	0.44
1:C:30:LEU:HD22	1:C:93:ASN:HD22	1.83	0.44
1:A:12:GLN:HB3	1:D:81:LEU:C	2.38	0.44
1:E:219:THR:O	1:E:220:ASN:HB2	2.17	0.44
1:E:161:GLU:HG3	1:E:222:HIS:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:ASP:HB2	1:H:221:GLY:H	1.82	0.44
1:I:185:ARG:HH11	1:I:185:ARG:CB	2.11	0.44
1:I:223:ILE:C	1:I:225:ASP:H	2.21	0.44
1:I:43:LYS:HZ2	1:I:46:GLN:HE22	1.65	0.44
1:J:91:MSE:SE	1:J:140:VAL:HG13	2.67	0.44
1:K:119:GLU:HB2	1:K:159:VAL:HA	2.00	0.44
1:A:119:GLU:HB2	1:A:159:VAL:HA	2.00	0.44
1:B:118:TRP:HA	1:B:155:THR:OG1	2.18	0.44
1:B:161:GLU:HG3	1:B:222:HIS:NE2	2.33	0.44
1:E:119:GLU:HB2	1:E:159:VAL:HA	2.00	0.44
1:E:161:GLU:HG3	1:E:222:HIS:NE2	2.33	0.44
1:F:161:GLU:HG3	1:F:222:HIS:NE2	2.33	0.44
1:F:330:LEU:O	1:F:334:GLN:HG3	2.17	0.44
1:G:330:LEU:O	1:G:334:GLN:HG3	2.17	0.44
1:J:119:GLU:HB2	1:J:159:VAL:HA	2.00	0.44
1:J:30:LEU:HD22	1:J:93:ASN:HD22	1.83	0.44
1:K:161:GLU:HG3	1:K:222:HIS:NE2	2.33	0.44
1:K:339:PHE:HB3	1:K:342:ARG:HB2	1.99	0.44
1:L:119:GLU:HB2	1:L:159:VAL:HA	2.00	0.44
1:A:30:LEU:HD22	1:A:93:ASN:HD22	1.83	0.44
1:B:195:GLU:HG2	1:B:207:VAL:HG11	1.99	0.44
1:B:325:ASP:O	1:B:328:ASP:HB2	2.18	0.44
1:C:108:ASN:OD1	1:C:112:ASP:HB2	2.18	0.44
1:C:161:GLU:HG3	1:C:222:HIS:NE2	2.33	0.44
1:C:325:ASP:O	1:C:328:ASP:HB2	2.18	0.44
1:C:95:ASP:HB2	1:C:131:TYR:CE2	2.53	0.44
1:D:174:LEU:HD23	1:D:208:LEU:HB2	1.99	0.44
1:E:30:LEU:HD22	1:E:93:ASN:HD22	1.83	0.44
1:F:108:ASN:OD1	1:F:112:ASP:HB2	2.18	0.44
1:F:174:LEU:HD23	1:F:208:LEU:HB2	1.99	0.44
1:G:174:LEU:HD23	1:G:208:LEU:HB2	1.99	0.44
1:J:325:ASP:O	1:J:328:ASP:HB2	2.18	0.44
1:J:95:ASP:HB2	1:J:131:TYR:CE2	2.53	0.44
1:A:329:GLN:H	1:A:329:GLN:CD	2.22	0.44
1:B:114:ARG:NH1	2:B:380:HOH:O	2.31	0.44
1:C:118:TRP:HA	1:C:155:THR:OG1	2.18	0.44
1:D:219:THR:O	1:D:220:ASN:HB2	2.17	0.44
1:D:325:ASP:O	1:D:328:ASP:HB2	2.18	0.44
1:F:223:ILE:C	1:F:225:ASP:H	2.21	0.44
1:G:234:GLU:OE1	1:G:270:LYS:HD3	2.17	0.44
1:I:108:ASN:OD1	1:I:112:ASP:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:215:ASP:HB2	1:I:221:GLY:HA2	1.98	0.44
1:I:325:ASP:O	1:I:328:ASP:HB2	2.18	0.44
1:K:118:TRP:HA	1:K:155:THR:OG1	2.18	0.44
1:L:118:TRP:HA	1:L:155:THR:OG1	2.18	0.44
1:L:95:ASP:HB2	1:L:131:TYR:CE2	2.53	0.44
1:B:119:GLU:HB2	1:B:159:VAL:HA	2.00	0.43
1:B:203:ASN:HD22	1:B:203:ASN:HA	1.50	0.43
1:B:38:TRP:HZ3	1:B:352:ILE:HA	1.82	0.43
1:E:330:LEU:O	1:E:334:GLN:HG3	2.17	0.43
1:F:118:TRP:HA	1:F:155:THR:OG1	2.18	0.43
1:F:142:ARG:N	2:F:388:HOH:O	2.46	0.43
1:G:161:GLU:HG3	1:G:222:HIS:NE2	2.33	0.43
1:H:121:ASN:O	1:H:125:GLY:HA2	2.18	0.43
1:J:223:ILE:C	1:J:225:ASP:H	2.21	0.43
1:K:174:LEU:HD23	1:K:208:LEU:HB2	1.99	0.43
1:A:91:MSE:SE	1:A:140:VAL:HG13	2.68	0.43
1:B:108:ASN:OD1	1:B:112:ASP:HB2	2.18	0.43
1:B:329:GLN:H	1:B:329:GLN:CD	2.22	0.43
1:D:118:TRP:HA	1:D:155:THR:OG1	2.18	0.43
1:E:91:MSE:SE	1:E:140:VAL:HG13	2.68	0.43
1:E:174:LEU:HD23	1:E:208:LEU:HB2	1.99	0.43
1:E:325:ASP:O	1:E:328:ASP:HB2	2.18	0.43
1:F:91:MSE:SE	1:F:140:VAL:HG13	2.68	0.43
1:G:167:VAL:HG12	1:G:168:ASP:N	2.32	0.43
1:G:195:GLU:HG2	1:G:207:VAL:HG11	1.99	0.43
1:K:91:MSE:SE	1:K:140:VAL:HG13	2.67	0.43
1:K:330:LEU:O	1:K:334:GLN:HG3	2.17	0.43
1:L:174:LEU:HD23	1:L:208:LEU:HB2	1.99	0.43
1:L:325:ASP:O	1:L:328:ASP:HB2	2.18	0.43
1:A:189:LEU:HA	1:A:189:LEU:HD12	1.84	0.43
1:B:95:ASP:HB2	1:B:131:TYR:CE2	2.53	0.43
1:D:95:ASP:HB2	1:D:131:TYR:CE2	2.53	0.43
1:D:195:GLU:HG2	1:D:207:VAL:HG11	1.99	0.43
1:E:118:TRP:HA	1:E:155:THR:OG1	2.18	0.43
1:E:95:ASP:HB2	1:E:131:TYR:CE2	2.53	0.43
1:F:119:GLU:HB2	1:F:159:VAL:HA	2.00	0.43
1:F:219:THR:O	1:F:220:ASN:HB2	2.17	0.43
1:G:325:ASP:O	1:G:328:ASP:HB2	2.18	0.43
1:I:167:VAL:HG12	1:I:168:ASP:N	2.33	0.43
1:I:189:LEU:HD12	1:I:189:LEU:HA	1.84	0.43
1:J:161:GLU:HG3	1:J:222:HIS:NE2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:339:PHE:HB3	1:J:342:ARG:HB2	1.99	0.43
1:K:329:GLN:CD	1:K:329:GLN:H	2.22	0.43
1:K:369:THR:O	1:K:370:LEU:CB	2.47	0.43
1:L:121:ASN:ND2	1:L:121:ASN:N	2.60	0.43
1:L:161:GLU:HG3	1:L:222:HIS:NE2	2.33	0.43
1:A:330:LEU:O	1:A:334:GLN:HG3	2.17	0.43
1:C:167:VAL:HG12	1:C:168:ASP:N	2.32	0.43
1:D:161:GLU:HG3	1:D:222:HIS:NE2	2.33	0.43
1:D:329:GLN:CD	1:D:329:GLN:H	2.22	0.43
1:E:195:GLU:HG2	1:E:207:VAL:HG11	1.99	0.43
1:F:30:LEU:HD22	1:F:93:ASN:HD22	1.83	0.43
1:J:321:PRO:HB3	1:J:358:ASN:ND2	2.34	0.43
1:K:167:VAL:HG12	1:K:168:ASP:N	2.33	0.43
1:L:167:VAL:HG12	1:L:168:ASP:N	2.33	0.43
1:L:330:LEU:O	1:L:334:GLN:HG3	2.17	0.43
1:L:91:MSE:SE	1:L:140:VAL:HG13	2.68	0.43
1:E:185:ARG:CB	1:E:185:ARG:HH11	2.11	0.43
1:E:236:ALA:O	1:E:237:CYS:HB2	2.19	0.43
1:H:5:ILE:HD13	1:H:153:TYR:CE2	2.54	0.43
1:H:80:GLU:C	1:H:82:GLY:H	2.22	0.43
1:I:329:GLN:CD	1:I:329:GLN:H	2.22	0.43
1:J:118:TRP:HA	1:J:155:THR:OG1	2.18	0.43
1:J:174:LEU:HD23	1:J:208:LEU:HB2	1.99	0.43
1:J:327:ASN:HD22	1:J:327:ASN:HA	1.63	0.43
1:K:95:ASP:HB2	1:K:131:TYR:CE2	2.53	0.43
1:B:236:ALA:O	1:B:237:CYS:HB2	2.19	0.43
1:B:321:PRO:HB3	1:B:358:ASN:ND2	2.34	0.43
1:C:330:LEU:O	1:C:334:GLN:HG3	2.17	0.43
1:E:329:GLN:CD	1:E:329:GLN:H	2.22	0.43
1:F:95:ASP:HB2	1:F:131:TYR:CE2	2.53	0.43
1:F:236:ALA:O	1:F:237:CYS:HB2	2.19	0.43
1:G:108:ASN:OD1	1:G:112:ASP:HB2	2.18	0.43
1:H:74:ALA:O	1:H:78:VAL:HG23	2.18	0.43
1:I:119:GLU:HB2	1:I:159:VAL:HA	2.00	0.43
1:J:329:GLN:H	1:J:329:GLN:CD	2.22	0.43
1:K:66:VAL:HG21	1:K:71:TYR:HA	2.01	0.43
1:C:327:ASN:HD22	1:C:327:ASN:HA	1.63	0.43
1:F:329:GLN:H	1:F:329:GLN:CD	2.22	0.43
1:H:132:PHE:HB3	1:H:133:PRO:CD	2.44	0.43
1:H:132:PHE:O	1:H:133:PRO:C	2.56	0.43
1:I:118:TRP:HA	1:I:155:THR:OG1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:95:ASP:HB2	1:I:131:TYR:CE2	2.53	0.43
1:K:236:ALA:O	1:K:237:CYS:HB2	2.19	0.43
1:L:30:LEU:HD22	1:L:93:ASN:HD22	1.83	0.43
1:L:329:GLN:H	1:L:329:GLN:CD	2.22	0.43
1:A:66:VAL:HG21	1:A:71:TYR:HA	2.01	0.43
1:C:329:GLN:H	1:C:329:GLN:CD	2.22	0.43
1:E:223:ILE:C	1:E:225:ASP:H	2.21	0.43
1:G:236:ALA:O	1:G:237:CYS:HB2	2.19	0.43
1:G:89:ILE:H	1:G:89:ILE:CD1	2.22	0.43
1:H:224:ASP:HB2	1:H:360:HIS:HD2	1.81	0.43
1:C:132:PHE:CD2	1:I:135:ASP:HB3	2.53	0.43
1:I:66:VAL:HG21	1:I:71:TYR:HA	2.01	0.43
1:K:108:ASN:OD1	1:K:112:ASP:HB2	2.18	0.43
1:K:327:ASN:HA	1:K:327:ASN:HD22	1.63	0.43
1:A:325:ASP:O	1:A:328:ASP:HB2	2.18	0.43
1:B:174:LEU:HD23	1:B:208:LEU:HB2	1.99	0.43
1:E:135:ASP:HB3	1:L:132:PHE:HE2	1.78	0.43
1:E:321:PRO:HB3	1:E:358:ASN:ND2	2.34	0.43
1:E:66:VAL:HG21	1:E:71:TYR:HA	2.01	0.43
1:G:118:TRP:HA	1:G:155:THR:OG1	2.18	0.43
1:I:195:GLU:HG2	1:I:207:VAL:HG11	1.99	0.43
1:A:118:TRP:HA	1:A:155:THR:OG1	2.18	0.43
1:A:121:ASN:H	1:A:121:ASN:ND2	2.07	0.43
1:A:43:LYS:HZ2	1:A:46:GLN:HE22	1.66	0.43
1:B:171:GLY:CA	1:B:204:CYS:HA	2.43	0.43
1:C:321:PRO:HB3	1:C:358:ASN:ND2	2.34	0.43
1:C:66:VAL:HG21	1:C:71:TYR:HA	2.01	0.43
1:E:40:LEU:HD22	1:E:288:THR:OG1	2.19	0.43
1:F:195:GLU:HG2	1:F:207:VAL:HG11	1.99	0.43
1:F:40:LEU:HD22	1:F:288:THR:OG1	2.19	0.43
1:F:98:ILE:HG22	2:F:379:HOH:O	2.18	0.43
1:G:95:ASP:HB2	1:G:131:TYR:CE2	2.53	0.43
1:H:15:PHE:CE2	1:H:108:ASN:HB3	2.54	0.43
1:J:108:ASN:OD1	1:J:112:ASP:HB2	2.18	0.43
1:J:185:ARG:CB	1:J:185:ARG:HH11	2.11	0.43
1:K:325:ASP:O	1:K:328:ASP:HB2	2.18	0.43
1:L:236:ALA:O	1:L:237:CYS:HB2	2.19	0.43
1:A:321:PRO:HB3	1:A:358:ASN:ND2	2.34	0.42
1:B:138:ALA:HB1	2:B:384:HOH:O	2.19	0.42
1:C:185:ARG:CB	1:C:185:ARG:HH11	2.11	0.42
1:C:311:PHE:HE1	1:C:313:ILE:HD11	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:ASN:HD22	1:D:203:ASN:HA	1.50	0.42
1:F:325:ASP:O	1:F:328:ASP:HB2	2.18	0.42
1:G:66:VAL:HG21	1:G:71:TYR:HA	2.01	0.42
1:H:20:GLU:OE1	1:H:360:HIS:HE1	2.02	0.42
1:I:236:ALA:O	1:I:237:CYS:HB2	2.19	0.42
1:J:203:ASN:HA	1:J:203:ASN:HD22	1.50	0.42
1:K:40:LEU:HD22	1:K:288:THR:OG1	2.19	0.42
1:L:108:ASN:OD1	1:L:112:ASP:HB2	2.18	0.42
1:L:311:PHE:HE1	1:L:313:ILE:HD11	1.84	0.42
1:A:95:ASP:HB2	1:A:131:TYR:CE2	2.53	0.42
1:B:30:LEU:HD22	1:B:93:ASN:HD22	1.83	0.42
1:B:40:LEU:HD22	1:B:288:THR:OG1	2.19	0.42
1:D:119:GLU:HB2	1:D:159:VAL:HA	2.00	0.42
1:H:223:ILE:HA	1:H:226:VAL:HG22	2.01	0.42
1:A:236:ALA:O	1:A:237:CYS:HB2	2.19	0.42
1:A:315:ASN:CB	2:A:379:HOH:O	2.63	0.42
1:D:311:PHE:HE1	1:D:313:ILE:HD11	1.84	0.42
1:D:321:PRO:HB3	1:D:358:ASN:ND2	2.34	0.42
1:C:291:TYR:OH	1:D:80:GLU:HB2	2.19	0.42
1:F:142:ARG:HB2	2:F:388:HOH:O	2.20	0.42
1:I:339:PHE:HB3	1:I:342:ARG:HB2	1.99	0.42
1:I:40:LEU:HD22	1:I:288:THR:OG1	2.19	0.42
1:B:66:VAL:HG21	1:B:71:TYR:HA	2.01	0.42
1:F:321:PRO:HB3	1:F:358:ASN:ND2	2.34	0.42
1:G:329:GLN:H	1:G:329:GLN:CD	2.22	0.42
1:H:263:ASP:C	1:H:265:LYS:H	2.23	0.42
1:A:127:VAL:HG12	2:A:382:HOH:O	2.19	0.42
1:D:66:VAL:HG21	1:D:71:TYR:HA	2.01	0.42
1:E:108:ASN:OD1	1:E:112:ASP:HB2	2.18	0.42
1:G:321:PRO:HB3	1:G:358:ASN:ND2	2.34	0.42
1:H:11:LYS:HG3	1:H:203:ASN:ND2	2.34	0.42
1:H:178:MSE:SE	1:H:221:GLY:HA3	2.69	0.42
1:H:339:PHE:C	1:H:341:ASP:H	2.21	0.42
1:I:321:PRO:HB3	1:I:358:ASN:ND2	2.34	0.42
1:J:66:VAL:HG21	1:J:71:TYR:HA	2.01	0.42
1:L:252:LYS:HE2	1:L:252:LYS:HB3	1.92	0.42
1:A:35:ASN:N	1:A:35:ASN:OD1	2.53	0.42
1:A:40:LEU:HD22	1:A:288:THR:OG1	2.19	0.42
1:B:311:PHE:HE1	1:B:313:ILE:HD11	1.84	0.42
1:D:108:ASN:OD1	1:D:112:ASP:HB2	2.18	0.42
1:D:236:ALA:O	1:D:237:CYS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:GLY:CA	1:E:204:CYS:HA	2.43	0.42
1:H:310:ASN:OD1	1:H:358:ASN:HB3	2.19	0.42
1:H:5:ILE:HD11	1:H:8:THR:OG1	2.19	0.42
1:J:40:LEU:HD22	1:J:288:THR:OG1	2.19	0.42
1:L:321:PRO:HB3	1:L:358:ASN:ND2	2.34	0.42
1:A:7:ASN:HB2	1:D:84:HIS:CD2	2.54	0.42
1:C:236:ALA:O	1:C:237:CYS:HB2	2.19	0.42
1:C:35:ASN:OD1	1:C:35:ASN:N	2.53	0.42
1:C:40:LEU:HD22	1:C:288:THR:OG1	2.19	0.42
1:C:71:TYR:CZ	1:J:143:LYS:HG2	2.54	0.42
1:F:185:ARG:CB	1:F:185:ARG:HH11	2.11	0.42
1:H:313:ILE:HD12	1:H:318:ILE:HD11	2.00	0.42
1:I:174:LEU:HB3	1:I:223:ILE:CD1	2.50	0.42
1:K:121:ASN:O	1:K:125:GLY:HA2	2.20	0.42
1:K:311:PHE:HE1	1:K:313:ILE:HD11	1.84	0.42
1:D:132:PHE:CE2	1:J:135:ASP:HB3	2.54	0.42
1:B:291:TYR:HH	1:F:80:GLU:HB2	1.83	0.42
1:H:230:ILE:O	1:H:231:ARG:HB2	2.20	0.42
1:H:325:ASP:N	1:H:328:ASP:OD1	2.50	0.42
1:A:203:ASN:HD22	1:A:203:ASN:HA	1.50	0.42
1:C:224:ASP:HB2	1:C:360:HIS:CD2	2.55	0.42
1:G:121:ASN:O	1:G:125:GLY:HA2	2.20	0.42
1:H:28:TRP:CZ3	1:H:144:VAL:HG23	2.54	0.42
1:J:236:ALA:O	1:J:237:CYS:HB2	2.19	0.42
1:I:40:LEU:HD12	1:J:40:LEU:HB3	2.02	0.42
1:K:321:PRO:HB3	1:K:358:ASN:ND2	2.34	0.42
1:B:121:ASN:O	1:B:125:GLY:HA2	2.20	0.42
1:B:182:HIS:ND1	1:B:183:PRO:HD2	2.35	0.42
1:E:121:ASN:O	1:E:125:GLY:HA2	2.20	0.42
1:F:121:ASN:O	1:F:125:GLY:HA2	2.20	0.42
1:F:182:HIS:ND1	1:F:183:PRO:HD2	2.35	0.42
1:G:182:HIS:ND1	1:G:183:PRO:HD2	2.35	0.42
1:G:40:LEU:HD22	1:G:288:THR:OG1	2.19	0.42
1:I:121:ASN:O	1:I:125:GLY:HA2	2.20	0.42
1:L:35:ASN:OD1	1:L:35:ASN:N	2.53	0.42
1:D:40:LEU:HD22	1:D:288:THR:OG1	2.19	0.41
1:F:121:ASN:N	1:F:121:ASN:ND2	2.60	0.41
1:F:311:PHE:HE1	1:F:313:ILE:HD11	1.84	0.41
1:G:185:ARG:CB	1:G:185:ARG:HH11	2.11	0.41
1:H:231:ARG:HB3	1:H:231:ARG:HH11	1.85	0.41
1:I:309:LEU:HD22	1:I:309:LEU:HA	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:121:ASN:O	1:J:125:GLY:HA2	2.20	0.41
1:J:311:PHE:HE1	1:J:313:ILE:HD11	1.84	0.41
1:K:189:LEU:HD12	1:K:189:LEU:HA	1.84	0.41
1:L:115:ALA:O	1:L:153:TYR:HD1	2.03	0.41
1:L:171:GLY:CA	1:L:204:CYS:HA	2.43	0.41
1:L:224:ASP:HB2	1:L:360:HIS:CD2	2.55	0.41
1:A:182:HIS:ND1	1:A:183:PRO:HD2	2.35	0.41
1:B:189:LEU:HD12	1:B:189:LEU:HA	1.84	0.41
1:B:35:ASN:N	1:B:35:ASN:OD1	2.53	0.41
1:G:215:ASP:N	1:G:216:PRO:HD3	2.36	0.41
1:H:94:ASP:OD2	1:H:136:GLN:HB2	2.20	0.41
1:I:215:ASP:N	1:I:216:PRO:HD3	2.36	0.41
1:L:121:ASN:O	1:L:125:GLY:HA2	2.20	0.41
1:F:189:LEU:HA	1:F:189:LEU:HD12	1.84	0.41
1:H:171:GLY:HA2	1:H:204:CYS:HA	2.01	0.41
1:I:311:PHE:HE1	1:I:313:ILE:HD11	1.84	0.41
1:J:224:ASP:HB2	1:J:360:HIS:CD2	2.55	0.41
1:K:35:ASN:N	1:K:35:ASN:OD1	2.53	0.41
1:B:215:ASP:N	1:B:216:PRO:HD3	2.36	0.41
1:B:56:ILE:HG12	1:B:56:ILE:H	1.67	0.41
1:D:121:ASN:O	1:D:125:GLY:HA2	2.20	0.41
1:D:215:ASP:N	1:D:216:PRO:HD3	2.36	0.41
1:D:35:ASN:OD1	1:D:35:ASN:N	2.53	0.41
1:F:174:LEU:HB3	1:F:223:ILE:CD1	2.50	0.41
1:J:189:LEU:HD12	1:J:189:LEU:HA	1.84	0.41
1:J:56:ILE:HG12	1:J:56:ILE:H	1.67	0.41
1:L:182:HIS:ND1	1:L:183:PRO:HD2	2.35	0.41
1:L:40:LEU:HD22	1:L:288:THR:OG1	2.19	0.41
1:A:115:ALA:O	1:A:153:TYR:HD1	2.03	0.41
1:E:115:ALA:O	1:E:153:TYR:HD1	2.03	0.41
1:E:215:ASP:N	1:E:216:PRO:HD3	2.36	0.41
1:G:35:ASN:OD1	1:G:35:ASN:N	2.53	0.41
1:A:40:LEU:HD12	1:G:40:LEU:HB3	2.02	0.41
1:I:182:HIS:ND1	1:I:183:PRO:HD2	2.35	0.41
1:J:35:ASN:N	1:J:35:ASN:OD1	2.53	0.41
1:K:103:PRO:CD	1:K:144:VAL:HG11	2.50	0.41
1:K:67:PRO:HA	1:K:68:PRO:HD3	1.80	0.41
1:L:43:LYS:HZ2	1:L:46:GLN:HE22	1.67	0.41
1:C:115:ALA:O	1:C:153:TYR:HD1	2.03	0.41
1:D:182:HIS:ND1	1:D:183:PRO:HD2	2.36	0.41
1:E:327:ASN:HD22	1:E:327:ASN:HA	1.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:105:PHE:CB	1:H:367:PRO:HD2	2.51	0.41
1:H:100:ASP:CB	1:H:161:GLU:HB2	2.49	0.41
1:H:198:LEU:CD2	1:H:202:LEU:HD22	2.48	0.41
1:H:8:THR:HB	1:H:13:ASP:OD1	2.20	0.41
1:L:174:LEU:HB3	1:L:223:ILE:CD1	2.50	0.41
1:L:215:ASP:N	1:L:216:PRO:HD3	2.36	0.41
1:B:224:ASP:HB2	1:B:360:HIS:CD2	2.55	0.41
1:D:115:ALA:O	1:D:153:TYR:HD1	2.03	0.41
1:G:171:GLY:CA	1:G:204:CYS:HA	2.43	0.41
1:G:161:GLU:HG3	1:G:222:HIS:HE2	1.86	0.41
1:L:66:VAL:HG21	1:L:71:TYR:HA	2.01	0.41
1:A:121:ASN:O	1:A:125:GLY:HA2	2.20	0.41
1:A:311:PHE:HE1	1:A:313:ILE:HD11	1.84	0.41
1:B:252:LYS:HB3	1:B:252:LYS:HE2	1.92	0.41
1:C:103:PRO:CD	1:C:144:VAL:HG11	2.50	0.41
1:D:67:PRO:HA	1:D:68:PRO:HD3	1.80	0.41
1:F:115:ALA:O	1:F:153:TYR:HD1	2.03	0.41
1:F:300:GLU:HG2	1:F:301:GLY:N	2.36	0.41
1:G:103:PRO:CD	1:G:144:VAL:HG11	2.50	0.41
1:G:224:ASP:HB2	1:G:360:HIS:CD2	2.55	0.41
1:G:300:GLU:HG2	1:G:301:GLY:N	2.36	0.41
1:H:121:ASN:O	1:H:125:GLY:N	2.51	0.41
1:H:172:THR:HG22	1:H:173:VAL:H	1.86	0.41
1:J:24:GLN:HA	1:J:368:ALA:N	2.33	0.41
1:A:252:LYS:HE2	1:A:252:LYS:HB3	1.92	0.41
1:B:103:PRO:CD	1:B:144:VAL:HG11	2.50	0.41
1:B:185:ARG:HH11	1:B:185:ARG:CB	2.11	0.41
1:B:300:GLU:HG2	1:B:301:GLY:N	2.36	0.41
1:B:43:LYS:HZ2	1:B:46:GLN:HE22	1.68	0.41
1:C:203:ASN:HA	1:C:203:ASN:HD22	1.50	0.41
1:F:66:VAL:HG21	1:F:71:TYR:HA	2.01	0.41
1:H:133:PRO:HG3	1:K:135:ASP:CG	2.41	0.41
1:H:173:VAL:HG12	1:H:206:LYS:O	2.20	0.41
1:I:300:GLU:HG2	1:I:301:GLY:N	2.36	0.41
1:A:124:GLY:O	1:A:127:VAL:HG13	2.21	0.41
1:A:215:ASP:N	1:A:216:PRO:HD3	2.36	0.41
1:A:24:GLN:HA	1:A:368:ALA:N	2.33	0.41
1:A:300:GLU:HG2	1:A:301:GLY:N	2.36	0.41
1:A:12:GLN:NE2	1:D:82:GLY:HA2	2.19	0.41
1:E:311:PHE:HE1	1:E:313:ILE:HD11	1.84	0.41
1:E:35:ASN:N	1:E:35:ASN:OD1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:GLN:NE2	1:H:314:VAL:HG12	2.36	0.41
1:I:103:PRO:CD	1:I:144:VAL:HG11	2.50	0.41
1:I:115:ALA:O	1:I:153:TYR:HD1	2.03	0.41
1:I:80:GLU:HB2	1:J:291:TYR:OH	2.21	0.41
1:J:182:HIS:ND1	1:J:183:PRO:HD2	2.36	0.41
1:L:300:GLU:HG2	1:L:301:GLY:N	2.36	0.41
1:A:174:LEU:HB3	1:A:223:ILE:CD1	2.50	0.41
1:B:233:GLY:N	2:B:397:HOH:O	2.54	0.41
1:B:327:ASN:HA	1:B:327:ASN:HD22	1.63	0.41
1:B:27:ILE:HG13	1:B:60:GLU:OE2	2.21	0.41
1:C:182:HIS:ND1	1:C:183:PRO:HD2	2.35	0.41
1:C:215:ASP:N	1:C:216:PRO:HD3	2.36	0.41
1:F:99:ARG:HD3	1:F:360:HIS:CD2	2.56	0.41
1:G:311:PHE:HE1	1:G:313:ILE:HD11	1.84	0.41
1:H:28:TRP:CZ3	1:H:147:ILE:HD11	2.56	0.41
1:K:224:ASP:HB2	1:K:360:HIS:CD2	2.55	0.41
1:C:124:GLY:O	1:C:127:VAL:HG13	2.21	0.40
1:E:224:ASP:HB2	1:E:360:HIS:CD2	2.55	0.40
1:F:124:GLY:O	1:F:127:VAL:HG13	2.21	0.40
1:F:215:ASP:N	1:F:216:PRO:HD3	2.36	0.40
1:H:231:ARG:HB2	1:H:231:ARG:NH1	2.36	0.40
1:H:296:ILE:O	1:H:296:ILE:HG23	2.20	0.40
1:H:4:ARG:NH1	1:H:142:ARG:HD3	2.35	0.40
1:J:215:ASP:N	1:J:216:PRO:HD3	2.36	0.40
1:J:27:ILE:HG13	1:J:60:GLU:OE2	2.21	0.40
1:K:171:GLY:CA	1:K:204:CYS:HA	2.43	0.40
1:L:124:GLY:O	1:L:127:VAL:HG13	2.21	0.40
1:L:327:ASN:HD22	1:L:327:ASN:HA	1.63	0.40
1:A:155:THR:HB	1:A:158:PHE:HB3	2.04	0.40
1:A:224:ASP:HB2	1:A:360:HIS:CD2	2.55	0.40
1:B:115:ALA:O	1:B:153:TYR:HD1	2.03	0.40
1:C:300:GLU:HG2	1:C:301:GLY:N	2.36	0.40
1:D:124:GLY:O	1:D:127:VAL:HG13	2.21	0.40
1:D:173:VAL:HG22	1:D:174:LEU:N	2.37	0.40
1:D:243:LYS:NZ	1:H:192:GLU:CG	2.73	0.40
1:E:182:HIS:ND1	1:E:183:PRO:HD2	2.35	0.40
1:F:173:VAL:HG22	1:F:174:LEU:N	2.37	0.40
1:G:27:ILE:HG13	1:G:60:GLU:OE2	2.21	0.40
1:H:100:ASP:OD1	1:H:100:ASP:N	2.54	0.40
1:H:113:LEU:O	1:H:150:VAL:HG23	2.20	0.40
1:I:173:VAL:HG22	1:I:174:LEU:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:300:GLU:HG2	1:K:301:GLY:N	2.36	0.40
1:C:27:ILE:HG13	1:C:60:GLU:OE2	2.21	0.40
1:E:124:GLY:O	1:E:127:VAL:HG13	2.21	0.40
1:E:300:GLU:HG2	1:E:301:GLY:N	2.36	0.40
1:E:99:ARG:HD3	1:E:360:HIS:CD2	2.56	0.40
1:G:115:ALA:O	1:G:153:TYR:HD1	2.04	0.40
1:G:99:ARG:HD3	1:G:360:HIS:CD2	2.56	0.40
1:H:17:MSE:HB2	1:H:106:LEU:CD2	2.51	0.40
1:I:30:LEU:HD22	1:I:93:ASN:ND2	2.37	0.40
1:I:99:ARG:HD3	1:I:360:HIS:CD2	2.56	0.40
1:J:300:GLU:HG2	1:J:301:GLY:N	2.36	0.40
1:K:115:ALA:O	1:K:153:TYR:HD1	2.03	0.40
1:L:189:LEU:HA	1:L:189:LEU:HD12	1.84	0.40
1:B:99:ARG:HD3	1:B:360:HIS:CD2	2.56	0.40
1:C:121:ASN:O	1:C:125:GLY:HA2	2.20	0.40
1:D:155:THR:HB	1:D:158:PHE:HB3	2.04	0.40
1:D:68:PRO:HG3	1:D:90:GLU:CG	2.52	0.40
1:E:103:PRO:CD	1:E:144:VAL:HG11	2.50	0.40
1:E:174:LEU:HB3	1:E:223:ILE:CD1	2.50	0.40
1:F:30:LEU:HD22	1:F:93:ASN:ND2	2.37	0.40
1:K:68:PRO:HG3	1:K:90:GLU:CG	2.52	0.40
1:L:99:ARG:HD3	1:L:360:HIS:CD2	2.56	0.40
1:H:226:VAL:HG23	1:H:227:ALA:N	2.37	0.40
1:I:35:ASN:N	1:I:35:ASN:OD1	2.53	0.40
1:K:182:HIS:ND1	1:K:183:PRO:HD2	2.35	0.40
1:K:27:ILE:HG13	1:K:60:GLU:OE2	2.21	0.40
1:L:27:ILE:HG13	1:L:60:GLU:OE2	2.21	0.40

All (35) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:LYS:NZ	1:K:284:GLN:NE2[1_556]	1.07	1.13
1:B:329:GLN:CB	1:D:282:TYR:OH[1_455]	1.18	1.02
1:A:329:GLN:CB	1:E:282:TYR:OH[2_646]	1.22	0.98
1:A:260:GLN:OE1	1:H:323:TYR:O[2_646]	1.34	0.86
1:E:217:TYR:OH	1:J:267:ARG:NE[2_655]	1.47	0.73
1:B:260:GLN:OE1	1:C:323:TYR:O[1_455]	1.56	0.64
1:E:217:TYR:OH	1:J:267:ARG:NH2[2_655]	1.70	0.50
1:E:217:TYR:OH	1:J:267:ARG:CZ[2_655]	1.71	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:23:LYS:NZ	1:L:188:HIS:O[2_645]	1.72	0.48
1:E:7:ASN:ND2	1:I:284:GLN:OE1[2_555]	1.78	0.42
1:A:285:GLU:OE2	1:J:243:LYS:NZ[1_556]	1.80	0.40
1:G:243:LYS:NZ	1:K:284:GLN:CD[1_556]	1.81	0.39
1:B:329:GLN:C	1:D:282:TYR:CE2[1_455]	1.86	0.34
1:C:244:GLU:OE2	1:H:217:TYR:OH[2_646]	1.86	0.34
1:A:329:GLN:C	1:E:282:TYR:CE2[2_646]	1.87	0.33
1:E:217:TYR:CZ	1:J:267:ARG:NE[2_655]	1.91	0.29
1:B:7:ASN:ND2	1:E:84:HIS:CE1[2_546]	1.93	0.27
1:E:217:TYR:CE2	1:J:267:ARG:NE[2_655]	1.95	0.25
1:E:341:ASP:C	1:G:84:HIS:NE2[2_556]	1.98	0.22
1:E:217:TYR:CE2	1:J:267:ARG:CD[2_655]	2.00	0.20
1:B:7:ASN:CG	1:E:84:HIS:CE1[2_546]	2.01	0.19
1:B:329:GLN:O	1:D:282:TYR:CE2[1_455]	2.04	0.16
1:F:211:LYS:CD	1:I:192:GLU:OE2[2_556]	2.04	0.16
1:A:329:GLN:CG	1:E:282:TYR:OH[2_646]	2.04	0.16
1:B:7:ASN:CB	1:E:84:HIS:CE1[2_546]	2.08	0.12
1:A:329:GLN:O	1:E:282:TYR:CE2[2_646]	2.10	0.10
1:B:329:GLN:CG	1:D:282:TYR:OH[1_455]	2.11	0.09
1:B:7:ASN:CB	1:E:84:HIS:ND1[2_546]	2.12	0.08
1:A:329:GLN:CB	1:E:282:TYR:CZ[2_646]	2.14	0.06
1:B:330:LEU:N	1:D:282:TYR:CE2[1_455]	2.16	0.04
1:G:243:LYS:NZ	1:K:284:GLN:OE1[1_556]	2.17	0.03
1:F:211:LYS:NZ	1:I:192:GLU:OE1[2_556]	2.18	0.02
1:B:329:GLN:CB	1:D:282:TYR:CZ[1_455]	2.19	0.01
1:E:342:ARG:N	1:G:84:HIS:NE2[2_556]	2.19	0.01
1:A:330:LEU:N	1:E:282:TYR:CE2[2_646]	2.19	0.01

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	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
1	C	358/377 (95%)	291 (81%)	60 (17%)	7 (2%)	7	27
1	D	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
1	E	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
1	F	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
1	G	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
1	H	367/377 (97%)	303 (83%)	54 (15%)	10 (3%)	5	19
1	I	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
1	J	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
1	K	358/377 (95%)	293 (82%)	58 (16%)	7 (2%)	7	27
1	L	358/377 (95%)	292 (82%)	59 (16%)	7 (2%)	7	27
All	All	4305/4524 (95%)	3515 (82%)	703 (16%)	87 (2%)	7	27

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	GLY
1	B	171	GLY
1	C	171	GLY
1	D	171	GLY
1	E	171	GLY
1	F	171	GLY
1	G	171	GLY
1	I	171	GLY
1	J	171	GLY
1	K	171	GLY
1	L	171	GLY
1	A	359	ILE
1	B	359	ILE
1	C	359	ILE
1	D	359	ILE
1	E	359	ILE
1	F	359	ILE
1	G	359	ILE
1	H	83	SER
1	I	359	ILE
1	J	359	ILE
1	K	359	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	359	ILE
1	A	248	TYR
1	B	248	TYR
1	C	248	TYR
1	D	248	TYR
1	E	248	TYR
1	F	248	TYR
1	G	248	TYR
1	H	81	LEU
1	H	171	GLY
1	H	211	LYS
1	H	216	PRO
1	H	264	ALA
1	I	248	TYR
1	J	248	TYR
1	K	248	TYR
1	L	248	TYR
1	A	169	GLY
1	B	169	GLY
1	C	169	GLY
1	D	169	GLY
1	E	169	GLY
1	F	169	GLY
1	G	169	GLY
1	I	169	GLY
1	J	169	GLY
1	K	169	GLY
1	L	169	GLY
1	H	132	PHE
1	A	232	PRO
1	B	232	PRO
1	C	232	PRO
1	D	232	PRO
1	E	232	PRO
1	F	232	PRO
1	G	232	PRO
1	H	138	ALA
1	H	293	GLU
1	I	232	PRO
1	J	232	PRO
1	K	232	PRO
1	L	232	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	98	ILE
1	A	132	PHE
1	B	98	ILE
1	B	132	PHE
1	C	98	ILE
1	C	132	PHE
1	D	98	ILE
1	D	132	PHE
1	E	98	ILE
1	E	132	PHE
1	F	98	ILE
1	F	132	PHE
1	G	98	ILE
1	G	132	PHE
1	I	98	ILE
1	I	132	PHE
1	J	98	ILE
1	J	132	PHE
1	K	98	ILE
1	K	132	PHE
1	L	98	ILE
1	L	132	PHE
1	H	5	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	B	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	C	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	D	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	E	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	F	310/316 (98%)	284 (92%)	26 (8%)	11	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	H	316/316 (100%)	286 (90%)	30 (10%)	8	26
1	I	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	J	310/316 (98%)	284 (92%)	26 (8%)	11	31
1	K	310/316 (98%)	285 (92%)	25 (8%)	11	33
1	L	310/316 (98%)	284 (92%)	26 (8%)	11	31
All	All	3726/3792 (98%)	3411 (92%)	315 (8%)	10	31

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	5	ILE
1	A	36	ASP
1	A	67	PRO
1	A	89	ILE
1	A	99	ARG
1	A	114	ARG
1	A	121	ASN
1	A	127	VAL
1	A	131	TYR
1	A	150	VAL
1	A	176	THR
1	A	178	MSE
1	A	185	ARG
1	A	189	LEU
1	A	192	GLU
1	A	197	LYS
1	A	203	ASN
1	A	212	ASP
1	A	225	ASP
1	A	278	LYS
1	A	309	LEU
1	A	327	ASN
1	A	350	GLU
1	A	358	ASN
1	A	370	LEU
1	B	4	ARG
1	B	5	ILE
1	B	36	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	67	PRO
1	B	89	ILE
1	B	99	ARG
1	B	114	ARG
1	B	121	ASN
1	B	127	VAL
1	B	131	TYR
1	B	150	VAL
1	B	176	THR
1	B	178	MSE
1	B	185	ARG
1	B	189	LEU
1	B	192	GLU
1	B	197	LYS
1	B	203	ASN
1	B	212	ASP
1	B	225	ASP
1	B	278	LYS
1	B	309	LEU
1	B	327	ASN
1	B	350	GLU
1	B	358	ASN
1	B	370	LEU
1	C	4	ARG
1	C	5	ILE
1	C	36	ASP
1	C	67	PRO
1	C	89	ILE
1	C	99	ARG
1	C	114	ARG
1	C	121	ASN
1	C	127	VAL
1	C	131	TYR
1	C	150	VAL
1	C	176	THR
1	C	178	MSE
1	C	185	ARG
1	C	189	LEU
1	C	192	GLU
1	C	197	LYS
1	C	203	ASN
1	C	212	ASP

Continued from previous page...

Mol	Chain	Res	Type
1	C	225	ASP
1	C	278	LYS
1	C	309	LEU
1	C	327	ASN
1	C	350	GLU
1	C	358	ASN
1	C	370	LEU
1	D	4	ARG
1	D	5	ILE
1	D	36	ASP
1	D	67	PRO
1	D	89	ILE
1	D	99	ARG
1	D	114	ARG
1	D	121	ASN
1	D	127	VAL
1	D	131	TYR
1	D	150	VAL
1	D	176	THR
1	D	178	MSE
1	D	185	ARG
1	D	189	LEU
1	D	192	GLU
1	D	197	LYS
1	D	203	ASN
1	D	212	ASP
1	D	225	ASP
1	D	278	LYS
1	D	309	LEU
1	D	327	ASN
1	D	350	GLU
1	D	358	ASN
1	D	370	LEU
1	E	4	ARG
1	E	5	ILE
1	E	36	ASP
1	E	67	PRO
1	E	89	ILE
1	E	99	ARG
1	E	114	ARG
1	E	121	ASN
1	E	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	131	TYR
1	E	150	VAL
1	E	176	THR
1	E	178	MSE
1	E	185	ARG
1	E	189	LEU
1	E	192	GLU
1	E	197	LYS
1	E	203	ASN
1	E	212	ASP
1	E	225	ASP
1	E	278	LYS
1	E	309	LEU
1	E	327	ASN
1	E	350	GLU
1	E	358	ASN
1	E	370	LEU
1	F	4	ARG
1	F	5	ILE
1	F	36	ASP
1	F	67	PRO
1	F	89	ILE
1	F	99	ARG
1	F	114	ARG
1	F	121	ASN
1	F	127	VAL
1	F	131	TYR
1	F	150	VAL
1	F	176	THR
1	F	178	MSE
1	F	185	ARG
1	F	189	LEU
1	F	192	GLU
1	F	197	LYS
1	F	203	ASN
1	F	212	ASP
1	F	225	ASP
1	F	278	LYS
1	F	309	LEU
1	F	327	ASN
1	F	350	GLU
1	F	358	ASN

Continued from previous page...

Mol	Chain	Res	Type
1	F	370	LEU
1	G	4	ARG
1	G	5	ILE
1	G	36	ASP
1	G	67	PRO
1	G	89	ILE
1	G	99	ARG
1	G	114	ARG
1	G	121	ASN
1	G	127	VAL
1	G	131	TYR
1	G	150	VAL
1	G	176	THR
1	G	178	MSE
1	G	185	ARG
1	G	189	LEU
1	G	192	GLU
1	G	197	LYS
1	G	203	ASN
1	G	212	ASP
1	G	225	ASP
1	G	278	LYS
1	G	309	LEU
1	G	327	ASN
1	G	350	GLU
1	G	358	ASN
1	G	370	LEU
1	H	4	ARG
1	H	13	ASP
1	H	52	VAL
1	H	66	VAL
1	H	80	GLU
1	H	89	ILE
1	H	121	ASN
1	H	127	VAL
1	H	161	GLU
1	H	176	THR
1	H	178	MSE
1	H	185	ARG
1	H	189	LEU
1	H	202	LEU
1	H	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	217	TYR
1	H	225	ASP
1	H	240	THR
1	H	241	ASP
1	H	262	THR
1	H	263	ASP
1	H	269	LEU
1	H	278	LYS
1	H	283	LEU
1	H	299	GLU
1	H	309	LEU
1	H	312	LEU
1	H	315	ASN
1	H	328	ASP
1	H	351	GLU
1	I	4	ARG
1	I	5	ILE
1	I	36	ASP
1	I	67	PRO
1	I	89	ILE
1	I	99	ARG
1	I	114	ARG
1	I	121	ASN
1	I	127	VAL
1	I	131	TYR
1	I	150	VAL
1	I	176	THR
1	I	178	MSE
1	I	185	ARG
1	I	189	LEU
1	I	192	GLU
1	I	197	LYS
1	I	203	ASN
1	I	212	ASP
1	I	225	ASP
1	I	278	LYS
1	I	309	LEU
1	I	327	ASN
1	I	350	GLU
1	I	358	ASN
1	I	370	LEU
1	J	4	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	5	ILE
1	J	36	ASP
1	J	67	PRO
1	J	89	ILE
1	J	99	ARG
1	J	114	ARG
1	J	121	ASN
1	J	127	VAL
1	J	131	TYR
1	J	150	VAL
1	J	176	THR
1	J	178	MSE
1	J	185	ARG
1	J	189	LEU
1	J	192	GLU
1	J	197	LYS
1	J	203	ASN
1	J	212	ASP
1	J	225	ASP
1	J	278	LYS
1	J	309	LEU
1	J	327	ASN
1	J	350	GLU
1	J	358	ASN
1	J	370	LEU
1	K	4	ARG
1	K	36	ASP
1	K	67	PRO
1	K	89	ILE
1	K	99	ARG
1	K	114	ARG
1	K	121	ASN
1	K	127	VAL
1	K	131	TYR
1	K	150	VAL
1	K	176	THR
1	K	178	MSE
1	K	185	ARG
1	K	189	LEU
1	K	192	GLU
1	K	197	LYS
1	K	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	212	ASP
1	K	225	ASP
1	K	278	LYS
1	K	309	LEU
1	K	327	ASN
1	K	350	GLU
1	K	358	ASN
1	K	370	LEU
1	L	4	ARG
1	L	5	ILE
1	L	36	ASP
1	L	67	PRO
1	L	89	ILE
1	L	99	ARG
1	L	114	ARG
1	L	121	ASN
1	L	127	VAL
1	L	131	TYR
1	L	150	VAL
1	L	176	THR
1	L	178	MSE
1	L	185	ARG
1	L	189	LEU
1	L	192	GLU
1	L	197	LYS
1	L	203	ASN
1	L	212	ASP
1	L	225	ASP
1	L	278	LYS
1	L	309	LEU
1	L	327	ASN
1	L	350	GLU
1	L	358	ASN
1	L	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (255) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	12	GLN
1	A	26	GLN
1	A	35	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	37	ASN
1	A	46	GLN
1	A	73	ASN
1	A	121	ASN
1	A	186	ASN
1	A	203	ASN
1	A	220	ASN
1	A	249	GLN
1	A	261	GLN
1	A	284	GLN
1	A	310	ASN
1	A	315	ASN
1	A	322	GLN
1	A	327	ASN
1	A	333	GLN
1	A	358	ASN
1	A	360	HIS
1	A	366	GLN
1	B	12	GLN
1	B	26	GLN
1	B	35	ASN
1	B	37	ASN
1	B	46	GLN
1	B	73	ASN
1	B	121	ASN
1	B	186	ASN
1	B	203	ASN
1	B	220	ASN
1	B	249	GLN
1	B	261	GLN
1	B	284	GLN
1	B	310	ASN
1	B	315	ASN
1	B	322	GLN
1	B	327	ASN
1	B	333	GLN
1	B	358	ASN
1	B	360	HIS
1	B	366	GLN
1	C	12	GLN
1	C	26	GLN
1	C	35	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	37	ASN
1	C	46	GLN
1	C	73	ASN
1	C	121	ASN
1	C	186	ASN
1	C	203	ASN
1	C	220	ASN
1	C	249	GLN
1	C	261	GLN
1	C	284	GLN
1	C	310	ASN
1	C	315	ASN
1	C	322	GLN
1	C	327	ASN
1	C	333	GLN
1	C	358	ASN
1	C	360	HIS
1	C	366	GLN
1	D	12	GLN
1	D	26	GLN
1	D	35	ASN
1	D	37	ASN
1	D	46	GLN
1	D	73	ASN
1	D	84	HIS
1	D	121	ASN
1	D	186	ASN
1	D	203	ASN
1	D	220	ASN
1	D	249	GLN
1	D	261	GLN
1	D	284	GLN
1	D	310	ASN
1	D	315	ASN
1	D	322	GLN
1	D	327	ASN
1	D	333	GLN
1	D	358	ASN
1	D	360	HIS
1	D	366	GLN
1	E	12	GLN
1	E	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	35	ASN
1	E	37	ASN
1	E	46	GLN
1	E	73	ASN
1	E	121	ASN
1	E	186	ASN
1	E	203	ASN
1	E	220	ASN
1	E	249	GLN
1	E	261	GLN
1	E	284	GLN
1	E	310	ASN
1	E	315	ASN
1	E	322	GLN
1	E	327	ASN
1	E	333	GLN
1	E	358	ASN
1	E	360	HIS
1	E	366	GLN
1	F	12	GLN
1	F	26	GLN
1	F	35	ASN
1	F	37	ASN
1	F	46	GLN
1	F	73	ASN
1	F	121	ASN
1	F	186	ASN
1	F	203	ASN
1	F	220	ASN
1	F	249	GLN
1	F	261	GLN
1	F	284	GLN
1	F	310	ASN
1	F	315	ASN
1	F	322	GLN
1	F	327	ASN
1	F	333	GLN
1	F	358	ASN
1	F	360	HIS
1	F	366	GLN
1	G	12	GLN
1	G	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	35	ASN
1	G	37	ASN
1	G	46	GLN
1	G	73	ASN
1	G	121	ASN
1	G	186	ASN
1	G	203	ASN
1	G	220	ASN
1	G	249	GLN
1	G	261	GLN
1	G	284	GLN
1	G	310	ASN
1	G	315	ASN
1	G	322	GLN
1	G	327	ASN
1	G	333	GLN
1	G	358	ASN
1	G	360	HIS
1	G	366	GLN
1	H	12	GLN
1	H	24	GLN
1	H	26	GLN
1	H	35	ASN
1	H	37	ASN
1	H	46	GLN
1	H	73	ASN
1	H	85	ASN
1	H	121	ASN
1	H	186	ASN
1	H	203	ASN
1	H	220	ASN
1	H	249	GLN
1	H	261	GLN
1	H	284	GLN
1	H	315	ASN
1	H	322	GLN
1	H	329	GLN
1	H	333	GLN
1	H	358	ASN
1	H	360	HIS
1	H	366	GLN
1	I	12	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	26	GLN
1	I	35	ASN
1	I	37	ASN
1	I	46	GLN
1	I	73	ASN
1	I	121	ASN
1	I	186	ASN
1	I	203	ASN
1	I	220	ASN
1	I	249	GLN
1	I	261	GLN
1	I	284	GLN
1	I	310	ASN
1	I	315	ASN
1	I	322	GLN
1	I	327	ASN
1	I	333	GLN
1	I	358	ASN
1	I	360	HIS
1	I	366	GLN
1	J	12	GLN
1	J	26	GLN
1	J	35	ASN
1	J	37	ASN
1	J	46	GLN
1	J	73	ASN
1	J	121	ASN
1	J	186	ASN
1	J	203	ASN
1	J	220	ASN
1	J	249	GLN
1	J	261	GLN
1	J	284	GLN
1	J	310	ASN
1	J	315	ASN
1	J	322	GLN
1	J	327	ASN
1	J	333	GLN
1	J	358	ASN
1	J	360	HIS
1	J	366	GLN
1	K	12	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	26	GLN
1	K	35	ASN
1	K	37	ASN
1	K	46	GLN
1	K	73	ASN
1	K	121	ASN
1	K	186	ASN
1	K	203	ASN
1	K	220	ASN
1	K	249	GLN
1	K	261	GLN
1	K	284	GLN
1	K	310	ASN
1	K	315	ASN
1	K	322	GLN
1	K	327	ASN
1	K	333	GLN
1	K	358	ASN
1	K	360	HIS
1	K	366	GLN
1	L	12	GLN
1	L	26	GLN
1	L	35	ASN
1	L	37	ASN
1	L	46	GLN
1	L	73	ASN
1	L	121	ASN
1	L	186	ASN
1	L	203	ASN
1	L	220	ASN
1	L	249	GLN
1	L	261	GLN
1	L	284	GLN
1	L	310	ASN
1	L	315	ASN
1	L	322	GLN
1	L	327	ASN
1	L	333	GLN
1	L	358	ASN
1	L	360	HIS
1	L	366	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.