



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:48 am BST

PDB ID : 1NY6  
Title : Crystal structure of sigm54 activator (AAA+ ATPase) in the active state  
Authors : Lee, S.Y.; de la Torre, A.; Kustu, S.; Nixon, B.T.; Wemmer, D.E.  
Deposited on : 2003-02-11  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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  
buster-report : 1.1.7 (2018)  
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

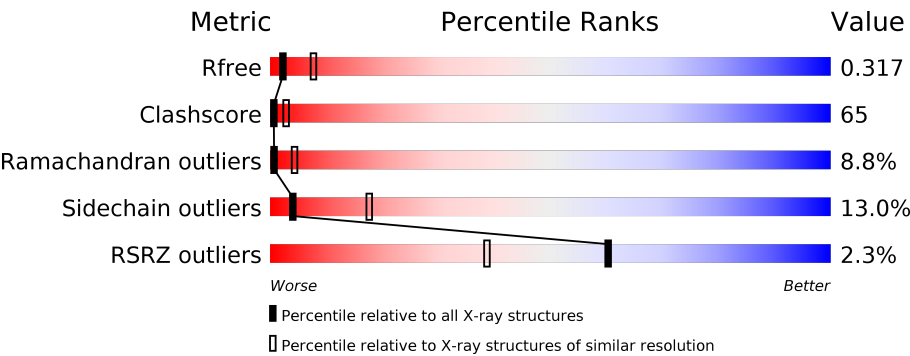
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	
1	B	267	
1	C	267	
1	D	267	
1	E	267	
1	F	267	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	267	<div><div></div><div>3%</div><div>23%</div><div>59%</div><div>10%</div><div>7%</div></div>
1	H	267	<div><div></div><div>5%</div><div>22%</div><div>57%</div><div>12%</div><div>8%</div></div>
1	I	267	<div><div></div><div>2%</div><div>28%</div><div>51%</div><div>13%</div><div>7%</div></div>
1	J	267	<div><div></div><div>6%</div><div>36%</div><div>48%</div><div>8%</div><div>7%</div></div>
1	K	267	<div><div></div><div>2%</div><div>27%</div><div>52%</div><div>13%</div><div>7%</div></div>
1	L	267	<div><div></div><div>%</div><div>13%</div><div>58%</div><div>19%</div><div>8%</div></div>
1	M	267	<div><div></div><div>%</div><div>21%</div><div>56%</div><div>14%</div><div>7%</div></div>
1	N	267	<div><div></div><div>%</div><div>27%</div><div>52%</div><div>11%</div><div>7%</div></div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 28041 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 transcriptional regulator (NtrC family).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1979	1278	333	364	4			
1	B	243	Total	C	N	O	S	0	0	0
			1940	1250	329	357	4			
1	C	248	Total	C	N	O	S	0	0	0
			1988	1283	334	367	4			
1	D	247	Total	C	N	O	S	0	0	0
			1979	1278	333	364	4			
1	E	248	Total	C	N	O	S	0	0	0
			1988	1283	334	367	4			
1	F	248	Total	C	N	O	S	0	0	0
			1988	1283	334	367	4			
1	G	248	Total	C	N	O	S	0	0	0
			1988	1283	334	367	4			
1	H	245	Total	C	N	O	S	0	0	0
			1954	1259	331	360	4			
1	I	247	Total	C	N	O	S	0	0	0
			1966	1268	333	361	4			
1	J	247	Total	C	N	O	S	0	0	0
			1975	1276	333	362	4			
1	K	248	Total	C	N	O	S	0	0	0
			1988	1283	334	367	4			
1	L	246	Total	C	N	O	S	0	0	0
			1972	1273	332	363	4			
1	M	247	Total	C	N	O	S	0	0	0
			1979	1278	333	364	4			
1	N	247	Total	C	N	O	S	0	0	0
			1979	1278	333	364	4			

There are 14 discrepancies between the modelled and reference sequences:

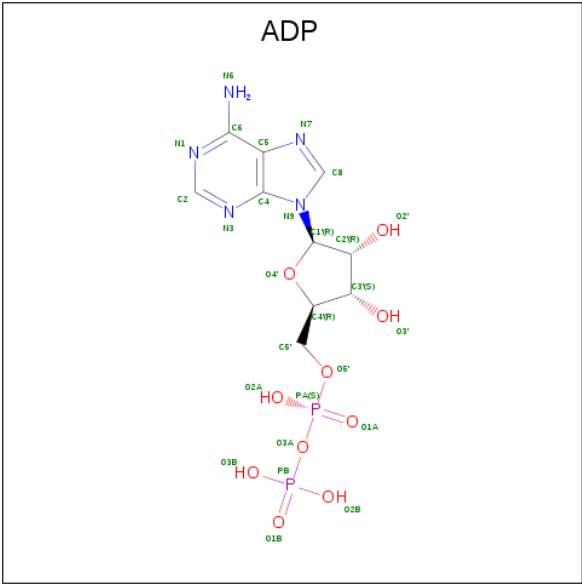
Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MET	-	INITIATING METHIONINE	UNP O67198

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	121	MET	-	INITIATING METHIONINE	UNP 067198
C	121	MET	-	INITIATING METHIONINE	UNP 067198
D	121	MET	-	INITIATING METHIONINE	UNP 067198
E	121	MET	-	INITIATING METHIONINE	UNP 067198
F	121	MET	-	INITIATING METHIONINE	UNP 067198
G	121	MET	-	INITIATING METHIONINE	UNP 067198
H	121	MET	-	INITIATING METHIONINE	UNP 067198
I	121	MET	-	INITIATING METHIONINE	UNP 067198
J	121	MET	-	INITIATING METHIONINE	UNP 067198
K	121	MET	-	INITIATING METHIONINE	UNP 067198
L	121	MET	-	INITIATING METHIONINE	UNP 067198
M	121	MET	-	INITIATING METHIONINE	UNP 067198
N	121	MET	-	INITIATING METHIONINE	UNP 067198

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

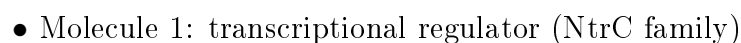
Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		



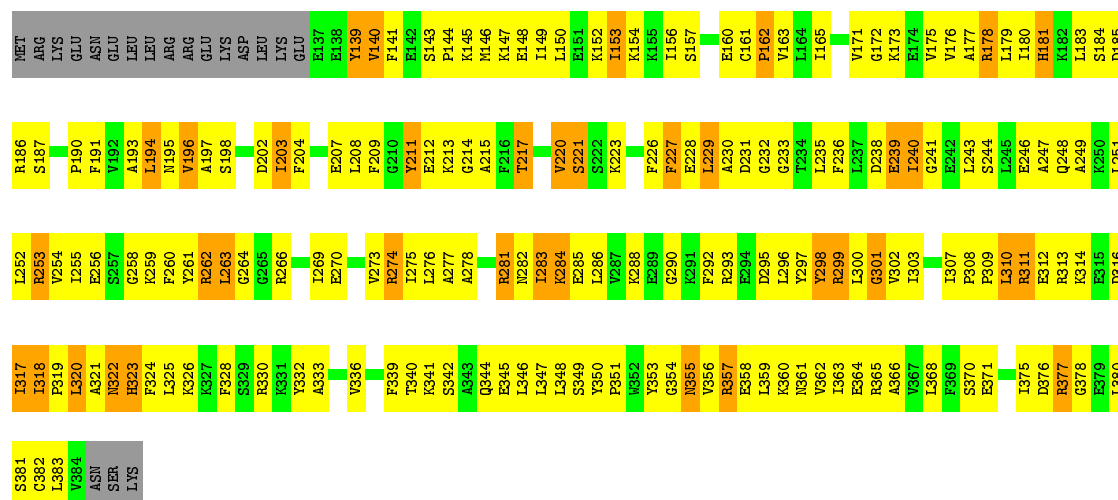
- Molecule 1: transcriptional regulator (NtrC family)



ASN  
SER  
LYS

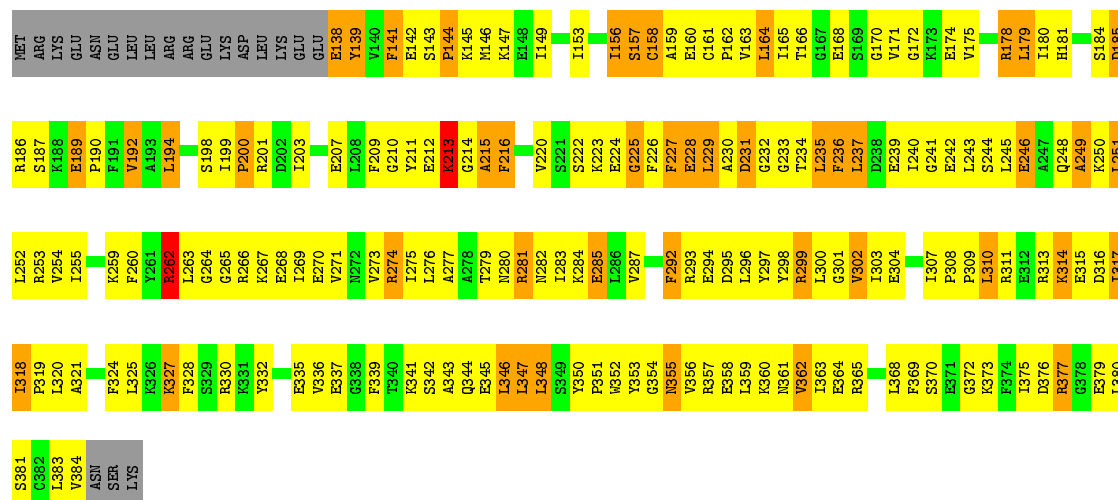
- Molecule 1: transcriptional regulator (NtrC family)

Chain C: 25% 54% 14% 7%



- Molecule 1: transcriptional regulator (NtrC family)

Chain D: 23% 52% 17% 7%

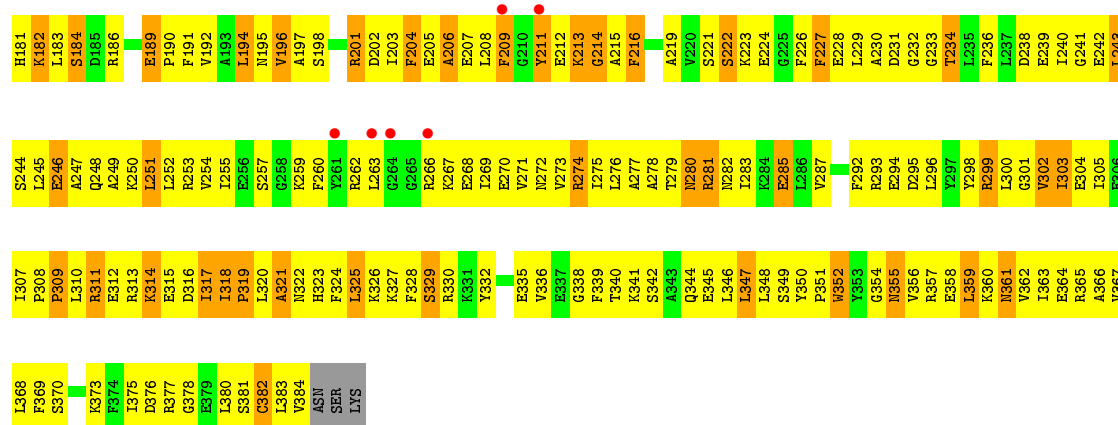


- Molecule 1: transcriptional regulator (NtrC family)

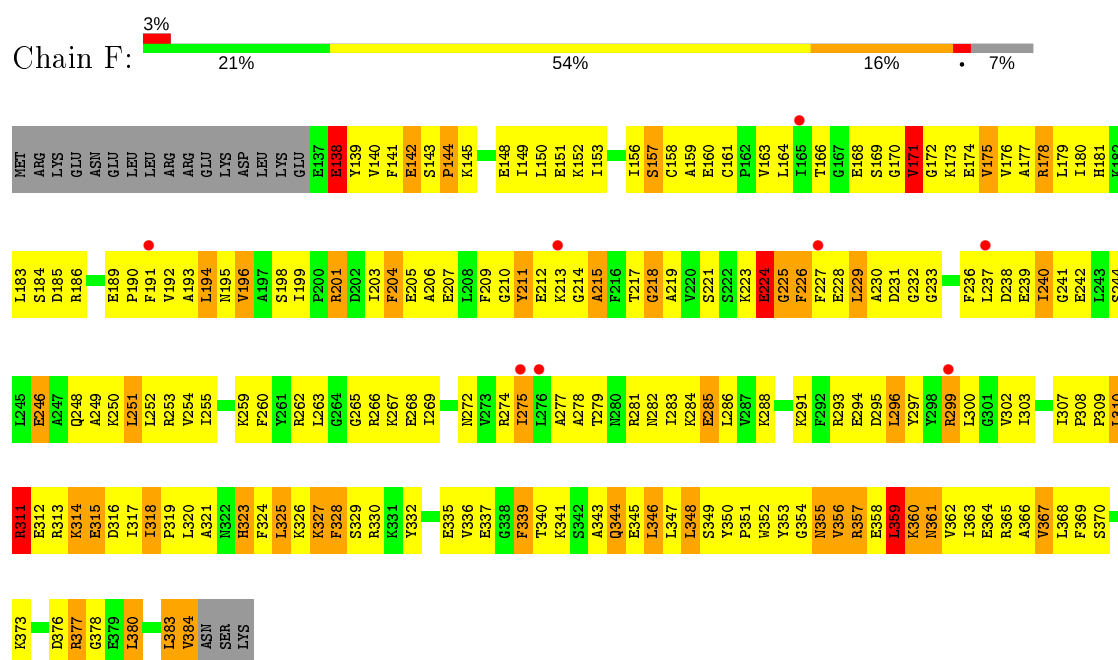
Chain E: 3% 16% 57% 19% 7%



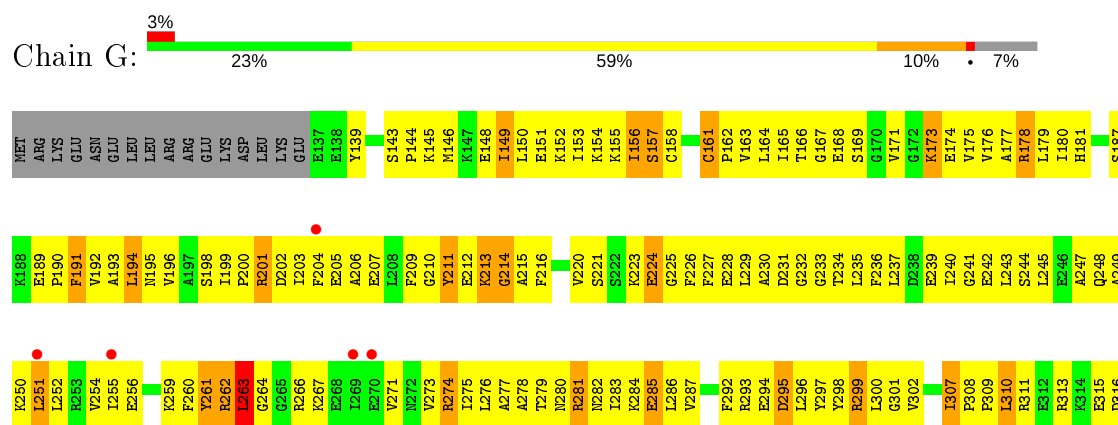


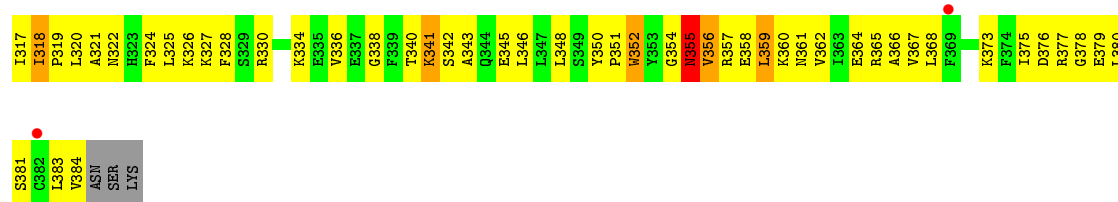


- Molecule 1: transcriptional regulator (NtrC family)

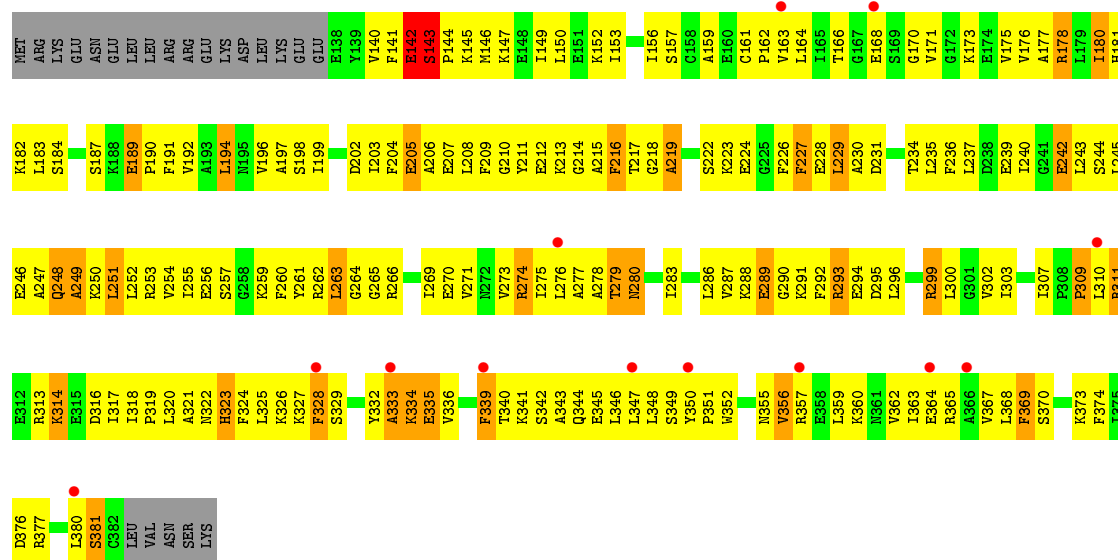


- Molecule 1: transcriptional regulator (NtrC family)

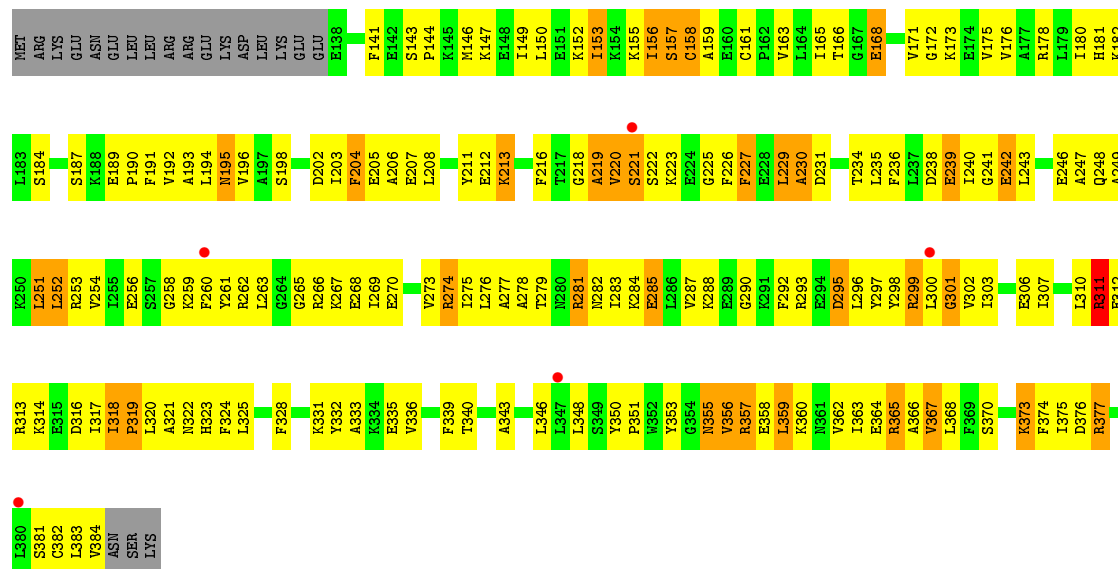




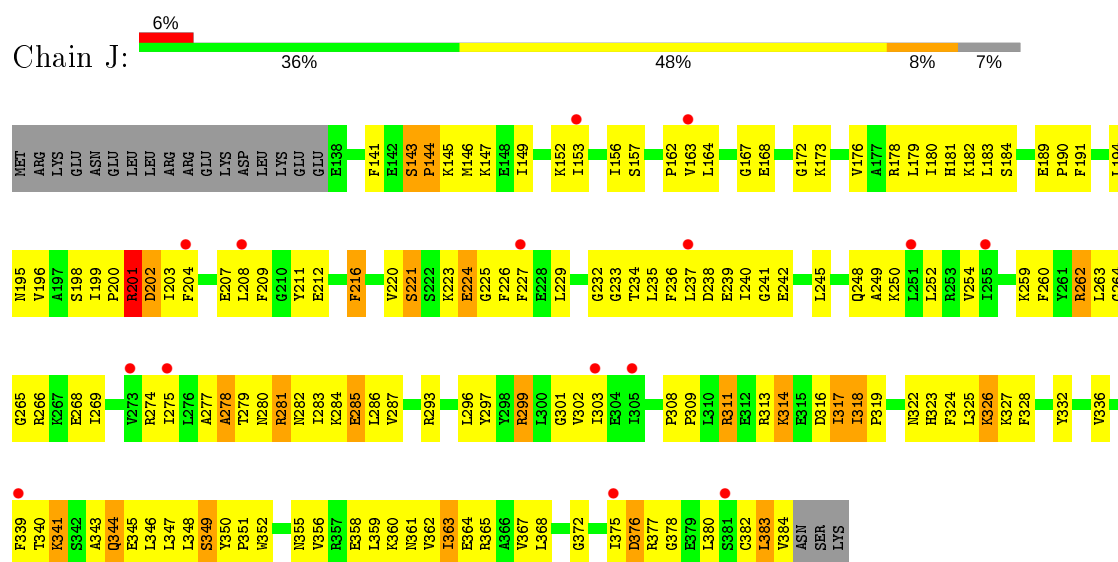
- Molecule 1: transcriptional regulator (NtrC family)



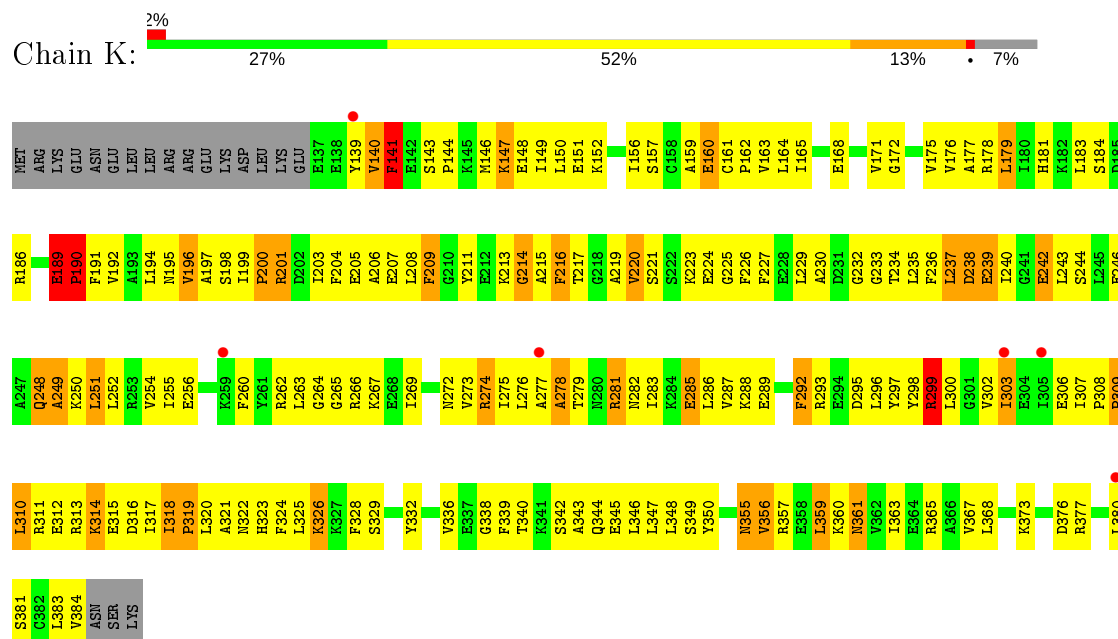
- Molecule 1: transcriptional regulator (NtrC family)



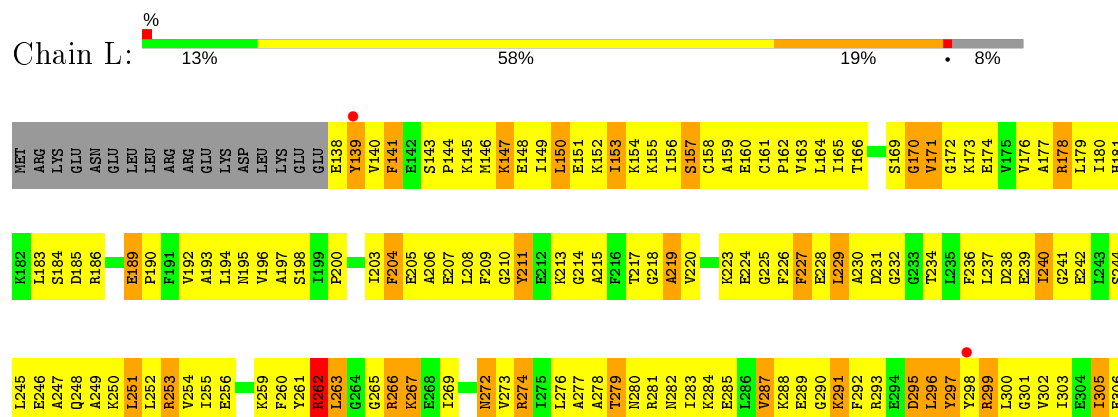
- Molecule 1: transcriptional regulator (NtrC family)

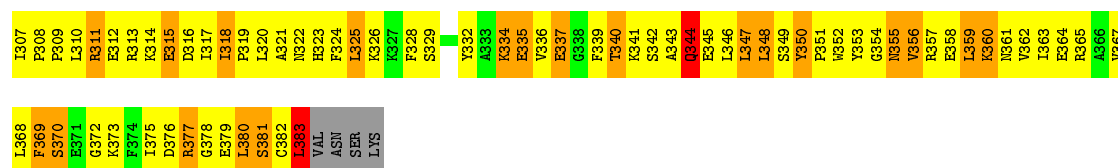


• Molecule 1: transcriptional regulator (NtrC family)

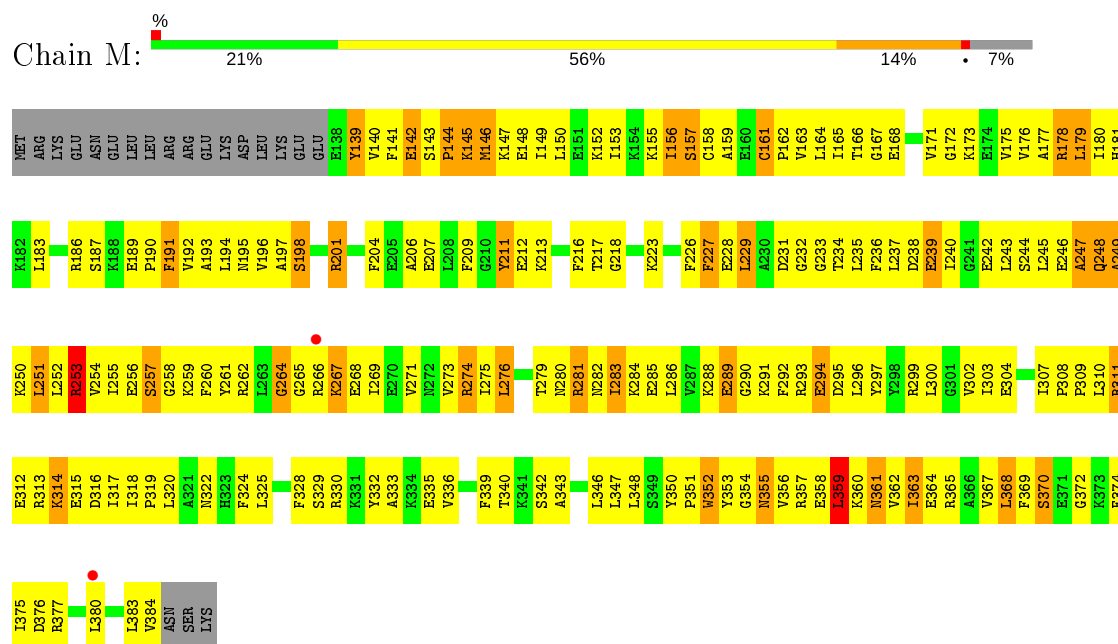


• Molecule 1: transcriptional regulator (NtrC family)

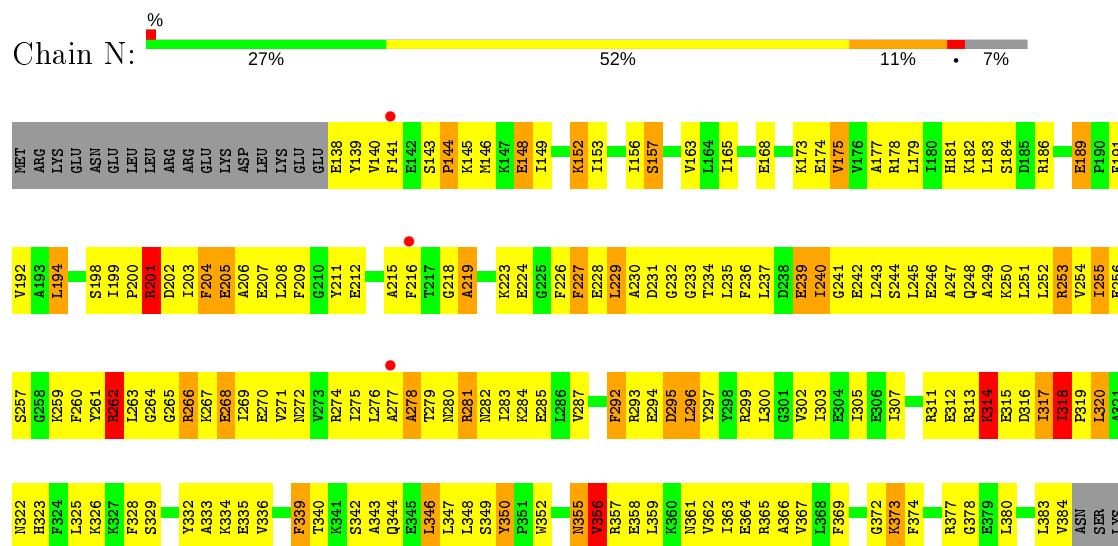




• Molecule 1: transcriptional regulator (NtrC family)



• Molecule 1: transcriptional regulator (NtrC family)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.79Å 108.27Å 110.02Å 70.25° 85.90° 73.27°	Depositor
Resolution (Å)	19.98 – 3.10 62.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.98-3.10) 97.5 (62.44-3.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.266 , 0.329 0.259 , 0.317	Depositor DCC
$R_{free}$ test set	8701 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.2	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 86.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	28041	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.45	0/2013	0.65	0/2700
1	B	0.48	0/1972	0.67	0/2644
1	C	0.55	0/2022	0.83	1/2712 (0.0%)
1	D	0.55	0/2013	0.78	1/2700 (0.0%)
1	E	0.62	0/2022	0.93	1/2712 (0.0%)
1	F	0.53	0/2022	0.73	0/2712
1	G	0.47	0/2022	0.69	1/2712 (0.0%)
1	H	0.45	0/1987	0.96	2/2665 (0.1%)
1	I	0.45	0/1999	0.68	0/2681
1	J	0.42	0/2009	0.63	0/2695
1	K	0.47	0/2022	0.70	1/2712 (0.0%)
1	L	0.63	0/2006	0.87	1/2690 (0.0%)
1	M	0.52	0/2013	0.74	0/2700
1	N	0.45	0/2013	0.69	1/2700 (0.0%)
All	All	0.51	0/28135	0.76	9/37735 (0.0%)

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

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

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	143	SER	C-N-CD	-34.04	45.71	120.60
1	E	190	PRO	CA-N-CD	-20.80	82.37	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	PRO	CA-N-CD	-16.92	87.81	111.50
1	H	142	GLU	O-C-N	-9.85	106.93	122.70
1	D	262	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	K	220	VAL	N-CA-C	5.84	126.76	111.00
1	L	383	LEU	CA-CB-CG	-5.49	102.68	115.30
1	G	354	GLY	N-CA-C	-5.48	99.40	113.10
1	N	262	ARG	N-CA-C	-5.25	96.83	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	142	GLU	Mainchain,Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1979	0	2040	214	0
1	B	1940	0	2007	249	0
1	C	1988	0	2046	268	0
1	D	1979	0	2040	276	0
1	E	1988	0	2046	359	0
1	F	1988	0	2046	296	0
1	G	1988	0	2046	245	0
1	H	1954	0	2009	281	0
1	I	1966	0	2022	250	0
1	J	1975	0	2036	193	0
1	K	1988	0	2046	246	0
1	L	1972	0	2031	382	0
1	M	1979	0	2040	301	0
1	N	1979	0	2040	271	0
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	4	0
2	D	27	0	12	6	0
2	E	27	0	12	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	27	0	12	7	0
2	G	27	0	12	0	0
2	H	27	0	12	3	0
2	I	27	0	12	5	0
2	J	27	0	12	1	0
2	K	27	0	12	1	0
2	L	27	0	12	6	0
2	M	27	0	12	6	0
2	N	27	0	12	2	0
All	All	28041	0	28663	3697	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 65.

All (3697) 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:D:235:LEU:HD12	1:D:236:PHE:N	1.44	1.30
1:L:334:LYS:NZ	1:L:367:VAL:HG13	1.51	1.24
1:E:177:ALA:CA	1:E:180:ILE:HD12	1.69	1.21
1:E:240:ILE:CD1	1:E:277:ALA:HB1	1.72	1.18
1:F:318:ILE:HG13	1:F:319:PRO:HD3	1.23	1.17
1:E:177:ALA:HA	1:E:180:ILE:CD1	1.76	1.15
1:E:240:ILE:HD11	1:E:277:ALA:CB	1.77	1.14
1:C:220:VAL:HG12	1:C:221:SER:H	1.11	1.14
1:L:350:TYR:CD2	1:L:351:PRO:HD2	1.82	1.13
1:D:262:ARG:HH11	1:D:262:ARG:HG2	1.05	1.13
1:F:340:THR:CG2	1:F:376:ASP:HB3	1.79	1.12
1:A:343:ALA:HB2	1:A:376:ASP:HA	1.24	1.12
1:E:344:GLN:O	1:E:348:LEU:HD12	1.48	1.11
1:B:283:ILE:HA	1:B:286:LEU:HD12	1.22	1.11
1:G:259:LYS:HB3	1:G:267:LYS:HG3	1.14	1.11
1:L:140:VAL:HG11	1:L:320:LEU:HG	1.21	1.10
1:L:343:ALA:HB2	1:L:376:ASP:HA	1.29	1.10
1:G:320:LEU:HD22	1:G:359:LEU:HD13	1.31	1.10
1:H:214:GLY:H	1:H:219:ALA:HB1	1.11	1.10
1:L:224:GLU:HA	1:L:262:ARG:HH21	1.17	1.10
1:D:318:ILE:HG13	1:D:319:PRO:HD3	1.31	1.09
1:G:318:ILE:HG12	1:G:348:LEU:HD21	1.30	1.09
1:J:189:GLU:HG3	1:J:190:PRO:HD2	1.34	1.09
1:L:362:VAL:HG13	1:L:383:LEU:HD13	1.31	1.09

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:318:ILE:HG13	1:M:319:PRO:HD3	1.15	1.09
1:E:139:TYR:HB3	1:E:141:PHE:HE1	1.18	1.08
1:C:181:HIS:CD2	1:C:191:PHE:HB2	1.89	1.08
1:M:201:ARG:HB2	1:M:201:ARG:HH11	1.01	1.07
1:D:275:ILE:HD12	1:D:275:ILE:H	1.20	1.07
1:M:194:LEU:HD21	1:M:237:LEU:HD23	1.34	1.06
1:C:178:ARG:HG3	1:C:178:ARG:HH11	1.16	1.06
1:C:318:ILE:HG13	1:C:319:PRO:HD3	1.33	1.06
1:N:240:ILE:HD11	1:N:277:ALA:HB1	1.09	1.06
1:B:275:ILE:H	1:B:275:ILE:HD12	1.18	1.05
1:G:189:GLU:HG3	1:G:190:PRO:HD2	1.38	1.05
1:F:240:ILE:HD11	1:F:277:ALA:HB1	1.07	1.04
1:F:340:THR:HG21	1:F:376:ASP:HB3	1.34	1.04
1:A:318:ILE:HG12	1:A:348:LEU:HD21	1.40	1.04
1:H:343:ALA:HB2	1:H:376:ASP:HA	1.34	1.03
1:E:176:VAL:HG12	1:E:180:ILE:HD11	1.32	1.03
1:H:293:ARG:HG2	1:H:293:ARG:HH11	1.21	1.03
1:L:143:SER:HB2	1:L:144:PRO:HD2	1.37	1.02
1:L:329:SER:HA	1:L:334:LYS:HE2	1.38	1.02
1:M:211:TYR:HE1	1:M:223:LYS:HB2	1.18	1.01
1:E:325:LEU:O	1:E:329:SER:HB2	1.59	1.01
1:D:164:LEU:HD12	1:D:165:ILE:H	1.20	1.01
1:E:282:ASN:ND2	1:E:285:GLU:HB2	1.76	1.01
1:L:334:LYS:NZ	1:L:367:VAL:CG1	2.24	1.01
1:L:139:TYR:HB3	1:L:141:PHE:CE2	1.95	1.01
1:D:240:ILE:HG13	1:D:277:ALA:HB1	1.44	1.00
1:E:309:PRO:HG2	1:E:312:GLU:HG3	1.40	1.00
1:H:318:ILE:HD11	1:H:348:LEU:HD11	1.43	1.00
1:I:318:ILE:HG13	1:I:319:PRO:HD3	1.44	1.00
1:N:282:ASN:HD22	1:N:285:GLU:HG2	1.26	0.99
1:K:198:SER:O	1:K:199:ILE:HG13	1.61	0.99
1:J:282:ASN:HD22	1:J:285:GLU:HB2	1.27	0.98
1:M:243:LEU:HD22	1:M:247:ALA:HB1	1.45	0.98
1:M:180:ILE:HG21	1:M:276:LEU:HD11	1.43	0.98
1:I:194:LEU:HD23	1:I:194:LEU:H	1.28	0.98
1:D:207:GLU:HB3	1:D:226:PHE:HE1	1.25	0.98
1:M:253:ARG:HG3	1:N:198:SER:HB2	1.47	0.97
1:A:325:LEU:O	1:A:325:LEU:HD23	1.63	0.97
1:G:168:GLU:O	1:G:171:VAL:HG23	1.63	0.97
1:J:224:GLU:HG2	1:J:225:GLY:H	1.28	0.97
1:E:363:ILE:O	1:E:367:VAL:HG23	1.63	0.97

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:201:ARG:HB2	1:J:201:ARG:HH11	1.27	0.97
1:C:235:LEU:HD12	1:C:236:PHE:N	1.79	0.97
1:I:220:VAL:HG12	1:I:221:SER:H	1.28	0.96
1:H:357:ARG:HH12	1:N:252:LEU:HD21	1.29	0.96
1:F:240:ILE:CD1	1:F:277:ALA:HB1	1.96	0.95
1:L:138:GLU:HG3	1:L:139:TYR:N	1.77	0.95
1:B:217:THR:HG23	1:B:218:GLY:H	1.30	0.95
1:E:201:ARG:HB2	1:E:201:ARG:HH11	1.32	0.95
1:L:334:LYS:HZ2	1:L:367:VAL:HG13	1.13	0.95
1:F:189:GLU:HG3	1:F:190:PRO:HD2	1.46	0.95
1:H:189:GLU:HG3	1:H:190:PRO:HD2	1.47	0.95
1:C:235:LEU:HD12	1:C:236:PHE:H	1.32	0.95
1:I:261:TYR:HE1	1:J:199:ILE:HG12	1.30	0.95
1:J:216:PHE:H	1:J:216:PHE:HD2	1.09	0.95
1:L:143:SER:HB2	1:L:144:PRO:CD	1.95	0.95
1:E:325:LEU:HD21	1:E:336:VAL:HG12	1.49	0.94
1:K:164:LEU:HD12	1:K:165:ILE:H	1.33	0.94
1:F:326:LYS:HE2	1:F:330:ARG:NH2	1.83	0.94
1:F:309:PRO:HG3	1:F:311:ARG:NH1	1.82	0.94
1:M:201:ARG:NH1	1:M:201:ARG:HB2	1.83	0.93
1:N:228:GLU:OE2	1:N:262:ARG:NE	2.01	0.93
1:H:214:GLY:N	1:H:219:ALA:HB1	1.81	0.93
1:N:281:ARG:HD3	1:N:281:ARG:H	1.31	0.93
1:D:228:GLU:OE2	1:D:262:ARG:NE	2.02	0.93
1:M:143:SER:HB2	1:M:144:PRO:HD2	1.51	0.93
1:H:302:VAL:HG12	1:H:303:ILE:HG13	1.49	0.93
1:B:314:LYS:HD2	1:B:314:LYS:H	1.33	0.93
1:M:308:PRO:HG2	1:M:313:ARG:HD2	1.51	0.93
1:N:240:ILE:HD11	1:N:277:ALA:CB	1.99	0.92
1:C:150:LEU:HG	1:C:154:LYS:NZ	1.83	0.92
1:N:201:ARG:HH11	1:N:201:ARG:HB2	1.33	0.92
1:H:176:VAL:HG21	1:H:307:ILE:HD11	1.50	0.92
1:E:214:GLY:HA2	1:E:219:ALA:HB3	1.52	0.92
1:I:343:ALA:HB2	1:I:376:ASP:HA	1.52	0.92
1:D:164:LEU:HD12	1:D:165:ILE:N	1.83	0.91
1:B:317:ILE:HB	1:B:348:LEU:HD23	1.53	0.91
1:E:302:VAL:HG12	1:E:303:ILE:HG12	1.52	0.91
1:H:362:VAL:HG22	1:H:365:ARG:NH2	1.85	0.91
1:H:362:VAL:HG22	1:H:365:ARG:HH21	1.34	0.91
1:M:211:TYR:CE1	1:M:223:LYS:HB2	2.05	0.91
1:D:262:ARG:NH1	1:D:262:ARG:HG2	1.80	0.91

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:362:VAL:HG13	1:L:383:LEU:CD1	1.99	0.91
1:B:362:VAL:HG13	1:B:384:VAL:HG21	1.51	0.91
1:G:149:ILE:O	1:G:153:ILE:HG12	1.69	0.91
1:G:212:GLU:HB2	1:G:262:ARG:O	1.69	0.91
1:E:152:LYS:HG2	1:F:369:PHE:CE1	2.05	0.91
1:H:194:LEU:HD21	1:H:237:LEU:HD23	1.53	0.91
1:D:235:LEU:HD12	1:D:236:PHE:H	1.16	0.91
1:K:264:GLY:HA2	1:L:207:GLU:OE2	1.71	0.91
1:E:177:ALA:HA	1:E:180:ILE:HD12	0.92	0.90
1:K:201:ARG:HH11	1:K:201:ARG:HB2	1.37	0.90
1:E:139:TYR:HB3	1:E:141:PHE:CE1	2.07	0.90
1:K:213:LYS:HD2	1:K:220:VAL:O	1.71	0.90
1:C:140:VAL:HG11	1:C:320:LEU:HD23	1.54	0.90
1:F:240:ILE:HD11	1:F:277:ALA:CB	1.98	0.90
1:H:214:GLY:H	1:H:219:ALA:CB	1.83	0.90
1:L:329:SER:CA	1:L:334:LYS:HE2	2.00	0.90
1:M:164:LEU:HD21	1:M:283:ILE:HG13	1.53	0.90
1:B:318:ILE:HG12	1:B:348:LEU:HD21	1.53	0.90
1:G:240:ILE:HG13	1:G:277:ALA:HB1	1.52	0.90
1:L:227:PHE:CE2	1:L:254:VAL:HG11	2.06	0.90
1:E:165:ILE:HD11	1:E:177:ALA:HB2	1.52	0.89
1:C:220:VAL:HG12	1:C:221:SER:N	1.86	0.89
1:E:171:VAL:HG12	1:E:355:ASN:OD1	1.71	0.89
1:H:255:ILE:HG12	1:H:275:ILE:CD1	2.03	0.89
1:L:165:ILE:H	1:L:278:ALA:HB2	1.35	0.89
1:E:354:GLY:HA3	1:E:358:GLU:HB2	1.54	0.88
1:E:365:ARG:HH11	1:E:383:LEU:HD22	1.38	0.88
1:H:234:THR:HG21	1:H:276:LEU:HD12	1.55	0.88
1:H:156:ILE:HD12	1:H:303:ILE:HD13	1.54	0.88
1:N:145:LYS:HA	1:N:148:GLU:HG2	1.55	0.88
1:C:251:LEU:HD22	1:C:255:ILE:HD11	1.55	0.88
1:H:255:ILE:HG12	1:H:275:ILE:HD13	1.55	0.88
1:H:198:SER:HB2	1:N:250:LYS:HB2	1.55	0.88
1:M:318:ILE:HG23	1:M:348:LEU:HD21	1.55	0.88
1:I:240:ILE:HD11	1:I:277:ALA:HB1	1.55	0.88
1:G:224:GLU:HG2	1:G:225:GLY:H	1.39	0.88
1:L:140:VAL:CG1	1:L:320:LEU:HG	2.03	0.88
1:N:251:LEU:HD22	1:N:296:LEU:HD21	1.54	0.88
1:A:275:ILE:HD12	1:A:275:ILE:H	1.38	0.88
1:E:240:ILE:HD11	1:E:277:ALA:HB1	0.91	0.88
1:E:227:PHE:CE2	1:E:254:VAL:HG11	2.09	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:343:ALA:HB2	1:J:376:ASP:HA	1.56	0.88
1:F:201:ARG:HB2	1:F:201:ARG:HH11	1.37	0.88
1:H:143:SER:HA	1:H:147:LYS:HE3	1.56	0.87
1:L:163:VAL:HG22	1:L:303:ILE:HG21	1.54	0.87
1:E:267:LYS:HD2	1:E:267:LYS:H	1.38	0.87
1:J:318:ILE:HG13	1:J:319:PRO:HD3	1.54	0.87
1:F:347:LEU:HD21	1:F:380:LEU:HD12	1.57	0.87
1:I:189:GLU:HB3	1:I:190:PRO:HD2	1.56	0.87
1:B:240:ILE:HG13	1:B:277:ALA:HB1	1.55	0.87
1:F:153:ILE:HG23	1:F:180:ILE:HG12	1.57	0.87
1:L:189:GLU:HG3	1:L:190:PRO:HD2	1.57	0.87
1:F:223:LYS:O	1:F:225:GLY:N	2.07	0.86
1:M:318:ILE:CG1	1:M:319:PRO:HD3	2.03	0.86
1:I:220:VAL:HG12	1:I:221:SER:N	1.90	0.86
1:L:347:LEU:O	1:L:349:SER:N	2.08	0.86
1:D:282:ASN:HD22	1:D:285:GLU:HB2	1.39	0.86
1:L:165:ILE:O	1:L:278:ALA:HB1	1.75	0.86
1:B:189:GLU:HG3	1:B:190:PRO:HD2	1.57	0.86
1:M:181:HIS:CE1	1:M:187:SER:HA	2.11	0.86
1:C:143:SER:O	1:C:147:LYS:HB2	1.75	0.86
1:I:284:LYS:HE2	1:I:297:TYR:OH	1.75	0.86
1:M:143:SER:O	1:M:147:LYS:HB2	1.76	0.86
1:I:141:PHE:CB	1:I:150:LEU:HD11	2.06	0.86
1:E:292:PHE:CZ	1:E:296:LEU:HD12	2.11	0.86
1:L:239:GLU:O	1:L:241:GLY:N	2.07	0.86
1:N:325:LEU:O	1:N:325:LEU:HD23	1.76	0.85
1:H:192:VAL:HG21	1:H:230:ALA:HB2	1.58	0.85
1:M:318:ILE:HG13	1:M:319:PRO:CD	2.03	0.85
1:N:259:LYS:HG2	1:N:270:GLU:HB2	1.58	0.85
1:B:275:ILE:HD12	1:B:275:ILE:N	1.91	0.85
1:F:143:SER:HB2	1:F:144:PRO:HD2	1.59	0.85
1:N:318:ILE:HG13	1:N:319:PRO:HD3	1.58	0.85
1:B:146:MET:HG3	1:B:313:ARG:HH21	1.41	0.85
1:A:362:VAL:HG13	1:A:383:LEU:HD12	1.59	0.85
1:D:143:SER:HB2	1:D:315:GLU:HB2	1.55	0.85
1:E:354:GLY:N	1:E:358:GLU:OE1	2.10	0.85
1:K:318:ILE:HG12	1:K:348:LEU:HD21	1.58	0.84
1:I:141:PHE:CD2	1:I:150:LEU:HD21	2.11	0.84
1:M:256:GLU:HG2	1:M:257:SER:H	1.41	0.84
1:E:150:LEU:HD12	1:E:150:LEU:O	1.76	0.84
1:F:153:ILE:HG21	1:F:179:LEU:HD22	1.60	0.84

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:200:PRO:HG2	1:N:203:ILE:HD12	1.59	0.84
1:C:365:ARG:NH1	1:C:383:LEU:HD22	1.93	0.84
1:D:284:LYS:HG2	1:D:297:TYR:OH	1.78	0.84
1:H:146:MET:HG2	1:H:313:ARG:CZ	2.08	0.84
1:N:139:TYR:CE2	1:N:175:VAL:HG13	2.12	0.84
1:K:209:PHE:CD2	1:K:250:LYS:HD3	2.12	0.84
1:L:376:ASP:O	1:L:378:GLY:N	2.10	0.84
1:D:357:ARG:HD3	2:D:2:ADP:H5'2	1.59	0.84
1:L:141:PHE:CE1	1:L:150:LEU:HG	2.12	0.84
1:L:334:LYS:CE	1:L:367:VAL:HG13	2.08	0.84
1:K:139:TYR:O	1:K:140:VAL:HG23	1.75	0.84
1:K:279:THR:HG21	1:K:283:ILE:HD11	1.59	0.84
1:N:146:MET:HE3	1:N:307:ILE:HG23	1.59	0.84
1:D:235:LEU:CD1	1:D:236:PHE:N	2.38	0.83
1:J:365:ARG:HD2	1:J:383:LEU:HD22	1.60	0.83
1:C:178:ARG:CG	1:C:178:ARG:HH11	1.90	0.83
1:C:300:LEU:O	1:C:302:VAL:N	2.10	0.83
1:L:229:LEU:C	1:L:229:LEU:HD13	1.98	0.83
1:D:207:GLU:HB3	1:D:226:PHE:CE1	2.14	0.83
1:I:194:LEU:HD13	1:I:226:PHE:HD1	1.44	0.83
1:J:318:ILE:HG12	1:J:348:LEU:HD21	1.58	0.83
1:L:141:PHE:CD1	1:L:150:LEU:HG	2.14	0.83
1:M:283:ILE:HA	1:M:286:LEU:HD12	1.58	0.83
1:A:358:GLU:O	1:A:362:VAL:HG23	1.78	0.83
1:H:194:LEU:H	1:H:194:LEU:HD23	1.44	0.83
1:A:143:SER:HB2	1:A:144:PRO:HD2	1.61	0.82
1:L:240:ILE:O	1:L:240:ILE:HG22	1.78	0.82
1:F:238:ASP:O	1:F:239:GLU:HG2	1.79	0.82
1:L:140:VAL:HG11	1:L:320:LEU:CG	2.07	0.82
1:L:240:ILE:HD11	1:L:277:ALA:HB3	1.59	0.82
1:L:163:VAL:HG22	1:L:303:ILE:CG2	2.09	0.82
1:F:240:ILE:O	1:F:242:GLU:N	2.13	0.82
1:G:263:LEU:CG	1:G:264:GLY:H	1.92	0.82
1:I:172:GLY:O	1:I:176:VAL:HG23	1.80	0.82
1:J:200:PRO:HG2	1:J:203:ILE:HD12	1.59	0.82
1:N:245:LEU:HD22	1:N:293:ARG:HG3	1.60	0.82
1:K:207:GLU:OE1	1:K:207:GLU:HA	1.78	0.82
1:C:181:HIS:HD2	1:C:191:PHE:CD1	1.98	0.82
1:F:343:ALA:O	1:F:345:GLU:N	2.12	0.82
1:H:168:GLU:HG3	1:H:311:ARG:HH22	1.44	0.82
1:K:186:ARG:HH22	1:K:272:ASN:ND2	1.78	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:TYR:CE1	1:D:223:LYS:HB3	2.14	0.82
1:F:194:LEU:HD23	1:F:194:LEU:H	1.42	0.82
1:B:324:PHE:HD1	1:B:363:ILE:HD12	1.44	0.81
1:E:354:GLY:CA	1:E:358:GLU:HB2	2.09	0.81
1:L:334:LYS:HE3	1:L:336:VAL:HB	1.60	0.81
1:C:150:LEU:HG	1:C:154:LYS:HZ2	1.43	0.81
1:N:146:MET:CE	1:N:307:ILE:HG23	2.10	0.81
1:C:240:ILE:HG12	1:C:277:ALA:HB1	1.60	0.81
1:D:309:PRO:HB2	1:D:311:ARG:HG2	1.61	0.81
1:E:309:PRO:HB2	1:E:311:ARG:HD3	1.61	0.81
1:H:197:ALA:O	1:N:246:GLU:HA	1.79	0.81
1:K:235:LEU:HB2	1:K:273:VAL:HG11	1.61	0.81
1:C:181:HIS:HD2	1:C:191:PHE:HB2	1.38	0.81
1:E:310:LEU:O	1:E:317:ILE:HD11	1.80	0.81
1:I:220:VAL:CG1	1:I:221:SER:H	1.93	0.81
1:F:172:GLY:HA2	2:F:4:ADP:PA	2.21	0.81
1:I:301:GLY:O	1:J:365:ARG:NH2	2.14	0.81
1:M:207:GLU:O	1:M:226:PHE:HD1	1.64	0.81
1:E:137:GLU:HG2	1:E:138:GLU:H	1.45	0.81
1:E:358:GLU:O	1:E:362:VAL:HG23	1.81	0.81
1:H:265:GLY:O	1:H:266:ARG:HD3	1.80	0.81
1:I:143:SER:HB3	1:I:316:ASP:OD2	1.81	0.81
1:L:138:GLU:HG3	1:L:139:TYR:H	1.44	0.81
1:I:240:ILE:CD1	1:I:277:ALA:HB1	2.10	0.81
1:K:216:PHE:CD1	1:K:219:ALA:HB2	2.16	0.81
1:C:227:PHE:CE2	1:C:254:VAL:HG11	2.15	0.81
1:A:240:ILE:HG13	1:A:277:ALA:HB1	1.61	0.81
1:E:138:GLU:HB2	1:E:323:HIS:NE2	1.95	0.81
1:G:231:ASP:OD1	1:G:271:VAL:HA	1.81	0.81
1:I:252:LEU:HD13	1:I:296:LEU:HA	1.60	0.81
1:K:204:PHE:HE2	1:K:208:LEU:HD12	1.47	0.80
1:B:321:ALA:HA	1:B:363:ILE:HD11	1.63	0.80
1:N:165:ILE:O	1:N:278:ALA:HA	1.81	0.80
1:K:216:PHE:HD1	1:K:219:ALA:HB2	1.46	0.80
1:I:267:LYS:H	1:I:267:LYS:HD2	1.46	0.80
1:M:249:ALA:HA	1:M:293:ARG:HH12	1.46	0.80
1:B:178:ARG:HD2	1:B:191:PHE:CE2	2.16	0.80
1:E:316:ASP:O	1:E:319:PRO:HD2	1.81	0.80
1:K:161:CYS:HB2	1:K:162:PRO:HD2	1.61	0.80
1:K:215:ALA:H	1:K:219:ALA:CB	1.95	0.80
1:L:350:TYR:CD2	1:L:351:PRO:CD	2.62	0.80

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:THR:HG21	1:E:283:ILE:HD11	1.64	0.79
1:G:209:PHE:O	1:G:225:GLY:HA3	1.82	0.79
1:L:141:PHE:HD2	1:L:141:PHE:N	1.79	0.79
1:H:189:GLU:CG	1:H:190:PRO:HD2	2.13	0.79
1:M:146:MET:HE3	1:M:146:MET:HA	1.62	0.79
1:D:350:TYR:CD1	1:D:351:PRO:HD2	2.17	0.79
1:J:200:PRO:CG	1:J:203:ILE:HD12	2.11	0.79
1:L:281:ARG:HD2	1:L:282:ASN:H	1.46	0.79
1:L:334:LYS:HZ2	1:L:367:VAL:CG1	1.88	0.79
1:N:328:PHE:O	1:N:367:VAL:HG11	1.82	0.79
1:C:181:HIS:CD2	1:C:191:PHE:HD1	2.01	0.79
1:L:339:PHE:CE2	1:L:375:ILE:HD11	2.18	0.79
1:N:359:LEU:O	1:N:363:ILE:HG13	1.83	0.79
1:M:191:PHE:HE2	1:M:193:ALA:HB2	1.46	0.79
1:D:235:LEU:HD11	1:D:237:LEU:HD23	1.63	0.79
1:H:145:LYS:HB2	1:H:313:ARG:HH21	1.45	0.79
1:J:316:ASP:O	1:J:319:PRO:HD2	1.80	0.79
1:K:143:SER:HB2	1:K:144:PRO:HD2	1.62	0.79
1:M:363:ILE:H	1:M:363:ILE:CD1	1.96	0.79
1:B:318:ILE:HG13	1:B:319:PRO:HD3	1.63	0.79
1:D:235:LEU:CD1	1:D:236:PHE:H	1.96	0.79
1:E:234:THR:HG23	1:E:274:ARG:HB3	1.65	0.79
1:M:167:GLY:O	1:M:280:ASN:HA	1.83	0.79
1:D:203:ILE:HG22	1:D:207:GLU:HG2	1.65	0.79
1:I:314:LYS:HA	1:I:317:ILE:CD1	2.13	0.79
1:M:246:GLU:O	1:M:249:ALA:HB3	1.83	0.79
1:C:153:ILE:HG21	1:C:179:LEU:HD22	1.64	0.79
1:F:309:PRO:HG3	1:F:311:ARG:HH12	1.47	0.79
1:E:196:VAL:HG12	1:E:196:VAL:O	1.83	0.78
1:H:350:TYR:HB3	1:H:351:PRO:HA	1.65	0.78
1:K:282:ASN:HD22	1:K:285:GLU:HB2	1.47	0.78
1:H:196:VAL:HA	1:H:204:PHE:CE1	2.19	0.78
1:C:172:GLY:O	1:C:176:VAL:HG23	1.83	0.78
1:L:195:ASN:HB3	1:L:198:SER:OG	1.84	0.78
1:E:269:ILE:H	1:E:269:ILE:HD12	1.49	0.78
1:F:178:ARG:HH11	1:F:178:ARG:HG3	1.46	0.78
1:G:340:THR:OG1	1:G:342:SER:HB3	1.82	0.78
1:K:205:GLU:OE1	1:K:246:GLU:HB2	1.83	0.78
1:K:249:ALA:HB2	1:K:293:ARG:HH11	1.49	0.78
1:L:138:GLU:CG	1:L:139:TYR:H	1.93	0.78
1:M:146:MET:HG3	1:M:313:ARG:HE	1.47	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:PHE:CD2	1:E:219:ALA:HB2	2.18	0.78
1:E:192:VAL:CG2	1:E:230:ALA:HB2	2.13	0.78
1:K:143:SER:HB2	1:K:315:GLU:HB2	1.64	0.78
1:M:281:ARG:HG2	1:M:286:LEU:HD21	1.66	0.78
1:A:189:GLU:HG3	1:A:190:PRO:HD2	1.66	0.78
1:N:200:PRO:CG	1:N:203:ILE:HD12	2.14	0.78
1:A:139:TYR:CD2	1:A:175:VAL:HG13	2.19	0.78
1:D:192:VAL:O	1:D:192:VAL:HG12	1.84	0.78
1:C:253:ARG:HH11	1:C:253:ARG:HG2	1.49	0.77
1:E:167:GLY:O	1:E:173:LYS:HE3	1.84	0.77
1:H:356:VAL:HG11	2:H:14:ADP:C8	2.20	0.77
1:E:165:ILE:CD1	1:E:177:ALA:HB2	2.14	0.77
1:F:325:LEU:HD21	1:F:336:VAL:HG12	1.66	0.77
1:C:314:LYS:HA	1:C:317:ILE:HG13	1.66	0.77
1:D:210:GLY:HA3	1:D:225:GLY:H	1.48	0.77
1:L:311:ARG:HG2	1:L:351:PRO:O	1.83	0.77
1:E:325:LEU:HD23	1:E:325:LEU:O	1.85	0.77
1:F:357:ARG:HH11	1:F:357:ARG:HG3	1.49	0.77
1:B:275:ILE:H	1:B:275:ILE:CD1	1.93	0.77
1:M:143:SER:CB	1:M:144:PRO:HD2	2.11	0.77
1:E:203:ILE:O	1:E:206:ALA:HB3	1.85	0.77
1:F:176:VAL:O	1:F:180:ILE:HG13	1.84	0.77
1:L:350:TYR:HD2	1:L:352:TRP:H	1.33	0.77
1:G:252:LEU:HB2	1:G:296:LEU:HD23	1.66	0.77
1:J:332:TYR:CE1	1:J:368:LEU:HD21	2.19	0.77
1:L:194:LEU:HD21	1:L:237:LEU:HD23	1.67	0.77
1:M:189:GLU:HG3	1:M:190:PRO:HD2	1.67	0.77
1:A:325:LEU:HD13	1:A:338:GLY:HA2	1.67	0.76
1:L:334:LYS:HZ3	1:L:367:VAL:CG1	1.95	0.76
1:N:245:LEU:HA	1:N:248:GLN:HE21	1.48	0.76
1:G:263:LEU:CD2	1:G:264:GLY:H	1.97	0.76
1:E:192:VAL:HG21	1:E:230:ALA:HB2	1.67	0.76
1:F:347:LEU:HD21	1:F:380:LEU:CD1	2.15	0.76
1:I:377:ARG:HD2	1:I:381:SER:HB3	1.68	0.76
1:L:140:VAL:O	1:L:140:VAL:HG12	1.84	0.76
1:N:208:LEU:HA	1:N:226:PHE:HB2	1.68	0.76
1:H:240:ILE:HG13	1:H:277:ALA:HB1	1.67	0.76
1:I:283:ILE:O	1:I:287:VAL:HG23	1.84	0.76
1:K:325:LEU:HD13	1:K:338:GLY:HA2	1.68	0.76
1:L:314:LYS:HA	1:L:317:ILE:CD1	2.15	0.76
1:A:252:LEU:HD13	1:A:296:LEU:HA	1.67	0.76

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:VAL:O	1:C:180:ILE:HG13	1.86	0.76
1:H:161:CYS:HB2	1:H:162:PRO:HD2	1.68	0.76
1:M:256:GLU:HG2	1:M:257:SER:N	2.01	0.76
1:E:138:GLU:HB2	1:E:323:HIS:HE2	1.49	0.76
1:H:250:LYS:HG3	1:I:198:SER:HB2	1.66	0.76
1:F:157:SER:OG	1:F:183:LEU:HB2	1.86	0.75
1:H:254:VAL:HG22	1:H:260:PHE:HB3	1.67	0.75
1:L:248:GLN:HE22	1:L:292:PHE:HA	1.49	0.75
1:N:209:PHE:CD1	1:N:250:LYS:HD3	2.20	0.75
1:N:281:ARG:N	1:N:281:ARG:HD3	1.99	0.75
1:I:173:LYS:HE3	2:I:8:ADP:O1B	1.87	0.75
1:J:350:TYR:CD1	1:J:351:PRO:HD2	2.22	0.75
1:D:158:CYS:HA	1:D:185:ASP:OD1	1.87	0.75
1:E:355:ASN:H	1:E:355:ASN:HD22	1.34	0.75
1:G:263:LEU:HD23	1:G:264:GLY:H	1.51	0.75
1:I:208:LEU:HD21	1:I:227:PHE:CD1	2.21	0.75
1:L:250:LYS:O	1:L:253:ARG:HB3	1.87	0.75
1:M:139:TYR:HB3	2:M:12:ADP:N1	2.02	0.75
1:D:237:LEU:HD12	1:D:243:LEU:HD11	1.68	0.75
1:E:292:PHE:HE2	1:E:296:LEU:HB3	1.50	0.75
1:F:355:ASN:OD1	1:F:355:ASN:N	2.17	0.75
1:L:141:PHE:CD2	1:L:141:PHE:N	2.49	0.75
1:L:340:THR:CG2	1:L:376:ASP:HB3	2.15	0.75
1:M:227:PHE:CE2	1:M:273:VAL:HG21	2.22	0.75
1:I:253:ARG:NE	1:J:198:SER:HB2	2.02	0.75
1:K:252:LEU:HB2	1:K:296:LEU:HD23	1.68	0.75
1:M:201:ARG:HH11	1:M:201:ARG:CB	1.91	0.75
1:N:153:ILE:HG21	1:N:179:LEU:HD22	1.67	0.75
1:B:192:VAL:HG21	1:B:230:ALA:HB2	1.69	0.75
1:B:201:ARG:NH1	1:B:201:ARG:HB2	2.00	0.75
1:F:275:ILE:HD12	1:F:275:ILE:H	1.52	0.75
1:G:245:LEU:HD22	1:G:248:GLN:NE2	2.01	0.75
1:I:297:TYR:HD2	1:I:298:TYR:CD1	2.04	0.75
1:J:282:ASN:ND2	1:J:285:GLU:HB2	2.00	0.75
1:J:365:ARG:HD2	1:J:383:LEU:CD2	2.16	0.75
1:K:302:VAL:HG21	1:L:361:ASN:HB3	1.68	0.75
1:N:240:ILE:CD1	1:N:277:ALA:HB1	2.05	0.75
1:B:176:VAL:O	1:B:180:ILE:HG13	1.86	0.75
1:D:235:LEU:HD11	1:D:237:LEU:CD2	2.17	0.75
1:L:281:ARG:HD2	1:L:282:ASN:N	2.01	0.75
1:N:143:SER:HB2	1:N:144:PRO:HD2	1.68	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:OG1	1:A:376:ASP:HB3	1.87	0.74
1:E:292:PHE:CE2	1:E:296:LEU:HD12	2.22	0.74
1:H:320:LEU:HB3	1:H:324:PHE:HE1	1.52	0.74
1:M:347:LEU:HD21	1:M:380:LEU:HG	1.69	0.74
1:F:311:ARG:HH11	1:F:311:ARG:HG2	1.52	0.74
1:I:176:VAL:O	1:I:180:ILE:HG13	1.87	0.74
1:F:163:VAL:HG13	1:F:303:ILE:HG22	1.69	0.74
1:L:314:LYS:HA	1:L:317:ILE:HD11	1.67	0.74
1:C:194:LEU:CD2	1:C:194:LEU:H	2.00	0.74
1:M:171:VAL:HB	1:M:307:ILE:HG22	1.68	0.74
1:G:189:GLU:HG2	1:G:232:GLY:O	1.87	0.74
1:M:168:GLU:OE1	1:M:309:PRO:HB3	1.87	0.74
1:E:157:SER:HB3	1:E:183:LEU:O	1.88	0.74
1:F:213:LYS:HD3	1:G:220:VAL:HG11	1.69	0.74
1:I:204:PHE:HE2	1:I:208:LEU:HD12	1.51	0.74
1:H:377:ARG:HG2	1:H:381:SER:HB3	1.70	0.74
1:I:256:GLU:HG2	1:I:299:ARG:HE	1.51	0.74
1:L:315:GLU:N	1:L:315:GLU:OE1	2.20	0.74
1:B:194:LEU:HD21	1:B:237:LEU:HD23	1.69	0.74
1:D:337:GLU:OE1	1:D:373:LYS:HD3	1.87	0.74
1:B:380:LEU:O	1:B:384:VAL:HB	1.88	0.74
1:C:165:ILE:HB	1:C:278:ALA:HB2	1.67	0.74
1:F:340:THR:HG23	1:F:376:ASP:HB3	1.69	0.74
1:J:208:LEU:HA	1:J:226:PHE:HB2	1.69	0.74
1:K:314:LYS:HA	1:K:317:ILE:HG13	1.70	0.74
1:E:205:GLU:OE2	1:E:246:GLU:HB2	1.87	0.73
1:I:194:LEU:HD23	1:I:194:LEU:N	2.02	0.73
1:J:172:GLY:O	1:J:176:VAL:HG23	1.88	0.73
1:M:192:VAL:O	1:M:235:LEU:HD12	1.87	0.73
1:L:176:VAL:O	1:L:180:ILE:HG13	1.88	0.73
1:L:224:GLU:HA	1:L:262:ARG:NH2	1.99	0.73
1:B:192:VAL:CG2	1:B:230:ALA:HB2	2.18	0.73
1:C:181:HIS:CE1	1:C:187:SER:HA	2.24	0.73
1:D:143:SER:HB2	1:D:144:PRO:HD2	1.70	0.73
1:D:266:ARG:HH22	1:E:207:GLU:HG2	1.54	0.73
1:L:298:TYR:CE1	1:M:354:GLY:HA3	2.23	0.73
1:B:227:PHE:CE2	1:B:254:VAL:HG11	2.23	0.73
1:E:365:ARG:NH1	1:E:383:LEU:HD22	2.02	0.73
1:H:311:ARG:HG2	1:H:352:TRP:HA	1.70	0.73
1:I:165:ILE:HB	1:I:278:ALA:HB2	1.70	0.73
1:M:265:GLY:HA2	1:N:203:ILE:HD13	1.70	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:ARG:HB2	1:E:201:ARG:NH1	2.03	0.73
1:F:321:ALA:HA	1:F:363:ILE:CD1	2.18	0.73
1:K:164:LEU:HD12	1:K:165:ILE:N	2.03	0.73
1:L:352:TRP:CH2	1:L:362:VAL:HG21	2.23	0.73
1:M:363:ILE:HD12	1:M:363:ILE:N	2.03	0.73
1:G:275:ILE:N	1:G:275:ILE:HD12	2.04	0.73
1:L:343:ALA:HB2	1:L:376:ASP:CA	2.15	0.73
1:N:357:ARG:HH12	1:N:361:ASN:CG	1.92	0.73
1:N:363:ILE:O	1:N:367:VAL:HG23	1.88	0.73
1:B:201:ARG:HB2	1:B:201:ARG:HH11	1.53	0.73
1:K:342:SER:OG	1:K:377:ARG:HB2	1.88	0.73
1:B:365:ARG:HH11	1:B:383:LEU:HB3	1.52	0.73
1:D:248:GLN:HE22	1:D:292:PHE:HA	1.54	0.73
1:E:236:PHE:HD1	1:E:276:LEU:O	1.71	0.73
1:C:283:ILE:HG21	1:C:297:TYR:CD1	2.23	0.73
1:I:165:ILE:HG22	1:I:173:LYS:HG2	1.70	0.73
1:L:283:ILE:HB	1:L:297:TYR:CZ	2.24	0.73
1:D:244:SER:O	1:D:248:GLN:HG3	1.88	0.72
1:A:309:PRO:HG3	1:A:311:ARG:NH1	2.04	0.72
1:C:140:VAL:HG12	1:C:140:VAL:O	1.89	0.72
1:C:162:PRO:HG2	1:C:302:VAL:HG23	1.70	0.72
1:D:189:GLU:HG3	1:D:190:PRO:HD2	1.71	0.72
1:D:194:LEU:O	1:D:194:LEU:HD23	1.89	0.72
1:H:321:ALA:HA	1:H:363:ILE:CD1	2.18	0.72
1:N:239:GLU:O	1:N:241:GLY:N	2.23	0.72
1:F:309:PRO:HA	1:F:355:ASN:HD22	1.51	0.72
1:L:240:ILE:HB	1:L:279:THR:HG22	1.71	0.72
1:B:161:CYS:HB2	1:B:162:PRO:HD2	1.71	0.72
1:E:176:VAL:HG21	1:E:307:ILE:HD11	1.71	0.72
1:G:299:ARG:HE	1:G:299:ARG:HA	1.54	0.72
1:J:189:GLU:CG	1:J:190:PRO:HD2	2.18	0.72
1:K:157:SER:OG	1:K:183:LEU:HB2	1.90	0.72
1:M:282:ASN:ND2	1:M:285:GLU:HB2	2.04	0.72
1:E:236:PHE:HE1	1:E:278:ALA:HB2	1.52	0.72
1:J:269:ILE:N	1:J:269:ILE:HD12	2.05	0.72
1:K:216:PHE:HD1	1:K:216:PHE:N	1.88	0.72
1:B:186:ARG:HD3	1:B:232:GLY:O	1.88	0.72
1:C:181:HIS:HD2	1:C:191:PHE:HD1	1.33	0.72
1:D:263:LEU:HD23	1:D:264:GLY:N	2.04	0.72
1:F:357:ARG:HG2	2:F:4:ADP:H5'2	1.70	0.72
1:G:194:LEU:HD21	1:G:237:LEU:HD22	1.71	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:143:SER:N	1:I:316:ASP:OD1	2.23	0.72
1:I:318:ILE:HG12	1:I:348:LEU:HD21	1.69	0.72
1:B:153:ILE:HG21	1:B:179:LEU:HD22	1.71	0.72
1:E:146:MET:CE	1:E:149:ILE:HD12	2.20	0.72
1:G:310:LEU:HB2	1:G:355:ASN:CB	2.19	0.72
1:H:208:LEU:HD23	1:H:209:PHE:CE1	2.25	0.72
1:I:261:TYR:CE1	1:J:199:ILE:HG12	2.20	0.72
1:M:265:GLY:HA2	1:N:203:ILE:CD1	2.20	0.72
1:N:357:ARG:HH12	1:N:361:ASN:ND2	1.88	0.72
1:F:279:THR:HG21	1:F:283:ILE:HD11	1.72	0.72
1:H:357:ARG:HG3	2:H:14:ADP:H5'2	1.72	0.72
1:J:201:ARG:CB	1:J:201:ARG:HH11	2.02	0.72
1:F:362:VAL:HG13	1:F:383:LEU:HD12	1.71	0.71
1:J:168:GLU:OE1	1:J:309:PRO:HB3	1.90	0.71
1:M:253:ARG:HG3	1:N:198:SER:CB	2.19	0.71
1:D:341:LYS:O	1:D:345:GLU:HG3	1.90	0.71
1:E:347:LEU:HD21	1:E:380:LEU:CD1	2.19	0.71
1:F:173:LYS:H	2:F:4:ADP:PB	2.14	0.71
1:G:313:ARG:HB3	1:G:316:ASP:OD2	1.89	0.71
1:E:149:ILE:O	1:E:152:LYS:N	2.23	0.71
1:G:189:GLU:CG	1:G:190:PRO:HD2	2.19	0.71
1:E:186:ARG:NH2	1:E:272:ASN:HD21	1.87	0.71
1:E:328:PHE:CE1	1:E:364:GLU:HB2	2.25	0.71
1:F:194:LEU:HD23	1:F:194:LEU:N	2.04	0.71
1:F:321:ALA:HA	1:F:363:ILE:HD11	1.72	0.71
1:I:254:VAL:HG22	1:I:260:PHE:HB3	1.71	0.71
1:I:335:GLU:O	1:I:373:LYS:HG2	1.89	0.71
1:J:194:LEU:HD21	1:J:237:LEU:HD23	1.73	0.71
1:J:340:THR:OG1	1:J:376:ASP:HB2	1.90	0.71
1:L:334:LYS:HD3	1:L:367:VAL:HG13	1.70	0.71
1:B:174:GLU:HB3	2:B:7:ADP:O1A	1.90	0.71
1:E:216:PHE:CE2	1:E:219:ALA:HB2	2.26	0.71
1:I:156:ILE:O	1:I:158:CYS:N	2.22	0.71
1:L:211:TYR:HE1	1:L:223:LYS:HD3	1.55	0.71
1:M:363:ILE:H	1:M:363:ILE:HD12	1.55	0.71
1:L:138:GLU:OE1	1:L:323:HIS:NE2	2.24	0.71
1:M:180:ILE:CG2	1:M:276:LEU:HD11	2.18	0.71
1:F:314:LYS:HA	1:F:317:ILE:HG13	1.72	0.71
1:K:269:ILE:H	1:K:269:ILE:HD12	1.56	0.71
1:N:201:ARG:NH1	1:N:201:ARG:HB2	2.06	0.71
1:N:246:GLU:H	1:N:246:GLU:CD	1.89	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:HG23	1:B:274:ARG:O	1.90	0.71
1:C:194:LEU:HD23	1:C:194:LEU:H	1.55	0.71
1:C:244:SER:O	1:C:248:GLN:HG3	1.89	0.71
1:D:316:ASP:O	1:D:319:PRO:HD2	1.90	0.71
1:N:145:LYS:CA	1:N:148:GLU:HG2	2.19	0.71
1:N:339:PHE:CE2	1:N:347:LEU:HD11	2.25	0.71
1:E:355:ASN:N	1:E:355:ASN:HD22	1.86	0.71
1:A:139:TYR:CE2	1:A:175:VAL:HG22	2.26	0.71
1:B:208:LEU:HG	1:B:209:PHE:CD1	2.26	0.71
1:E:181:HIS:CD2	1:E:234:THR:OG1	2.43	0.71
1:F:201:ARG:HB2	1:F:201:ARG:NH1	2.06	0.71
1:G:178:ARG:HA	1:G:191:PHE:HE1	1.56	0.71
1:D:308:PRO:HG2	1:D:313:ARG:HD2	1.72	0.70
1:E:236:PHE:HE1	1:E:278:ALA:CB	2.03	0.70
1:K:282:ASN:ND2	1:K:285:GLU:HB2	2.06	0.70
1:E:231:ASP:OD2	1:E:271:VAL:HG12	1.90	0.70
1:F:153:ILE:HD12	1:F:180:ILE:HG12	1.73	0.70
1:I:239:GLU:HG2	1:I:281:ARG:HH21	1.56	0.70
1:A:254:VAL:HG22	1:A:260:PHE:HB3	1.73	0.70
1:C:220:VAL:CG1	1:C:221:SER:H	1.90	0.70
1:E:267:LYS:N	1:E:267:LYS:HD2	2.06	0.70
1:H:146:MET:HG2	1:H:313:ARG:NH1	2.05	0.70
1:M:211:TYR:HE1	1:M:223:LYS:CB	2.02	0.70
1:E:214:GLY:HA2	1:E:219:ALA:CB	2.20	0.70
1:B:204:PHE:HE2	1:B:208:LEU:HD22	1.55	0.70
1:E:173:LYS:NZ	2:E:3:ADP:O1B	2.23	0.70
1:B:194:LEU:HD21	1:B:237:LEU:CD2	2.22	0.70
1:B:337:GLU:HG2	1:B:373:LYS:HB3	1.73	0.70
1:C:252:LEU:HD13	1:C:296:LEU:HA	1.73	0.70
1:E:137:GLU:HG2	1:E:138:GLU:HG2	1.74	0.70
1:E:310:LEU:HG	1:E:317:ILE:HG12	1.72	0.70
1:E:313:ARG:HB3	1:E:316:ASP:OD2	1.91	0.70
1:L:211:TYR:CE1	1:L:223:LYS:HD3	2.27	0.70
1:M:249:ALA:HA	1:M:293:ARG:NH1	2.07	0.70
1:H:215:ALA:HA	1:I:211:TYR:OH	1.92	0.70
1:K:302:VAL:HG13	1:L:365:ARG:HB2	1.73	0.70
1:G:198:SER:O	1:G:199:ILE:HG13	1.91	0.70
1:L:138:GLU:CG	1:L:139:TYR:N	2.47	0.70
1:L:343:ALA:O	1:L:345:GLU:N	2.25	0.70
1:M:314:LYS:HA	1:M:317:ILE:CD1	2.22	0.70
1:N:325:LEU:C	1:N:325:LEU:HD23	2.11	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:ALA:CB	1:E:300:LEU:HD13	2.22	0.70
1:J:284:LYS:HE2	1:J:297:TYR:OH	1.92	0.70
1:K:361:ASN:HD22	1:K:361:ASN:N	1.90	0.70
1:C:162:PRO:HG2	1:C:302:VAL:CG2	2.22	0.70
1:G:320:LEU:HD11	1:G:356:VAL:HG13	1.74	0.70
1:K:216:PHE:CD1	1:K:216:PHE:N	2.58	0.70
1:N:235:LEU:HD12	1:N:236:PHE:N	2.06	0.70
1:H:198:SER:HB2	1:N:250:LYS:CB	2.22	0.69
1:B:244:SER:O	1:B:248:GLN:HG3	1.92	0.69
1:L:207:GLU:OE1	1:L:207:GLU:HA	1.90	0.69
1:M:299:ARG:HD3	1:N:357:ARG:NH2	2.08	0.69
1:J:254:VAL:HG22	1:J:260:PHE:HB3	1.74	0.69
1:A:189:GLU:CG	1:A:190:PRO:HD2	2.22	0.69
1:J:383:LEU:HD23	1:J:383:LEU:N	2.07	0.69
1:B:208:LEU:HG	1:B:209:PHE:CE1	2.26	0.69
1:B:266:ARG:HB3	1:C:229:LEU:CD2	2.22	0.69
1:B:317:ILE:HB	1:B:348:LEU:CD2	2.22	0.69
1:F:149:ILE:HD13	1:F:307:ILE:HD13	1.73	0.69
1:H:215:ALA:HB2	1:I:223:LYS:NZ	2.07	0.69
1:E:303:ILE:HG22	1:E:303:ILE:O	1.92	0.69
1:H:234:THR:HG21	1:H:276:LEU:CD1	2.21	0.69
1:I:240:ILE:HD11	1:I:277:ALA:CB	2.22	0.69
1:L:322:ASN:HA	1:L:339:PHE:HE1	1.55	0.69
1:L:340:THR:HG23	1:L:376:ASP:HB3	1.72	0.69
1:N:165:ILE:HB	1:N:278:ALA:HB2	1.73	0.69
1:N:283:ILE:O	1:N:287:VAL:HG23	1.91	0.69
1:C:161:CYS:HB2	1:C:302:VAL:HG11	1.74	0.69
1:C:300:LEU:O	1:C:302:VAL:HG23	1.93	0.69
1:E:308:PRO:HG2	1:E:313:ARG:HD2	1.75	0.69
1:F:267:LYS:HD2	1:F:267:LYS:N	2.08	0.69
1:I:172:GLY:HA2	2:I:8:ADP:O1A	1.93	0.69
1:J:240:ILE:O	1:J:242:GLU:N	2.25	0.69
1:D:210:GLY:CA	1:D:225:GLY:H	2.04	0.69
1:E:171:VAL:HB	1:E:307:ILE:HG22	1.75	0.69
1:F:346:LEU:HG	1:F:377:ARG:HH11	1.56	0.69
1:I:207:GLU:HA	1:I:207:GLU:OE1	1.92	0.69
1:M:350:TYR:CG	1:M:351:PRO:HD2	2.27	0.69
1:B:189:GLU:CG	1:B:190:PRO:HD2	2.23	0.69
1:G:310:LEU:HD22	1:G:317:ILE:HG12	1.74	0.69
1:D:227:PHE:HD2	1:D:273:VAL:HG21	1.58	0.69
1:A:369:PHE:HA	1:G:155:LYS:HD3	1.75	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:144:PRO:HG2	1:J:145:LYS:H	1.58	0.69
1:C:266:ARG:NH1	1:D:216:PHE:CZ	2.58	0.69
1:F:172:GLY:O	1:F:176:VAL:HG23	1.92	0.69
1:I:365:ARG:NE	1:I:383:LEU:HD22	2.08	0.69
1:L:302:VAL:O	1:M:365:ARG:HD3	1.93	0.69
1:C:236:PHE:CE2	1:C:238:ASP:HB2	2.28	0.68
1:I:256:GLU:HG2	1:I:299:ARG:NE	2.08	0.68
1:K:208:LEU:HD22	1:K:209:PHE:CD1	2.28	0.68
1:A:237:LEU:HB2	1:A:240:ILE:CD1	2.23	0.68
1:A:325:LEU:CD1	1:A:338:GLY:HA2	2.23	0.68
1:B:178:ARG:HD2	1:B:191:PHE:HE2	1.59	0.68
1:E:186:ARG:HB2	1:E:189:GLU:HB2	1.75	0.68
1:E:313:ARG:O	1:E:315:GLU:N	2.26	0.68
1:G:308:PRO:HG2	1:G:313:ARG:HD2	1.75	0.68
1:H:227:PHE:CE2	1:H:254:VAL:HG11	2.28	0.68
1:H:359:LEU:HD23	1:H:359:LEU:O	1.94	0.68
1:J:220:VAL:HG12	1:J:221:SER:N	2.09	0.68
1:M:244:SER:O	1:M:247:ALA:HB3	1.92	0.68
1:A:161:CYS:O	1:A:274:ARG:NH1	2.25	0.68
1:B:260:PHE:C	1:B:260:PHE:HD1	1.97	0.68
1:D:302:VAL:HG12	1:D:303:ILE:HD13	1.75	0.68
1:E:350:TYR:CD1	1:E:384:VAL:HG13	2.28	0.68
1:F:242:GLU:HG2	1:F:281:ARG:HH22	1.58	0.68
1:M:216:PHE:O	1:M:218:GLY:N	2.26	0.68
1:M:240:ILE:HG23	1:M:243:LEU:HD12	1.75	0.68
1:N:240:ILE:HG23	1:N:243:LEU:HD12	1.74	0.68
1:B:246:GLU:HG3	1:C:197:ALA:O	1.93	0.68
1:G:350:TYR:CD1	1:G:351:PRO:HD2	2.28	0.68
1:H:296:LEU:HD23	1:H:296:LEU:O	1.92	0.68
1:H:318:ILE:HG13	1:H:348:LEU:HD21	1.75	0.68
1:I:350:TYR:CD1	1:I:351:PRO:HD2	2.28	0.68
1:B:321:ALA:HA	1:B:363:ILE:CD1	2.23	0.68
1:D:240:ILE:CG1	1:D:277:ALA:HB1	2.22	0.68
1:E:365:ARG:NH1	1:E:383:LEU:HB3	2.08	0.68
1:M:175:VAL:HG23	2:M:12:ADP:O1A	1.94	0.68
1:G:245:LEU:HD22	1:G:248:GLN:HE22	1.56	0.68
1:H:192:VAL:CG2	1:H:230:ALA:HB2	2.24	0.68
1:L:334:LYS:CD	1:L:367:VAL:HG13	2.23	0.68
1:J:325:LEU:HD23	1:J:326:LYS:N	2.09	0.68
1:M:261:TYR:HE2	1:N:199:ILE:HG12	1.58	0.68
1:N:140:VAL:HG11	1:N:320:LEU:HD23	1.75	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ARG:HH22	1:E:272:ASN:ND2	1.91	0.68
1:G:320:LEU:O	1:G:320:LEU:HD23	1.93	0.68
1:D:161:CYS:O	1:D:274:ARG:NH1	2.26	0.68
1:F:299:ARG:HE	1:F:299:ARG:HA	1.59	0.68
1:H:318:ILE:HD13	1:H:344:GLN:HE21	1.59	0.68
1:C:181:HIS:CD2	1:C:191:PHE:CD1	2.78	0.68
1:H:170:GLY:C	1:H:355:ASN:HB2	2.14	0.68
1:L:285:GLU:OE2	1:L:289:GLU:HB2	1.94	0.68
1:L:149:ILE:HD11	1:L:306:GLU:O	1.93	0.68
1:N:139:TYR:CD2	1:N:175:VAL:HG13	2.29	0.68
1:A:170:GLY:O	1:A:355:ASN:HB2	1.93	0.67
1:C:318:ILE:CG1	1:C:319:PRO:HD3	2.19	0.67
1:F:317:ILE:HG21	1:F:347:LEU:O	1.94	0.67
1:K:196:VAL:HG22	1:K:204:PHE:CZ	2.29	0.67
1:M:253:ARG:HD2	1:M:259:LYS:O	1.93	0.67
1:A:292:PHE:CZ	1:A:296:LEU:HD12	2.30	0.67
1:D:310:LEU:HD22	1:D:317:ILE:HG12	1.76	0.67
1:H:140:VAL:HG12	1:H:141:PHE:H	1.60	0.67
1:I:208:LEU:HD21	1:I:227:PHE:HD1	1.57	0.67
1:M:267:LYS:H	1:M:267:LYS:HD2	1.58	0.67
1:B:210:GLY:O	1:B:263:LEU:N	2.23	0.67
1:F:282:ASN:HD22	1:F:285:GLU:HB2	1.58	0.67
1:G:191:PHE:HE2	1:G:236:PHE:HB3	1.60	0.67
1:G:259:LYS:HB3	1:G:267:LYS:CG	2.08	0.67
1:H:143:SER:HB2	1:H:316:ASP:OD1	1.95	0.67
1:I:314:LYS:HA	1:I:317:ILE:HG13	1.76	0.67
1:L:350:TYR:CG	1:L:351:PRO:HD2	2.29	0.67
1:L:365:ARG:CZ	1:L:383:LEU:HD21	2.24	0.67
1:C:140:VAL:CG1	1:C:320:LEU:HD23	2.24	0.67
1:D:207:GLU:O	1:D:225:GLY:HA2	1.94	0.67
1:E:320:LEU:O	1:E:322:ASN:N	2.27	0.67
1:H:216:PHE:CG	1:H:216:PHE:O	2.47	0.67
1:M:141:PHE:HD2	1:M:150:LEU:HB2	1.57	0.67
1:E:319:PRO:O	1:E:322:ASN:HB2	1.94	0.67
1:L:240:ILE:CG2	1:L:240:ILE:O	2.42	0.67
1:L:324:PHE:O	1:L:328:PHE:HD1	1.77	0.67
1:B:164:LEU:HD12	1:B:165:ILE:H	1.59	0.67
1:C:178:ARG:HG3	1:C:178:ARG:NH1	1.97	0.67
1:D:282:ASN:ND2	1:D:285:GLU:HB2	2.09	0.67
1:E:314:LYS:HA	1:E:317:ILE:HD12	1.77	0.67
1:E:346:LEU:C	1:E:348:LEU:H	1.96	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:ARG:HH22	1:H:261:TYR:HE1	1.41	0.67
1:H:215:ALA:N	1:I:223:LYS:NZ	2.42	0.67
1:L:291:LYS:O	1:L:291:LYS:HD3	1.94	0.67
1:D:362:VAL:O	1:D:362:VAL:HG12	1.93	0.67
1:M:172:GLY:HA2	2:M:12:ADP:O1A	1.94	0.67
1:I:141:PHE:CG	1:I:150:LEU:HD11	2.29	0.67
1:N:152:LYS:HA	1:N:152:LYS:HE3	1.77	0.67
1:N:363:ILE:HA	1:N:366:ALA:HB3	1.76	0.67
1:E:212:GLU:O	1:E:222:SER:HA	1.95	0.67
1:F:138:GLU:CG	1:F:139:TYR:H	2.08	0.67
1:F:194:LEU:HD21	1:F:237:LEU:HD23	1.76	0.67
1:F:376:ASP:O	1:F:378:GLY:N	2.28	0.67
1:K:209:PHE:CE2	1:K:250:LYS:HD3	2.30	0.67
1:M:191:PHE:CE2	1:M:193:ALA:HB2	2.30	0.67
1:N:318:ILE:HG12	1:N:348:LEU:HD21	1.77	0.67
1:E:282:ASN:HD22	1:E:285:GLU:HB2	1.56	0.67
1:K:208:LEU:HD22	1:K:209:PHE:CE1	2.30	0.67
1:L:239:GLU:C	1:L:241:GLY:H	1.97	0.67
1:N:342:SER:OG	1:N:377:ARG:HB2	1.94	0.67
1:F:308:PRO:HG2	1:F:313:ARG:HD2	1.77	0.66
1:J:324:PHE:CD1	1:J:360:LYS:HA	2.30	0.66
1:K:206:ALA:HB1	1:K:211:TYR:HB3	1.76	0.66
1:K:240:ILE:HG13	1:K:277:ALA:HB1	1.77	0.66
1:K:266:ARG:HH22	1:L:207:GLU:CD	1.97	0.66
1:L:229:LEU:O	1:L:229:LEU:HD22	1.94	0.66
1:B:314:LYS:CD	1:B:314:LYS:H	2.03	0.66
1:D:316:ASP:C	1:D:319:PRO:HD2	2.16	0.66
1:N:228:GLU:O	1:N:231:ASP:N	2.27	0.66
1:N:262:ARG:HG2	1:N:262:ARG:HH11	1.60	0.66
1:A:320:LEU:O	1:A:323:HIS:N	2.27	0.66
1:B:204:PHE:CE2	1:B:208:LEU:HD22	2.30	0.66
1:D:170:GLY:O	1:D:355:ASN:HB2	1.96	0.66
1:D:296:LEU:O	1:D:300:LEU:HG	1.96	0.66
1:L:161:CYS:HB3	1:M:364:GLU:OE1	1.94	0.66
1:D:156:ILE:HD11	1:D:303:ILE:HG21	1.76	0.66
1:G:263:LEU:HG	1:G:264:GLY:H	1.58	0.66
1:G:315:GLU:N	1:G:315:GLU:OE1	2.27	0.66
1:H:176:VAL:HG21	1:H:307:ILE:CD1	2.23	0.66
1:H:334:LYS:HG2	1:H:335:GLU:N	2.11	0.66
1:M:149:ILE:O	1:M:153:ILE:HG12	1.95	0.66
1:M:171:VAL:HB	1:M:307:ILE:CG2	2.24	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:PHE:CZ	1:C:296:LEU:HD12	2.30	0.66
1:F:178:ARG:NH1	1:F:178:ARG:HG3	2.09	0.66
1:F:196:VAL:HG13	1:F:204:PHE:HE1	1.61	0.66
1:I:141:PHE:CE2	1:I:150:LEU:HD21	2.30	0.66
1:I:153:ILE:HD11	1:I:176:VAL:HG13	1.78	0.66
1:I:269:ILE:N	1:I:269:ILE:HD12	2.10	0.66
1:K:269:ILE:N	1:K:269:ILE:HD12	2.10	0.66
1:L:153:ILE:HD11	1:L:176:VAL:HG13	1.78	0.66
1:L:318:ILE:HD12	1:L:319:PRO:HD3	1.76	0.66
1:M:254:VAL:HG22	1:M:260:PHE:HB3	1.77	0.66
1:J:212:GLU:HG3	1:J:265:GLY:HA2	1.78	0.66
1:N:346:LEU:HD12	1:N:377:ARG:HD2	1.76	0.66
1:C:236:PHE:HA	1:C:276:LEU:O	1.95	0.66
1:E:345:GLU:O	1:E:348:LEU:HB2	1.94	0.66
1:G:252:LEU:HD22	1:G:293:ARG:HH12	1.61	0.66
1:H:215:ALA:H	1:I:223:LYS:NZ	1.94	0.66
1:K:309:PRO:O	1:K:313:ARG:HD3	1.96	0.66
1:M:352:TRP:HA	1:M:352:TRP:CE3	2.30	0.66
1:A:149:ILE:O	1:A:153:ILE:HG12	1.96	0.66
1:H:309:PRO:O	1:H:313:ARG:HG3	1.96	0.66
1:M:299:ARG:HD3	1:N:357:ARG:HH21	1.59	0.66
1:N:157:SER:HB3	1:N:184:SER:HA	1.76	0.66
1:N:259:LYS:HD2	1:N:268:GLU:HG2	1.78	0.66
1:D:235:LEU:C	1:D:235:LEU:HD12	2.16	0.65
1:E:146:MET:HE3	1:E:149:ILE:HD12	1.78	0.65
1:G:318:ILE:HG13	1:G:319:PRO:HD3	1.76	0.65
1:H:227:PHE:HE2	1:H:254:VAL:HG21	1.61	0.65
1:H:321:ALA:HA	1:H:363:ILE:HD11	1.76	0.65
1:I:318:ILE:HG13	1:I:319:PRO:CD	2.24	0.65
1:K:201:ARG:NH1	1:K:201:ARG:HB2	2.07	0.65
1:L:163:VAL:HB	1:L:276:LEU:CD2	2.26	0.65
1:L:350:TYR:HD2	1:L:352:TRP:N	1.95	0.65
1:L:352:TRP:HH2	1:L:362:VAL:HG21	1.60	0.65
1:B:204:PHE:O	1:B:206:ALA:N	2.29	0.65
1:B:330:ARG:HH11	1:B:330:ARG:HG3	1.61	0.65
1:C:150:LEU:HG	1:C:154:LYS:HZ1	1.60	0.65
1:H:328:PHE:CD1	1:H:364:GLU:HG2	2.32	0.65
1:L:283:ILE:HG22	1:L:287:VAL:HG23	1.78	0.65
1:L:314:LYS:HA	1:L:317:ILE:HG13	1.79	0.65
1:N:267:LYS:N	1:N:267:LYS:HD2	2.12	0.65
1:A:282:ASN:ND2	1:A:285:GLU:HB2	2.11	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:PRO:HG2	1:C:313:ARG:HD2	1.78	0.65
1:D:236:PHE:O	1:D:236:PHE:CG	2.48	0.65
1:E:354:GLY:C	1:E:358:GLU:HB2	2.17	0.65
1:I:143:SER:HB3	1:I:316:ASP:CG	2.15	0.65
1:K:204:PHE:CE2	1:K:208:LEU:HD12	2.29	0.65
1:M:178:ARG:HG3	1:M:178:ARG:HH11	1.61	0.65
1:N:206:ALA:HB2	1:N:216:PHE:CZ	2.31	0.65
1:A:363:ILE:O	1:A:367:VAL:HG23	1.95	0.65
1:B:143:SER:HB2	1:B:144:PRO:HD2	1.78	0.65
1:E:177:ALA:N	1:E:180:ILE:HD12	2.12	0.65
1:L:265:GLY:C	1:L:266:ARG:HG2	2.17	0.65
1:M:146:MET:HE3	1:M:149:ILE:HD12	1.78	0.65
1:M:363:ILE:CD1	1:M:363:ILE:N	2.59	0.65
1:H:270:GLU:O	1:H:271:VAL:HG23	1.95	0.65
1:I:141:PHE:HB3	1:I:150:LEU:HD11	1.77	0.65
1:K:249:ALA:CB	1:K:293:ARG:HH11	2.09	0.65
1:K:186:ARG:NH2	1:K:272:ASN:ND2	2.44	0.65
1:L:247:ALA:O	1:L:251:LEU:HB2	1.97	0.65
1:N:251:LEU:C	1:N:251:LEU:HD23	2.16	0.65
1:C:160:GLU:HA	1:C:274:ARG:NH1	2.12	0.65
1:J:352:TRP:CZ2	1:J:359:LEU:HD23	2.32	0.65
1:A:139:TYR:HD2	1:A:175:VAL:HG13	1.60	0.65
1:C:318:ILE:HG13	1:C:319:PRO:CD	2.20	0.65
1:E:176:VAL:O	1:E:180:ILE:CD1	2.45	0.65
1:E:186:ARG:HH22	1:E:272:ASN:HD21	1.42	0.65
1:F:311:ARG:HB3	1:F:351:PRO:O	1.97	0.65
1:A:244:SER:HB2	1:A:247:ALA:H	1.61	0.65
1:E:316:ASP:C	1:E:319:PRO:HD2	2.17	0.65
1:J:153:ILE:HG21	1:J:179:LEU:HD22	1.76	0.65
1:K:143:SER:CB	1:K:315:GLU:HB2	2.27	0.65
1:L:314:LYS:HA	1:L:317:ILE:CG1	2.27	0.65
1:A:145:LYS:O	1:A:149:ILE:HG13	1.96	0.65
1:E:309:PRO:CG	1:E:312:GLU:HG3	2.22	0.65
1:H:339:PHE:CD1	1:H:339:PHE:N	2.65	0.65
1:H:360:LYS:O	1:H:364:GLU:HG3	1.96	0.65
1:C:143:SER:OG	1:C:144:PRO:HD2	1.97	0.65
1:C:181:HIS:HD2	1:C:191:PHE:CB	2.09	0.65
1:D:181:HIS:HD2	1:D:234:THR:CB	2.10	0.65
1:F:206:ALA:O	1:F:210:GLY:N	2.28	0.65
1:F:326:LYS:HE2	1:F:330:ARG:HH22	1.61	0.65
1:G:310:LEU:HD12	1:G:356:VAL:H	1.61	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:196:VAL:HA	1:H:204:PHE:HE1	1.62	0.65
1:K:310:LEU:CD2	1:K:317:ILE:HG12	2.27	0.65
1:N:358:GLU:O	1:N:362:VAL:HG23	1.97	0.65
1:D:181:HIS:HD2	1:D:234:THR:HB	1.61	0.64
1:E:143:SER:O	1:E:147:LYS:HB2	1.97	0.64
1:G:209:PHE:CE1	1:G:250:LYS:HD3	2.32	0.64
1:G:340:THR:HG21	1:G:376:ASP:HB3	1.78	0.64
1:I:267:LYS:N	1:I:267:LYS:HD2	2.11	0.64
1:K:240:ILE:HG22	1:K:292:PHE:HE1	1.62	0.64
1:L:178:ARG:HH11	1:L:178:ARG:HG3	1.62	0.64
1:L:194:LEU:HD23	1:L:194:LEU:H	1.62	0.64
1:M:316:ASP:O	1:M:320:LEU:HG	1.97	0.64
1:A:259:LYS:HD3	1:A:268:GLU:OE1	1.96	0.64
1:B:283:ILE:CA	1:B:286:LEU:HD12	2.14	0.64
1:C:191:PHE:CE2	1:C:193:ALA:HB2	2.31	0.64
1:E:137:GLU:HG2	1:E:138:GLU:N	2.11	0.64
1:E:292:PHE:HZ	1:E:296:LEU:HD12	1.58	0.64
1:F:157:SER:HB3	1:F:183:LEU:C	2.17	0.64
1:G:178:ARG:HG2	1:G:191:PHE:CE1	2.33	0.64
1:A:377:ARG:HH21	1:L:285:GLU:HG2	1.62	0.64
1:A:180:ILE:O	1:A:180:ILE:HG22	1.98	0.64
1:B:260:PHE:C	1:B:260:PHE:CD1	2.68	0.64
1:D:246:GLU:H	1:D:246:GLU:CD	2.00	0.64
1:D:302:VAL:HG12	1:D:303:ILE:CD1	2.27	0.64
1:E:346:LEU:O	1:E:348:LEU:N	2.29	0.64
1:H:283:ILE:O	1:H:287:VAL:HG23	1.96	0.64
1:J:308:PRO:HG2	1:J:313:ARG:HD2	1.78	0.64
1:K:275:ILE:N	1:K:275:ILE:HD12	2.11	0.64
1:L:153:ILE:HG21	1:L:179:LEU:HD22	1.80	0.64
1:D:200:PRO:HG2	1:D:203:ILE:HB	1.79	0.64
1:E:181:HIS:HD2	1:E:234:THR:OG1	1.80	0.64
1:F:163:VAL:HG13	1:F:303:ILE:CG2	2.27	0.64
1:F:356:VAL:HG11	2:F:4:ADP:C8	2.33	0.64
1:I:168:GLU:O	1:I:171:VAL:HG23	1.97	0.64
1:L:160:GLU:C	1:L:274:ARG:HE	2.00	0.64
1:M:228:GLU:OE2	1:M:262:ARG:NH2	2.22	0.64
1:N:311:ARG:HH11	1:N:311:ARG:HG3	1.61	0.64
1:B:176:VAL:O	1:B:179:LEU:HB3	1.96	0.64
1:A:266:ARG:NH1	1:B:224:GLU:O	2.30	0.64
1:B:254:VAL:HG22	1:B:260:PHE:HB3	1.78	0.64
1:D:262:ARG:O	1:D:265:GLY:N	2.31	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:LEU:HD13	1:F:226:PHE:CD1	2.32	0.64
1:G:355:ASN:ND2	1:G:355:ASN:N	2.45	0.64
1:I:208:LEU:C	1:I:208:LEU:HD23	2.18	0.64
1:I:317:ILE:HB	1:I:348:LEU:HD23	1.80	0.64
1:J:201:ARG:HB2	1:J:201:ARG:NH1	2.06	0.64
1:M:259:LYS:HA	1:M:269:ILE:O	1.98	0.64
1:A:292:PHE:CE2	1:A:296:LEU:HD12	2.32	0.64
1:B:284:LYS:H	1:B:284:LYS:HD3	1.62	0.64
1:D:361:ASN:O	1:D:363:ILE:N	2.30	0.64
1:K:328:PHE:HB2	1:K:367:VAL:HG21	1.78	0.64
1:L:334:LYS:NZ	1:L:367:VAL:HG22	2.12	0.64
1:N:282:ASN:O	1:N:285:GLU:HB2	1.96	0.64
1:C:325:LEU:C	1:C:325:LEU:HD23	2.18	0.64
1:E:310:LEU:HD23	1:E:352:TRP:CD1	2.33	0.64
1:L:172:GLY:O	1:L:176:VAL:HG23	1.98	0.64
1:L:310:LEU:O	1:L:313:ARG:N	2.20	0.64
1:M:339:PHE:HB3	1:M:343:ALA:HB3	1.78	0.64
1:C:207:GLU:HG3	1:C:226:PHE:HE1	1.63	0.64
1:E:279:THR:OG1	1:E:280:ASN:N	2.29	0.64
1:H:162:PRO:HB2	1:H:300:LEU:HD22	1.80	0.64
1:F:326:LYS:HE2	1:F:330:ARG:HH21	1.58	0.64
1:H:293:ARG:CG	1:H:293:ARG:HH11	2.02	0.64
1:I:168:GLU:O	1:I:173:LYS:HE2	1.98	0.64
1:I:299:ARG:O	1:I:302:VAL:HG23	1.98	0.64
1:I:314:LYS:HA	1:I:317:ILE:HD11	1.79	0.64
1:J:163:VAL:HG13	1:J:303:ILE:O	1.98	0.64
1:K:303:ILE:HD11	1:L:368:LEU:HD13	1.79	0.64
1:N:245:LEU:HD23	1:N:248:GLN:NE2	2.13	0.64
1:B:236:PHE:HD1	1:B:276:LEU:O	1.80	0.63
1:B:337:GLU:OE1	1:B:373:LYS:HD3	1.98	0.63
1:J:346:LEU:HD23	1:J:346:LEU:O	1.97	0.63
1:F:335:GLU:O	1:F:373:LYS:HA	1.99	0.63
1:H:334:LYS:CG	1:H:335:GLU:N	2.62	0.63
1:I:153:ILE:HG23	1:I:180:ILE:HG12	1.79	0.63
1:L:171:VAL:HB	1:L:307:ILE:HG22	1.81	0.63
1:N:194:LEU:HD23	1:N:194:LEU:O	1.98	0.63
1:A:143:SER:HB3	1:A:316:ASP:OD1	1.98	0.63
1:J:189:GLU:HG2	1:J:232:GLY:O	1.98	0.63
1:D:284:LYS:HG2	1:D:297:TYR:CZ	2.33	0.63
1:F:337:GLU:OE1	1:F:373:LYS:HD3	1.99	0.63
1:G:280:ASN:OD1	1:G:281:ARG:HD3	1.97	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:293:ARG:HG2	1:H:293:ARG:NH1	2.01	0.63
1:H:309:PRO:HB3	1:H:311:ARG:CZ	2.28	0.63
1:L:208:LEU:HD21	1:L:227:PHE:CD1	2.33	0.63
1:M:166:THR:O	1:M:307:ILE:N	2.29	0.63
1:A:204:PHE:HE2	1:A:243:LEU:HD21	1.63	0.63
1:B:143:SER:OG	1:B:146:MET:HB2	1.97	0.63
1:C:365:ARG:HH11	1:C:383:LEU:HD22	1.63	0.63
1:D:163:VAL:HB	1:D:276:LEU:HD22	1.80	0.63
1:D:365:ARG:HD2	1:D:383:LEU:CD2	2.29	0.63
1:E:259:LYS:HG2	1:E:270:GLU:HB2	1.81	0.63
1:F:196:VAL:HG13	1:F:204:PHE:CE1	2.34	0.63
1:K:157:SER:HB3	1:K:183:LEU:O	1.98	0.63
1:M:181:HIS:HD2	1:M:234:THR:HB	1.64	0.63
1:N:282:ASN:HD21	1:N:284:LYS:HB2	1.62	0.63
1:A:165:ILE:O	1:A:278:ALA:HA	1.99	0.63
1:A:377:ARG:HH21	1:L:285:GLU:CG	2.11	0.63
1:B:204:PHE:O	1:B:205:GLU:C	2.37	0.63
1:B:250:LYS:HG3	1:C:198:SER:HB2	1.81	0.63
1:B:324:PHE:CD1	1:B:363:ILE:HD12	2.29	0.63
1:E:176:VAL:HG21	1:E:307:ILE:CD1	2.27	0.63
1:F:170:GLY:O	1:F:172:GLY:N	2.32	0.63
1:K:303:ILE:HG22	1:K:303:ILE:O	1.98	0.63
1:L:165:ILE:N	1:L:278:ALA:HB2	2.13	0.63
1:N:251:LEU:O	1:N:251:LEU:HD23	1.98	0.63
1:F:313:ARG:O	1:F:315:GLU:N	2.32	0.63
1:I:211:TYR:CE1	1:I:223:LYS:HB2	2.33	0.63
1:K:201:ARG:HH11	1:K:201:ARG:CB	2.09	0.63
1:B:237:LEU:HB2	1:B:240:ILE:HD11	1.79	0.63
1:B:264:GLY:HA2	1:C:207:GLU:OE2	1.98	0.63
1:C:275:ILE:N	1:C:275:ILE:HD12	2.13	0.63
1:F:343:ALA:HB2	1:F:376:ASP:HA	1.79	0.63
1:G:320:LEU:HD23	1:G:320:LEU:C	2.20	0.63
1:K:161:CYS:O	1:K:274:ARG:NH1	2.32	0.63
1:K:279:THR:HG21	1:K:283:ILE:CD1	2.27	0.63
1:M:354:GLY:O	1:M:357:ARG:HB3	1.99	0.63
1:A:144:PRO:HG2	1:A:145:LYS:H	1.63	0.63
1:D:161:CYS:HB2	1:D:162:PRO:HD2	1.81	0.63
1:E:269:ILE:N	1:E:269:ILE:HD12	2.13	0.63
1:I:367:VAL:HG12	1:I:367:VAL:O	1.98	0.63
1:L:336:VAL:HG21	1:L:370:SER:OG	1.99	0.63
1:N:311:ARG:O	1:N:312:GLU:HG2	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:HH21	1:A:302:VAL:HG21	1.63	0.62
1:E:173:LYS:HB2	1:E:173:LYS:NZ	2.14	0.62
1:F:309:PRO:CG	1:F:311:ARG:NH1	2.60	0.62
1:L:200:PRO:HG2	1:L:203:ILE:HD12	1.81	0.62
1:M:243:LEU:HD22	1:M:247:ALA:CB	2.26	0.62
1:M:357:ARG:O	1:M:361:ASN:HB2	2.00	0.62
1:C:160:GLU:OE2	1:C:186:ARG:NH2	2.32	0.62
1:E:344:GLN:O	1:E:348:LEU:CD1	2.36	0.62
1:H:216:PHE:O	1:H:218:GLY:N	2.26	0.62
1:J:262:ARG:HG2	1:J:262:ARG:HH11	1.64	0.62
1:K:266:ARG:NH1	1:L:224:GLU:O	2.32	0.62
1:M:186:ARG:HD3	1:M:233:GLY:HA2	1.80	0.62
1:M:281:ARG:CG	1:M:286:LEU:HD21	2.29	0.62
1:N:234:THR:HG23	1:N:274:ARG:O	1.99	0.62
1:A:234:THR:HG23	1:A:274:ARG:O	1.99	0.62
1:B:207:GLU:O	1:B:225:GLY:HA2	1.99	0.62
1:B:217:THR:HG23	1:B:218:GLY:N	2.10	0.62
1:C:347:LEU:HD21	1:C:380:LEU:CD1	2.28	0.62
1:E:156:ILE:CD1	1:F:368:LEU:HD13	2.30	0.62
1:I:314:LYS:HA	1:I:317:ILE:CG1	2.29	0.62
1:K:310:LEU:HD22	1:K:317:ILE:HG12	1.80	0.62
1:L:248:GLN:NE2	1:L:292:PHE:HA	2.15	0.62
1:L:350:TYR:CD2	1:L:352:TRP:N	2.66	0.62
1:N:282:ASN:HD22	1:N:285:GLU:CG	2.08	0.62
1:A:157:SER:HB3	1:A:184:SER:HA	1.81	0.62
1:E:196:VAL:HG11	1:E:243:LEU:HD23	1.82	0.62
1:F:365:ARG:HG2	1:F:369:PHE:CE2	2.34	0.62
1:H:142:GLU:HB3	1:H:146:MET:HB2	1.81	0.62
1:J:302:VAL:O	1:J:303:ILE:HD13	2.00	0.62
1:C:228:GLU:O	1:C:231:ASP:HB2	1.99	0.62
1:L:240:ILE:HD13	1:L:300:LEU:CD1	2.30	0.62
1:M:253:ARG:HH21	1:M:259:LYS:HE3	1.63	0.62
1:N:251:LEU:CD2	1:N:296:LEU:HD21	2.29	0.62
1:D:156:ILE:CD1	1:D:303:ILE:HG21	2.29	0.62
1:D:275:ILE:H	1:D:275:ILE:CD1	2.00	0.62
1:I:189:GLU:HA	1:I:189:GLU:OE1	1.99	0.62
1:J:341:LYS:O	1:J:345:GLU:HG3	1.99	0.62
1:M:146:MET:CE	1:M:146:MET:HA	2.29	0.62
1:N:181:HIS:CD2	1:N:234:THR:HB	2.35	0.62
1:B:250:LYS:O	1:B:253:ARG:HG2	2.00	0.62
1:F:316:ASP:C	1:F:319:PRO:HD2	2.19	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:240:ILE:CG1	1:G:277:ALA:HB1	2.25	0.62
1:I:171:VAL:HG11	1:I:307:ILE:O	1.99	0.62
1:D:352:TRP:O	1:D:355:ASN:N	2.33	0.62
1:E:201:ARG:CB	1:E:201:ARG:HH11	2.11	0.62
1:B:194:LEU:H	1:B:194:LEU:HD23	1.64	0.62
1:C:178:ARG:CG	1:C:178:ARG:NH1	2.53	0.62
1:E:189:GLU:HG2	1:E:232:GLY:O	1.99	0.62
1:E:238:ASP:O	1:E:239:GLU:HG2	1.99	0.62
1:K:316:ASP:O	1:K:319:PRO:HD2	1.99	0.62
1:A:174:GLU:HG3	1:A:236:PHE:HE2	1.65	0.61
1:A:316:ASP:C	1:A:319:PRO:HD2	2.20	0.61
1:B:251:LEU:HD22	1:B:255:ILE:HD11	1.82	0.61
1:F:326:LYS:O	1:F:329:SER:HB3	2.00	0.61
1:H:309:PRO:HB2	1:H:311:ARG:HD2	1.82	0.61
1:I:171:VAL:HG12	1:I:307:ILE:CG2	2.30	0.61
1:J:157:SER:HB3	1:J:183:LEU:C	2.19	0.61
1:L:266:ARG:NH2	1:M:207:GLU:OE2	2.33	0.61
1:M:157:SER:C	1:M:159:ALA:H	2.03	0.61
1:A:316:ASP:O	1:A:319:PRO:HD2	2.00	0.61
1:D:143:SER:CB	1:D:144:PRO:HD2	2.30	0.61
1:E:352:TRP:HE3	1:E:358:GLU:HG2	1.65	0.61
1:F:172:GLY:HA2	2:F:4:ADP:O3A	1.99	0.61
1:G:320:LEU:HD21	1:G:324:PHE:CE1	2.36	0.61
1:A:240:ILE:HG12	1:A:278:ALA:O	2.01	0.61
1:A:323:HIS:O	1:A:326:LYS:HB3	2.00	0.61
1:C:266:ARG:NE	1:D:203:ILE:HD12	2.15	0.61
1:D:236:PHE:C	1:D:236:PHE:CD1	2.74	0.61
1:D:296:LEU:CD1	1:D:300:LEU:HD11	2.30	0.61
1:G:169:SER:O	1:G:355:ASN:ND2	2.32	0.61
1:H:168:GLU:HG3	1:H:311:ARG:NH2	2.15	0.61
1:K:275:ILE:H	1:K:275:ILE:HD12	1.63	0.61
1:K:163:VAL:HB	1:K:276:LEU:HD22	1.82	0.61
1:K:340:THR:HG21	1:K:376:ASP:HB3	1.82	0.61
1:E:236:PHE:CE1	1:E:278:ALA:CB	2.83	0.61
1:H:236:PHE:HD1	1:H:276:LEU:O	1.83	0.61
1:I:157:SER:HB2	1:I:184:SER:HA	1.82	0.61
1:I:259:LYS:HD3	1:I:268:GLU:OE1	2.00	0.61
1:K:340:THR:O	1:K:344:GLN:HG3	2.00	0.61
1:N:322:ASN:O	1:N:326:LYS:HB2	2.00	0.61
1:A:318:ILE:CG1	1:A:348:LEU:HD21	2.25	0.61
1:D:318:ILE:CG1	1:D:319:PRO:HD3	2.19	0.61

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:266:ARG:HA	1:E:266:ARG:HE	1.66	0.61
1:L:195:ASN:O	1:L:197:ALA:N	2.33	0.61
1:M:140:VAL:HB	1:M:320:LEU:CD2	2.30	0.61
1:A:194:LEU:H	1:A:194:LEU:HD23	1.64	0.61
1:C:139:TYR:HB2	1:C:141:PHE:CE1	2.36	0.61
1:E:216:PHE:H	1:E:216:PHE:HD2	1.47	0.61
1:E:155:LYS:HD3	1:F:369:PHE:HA	1.83	0.61
1:G:340:THR:C	1:G:342:SER:N	2.54	0.61
1:I:358:GLU:O	1:I:362:VAL:HG23	2.00	0.61
1:K:163:VAL:HB	1:K:276:LEU:CD2	2.31	0.61
1:M:248:GLN:HG3	1:M:293:ARG:HB2	1.81	0.61
1:N:200:PRO:HB2	1:N:202:ASP:OD1	2.01	0.61
1:N:303:ILE:O	1:N:305:ILE:HG13	2.01	0.61
1:B:325:LEU:HD21	1:B:336:VAL:CG1	2.31	0.61
1:D:178:ARG:HH11	1:D:178:ARG:HG3	1.66	0.61
1:F:223:LYS:C	1:F:225:GLY:H	2.03	0.61
1:F:269:ILE:HD12	1:F:269:ILE:H	1.66	0.61
1:F:314:LYS:O	1:F:317:ILE:HG13	2.00	0.61
1:L:152:LYS:O	1:L:155:LYS:N	2.30	0.61
1:L:322:ASN:O	1:L:325:LEU:N	2.33	0.61
1:N:274:ARG:HH11	1:N:274:ARG:HG2	1.64	0.61
1:C:172:GLY:HA2	2:C:1:ADP:O1A	2.00	0.61
1:C:266:ARG:HH21	1:D:203:ILE:HD11	1.66	0.61
1:E:316:ASP:O	1:E:319:PRO:CD	2.47	0.61
1:G:164:LEU:HD12	1:G:165:ILE:N	2.16	0.61
1:G:261:TYR:N	1:G:261:TYR:CD1	2.68	0.61
1:G:294:GLU:O	1:G:297:TYR:HB3	2.00	0.61
1:N:383:LEU:O	1:N:384:VAL:HG23	2.01	0.61
1:A:282:ASN:HD22	1:A:285:GLU:HB2	1.66	0.61
1:A:324:PHE:CE2	1:A:360:LYS:HG3	2.36	0.61
1:C:156:ILE:HD13	1:C:303:ILE:HG21	1.81	0.61
1:G:252:LEU:HD13	1:G:296:LEU:HA	1.83	0.61
1:G:263:LEU:HD23	1:G:264:GLY:N	2.16	0.61
1:F:284:LYS:HE2	1:F:297:TYR:OH	2.00	0.61
1:I:181:HIS:CE1	1:I:191:PHE:HB2	2.36	0.61
1:J:216:PHE:CD2	1:J:216:PHE:N	2.63	0.61
1:L:146:MET:CE	1:L:313:ARG:HE	2.13	0.61
1:L:143:SER:HB3	1:L:316:ASP:OD2	2.01	0.61
1:L:334:LYS:CE	1:L:336:VAL:HB	2.29	0.61
1:H:215:ALA:HB2	1:I:223:LYS:HZ3	1.64	0.60
1:H:323:HIS:O	1:H:327:LYS:HB2	2.00	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:204:PHE:O	1:I:207:GLU:N	2.32	0.60
1:I:159:ALA:HB1	1:J:332:TYR:OH	2.01	0.60
1:K:181:HIS:HD2	1:K:234:THR:OG1	1.84	0.60
1:K:316:ASP:O	1:K:320:LEU:HG	2.01	0.60
1:K:340:THR:CG2	1:K:376:ASP:HB3	2.31	0.60
1:L:365:ARG:HG3	1:L:369:PHE:HE2	1.66	0.60
1:N:178:ARG:HG3	1:N:178:ARG:HH11	1.65	0.60
1:F:209:PHE:HE2	1:F:254:VAL:HG21	1.67	0.60
1:G:318:ILE:O	1:G:321:ALA:HB3	2.00	0.60
1:I:204:PHE:CE2	1:I:208:LEU:HD12	2.36	0.60
1:K:302:VAL:HG12	1:K:302:VAL:O	2.01	0.60
1:M:195:ASN:HB3	1:M:198:SER:OG	2.01	0.60
1:D:314:LYS:HA	1:D:317:ILE:HG13	1.83	0.60
1:D:324:PHE:CD1	1:D:359:LEU:HD22	2.36	0.60
1:E:195:ASN:O	1:E:197:ALA:N	2.33	0.60
1:H:234:THR:CG2	1:H:276:LEU:HD12	2.29	0.60
1:I:203:ILE:O	1:I:206:ALA:HB3	2.01	0.60
1:B:314:LYS:HD2	1:B:314:LYS:N	2.12	0.60
1:C:163:VAL:HB	1:C:276:LEU:CD2	2.31	0.60
1:C:303:ILE:HD13	1:D:365:ARG:HG3	1.84	0.60
1:D:189:GLU:CG	1:D:190:PRO:HD2	2.30	0.60
1:I:171:VAL:HG12	1:I:307:ILE:HG22	1.81	0.60
1:J:313:ARG:HB3	1:J:316:ASP:OD2	2.02	0.60
1:J:365:ARG:CD	1:J:383:LEU:HD22	2.30	0.60
1:B:235:LEU:HG	1:B:237:LEU:HD21	1.82	0.60
1:B:256:GLU:OE2	1:C:357:ARG:HD3	2.01	0.60
1:B:328:PHE:HB2	1:B:367:VAL:HG21	1.83	0.60
1:C:311:ARG:HH21	1:C:353:TYR:HD2	1.46	0.60
1:J:262:ARG:HG2	1:J:262:ARG:NH1	2.16	0.60
1:K:302:VAL:CG2	1:L:361:ASN:HB3	2.31	0.60
1:L:314:LYS:O	1:L:317:ILE:HG13	2.01	0.60
1:L:140:VAL:HG21	1:L:320:LEU:HD23	1.84	0.60
1:M:252:LEU:HD11	1:M:299:ARG:HG3	1.83	0.60
1:B:142:GLU:HG3	1:B:142:GLU:O	2.01	0.60
1:E:189:GLU:CG	1:E:232:GLY:O	2.49	0.60
1:F:201:ARG:CB	1:F:201:ARG:HH11	2.11	0.60
1:F:213:LYS:HB3	1:G:220:VAL:HG11	1.82	0.60
1:F:229:LEU:HD13	1:F:229:LEU:O	2.02	0.60
1:G:310:LEU:HB2	1:G:355:ASN:HB2	1.83	0.60
1:K:176:VAL:HG21	1:K:307:ILE:HD11	1.84	0.60
1:K:248:GLN:O	1:K:250:LYS:N	2.35	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:GLU:HG3	1:C:226:PHE:CE1	2.36	0.60
1:C:194:LEU:CD2	1:C:235:LEU:HD11	2.32	0.60
1:G:263:LEU:CG	1:G:264:GLY:N	2.64	0.60
1:H:176:VAL:CG2	1:H:307:ILE:HD11	2.30	0.60
1:H:334:LYS:HE3	1:H:336:VAL:O	2.00	0.60
1:L:138:GLU:O	1:L:139:TYR:CG	2.54	0.60
1:L:329:SER:CB	1:L:334:LYS:HE2	2.30	0.60
1:N:283:ILE:HG23	1:N:292:PHE:CD1	2.37	0.60
1:A:339:PHE:CD1	1:A:339:PHE:N	2.68	0.60
1:B:269:ILE:CG2	1:B:270:GLU:N	2.64	0.60
1:C:172:GLY:HA2	2:C:1:ADP:PA	2.41	0.60
1:E:168:GLU:HB2	1:E:171:VAL:CG1	2.32	0.60
1:F:350:TYR:HD2	1:F:352:TRP:CD2	2.19	0.60
1:N:282:ASN:ND2	1:N:285:GLU:HG2	2.09	0.60
1:A:237:LEU:HB2	1:A:240:ILE:HD13	1.84	0.60
1:E:239:GLU:HA	1:E:279:THR:HA	1.83	0.60
1:E:346:LEU:C	1:E:348:LEU:N	2.54	0.60
1:F:309:PRO:HA	1:F:355:ASN:ND2	2.17	0.60
1:K:322:ASN:O	1:K:326:LYS:HB2	2.02	0.60
1:M:339:PHE:HA	1:M:375:ILE:O	2.02	0.60
1:N:339:PHE:CD2	1:N:347:LEU:HD11	2.37	0.60
1:A:220:VAL:O	1:A:221:SER:HB3	2.02	0.60
1:G:252:LEU:HD11	1:G:299:ARG:HG3	1.83	0.60
1:K:316:ASP:C	1:K:319:PRO:HD2	2.22	0.60
1:L:347:LEU:HD21	1:L:380:LEU:HD11	1.84	0.60
1:N:194:LEU:H	1:N:194:LEU:CD2	2.15	0.60
1:N:313:ARG:O	1:N:315:GLU:N	2.35	0.60
1:N:357:ARG:NH1	1:N:361:ASN:OD1	2.35	0.60
1:B:224:GLU:HG2	1:B:228:GLU:HB2	1.83	0.59
1:F:164:LEU:HD12	1:F:277:ALA:O	2.02	0.59
1:F:341:LYS:O	1:F:345:GLU:HG3	2.02	0.59
1:I:194:LEU:CD2	1:I:235:LEU:HD11	2.31	0.59
1:I:249:ALA:HB2	1:I:293:ARG:NH1	2.17	0.59
1:M:228:GLU:CD	1:M:262:ARG:HH21	2.05	0.59
1:M:164:LEU:CD2	1:M:283:ILE:HG13	2.31	0.59
1:C:318:ILE:O	1:C:321:ALA:HB3	2.02	0.59
1:D:283:ILE:HD12	1:D:292:PHE:CE1	2.37	0.59
1:D:341:LYS:HD2	1:D:345:GLU:OE2	2.01	0.59
1:G:163:VAL:HB	1:G:276:LEU:CD2	2.32	0.59
1:G:341:LYS:O	1:G:345:GLU:HG3	2.01	0.59
1:H:288:LYS:C	1:H:290:GLY:H	2.05	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:318:ILE:CG1	1:I:319:PRO:HD3	2.28	0.59
1:K:325:LEU:HD21	1:K:336:VAL:HG12	1.83	0.59
1:L:252:LEU:HD11	1:L:256:GLU:OE1	2.01	0.59
1:L:240:ILE:HD13	1:L:300:LEU:HD13	1.84	0.59
1:N:316:ASP:C	1:N:319:PRO:HD2	2.23	0.59
1:A:328:PHE:HA	1:A:331:LYS:HB3	1.83	0.59
1:B:150:LEU:HD11	1:B:154:LYS:HZ2	1.67	0.59
1:G:146:MET:CE	1:G:149:ILE:HD12	2.31	0.59
1:G:210:GLY:HA2	1:G:224:GLU:O	2.02	0.59
1:G:249:ALA:HA	1:G:293:ARG:NH1	2.16	0.59
1:J:352:TRP:CZ3	1:J:358:GLU:HG2	2.37	0.59
1:K:165:ILE:HG22	1:K:165:ILE:O	2.01	0.59
1:L:343:ALA:O	1:L:344:GLN:C	2.40	0.59
1:M:140:VAL:O	1:M:141:PHE:HD1	1.85	0.59
1:M:145:LYS:O	1:M:148:GLU:HB3	2.02	0.59
1:C:173:LYS:H	2:C:1:ADP:PB	2.25	0.59
1:C:322:ASN:O	1:C:325:LEU:N	2.35	0.59
1:C:365:ARG:O	1:C:368:LEU:HB2	2.02	0.59
1:D:227:PHE:CD2	1:D:273:VAL:HG21	2.36	0.59
1:E:283:ILE:O	1:E:287:VAL:HG23	2.01	0.59
1:E:171:VAL:O	1:E:307:ILE:HG21	2.02	0.59
1:E:325:LEU:HD21	1:E:336:VAL:CG1	2.29	0.59
1:H:248:GLN:O	1:H:249:ALA:C	2.37	0.59
1:L:209:PHE:HE2	1:L:254:VAL:HG21	1.67	0.59
1:L:342:SER:OG	1:L:376:ASP:HB2	2.02	0.59
1:N:139:TYR:HB3	1:N:141:PHE:HE1	1.67	0.59
1:N:267:LYS:O	1:N:269:ILE:N	2.35	0.59
1:N:335:GLU:O	1:N:373:LYS:HA	2.01	0.59
1:D:252:LEU:O	1:D:255:ILE:HG13	2.01	0.59
1:F:346:LEU:HG	1:F:377:ARG:NH1	2.17	0.59
1:H:145:LYS:HB2	1:H:313:ARG:NH2	2.17	0.59
1:I:310:LEU:HD22	1:I:317:ILE:HG12	1.83	0.59
1:N:320:LEU:O	1:N:323:HIS:N	2.35	0.59
1:A:191:PHE:CE2	1:A:193:ALA:HB2	2.36	0.59
1:B:210:GLY:C	1:B:262:ARG:HG3	2.23	0.59
1:D:281:ARG:HH11	1:D:281:ARG:HG2	1.66	0.59
1:E:176:VAL:O	1:E:180:ILE:HD12	2.03	0.59
1:E:176:VAL:CG1	1:E:180:ILE:HD11	2.21	0.59
1:G:325:LEU:C	1:G:325:LEU:HD23	2.22	0.59
1:K:141:PHE:CE1	1:K:150:LEU:HD13	2.38	0.59
1:B:330:ARG:NH1	1:B:330:ARG:HG3	2.17	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:TYR:CD2	1:E:179:LEU:HD11	2.37	0.59
1:H:266:ARG:HB3	1:I:229:LEU:HD23	1.84	0.59
1:I:302:VAL:HG12	1:I:303:ILE:HG12	1.83	0.59
1:M:353:TYR:C	1:M:355:ASN:H	2.05	0.59
1:N:178:ARG:NE	1:N:191:PHE:CE2	2.70	0.59
1:D:275:ILE:HD12	1:D:275:ILE:N	2.04	0.59
1:F:318:ILE:HG13	1:F:319:PRO:CD	2.16	0.59
1:H:194:LEU:N	1:H:194:LEU:HD23	2.15	0.59
1:I:146:MET:SD	1:I:313:ARG:CZ	2.91	0.59
1:K:143:SER:O	1:K:147:LYS:HB2	2.02	0.59
1:L:337:GLU:OE1	1:L:373:LYS:HD3	2.01	0.59
1:A:296:LEU:C	1:A:296:LEU:HD13	2.23	0.59
1:E:347:LEU:HD21	1:E:380:LEU:HD13	1.84	0.59
1:H:339:PHE:H	1:H:339:PHE:HD1	1.51	0.59
1:I:318:ILE:O	1:I:321:ALA:HB3	2.02	0.59
1:A:164:LEU:HD12	1:A:165:ILE:N	2.16	0.59
1:C:163:VAL:HB	1:C:276:LEU:HD23	1.85	0.59
1:D:252:LEU:HA	1:D:255:ILE:CD1	2.33	0.59
1:J:269:ILE:HD12	1:J:269:ILE:H	1.68	0.59
1:M:161:CYS:HB2	1:M:302:VAL:HG11	1.83	0.59
1:M:191:PHE:C	1:M:191:PHE:CD2	2.77	0.59
1:B:317:ILE:CB	1:B:348:LEU:HD23	2.32	0.58
1:B:359:LEU:C	1:B:361:ASN:H	2.06	0.58
1:C:336:VAL:HG21	1:C:370:SER:CB	2.33	0.58
1:H:214:GLY:N	1:H:219:ALA:CB	2.55	0.58
1:J:239:GLU:N	1:J:278:ALA:O	2.35	0.58
1:L:315:GLU:O	1:L:319:PRO:HG2	2.03	0.58
1:L:343:ALA:O	1:L:346:LEU:N	2.36	0.58
1:N:325:LEU:HD12	1:N:339:PHE:CE1	2.38	0.58
1:A:194:LEU:HD21	1:A:237:LEU:HD22	1.86	0.58
1:E:166:THR:HG22	1:E:167:GLY:N	2.18	0.58
1:E:209:PHE:HD1	1:E:209:PHE:H	1.51	0.58
1:F:341:LYS:HA	1:F:344:GLN:HB2	1.84	0.58
1:G:320:LEU:CD2	1:G:359:LEU:HD13	2.22	0.58
1:I:208:LEU:CD2	1:I:227:PHE:HD1	2.16	0.58
1:J:157:SER:HB3	1:J:184:SER:N	2.18	0.58
1:L:145:LYS:O	1:L:148:GLU:HB3	2.03	0.58
1:L:213:LYS:O	1:L:219:ALA:HB1	2.03	0.58
1:A:172:GLY:O	1:A:173:LYS:C	2.40	0.58
1:B:171:VAL:HG21	1:B:307:ILE:HB	1.84	0.58
1:C:249:ALA:O	1:C:252:LEU:HB3	2.02	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:ARG:HG3	1:E:253:ARG:HH11	1.68	0.58
1:E:170:GLY:O	1:E:356:VAL:HG23	2.03	0.58
1:F:252:LEU:HD13	1:F:296:LEU:HA	1.84	0.58
1:F:359:LEU:O	1:F:361:ASN:N	2.35	0.58
1:N:192:VAL:CG2	1:N:230:ALA:HB2	2.34	0.58
1:B:208:LEU:CD2	1:B:209:PHE:HE1	2.16	0.58
1:B:292:PHE:CE2	1:B:296:LEU:HD12	2.37	0.58
1:D:266:ARG:HH22	1:E:207:GLU:CG	2.16	0.58
1:E:342:SER:OG	1:E:377:ARG:HB2	2.04	0.58
1:F:170:GLY:C	1:F:172:GLY:H	2.06	0.58
1:M:248:GLN:O	1:M:252:LEU:N	2.31	0.58
1:M:266:ARG:HH21	1:M:267:LYS:NZ	2.01	0.58
1:D:324:PHE:HD1	1:D:359:LEU:HD22	1.68	0.58
1:E:365:ARG:HD2	1:E:383:LEU:HD13	1.85	0.58
1:H:350:TYR:HB3	1:H:351:PRO:CA	2.33	0.58
1:J:352:TRP:CE3	1:J:358:GLU:HG2	2.39	0.58
1:K:215:ALA:H	1:K:219:ALA:HB1	1.66	0.58
1:M:164:LEU:HD21	1:M:283:ILE:CG1	2.31	0.58
1:A:143:SER:CB	1:A:144:PRO:HD2	2.32	0.58
1:B:318:ILE:HD13	1:B:348:LEU:HD11	1.84	0.58
1:I:189:GLU:HB3	1:I:190:PRO:CD	2.27	0.58
1:K:216:PHE:H	1:K:219:ALA:CB	2.17	0.58
1:K:314:LYS:HA	1:K:317:ILE:CD1	2.34	0.58
1:L:146:MET:SD	1:L:313:ARG:NE	2.77	0.58
1:L:240:ILE:HB	1:L:279:THR:CG2	2.33	0.58
1:L:315:GLU:H	1:L:315:GLU:CD	2.06	0.58
1:A:365:ARG:HD2	1:A:383:LEU:CD1	2.34	0.58
1:B:156:ILE:O	1:B:158:CYS:N	2.36	0.58
1:C:328:PHE:CE1	1:C:364:GLU:HB2	2.38	0.58
1:D:181:HIS:CD2	1:D:234:THR:OG1	2.57	0.58
1:D:301:GLY:O	1:D:302:VAL:C	2.41	0.58
1:G:242:GLU:HG2	1:G:281:ARG:NH2	2.19	0.58
1:K:237:LEU:HB2	1:K:240:ILE:HD11	1.85	0.58
1:N:186:ARG:HD3	1:N:232:GLY:O	2.04	0.58
1:E:259:LYS:HE2	1:E:270:GLU:OE2	2.03	0.58
1:E:354:GLY:C	1:E:358:GLU:CB	2.72	0.58
1:F:149:ILE:CD1	1:F:307:ILE:HD13	2.32	0.58
1:G:231:ASP:HA	1:G:273:VAL:HG22	1.85	0.58
1:H:311:ARG:O	1:H:314:LYS:HE2	2.03	0.58
1:I:350:TYR:CG	1:I:351:PRO:HD2	2.39	0.58
1:I:355:ASN:O	1:I:358:GLU:N	2.27	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:PRO:HG3	1:J:203:ILE:HD12	1.86	0.58
1:K:314:LYS:HA	1:K:317:ILE:CG1	2.33	0.58
1:L:156:ILE:O	1:L:158:CYS:N	2.36	0.58
1:L:208:LEU:HD22	1:L:209:PHE:CD1	2.39	0.58
1:M:350:TYR:CD1	1:M:351:PRO:HD2	2.39	0.58
1:D:325:LEU:HD23	1:D:325:LEU:C	2.23	0.58
1:H:332:TYR:O	1:H:333:ALA:HB3	2.02	0.58
1:J:167:GLY:O	1:J:280:ASN:HA	2.04	0.58
1:M:140:VAL:C	1:M:141:PHE:HD1	2.07	0.58
1:M:172:GLY:O	1:M:176:VAL:HG23	2.04	0.58
1:M:352:TRP:HA	1:M:352:TRP:HE3	1.69	0.58
1:M:324:PHE:CD1	1:M:359:LEU:HD23	2.38	0.58
1:N:146:MET:HE3	1:N:307:ILE:CG2	2.33	0.58
1:E:335:GLU:O	1:E:335:GLU:HG3	2.04	0.58
1:K:265:GLY:O	1:K:266:ARG:NE	2.36	0.58
1:N:211:TYR:OH	1:N:223:LYS:HG3	2.04	0.58
1:B:142:GLU:HG2	1:B:319:PRO:HG2	1.85	0.57
1:C:244:SER:O	1:C:247:ALA:HB3	2.04	0.57
1:D:157:SER:C	1:D:159:ALA:H	2.07	0.57
1:E:214:GLY:CA	1:E:219:ALA:HB3	2.29	0.57
1:F:194:LEU:HD13	1:F:226:PHE:HD1	1.67	0.57
1:G:211:TYR:HE1	1:G:263:LEU:HD13	1.69	0.57
1:G:318:ILE:CG1	1:G:319:PRO:HD3	2.34	0.57
1:J:211:TYR:CE2	1:J:223:LYS:HB3	2.39	0.57
1:K:349:SER:OG	1:K:350:TYR:N	2.36	0.57
1:D:296:LEU:HD11	1:D:300:LEU:HD11	1.86	0.57
1:M:246:GLU:H	1:M:246:GLU:CD	2.07	0.57
1:D:351:PRO:HB2	1:D:353:TYR:CE2	2.39	0.57
1:E:294:GLU:OE2	1:F:169:SER:HB3	2.05	0.57
1:F:160:GLU:OE2	1:F:186:ARG:NH2	2.37	0.57
1:F:275:ILE:N	1:F:275:ILE:HD12	2.19	0.57
1:G:211:TYR:CE1	1:G:263:LEU:HD13	2.39	0.57
1:G:279:THR:HG21	1:G:283:ILE:HD11	1.86	0.57
1:I:196:VAL:HG13	1:I:204:PHE:CE1	2.39	0.57
1:L:376:ASP:C	1:L:378:GLY:N	2.58	0.57
1:M:340:THR:OG1	1:M:376:ASP:HA	2.04	0.57
1:N:227:PHE:O	1:N:228:GLU:C	2.42	0.57
1:N:314:LYS:NZ	1:N:314:LYS:HB2	2.19	0.57
1:A:158:CYS:HA	1:A:185:ASP:OD2	2.04	0.57
1:A:275:ILE:CD1	1:A:275:ILE:H	2.15	0.57
1:B:230:ALA:O	1:B:273:VAL:HG22	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ARG:NH2	1:C:207:GLU:OE2	2.34	0.57
1:H:140:VAL:HG12	1:H:141:PHE:N	2.19	0.57
1:H:334:LYS:CG	1:H:335:GLU:H	2.18	0.57
1:K:192:VAL:HB	1:K:230:ALA:HB2	1.87	0.57
1:L:334:LYS:NZ	1:L:367:VAL:CG2	2.67	0.57
1:M:314:LYS:HA	1:M:317:ILE:HD11	1.86	0.57
1:M:336:VAL:HG11	1:M:375:ILE:HG13	1.86	0.57
1:A:194:LEU:HD21	1:A:237:LEU:CD2	2.34	0.57
1:C:251:LEU:CD2	1:C:255:ILE:HD11	2.32	0.57
1:G:282:ASN:ND2	1:G:285:GLU:HB2	2.20	0.57
1:G:355:ASN:O	1:G:357:ARG:N	2.35	0.57
1:K:194:LEU:HD22	1:K:226:PHE:CD1	2.38	0.57
1:M:206:ALA:HB2	1:M:216:PHE:CZ	2.39	0.57
1:N:201:ARG:HH11	1:N:201:ARG:CB	2.11	0.57
1:E:176:VAL:O	1:E:180:ILE:HG13	2.04	0.57
1:E:324:PHE:O	1:E:326:LYS:N	2.38	0.57
1:F:145:LYS:O	1:F:148:GLU:HB3	2.05	0.57
1:F:343:ALA:C	1:F:345:GLU:N	2.58	0.57
1:F:359:LEU:O	1:F:362:VAL:N	2.38	0.57
1:H:324:PHE:HB2	1:H:363:ILE:HG21	1.86	0.57
1:I:340:THR:OG1	1:I:376:ASP:HB3	2.04	0.57
1:J:224:GLU:HG2	1:J:225:GLY:N	2.10	0.57
1:H:146:MET:CG	1:H:313:ARG:CZ	2.82	0.57
1:H:161:CYS:SG	1:H:303:ILE:CD1	2.93	0.57
1:H:235:LEU:HD23	1:H:236:PHE:N	2.19	0.57
1:H:161:CYS:SG	1:H:303:ILE:HD12	2.45	0.57
1:J:201:ARG:NH2	1:J:242:GLU:O	2.38	0.57
1:B:315:GLU:N	1:B:315:GLU:OE1	2.35	0.57
1:B:321:ALA:HB1	1:B:339:PHE:CZ	2.40	0.57
1:F:143:SER:HB2	1:F:144:PRO:CD	2.33	0.57
1:F:365:ARG:HD2	1:F:383:LEU:CD2	2.35	0.57
1:H:363:ILE:O	1:H:367:VAL:HG23	2.04	0.57
1:J:181:HIS:CD2	1:J:191:PHE:HD1	2.23	0.57
1:N:146:MET:HE2	1:N:149:ILE:HD12	1.86	0.57
1:N:194:LEU:H	1:N:194:LEU:HD23	1.70	0.57
1:C:310:LEU:HD22	1:C:317:ILE:HG12	1.86	0.57
1:D:181:HIS:HD2	1:D:234:THR:OG1	1.88	0.57
1:E:203:ILE:O	1:E:203:ILE:HG22	2.05	0.57
1:E:355:ASN:ND2	1:E:355:ASN:N	2.53	0.57
1:F:157:SER:O	1:F:184:SER:HA	2.05	0.57
1:I:263:LEU:C	1:I:263:LEU:HD23	2.25	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:352:TRP:CH2	1:J:359:LEU:HD23	2.39	0.57
1:L:138:GLU:O	1:L:139:TYR:CD1	2.58	0.57
1:L:218:GLY:O	1:L:220:VAL:HG23	2.05	0.57
1:L:237:LEU:HB2	1:L:277:ALA:HB2	1.86	0.57
1:N:174:GLU:O	1:N:177:ALA:N	2.38	0.57
1:B:359:LEU:O	1:B:361:ASN:N	2.38	0.57
1:C:299:ARG:HG2	1:C:299:ARG:HH11	1.70	0.57
1:C:347:LEU:HD21	1:C:380:LEU:HD11	1.87	0.57
1:E:211:TYR:HD1	1:E:223:LYS:HE2	1.70	0.57
1:F:242:GLU:CG	1:F:281:ARG:HH22	2.18	0.57
1:G:224:GLU:HG2	1:G:225:GLY:N	2.16	0.57
1:I:182:LYS:O	1:I:187:SER:HB3	2.04	0.57
1:J:363:ILE:O	1:J:367:VAL:HG23	2.05	0.57
1:K:275:ILE:H	1:K:275:ILE:CD1	2.18	0.57
1:M:244:SER:O	1:M:248:GLN:NE2	2.38	0.57
1:N:352:TRP:HZ3	1:N:362:VAL:HG21	1.70	0.57
1:B:250:LYS:HZ3	1:B:253:ARG:NH2	2.02	0.56
1:B:325:LEU:O	1:B:325:LEU:HD23	2.03	0.56
1:C:293:ARG:NH2	1:C:295:ASP:OD2	2.37	0.56
1:H:266:ARG:HB3	1:I:229:LEU:CD2	2.35	0.56
1:H:346:LEU:HD23	1:H:346:LEU:O	2.04	0.56
1:I:351:PRO:HB2	1:I:353:TYR:CE2	2.40	0.56
1:K:143:SER:CB	1:K:144:PRO:HD2	2.34	0.56
1:D:209:PHE:CD1	1:D:250:LYS:HD3	2.40	0.56
1:I:328:PHE:CZ	1:I:364:GLU:HB2	2.40	0.56
1:A:232:GLY:HA2	1:A:272:ASN:HD22	1.69	0.56
1:C:324:PHE:CD1	1:C:360:LYS:HA	2.41	0.56
1:E:152:LYS:HG2	1:F:369:PHE:HE1	1.66	0.56
1:H:347:LEU:HD21	1:H:380:LEU:HD13	1.87	0.56
1:K:190:PRO:HD2	1:K:233:GLY:HA3	1.86	0.56
1:B:285:GLU:OE2	1:K:349:SER:HB3	2.04	0.56
1:L:359:LEU:O	1:L:362:VAL:N	2.38	0.56
1:N:260:PHE:C	1:N:260:PHE:CD1	2.78	0.56
1:A:139:TYR:CE2	1:A:175:VAL:HG13	2.41	0.56
1:B:358:GLU:O	1:B:362:VAL:HG23	2.05	0.56
1:B:343:ALA:HB2	1:B:376:ASP:HA	1.87	0.56
1:C:231:ASP:C	1:C:233:GLY:H	2.09	0.56
1:E:226:PHE:O	1:E:227:PHE:C	2.44	0.56
1:E:254:VAL:HG22	1:E:260:PHE:HB3	1.88	0.56
1:G:207:GLU:HG2	1:G:226:PHE:CE1	2.41	0.56
1:L:287:VAL:HG12	1:L:288:LYS:N	2.19	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:308:PRO:HG2	1:M:313:ARG:CD	2.28	0.56
1:N:296:LEU:HD13	1:N:300:LEU:HG	1.88	0.56
1:N:302:VAL:O	1:N:303:ILE:HD13	2.05	0.56
1:A:172:GLY:O	1:A:175:VAL:N	2.38	0.56
1:A:275:ILE:O	1:A:276:LEU:HD23	2.05	0.56
1:A:285:GLU:O	1:A:289:GLU:HG3	2.06	0.56
1:C:382:CYS:O	1:C:383:LEU:HD23	2.06	0.56
1:D:163:VAL:HB	1:D:276:LEU:CD2	2.36	0.56
1:E:171:VAL:CG1	1:E:355:ASN:OD1	2.51	0.56
1:I:152:LYS:O	1:I:155:LYS:N	2.37	0.56
1:K:178:ARG:HE	1:K:191:PHE:HD2	1.51	0.56
1:L:251:LEU:O	1:L:252:LEU:C	2.42	0.56
1:M:194:LEU:HD21	1:M:237:LEU:CD2	2.23	0.56
1:M:280:ASN:OD1	1:M:281:ARG:N	2.38	0.56
1:M:261:TYR:CE2	1:N:199:ILE:HG12	2.39	0.56
1:D:303:ILE:CD1	1:E:365:ARG:HG3	2.35	0.56
1:E:365:ARG:HG2	1:E:369:PHE:CE2	2.41	0.56
1:G:310:LEU:HB2	1:G:355:ASN:HB3	1.87	0.56
1:L:173:LYS:NZ	1:L:173:LYS:HB2	2.21	0.56
1:M:244:SER:O	1:M:247:ALA:CB	2.53	0.56
1:A:179:LEU:C	1:A:181:HIS:H	2.07	0.56
1:B:366:ALA:O	1:B:370:SER:HB3	2.06	0.56
1:E:186:ARG:NH2	1:E:272:ASN:ND2	2.50	0.56
1:F:366:ALA:O	1:F:368:LEU:N	2.39	0.56
1:G:275:ILE:N	1:G:275:ILE:CD1	2.67	0.56
1:H:271:VAL:CG1	1:H:273:VAL:HG23	2.35	0.56
1:I:266:ARG:HH11	1:J:216:PHE:HE1	1.54	0.56
1:N:228:GLU:O	1:N:230:ALA:N	2.39	0.56
1:N:255:ILE:O	1:N:255:ILE:HG22	2.05	0.56
1:A:376:ASP:O	1:A:378:GLY:N	2.38	0.56
1:B:365:ARG:NH1	1:B:383:LEU:O	2.39	0.56
1:J:143:SER:O	1:J:147:LYS:HB2	2.06	0.56
1:N:277:ALA:O	1:N:278:ALA:HB2	2.05	0.56
1:N:303:ILE:O	1:N:303:ILE:HG22	2.05	0.56
1:A:299:ARG:CA	1:A:299:ARG:HE	2.19	0.56
1:G:324:PHE:CD1	1:G:360:LYS:HA	2.41	0.56
1:H:152:LYS:O	1:H:156:ILE:HG12	2.05	0.56
1:H:194:LEU:HD13	1:H:226:PHE:CD2	2.40	0.56
1:H:324:PHE:CB	1:H:363:ILE:HG21	2.36	0.56
1:K:157:SER:HB3	1:K:183:LEU:C	2.26	0.56
1:K:178:ARG:NE	1:K:191:PHE:CE2	2.74	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:200:PRO:HG2	1:K:203:ILE:CG1	2.35	0.56
1:H:357:ARG:NH1	1:N:252:LEU:HD21	2.10	0.56
1:B:203:ILE:O	1:B:203:ILE:HG22	2.06	0.56
1:B:251:LEU:HD22	1:B:255:ILE:CD1	2.36	0.56
1:C:208:LEU:HD11	1:C:227:PHE:CD1	2.41	0.56
1:H:157:SER:OG	1:H:183:LEU:HB2	2.06	0.56
1:H:254:VAL:CG2	1:H:260:PHE:HB3	2.34	0.56
1:M:176:VAL:O	1:M:177:ALA:C	2.44	0.56
1:N:316:ASP:O	1:N:319:PRO:HD2	2.06	0.56
1:B:152:LYS:O	1:B:156:ILE:HG12	2.06	0.56
1:C:252:LEU:HB2	1:C:296:LEU:HD23	1.88	0.56
1:D:186:ARG:O	1:D:189:GLU:HB2	2.06	0.56
1:F:174:GLU:HG2	1:F:178:ARG:NH1	2.21	0.56
1:F:321:ALA:HB1	1:F:339:PHE:CZ	2.41	0.56
1:F:357:ARG:CG	1:F:357:ARG:HH11	2.17	0.56
1:G:173:LYS:O	1:G:175:VAL:N	2.38	0.56
1:J:152:LYS:O	1:J:156:ILE:HG12	2.05	0.56
1:L:240:ILE:HD11	1:L:277:ALA:CB	2.31	0.56
1:M:310:LEU:HD22	1:M:317:ILE:HG12	1.88	0.56
1:B:204:PHE:C	1:B:206:ALA:N	2.55	0.55
1:B:266:ARG:HB3	1:C:229:LEU:HD21	1.87	0.55
1:B:248:GLN:OE1	1:B:293:ARG:HG3	2.05	0.55
1:C:299:ARG:HH12	1:D:357:ARG:NH1	2.03	0.55
1:D:292:PHE:CE2	1:D:296:LEU:HD12	2.40	0.55
1:G:168:GLU:OE1	1:G:309:PRO:HB3	2.05	0.55
1:I:252:LEU:HD21	1:I:295:ASP:HB2	1.88	0.55
1:L:184:SER:O	1:L:186:ARG:N	2.39	0.55
1:M:253:ARG:CG	1:N:198:SER:CB	2.84	0.55
1:B:269:ILE:HG22	1:B:270:GLU:N	2.19	0.55
1:G:203:ILE:HG22	1:G:203:ILE:O	2.06	0.55
1:I:196:VAL:HA	1:I:204:PHE:HE1	1.72	0.55
1:I:205:GLU:HG2	1:I:247:ALA:HB2	1.86	0.55
1:L:149:ILE:HD13	1:L:307:ILE:CD1	2.36	0.55
1:N:143:SER:CB	1:N:144:PRO:HD2	2.31	0.55
1:C:253:ARG:CG	1:C:253:ARG:HH11	2.19	0.55
1:D:171:VAL:HG21	1:D:307:ILE:HB	1.89	0.55
1:F:347:LEU:CD2	1:F:380:LEU:HD12	2.34	0.55
1:H:299:ARG:O	1:H:302:VAL:HG23	2.06	0.55
1:I:350:TYR:CE1	1:I:384:VAL:HB	2.42	0.55
1:I:172:GLY:HA2	2:I:8:ADP:PA	2.46	0.55
1:J:339:PHE:HB3	1:J:343:ALA:HB3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:139:TYR:CE1	1:K:175:VAL:HG13	2.41	0.55
1:K:321:ALA:HA	1:K:363:ILE:CD1	2.36	0.55
1:N:245:LEU:HD23	1:N:248:GLN:HE21	1.70	0.55
1:A:192:VAL:CG2	1:A:230:ALA:HB2	2.37	0.55
1:B:296:LEU:HD13	1:B:296:LEU:C	2.26	0.55
1:F:355:ASN:O	1:F:357:ARG:N	2.34	0.55
1:F:365:ARG:HD2	1:F:383:LEU:HD21	1.88	0.55
1:J:216:PHE:N	1:J:216:PHE:HD2	1.90	0.55
1:J:281:ARG:HH11	1:J:281:ARG:HG2	1.71	0.55
1:K:189:GLU:OE1	1:K:189:GLU:HA	2.04	0.55
1:L:173:LYS:H	2:L:11:ADP:PB	2.29	0.55
1:M:211:TYR:N	1:M:211:TYR:CD1	2.74	0.55
1:M:294:GLU:HG2	1:M:295:ASP:N	2.22	0.55
1:A:143:SER:HB3	1:A:316:ASP:CG	2.26	0.55
1:B:261:TYR:O	1:B:262:ARG:C	2.43	0.55
1:E:168:GLU:HB2	1:E:171:VAL:HG11	1.88	0.55
1:E:236:PHE:CE1	1:E:278:ALA:HB2	2.38	0.55
1:E:326:LYS:HE2	1:E:330:ARG:HH21	1.71	0.55
1:I:249:ALA:HB2	1:I:293:ARG:HH11	1.71	0.55
1:I:311:ARG:HG3	1:I:312:GLU:HG3	1.88	0.55
1:I:313:ARG:HB3	1:I:316:ASP:OD2	2.06	0.55
1:K:240:ILE:HG22	1:K:292:PHE:CE1	2.41	0.55
1:L:157:SER:HB2	1:L:183:LEU:O	2.06	0.55
1:L:225:GLY:O	1:L:226:PHE:C	2.44	0.55
1:B:362:VAL:HG11	1:B:384:VAL:HG11	1.88	0.55
1:E:162:PRO:HG3	1:E:299:ARG:O	2.06	0.55
1:F:194:LEU:HD23	1:F:236:PHE:O	2.06	0.55
1:F:283:ILE:O	1:F:286:LEU:N	2.40	0.55
1:G:150:LEU:O	1:G:153:ILE:HB	2.06	0.55
1:H:346:LEU:HD12	1:H:377:ARG:HE	1.71	0.55
1:I:195:ASN:ND2	1:I:238:ASP:OD2	2.38	0.55
1:I:161:CYS:O	1:I:274:ARG:NH1	2.40	0.55
1:L:267:LYS:O	1:L:269:ILE:HD12	2.05	0.55
1:L:328:PHE:CE2	1:L:364:GLU:HB2	2.41	0.55
1:L:342:SER:O	1:L:377:ARG:HD2	2.07	0.55
1:A:325:LEU:C	1:A:325:LEU:HD23	2.25	0.55
1:B:253:ARG:HG3	1:B:254:VAL:N	2.21	0.55
1:C:292:PHE:CE2	1:C:296:LEU:HD12	2.41	0.55
1:D:203:ILE:CG2	1:D:207:GLU:HG2	2.37	0.55
1:D:332:TYR:CD1	1:D:368:LEU:HD21	2.41	0.55
1:F:142:GLU:OE1	1:F:142:GLU:HA	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:VAL:CG1	1:J:221:SER:N	2.68	0.55
1:L:339:PHE:CD2	1:L:375:ILE:HD11	2.41	0.55
1:M:141:PHE:CD2	1:M:150:LEU:HB2	2.41	0.55
1:B:164:LEU:HD12	1:B:165:ILE:N	2.22	0.55
1:D:141:PHE:HE1	1:D:179:LEU:HD12	1.70	0.55
1:E:209:PHE:CD1	1:E:209:PHE:N	2.74	0.55
1:E:244:SER:O	1:E:246:GLU:N	2.39	0.55
1:E:298:TYR:CE1	1:F:354:GLY:CA	2.90	0.55
1:H:215:ALA:HB3	1:H:264:GLY:HA3	1.88	0.55
1:K:346:LEU:HD23	1:K:346:LEU:O	2.07	0.55
1:L:311:ARG:HH11	1:L:353:TYR:HE2	1.53	0.55
1:N:192:VAL:HB	1:N:230:ALA:HB2	1.87	0.55
1:D:149:ILE:O	1:D:153:ILE:HG12	2.06	0.55
1:E:177:ALA:HB1	1:E:276:LEU:HD12	1.88	0.55
1:E:341:LYS:HD3	1:E:341:LYS:O	2.07	0.55
1:F:156:ILE:O	1:F:158:CYS:N	2.39	0.55
1:G:153:ILE:HG23	1:G:180:ILE:HG12	1.89	0.55
1:G:252:LEU:CD1	1:G:299:ARG:HG3	2.37	0.55
1:H:271:VAL:HG12	1:H:273:VAL:HG23	1.88	0.55
1:C:240:ILE:HD12	1:C:243:LEU:HD12	1.88	0.55
1:E:267:LYS:CD	1:E:267:LYS:H	2.15	0.55
1:G:310:LEU:CD2	1:G:317:ILE:HG12	2.37	0.55
1:H:247:ALA:O	1:H:248:GLN:C	2.45	0.55
1:I:143:SER:HB2	1:I:144:PRO:HD2	1.89	0.55
1:I:292:PHE:HE2	1:I:296:LEU:HB3	1.71	0.55
1:I:336:VAL:HA	1:I:373:LYS:O	2.07	0.55
1:J:349:SER:OG	1:J:350:TYR:N	2.40	0.55
1:M:211:TYR:N	1:M:211:TYR:HD1	2.05	0.55
1:M:256:GLU:O	1:M:258:GLY:N	2.40	0.55
1:D:271:VAL:HG23	1:D:273:VAL:HG23	1.88	0.54
1:G:191:PHE:CE2	1:G:193:ALA:HB2	2.42	0.54
1:G:261:TYR:HB3	1:G:266:ARG:C	2.26	0.54
1:H:328:PHE:C	1:H:367:VAL:HG11	2.27	0.54
1:L:165:ILE:HG22	1:L:173:LYS:HG2	1.89	0.54
1:N:152:LYS:O	1:N:156:ILE:HG12	2.08	0.54
1:B:192:VAL:CG2	1:B:229:LEU:HD12	2.37	0.54
1:C:150:LEU:CG	1:C:154:LYS:HZ1	2.20	0.54
1:C:376:ASP:O	1:C:378:GLY:N	2.41	0.54
1:F:311:ARG:HH11	1:F:311:ARG:CG	2.18	0.54
1:G:235:LEU:HD21	1:G:237:LEU:HD21	1.89	0.54
1:J:318:ILE:CG1	1:J:348:LEU:HD21	2.34	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:234:THR:HG23	1:K:274:ARG:O	2.07	0.54
1:K:325:LEU:CD1	1:K:338:GLY:HA2	2.35	0.54
1:L:152:LYS:O	1:L:154:LYS:N	2.40	0.54
1:A:208:LEU:HD22	1:A:209:PHE:CE1	2.43	0.54
1:C:258:GLY:O	1:C:270:GLU:HA	2.07	0.54
1:E:161:CYS:HB2	1:E:302:VAL:HG11	1.88	0.54
1:E:249:ALA:HA	1:E:293:ARG:HH11	1.73	0.54
1:E:320:LEU:C	1:E:322:ASN:N	2.60	0.54
1:F:171:VAL:HG21	1:F:307:ILE:HB	1.88	0.54
1:F:171:VAL:HG22	1:F:173:LYS:HG3	1.89	0.54
1:H:343:ALA:HB2	1:H:376:ASP:CA	2.23	0.54
1:I:366:ALA:C	1:I:368:LEU:H	2.09	0.54
1:C:322:ASN:O	1:C:323:HIS:C	2.46	0.54
1:C:326:LYS:HE2	1:C:330:ARG:HH22	1.72	0.54
1:F:239:GLU:N	1:F:278:ALA:O	2.39	0.54
1:F:316:ASP:O	1:F:319:PRO:HD2	2.07	0.54
1:G:260:PHE:HE2	1:G:271:VAL:HG11	1.73	0.54
1:H:226:PHE:O	1:H:229:LEU:N	2.41	0.54
1:H:287:VAL:CG1	1:H:294:GLU:HG2	2.38	0.54
1:H:316:ASP:HB3	1:H:320:LEU:HD11	1.90	0.54
1:I:251:LEU:O	1:I:253:ARG:N	2.40	0.54
1:I:279:THR:HG21	1:I:283:ILE:HD11	1.89	0.54
1:L:337:GLU:N	1:L:373:LYS:O	2.40	0.54
1:A:179:LEU:C	1:A:181:HIS:N	2.61	0.54
1:A:194:LEU:H	1:A:194:LEU:CD2	2.21	0.54
1:B:235:LEU:CG	1:B:237:LEU:HD21	2.38	0.54
1:C:324:PHE:CZ	1:C:360:LYS:HB2	2.42	0.54
1:C:340:THR:HG21	1:C:376:ASP:HB3	1.89	0.54
1:D:157:SER:HB3	1:D:184:SER:HA	1.89	0.54
1:E:196:VAL:CG1	1:E:196:VAL:O	2.55	0.54
1:E:346:LEU:HB2	1:E:377:ARG:NH1	2.22	0.54
1:F:153:ILE:HD12	1:F:180:ILE:CG1	2.37	0.54
1:I:163:VAL:HB	1:I:276:LEU:HD23	1.89	0.54
1:I:355:ASN:O	1:I:357:ARG:N	2.40	0.54
1:J:202:ASP:CG	1:J:202:ASP:O	2.45	0.54
1:K:216:PHE:H	1:K:219:ALA:HB2	1.73	0.54
1:L:296:LEU:O	1:L:299:ARG:N	2.36	0.54
1:D:343:ALA:HB2	1:D:376:ASP:HA	1.90	0.54
1:M:293:ARG:O	1:M:296:LEU:HB3	2.07	0.54
1:M:347:LEU:HD21	1:M:380:LEU:CG	2.36	0.54
1:N:204:PHE:CD2	1:N:204:PHE:O	2.61	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HD13	1:A:317:ILE:HG12	1.90	0.54
1:B:160:GLU:CA	1:B:274:ARG:HH12	2.21	0.54
1:C:251:LEU:O	1:C:255:ILE:HG13	2.07	0.54
1:E:173:LYS:HB2	1:E:173:LYS:HZ3	1.73	0.54
1:F:194:LEU:N	1:F:194:LEU:CD2	2.71	0.54
1:F:199:ILE:HD13	1:F:207:GLU:HG2	1.89	0.54
1:F:195:ASN:HA	1:F:238:ASP:HB3	1.88	0.54
1:F:325:LEU:CD2	1:F:336:VAL:HG12	2.36	0.54
1:G:296:LEU:O	1:G:296:LEU:HD13	2.08	0.54
1:L:174:GLU:O	1:L:177:ALA:HB3	2.07	0.54
1:N:186:ARG:NH1	1:N:232:GLY:O	2.40	0.54
1:B:227:PHE:O	1:B:230:ALA:N	2.40	0.54
1:B:365:ARG:NH1	1:B:383:LEU:HB3	2.22	0.54
1:E:311:ARG:CG	1:E:351:PRO:O	2.56	0.54
1:G:144:PRO:HG2	1:G:145:LYS:H	1.73	0.54
1:G:211:TYR:HE1	1:G:215:ALA:HB3	1.71	0.54
1:H:339:PHE:N	1:H:339:PHE:HD1	2.04	0.54
1:K:192:VAL:O	1:K:192:VAL:HG12	2.06	0.54
1:K:162:PRO:HG3	1:K:299:ARG:O	2.08	0.54
1:K:361:ASN:N	1:K:361:ASN:ND2	2.54	0.54
1:L:339:PHE:HE2	1:L:375:ILE:HD11	1.70	0.54
1:A:234:THR:HG21	1:A:276:LEU:CD1	2.38	0.54
1:A:244:SER:O	1:A:248:GLN:HG3	2.07	0.54
1:A:309:PRO:HG3	1:A:311:ARG:HH11	1.70	0.54
1:B:249:ALA:HB2	1:B:293:ARG:HH11	1.73	0.54
1:D:294:GLU:OE1	1:D:298:TYR:HE1	1.90	0.54
1:E:351:PRO:O	1:E:352:TRP:C	2.46	0.54
1:F:315:GLU:N	1:F:315:GLU:OE1	2.31	0.54
1:G:181:HIS:HE1	1:G:187:SER:O	1.91	0.54
1:I:253:ARG:NE	1:J:198:SER:CB	2.71	0.54
1:L:165:ILE:HB	1:L:278:ALA:CB	2.38	0.54
1:B:292:PHE:CZ	1:B:296:LEU:HD12	2.43	0.54
1:F:343:ALA:O	1:F:344:GLN:C	2.46	0.54
1:G:252:LEU:CD2	1:G:293:ARG:HH12	2.21	0.54
1:I:321:ALA:HA	1:I:363:ILE:CD1	2.38	0.54
1:I:336:VAL:HG11	1:I:375:ILE:HD11	1.90	0.54
1:K:275:ILE:O	1:K:276:LEU:HD23	2.07	0.54
1:L:329:SER:HA	1:L:334:LYS:HG3	1.88	0.54
1:M:191:PHE:HD2	1:M:191:PHE:C	2.10	0.54
1:M:274:ARG:HD3	1:M:276:LEU:HD21	1.90	0.54
1:M:281:ARG:HG2	1:M:281:ARG:HH11	1.72	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:279:THR:HG23	1:N:280:ASN:N	2.22	0.54
1:C:150:LEU:O	1:C:154:LYS:HG3	2.07	0.53
1:C:298:TYR:HE2	1:D:358:GLU:OE2	1.90	0.53
1:L:305:ILE:HG23	1:L:307:ILE:HD11	1.90	0.53
1:L:329:SER:HA	1:L:334:LYS:CG	2.38	0.53
1:N:313:ARG:C	1:N:315:GLU:H	2.12	0.53
1:A:275:ILE:HD12	1:A:275:ILE:N	2.16	0.53
1:C:243:LEU:O	1:C:248:GLN:NE2	2.37	0.53
1:C:261:TYR:O	1:C:262:ARG:C	2.46	0.53
1:E:211:TYR:CD2	1:E:263:LEU:HB2	2.43	0.53
1:G:152:LYS:O	1:G:156:ILE:HG12	2.08	0.53
1:G:176:VAL:O	1:G:177:ALA:C	2.46	0.53
1:I:230:ALA:O	1:I:273:VAL:HG22	2.08	0.53
1:L:204:PHE:CE2	1:L:208:LEU:HD12	2.43	0.53
1:L:342:SER:O	1:L:377:ARG:HB2	2.09	0.53
1:M:176:VAL:O	1:M:179:LEU:N	2.39	0.53
1:M:195:ASN:ND2	1:M:238:ASP:OD2	2.41	0.53
1:D:209:PHE:HE2	1:D:227:PHE:CE1	2.27	0.53
1:E:269:ILE:H	1:E:269:ILE:CD1	2.19	0.53
1:D:159:ALA:CB	1:E:332:TYR:HE2	2.21	0.53
1:F:153:ILE:HG21	1:F:179:LEU:CD2	2.36	0.53
1:I:211:TYR:CZ	1:I:223:LYS:HB2	2.43	0.53
1:I:266:ARG:HD2	1:J:216:PHE:HE1	1.74	0.53
1:L:139:TYR:HB3	1:L:141:PHE:CD2	2.41	0.53
1:L:326:LYS:O	1:L:329:SER:HB3	2.08	0.53
1:L:376:ASP:C	1:L:378:GLY:H	2.11	0.53
1:M:286:LEU:HA	1:M:289:GLU:OE1	2.07	0.53
1:N:209:PHE:CE1	1:N:250:LYS:HB3	2.43	0.53
1:A:252:LEU:HD22	1:A:295:ASP:OD1	2.09	0.53
1:A:325:LEU:HD12	1:A:339:PHE:CE1	2.43	0.53
1:D:259:LYS:HE2	1:D:270:GLU:OE2	2.07	0.53
1:D:308:PRO:O	1:D:313:ARG:HD2	2.08	0.53
1:F:365:ARG:NH1	1:F:383:LEU:HD22	2.24	0.53
1:I:194:LEU:HD13	1:I:226:PHE:CD1	2.32	0.53
1:J:262:ARG:HD3	1:J:269:ILE:HD11	1.90	0.53
1:K:384:VAL:O	1:K:384:VAL:HG12	2.07	0.53
1:L:159:ALA:CB	1:M:368:LEU:HD21	2.38	0.53
1:A:237:LEU:HB2	1:A:240:ILE:HD11	1.91	0.53
1:A:313:ARG:HB3	1:A:316:ASP:OD2	2.08	0.53
1:A:347:LEU:HD21	1:A:380:LEU:HD11	1.91	0.53
1:B:160:GLU:HA	1:B:274:ARG:NH1	2.23	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ARG:CB	1:B:201:ARG:HH11	2.20	0.53
1:C:215:ALA:C	1:C:217:THR:H	2.12	0.53
1:C:236:PHE:HE2	1:C:238:ASP:HB2	1.71	0.53
1:G:261:TYR:HD2	1:G:263:LEU:O	1.91	0.53
1:H:240:ILE:HG23	1:H:243:LEU:HD12	1.90	0.53
1:I:325:LEU:C	1:I:325:LEU:HD23	2.28	0.53
1:J:224:GLU:CG	1:J:225:GLY:H	2.06	0.53
1:J:309:PRO:CB	1:J:311:ARG:NH1	2.72	0.53
1:K:269:ILE:H	1:K:269:ILE:CD1	2.20	0.53
1:B:240:ILE:HG13	1:B:277:ALA:CB	2.32	0.53
1:B:251:LEU:O	1:B:252:LEU:C	2.47	0.53
1:C:309:PRO:CB	1:C:311:ARG:NH1	2.72	0.53
1:F:215:ALA:HB3	1:F:219:ALA:HB3	1.91	0.53
1:F:343:ALA:C	1:F:345:GLU:H	2.12	0.53
1:I:194:LEU:N	1:I:194:LEU:CD2	2.72	0.53
1:K:148:GLU:O	1:K:151:GLU:HB2	2.08	0.53
1:L:173:LYS:NZ	2:L:11:ADP:PB	2.81	0.53
1:L:228:GLU:O	1:L:231:ASP:N	2.40	0.53
1:L:267:LYS:O	1:L:269:ILE:CD1	2.57	0.53
1:M:252:LEU:HA	1:M:255:ILE:HD12	1.90	0.53
1:C:140:VAL:CB	1:C:320:LEU:HD23	2.39	0.53
1:E:156:ILE:HD11	1:E:303:ILE:HD12	1.91	0.53
1:E:239:GLU:C	1:E:241:GLY:H	2.11	0.53
1:H:340:THR:HG22	1:H:341:LYS:N	2.23	0.53
1:I:216:PHE:CZ	1:I:218:GLY:HA3	2.44	0.53
1:J:195:ASN:HB3	1:J:198:SER:OG	2.08	0.53
1:L:354:GLY:HA3	1:L:358:GLU:HB2	1.91	0.53
1:M:358:GLU:O	1:M:359:LEU:C	2.46	0.53
1:A:142:GLU:HA	1:A:147:LYS:HE2	1.91	0.53
1:A:346:LEU:HD21	1:A:384:VAL:O	2.08	0.53
1:C:259:LYS:HA	1:C:269:ILE:O	2.08	0.53
1:E:292:PHE:CE2	1:E:296:LEU:HB3	2.37	0.53
1:A:223:LYS:NZ	1:G:266:ARG:HD2	2.24	0.53
1:G:340:THR:C	1:G:342:SER:H	2.12	0.53
1:H:355:ASN:O	1:H:357:ARG:N	2.42	0.53
1:I:300:LEU:O	1:I:302:VAL:N	2.42	0.53
1:L:173:LYS:NZ	2:L:11:ADP:O1B	2.41	0.53
1:L:318:ILE:CD1	1:L:319:PRO:HD3	2.39	0.53
1:N:292:PHE:CZ	1:N:296:LEU:HD12	2.43	0.53
1:B:191:PHE:HE1	1:B:276:LEU:HD12	1.74	0.53
1:B:359:LEU:C	1:B:361:ASN:N	2.61	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:MET:CE	1:C:313:ARG:NH2	2.72	0.53
1:C:314:LYS:HA	1:C:317:ILE:CG1	2.37	0.53
1:C:336:VAL:HG21	1:C:370:SER:HB2	1.91	0.53
1:D:335:GLU:O	1:D:373:LYS:HA	2.09	0.53
1:E:166:THR:HG22	1:E:167:GLY:H	1.74	0.53
1:E:282:ASN:ND2	1:E:285:GLU:CB	2.64	0.53
1:E:279:THR:CG2	1:E:283:ILE:HD11	2.36	0.53
1:E:305:ILE:O	1:E:305:ILE:HG22	2.08	0.53
1:F:282:ASN:ND2	1:F:285:GLU:HB2	2.24	0.53
1:F:300:LEU:C	1:F:302:VAL:H	2.12	0.53
1:F:354:GLY:O	1:F:358:GLU:N	2.36	0.53
1:G:340:THR:O	1:G:342:SER:N	2.41	0.53
1:I:213:LYS:O	1:I:220:VAL:O	2.26	0.53
1:M:181:HIS:ND1	1:M:187:SER:HA	2.24	0.53
1:A:325:LEU:HD21	1:A:336:VAL:HG12	1.90	0.53
1:D:284:LYS:HE2	1:D:297:TYR:OH	2.09	0.53
1:D:299:ARG:NH2	1:D:302:VAL:HG21	2.24	0.53
1:H:309:PRO:HB2	1:H:311:ARG:CD	2.39	0.53
1:J:200:PRO:HG2	1:J:203:ILE:CD1	2.36	0.53
1:J:245:LEU:HD23	1:J:248:GLN:NE2	2.24	0.53
1:J:266:ARG:NH1	1:K:224:GLU:O	2.41	0.53
1:L:152:LYS:C	1:L:154:LYS:N	2.60	0.53
1:L:229:LEU:C	1:L:229:LEU:CD1	2.74	0.53
1:L:248:GLN:OE1	1:L:293:ARG:N	2.34	0.53
1:L:318:ILE:CG1	1:L:319:PRO:HD3	2.39	0.53
1:L:318:ILE:O	1:L:321:ALA:HB3	2.09	0.53
1:A:283:ILE:O	1:A:287:VAL:HG23	2.09	0.52
1:B:284:LYS:CD	1:B:284:LYS:H	2.18	0.52
1:C:254:VAL:CG2	1:C:260:PHE:HB3	2.38	0.52
1:E:176:VAL:C	1:E:180:ILE:HD12	2.28	0.52
1:G:322:ASN:O	1:G:326:LYS:HB2	2.09	0.52
1:H:226:PHE:O	1:H:227:PHE:C	2.46	0.52
1:H:286:LEU:HD22	1:H:291:LYS:HD3	1.91	0.52
1:L:229:LEU:O	1:L:229:LEU:HD13	2.08	0.52
1:L:250:LYS:NZ	1:L:263:LEU:HG	2.23	0.52
1:M:141:PHE:O	1:M:142:GLU:C	2.47	0.52
1:M:195:ASN:O	1:M:197:ALA:N	2.42	0.52
1:M:204:PHE:HE2	1:M:243:LEU:HD21	1.74	0.52
1:M:234:THR:HG23	1:M:276:LEU:HD23	1.91	0.52
1:C:365:ARG:NE	1:C:383:LEU:HD13	2.24	0.52
1:E:273:VAL:O	1:E:275:ILE:HD12	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:VAL:O	1:F:171:VAL:HG23	2.07	0.52
1:H:250:LYS:O	1:H:251:LEU:C	2.47	0.52
1:I:171:VAL:CG1	1:I:307:ILE:HG22	2.39	0.52
1:J:145:LYS:O	1:J:149:ILE:HG13	2.10	0.52
1:J:178:ARG:HG3	1:J:178:ARG:HH11	1.74	0.52
1:J:336:VAL:HG21	1:J:367:VAL:HG13	1.90	0.52
1:K:296:LEU:HD13	1:K:296:LEU:O	2.09	0.52
1:M:238:ASP:O	1:M:239:GLU:HB3	2.10	0.52
1:B:150:LEU:HD11	1:B:154:LYS:NZ	2.24	0.52
1:C:145:LYS:O	1:C:148:GLU:HB3	2.08	0.52
1:C:181:HIS:ND1	1:C:181:HIS:C	2.63	0.52
1:E:318:ILE:O	1:E:322:ASN:ND2	2.42	0.52
1:F:203:ILE:O	1:F:206:ALA:HB3	2.09	0.52
1:G:229:LEU:O	1:G:229:LEU:HD13	2.09	0.52
1:G:343:ALA:O	1:G:346:LEU:HB3	2.09	0.52
1:M:155:LYS:O	1:M:156:ILE:C	2.48	0.52
1:C:139:TYR:O	1:C:139:TYR:HD1	1.92	0.52
1:E:381:SER:C	1:E:383:LEU:H	2.13	0.52
1:F:140:VAL:HG11	1:F:320:LEU:HG	1.90	0.52
1:J:194:LEU:HD23	1:J:236:PHE:O	2.09	0.52
1:J:350:TYR:HD2	1:J:352:TRP:CD2	2.27	0.52
1:L:172:GLY:HA2	2:L:11:ADP:O1A	2.09	0.52
1:B:288:LYS:C	1:B:290:GLY:H	2.13	0.52
1:E:195:ASN:C	1:E:197:ALA:H	2.13	0.52
1:F:240:ILE:C	1:F:242:GLU:H	2.12	0.52
1:F:313:ARG:O	1:F:314:LYS:C	2.46	0.52
1:G:263:LEU:HG	1:G:264:GLY:N	2.23	0.52
1:I:163:VAL:HB	1:I:276:LEU:CD2	2.40	0.52
1:J:352:TRP:HZ3	1:J:362:VAL:HG21	1.74	0.52
1:K:208:LEU:HD21	1:K:227:PHE:CE1	2.45	0.52
1:L:252:LEU:HD12	1:L:252:LEU:O	2.10	0.52
1:L:143:SER:CB	1:L:316:ASP:OD2	2.57	0.52
1:M:236:PHE:HA	1:M:276:LEU:O	2.10	0.52
1:M:351:PRO:O	1:M:352:TRP:HB2	2.09	0.52
1:N:163:VAL:HB	1:N:276:LEU:CD2	2.39	0.52
1:A:212:GLU:O	1:A:213:LYS:C	2.48	0.52
1:A:251:LEU:O	1:A:255:ILE:HG13	2.10	0.52
1:A:299:ARG:HA	1:A:299:ARG:HE	1.74	0.52
1:B:215:ALA:HB1	1:B:264:GLY:HA3	1.92	0.52
1:E:139:TYR:HE2	1:E:179:LEU:HD21	1.74	0.52
1:F:175:VAL:HG12	1:F:176:VAL:N	2.23	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:LYS:O	1:G:176:VAL:N	2.40	0.52
1:G:228:GLU:HG3	1:G:260:PHE:HZ	1.74	0.52
1:G:346:LEU:HD21	1:G:384:VAL:HG21	1.91	0.52
1:I:252:LEU:HD13	1:I:296:LEU:CA	2.37	0.52
1:J:194:LEU:HD23	1:J:194:LEU:H	1.75	0.52
1:K:208:LEU:HD11	1:K:237:LEU:HD11	1.91	0.52
1:L:194:LEU:HD13	1:L:226:PHE:CD1	2.45	0.52
1:L:308:PRO:O	1:L:313:ARG:HD3	2.10	0.52
1:L:171:VAL:HG12	1:L:309:PRO:HA	1.90	0.52
1:M:248:GLN:HG3	1:M:293:ARG:CB	2.39	0.52
1:N:355:ASN:O	1:N:358:GLU:N	2.41	0.52
1:A:240:ILE:C	1:A:242:GLU:H	2.13	0.52
1:E:320:LEU:O	1:E:321:ALA:C	2.47	0.52
1:E:359:LEU:HD22	1:E:363:ILE:CG1	2.39	0.52
1:E:332:TYR:OH	1:E:364:GLU:OE1	2.21	0.52
1:F:223:LYS:HG3	1:F:223:LYS:O	2.10	0.52
1:F:186:ARG:HD3	1:F:232:GLY:O	2.09	0.52
1:H:194:LEU:N	1:H:194:LEU:CD2	2.72	0.52
1:I:204:PHE:O	1:I:207:GLU:HB2	2.10	0.52
1:I:366:ALA:O	1:I:370:SER:HB3	2.09	0.52
1:L:237:LEU:HB2	1:L:277:ALA:CB	2.39	0.52
1:L:171:VAL:HG23	1:L:307:ILE:HG21	1.92	0.52
1:L:325:LEU:O	1:L:329:SER:HB2	2.10	0.52
1:N:254:VAL:C	1:N:256:GLU:H	2.12	0.52
1:A:310:LEU:HD11	1:A:359:LEU:HD12	1.92	0.52
1:B:179:LEU:O	1:B:181:HIS:N	2.43	0.52
1:D:209:PHE:O	1:D:262:ARG:HD2	2.10	0.52
1:E:303:ILE:HD13	1:F:365:ARG:HG3	1.91	0.52
1:F:383:LEU:N	1:F:383:LEU:HD23	2.23	0.52
1:H:362:VAL:CG2	1:H:365:ARG:HH21	2.14	0.52
1:K:149:ILE:HA	1:K:152:LYS:HE3	1.90	0.52
1:K:299:ARG:HA	1:L:361:ASN:ND2	2.25	0.52
1:K:323:HIS:O	1:K:326:LYS:HB3	2.10	0.52
1:A:144:PRO:HD3	1:A:315:GLU:OE2	2.09	0.52
1:E:236:PHE:CE1	1:E:278:ALA:HB3	2.44	0.52
1:H:223:LYS:NZ	1:N:264:GLY:HA3	2.25	0.52
1:I:302:VAL:O	1:J:365:ARG:NE	2.43	0.52
1:K:324:PHE:CD1	1:K:360:LYS:HA	2.45	0.52
1:L:218:GLY:O	1:L:220:VAL:N	2.35	0.52
1:L:382:CYS:HB2	1:L:383:LEU:HG	1.92	0.52
1:M:141:PHE:CE2	1:M:150:LEU:HD13	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:294:GLU:HG2	1:M:295:ASP:H	1.75	0.52
1:N:262:ARG:NH1	1:N:262:ARG:HG2	2.22	0.52
1:N:305:ILE:HG22	1:N:307:ILE:HD11	1.92	0.52
1:A:139:TYR:CD2	1:A:175:VAL:CG1	2.92	0.52
1:D:368:LEU:C	1:D:370:SER:H	2.13	0.52
1:E:213:LYS:NZ	1:E:213:LYS:HB2	2.25	0.52
1:E:326:LYS:HE2	1:E:330:ARG:NH2	2.25	0.52
1:G:166:THR:HG22	1:G:279:THR:HG22	1.92	0.52
1:J:173:LYS:O	1:J:176:VAL:HB	2.10	0.52
1:J:176:VAL:O	1:J:180:ILE:HG13	2.10	0.52
1:K:347:LEU:HD21	1:K:380:LEU:HD11	1.91	0.52
1:L:310:LEU:O	1:L:312:GLU:N	2.43	0.52
1:M:273:VAL:HG23	1:M:273:VAL:O	2.10	0.52
1:M:340:THR:C	1:M:342:SER:H	2.13	0.52
1:N:146:MET:CE	1:N:149:ILE:HD12	2.40	0.52
1:N:350:TYR:HD2	1:N:352:TRP:H	1.58	0.52
1:A:166:THR:HG22	1:A:279:THR:HG22	1.92	0.51
1:B:146:MET:HG3	1:B:313:ARG:NH2	2.20	0.51
1:B:192:VAL:HG21	1:B:229:LEU:HD12	1.92	0.51
1:C:321:ALA:HA	1:C:363:ILE:CD1	2.40	0.51
1:D:350:TYR:CD1	1:D:384:VAL:HG13	2.45	0.51
1:H:342:SER:OG	1:H:376:ASP:HB2	2.09	0.51
1:J:340:THR:HG1	1:J:376:ASP:HB2	1.76	0.51
1:K:152:LYS:O	1:K:156:ILE:HG12	2.10	0.51
1:K:198:SER:O	1:K:199:ILE:CG1	2.47	0.51
1:K:227:PHE:CZ	1:K:254:VAL:HG11	2.44	0.51
1:K:279:THR:CG2	1:K:283:ILE:HD11	2.36	0.51
1:L:288:LYS:C	1:L:290:GLY:H	2.12	0.51
1:L:355:ASN:O	1:L:358:GLU:N	2.43	0.51
1:M:139:TYR:N	1:M:139:TYR:CD1	2.77	0.51
1:N:365:ARG:HG3	1:N:369:PHE:CE2	2.45	0.51
1:D:350:TYR:CG	1:D:384:VAL:HG13	2.46	0.51
1:D:159:ALA:CB	1:E:332:TYR:CE2	2.93	0.51
1:E:361:ASN:N	1:E:361:ASN:ND2	2.57	0.51
1:F:239:GLU:HA	1:F:279:THR:HA	1.93	0.51
1:F:351:PRO:HB2	1:F:353:TYR:CE2	2.45	0.51
1:H:255:ILE:HD13	1:H:300:LEU:HD21	1.93	0.51
1:I:275:ILE:HD12	1:I:275:ILE:N	2.26	0.51
1:J:209:PHE:HE2	1:J:254:VAL:HG21	1.74	0.51
1:A:365:ARG:HH11	1:A:383:LEU:HD22	1.76	0.51
1:B:168:GLU:OE2	1:B:311:ARG:NH2	2.44	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:PHE:HA	1:D:229:LEU:HB2	1.92	0.51
1:D:281:ARG:HG2	1:D:281:ARG:NH1	2.23	0.51
1:F:283:ILE:HG21	1:F:297:TYR:HD1	1.76	0.51
1:J:299:ARG:HA	1:J:299:ARG:HE	1.76	0.51
1:K:143:SER:HB2	1:K:315:GLU:CB	2.37	0.51
1:M:324:PHE:HD1	1:M:359:LEU:HD23	1.75	0.51
1:M:324:PHE:CE1	1:M:360:LYS:HB2	2.45	0.51
1:N:174:GLU:O	1:N:175:VAL:C	2.49	0.51
1:N:204:PHE:CG	1:N:204:PHE:O	2.60	0.51
1:A:192:VAL:HG21	1:A:230:ALA:HB2	1.91	0.51
1:B:178:ARG:NH1	1:B:191:PHE:CD2	2.79	0.51
1:B:285:GLU:O	1:B:288:LYS:N	2.42	0.51
1:C:181:HIS:HE1	1:C:187:SER:HA	1.69	0.51
1:D:240:ILE:O	1:D:242:GLU:N	2.43	0.51
1:E:156:ILE:O	1:E:158:CYS:N	2.40	0.51
1:E:241:GLY:HA3	1:E:281:ARG:NH2	2.24	0.51
1:E:302:VAL:HG23	1:F:361:ASN:OD1	2.09	0.51
1:F:171:VAL:HG12	1:F:355:ASN:HD22	1.75	0.51
1:G:352:TRP:HA	1:G:358:GLU:OE1	2.11	0.51
1:H:194:LEU:H	1:H:194:LEU:CD2	2.18	0.51
1:H:227:PHE:CD1	1:H:235:LEU:CD1	2.93	0.51
1:H:360:LYS:HG2	1:H:364:GLU:OE2	2.10	0.51
1:J:269:ILE:CD1	1:J:269:ILE:N	2.74	0.51
1:L:174:GLU:O	1:L:177:ALA:N	2.43	0.51
1:L:204:PHE:O	1:L:207:GLU:N	2.42	0.51
1:A:365:ARG:HD2	1:A:383:LEU:HD11	1.92	0.51
1:H:255:ILE:HG12	1:H:275:ILE:HD11	1.89	0.51
1:H:231:ASP:CG	1:H:271:VAL:HG13	2.31	0.51
1:H:346:LEU:HD12	1:H:377:ARG:HG2	1.93	0.51
1:I:300:LEU:C	1:I:302:VAL:H	2.13	0.51
1:I:321:ALA:HA	1:I:363:ILE:HD11	1.91	0.51
1:L:181:HIS:HD2	1:L:234:THR:HB	1.73	0.51
1:A:143:SER:HB2	1:A:144:PRO:CD	2.37	0.51
1:D:356:VAL:HG11	2:D:2:ADP:C8	2.45	0.51
1:F:174:GLU:O	1:F:177:ALA:N	2.44	0.51
1:F:239:GLU:HG3	1:F:239:GLU:O	2.11	0.51
1:H:177:ALA:O	1:H:178:ARG:C	2.49	0.51
1:H:227:PHE:HD1	1:H:235:LEU:HD12	1.74	0.51
1:H:256:GLU:OE2	1:I:357:ARG:HD3	2.11	0.51
1:H:332:TYR:CZ	1:H:370:SER:HB2	2.44	0.51
1:K:209:PHE:C	1:K:225:GLY:HA3	2.31	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:322:ASN:HA	1:L:339:PHE:CE1	2.40	0.51
1:M:266:ARG:HH21	1:M:267:LYS:HZ3	1.58	0.51
1:M:368:LEU:O	1:M:368:LEU:HD13	2.10	0.51
1:B:189:GLU:HB3	1:B:233:GLY:HA2	1.92	0.51
1:F:192:VAL:CG2	1:F:230:ALA:HB2	2.40	0.51
1:F:376:ASP:O	1:F:377:ARG:C	2.49	0.51
1:J:365:ARG:HD2	1:J:383:LEU:CD1	2.41	0.51
1:K:147:LYS:HD3	1:K:150:LEU:HD23	1.93	0.51
1:L:170:GLY:C	1:L:172:GLY:H	2.14	0.51
1:M:157:SER:O	1:M:159:ALA:N	2.43	0.51
1:N:240:ILE:HG23	1:N:243:LEU:CD1	2.40	0.51
1:N:334:LYS:HB3	1:N:336:VAL:HG23	1.92	0.51
1:C:230:ALA:O	1:C:233:GLY:N	2.41	0.51
1:E:249:ALA:HB2	1:E:293:ARG:HD2	1.92	0.51
1:E:262:ARG:HG3	1:E:269:ILE:CD1	2.41	0.51
1:F:323:HIS:C	1:F:323:HIS:HD1	2.15	0.51
1:E:298:TYR:CE1	1:F:354:GLY:HA3	2.46	0.51
1:I:256:GLU:CG	1:I:299:ARG:HE	2.23	0.51
1:D:265:GLY:O	1:D:266:ARG:NE	2.27	0.51
1:E:178:ARG:O	1:E:181:HIS:HB3	2.11	0.51
1:E:279:THR:HG21	1:E:283:ILE:CD1	2.38	0.51
1:F:315:GLU:O	1:F:319:PRO:HG2	2.11	0.51
1:H:150:LEU:HD12	1:H:150:LEU:O	2.10	0.51
1:I:192:VAL:CG2	1:I:230:ALA:HB2	2.41	0.51
1:I:203:ILE:HG22	1:I:207:GLU:HG2	1.92	0.51
1:J:309:PRO:HB2	1:J:311:ARG:NH1	2.26	0.51
1:J:346:LEU:HD23	1:J:346:LEU:C	2.31	0.51
1:J:340:THR:CG2	1:J:376:ASP:HB3	2.41	0.51
1:K:273:VAL:O	1:K:275:ILE:HD12	2.11	0.51
1:N:243:LEU:HB3	1:N:248:GLN:HG2	1.92	0.51
1:B:236:PHE:CD1	1:B:276:LEU:O	2.62	0.51
1:C:360:LYS:HG2	1:C:361:ASN:ND2	2.25	0.51
1:D:318:ILE:HG12	1:D:348:LEU:HD21	1.92	0.51
1:F:209:PHE:C	1:F:225:GLY:HA3	2.31	0.51
1:F:223:LYS:C	1:F:225:GLY:N	2.63	0.51
1:F:310:LEU:C	1:F:312:GLU:H	2.14	0.51
1:G:198:SER:C	1:G:199:ILE:HG13	2.31	0.51
1:G:359:LEU:O	1:G:359:LEU:HD23	2.11	0.51
1:G:340:THR:HG23	1:G:375:ILE:O	2.11	0.51
1:H:182:LYS:HA	1:H:187:SER:HB2	1.93	0.51
1:M:248:GLN:HA	1:M:251:LEU:HB3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:325:LEU:HD11	1:N:336:VAL:HG12	1.93	0.51
1:A:339:PHE:CZ	1:A:363:ILE:HD13	2.46	0.50
1:B:176:VAL:HG12	1:B:180:ILE:HD11	1.93	0.50
1:B:181:HIS:O	1:B:184:SER:N	2.39	0.50
1:E:340:THR:O	1:E:344:GLN:HG3	2.11	0.50
1:E:357:ARG:O	1:E:358:GLU:C	2.46	0.50
1:F:209:PHE:CE2	1:F:254:VAL:HG21	2.46	0.50
1:G:256:GLU:HG2	1:G:299:ARG:HH11	1.76	0.50
1:G:336:VAL:HA	1:G:373:LYS:O	2.11	0.50
1:J:157:SER:OG	1:J:183:LEU:HB2	2.11	0.50
1:J:220:VAL:CG1	1:J:221:SER:H	2.25	0.50
1:K:209:PHE:CD1	1:K:209:PHE:N	2.79	0.50
1:L:181:HIS:HA	1:L:184:SER:OG	2.11	0.50
1:L:352:TRP:CZ3	1:L:358:GLU:HG2	2.46	0.50
1:N:145:LYS:HA	1:N:148:GLU:CG	2.36	0.50
1:N:292:PHE:HZ	1:N:296:LEU:HD12	1.76	0.50
1:F:214:GLY:O	1:F:215:ALA:HB2	2.11	0.50
1:F:363:ILE:O	1:F:366:ALA:N	2.44	0.50
1:H:149:ILE:O	1:H:153:ILE:HG12	2.11	0.50
1:H:170:GLY:O	1:H:355:ASN:HB2	2.12	0.50
1:J:143:SER:CB	1:J:144:PRO:HD2	2.40	0.50
1:J:157:SER:O	1:J:184:SER:HA	2.12	0.50
1:L:283:ILE:HG21	1:L:297:TYR:CD1	2.46	0.50
1:L:328:PHE:O	1:L:332:TYR:HD1	1.94	0.50
1:L:358:GLU:O	1:L:362:VAL:HG23	2.11	0.50
1:M:143:SER:CB	1:M:144:PRO:CD	2.85	0.50
1:M:209:PHE:HE2	1:M:227:PHE:HE1	1.59	0.50
1:M:251:LEU:HD22	1:M:255:ILE:HG13	1.93	0.50
1:M:346:LEU:HD12	1:M:380:LEU:HB3	1.93	0.50
1:N:311:ARG:HG3	1:N:311:ARG:NH1	2.25	0.50
1:B:249:ALA:CB	1:B:293:ARG:HH11	2.25	0.50
1:B:310:LEU:CD1	1:B:359:LEU:HD12	2.41	0.50
1:D:186:ARG:HD3	1:D:233:GLY:HA2	1.93	0.50
1:D:315:GLU:N	1:D:315:GLU:OE1	2.41	0.50
1:F:223:LYS:CG	1:F:223:LYS:O	2.59	0.50
1:G:167:GLY:H	1:G:173:LYS:HD3	1.76	0.50
1:G:178:ARG:HA	1:G:191:PHE:CE1	2.42	0.50
1:H:230:ALA:O	1:H:273:VAL:HG22	2.11	0.50
1:K:186:ARG:HB2	1:K:189:GLU:HB2	1.94	0.50
1:M:145:LYS:HD2	1:M:308:PRO:HG3	1.92	0.50
1:N:211:TYR:CZ	1:N:223:LYS:HB2	2.46	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:THR:HB	1:B:306:GLU:OE2	2.11	0.50
1:C:309:PRO:HB2	1:C:311:ARG:NH1	2.26	0.50
1:C:347:LEU:HD21	1:C:380:LEU:HD12	1.92	0.50
1:E:176:VAL:C	1:E:180:ILE:CD1	2.80	0.50
1:E:191:PHE:HD1	1:E:234:THR:HB	1.75	0.50
1:F:310:LEU:O	1:F:312:GLU:N	2.41	0.50
1:G:154:LYS:O	1:G:157:SER:OG	2.18	0.50
1:H:255:ILE:CG1	1:H:275:ILE:HD13	2.34	0.50
1:K:227:PHE:CE2	1:K:254:VAL:HG11	2.47	0.50
1:M:254:VAL:CG2	1:M:260:PHE:HB3	2.42	0.50
1:N:181:HIS:HD2	1:N:234:THR:CB	2.24	0.50
1:F:179:LEU:O	1:F:183:LEU:HG	2.12	0.50
1:H:302:VAL:O	1:I:365:ARG:HG3	2.11	0.50
1:H:171:VAL:HB	1:H:307:ILE:CG2	2.41	0.50
1:I:194:LEU:HD22	1:I:235:LEU:HD11	1.93	0.50
1:K:267:LYS:O	1:K:269:ILE:HD12	2.12	0.50
1:K:355:ASN:O	1:K:356:VAL:C	2.50	0.50
1:N:274:ARG:HG2	1:N:274:ARG:NH1	2.24	0.50
1:A:213:LYS:HG2	1:A:221:SER:N	2.27	0.50
1:B:381:SER:O	1:B:382:CYS:C	2.49	0.50
1:D:189:GLU:CB	1:D:190:PRO:HD2	2.42	0.50
1:D:342:SER:OG	1:D:377:ARG:HB2	2.11	0.50
1:G:191:PHE:C	1:G:191:PHE:HD2	2.15	0.50
1:G:224:GLU:CG	1:G:225:GLY:H	2.18	0.50
1:H:349:SER:HB2	1:H:350:TYR:CD1	2.46	0.50
1:I:189:GLU:OE1	1:I:190:PRO:HD3	2.11	0.50
1:I:311:ARG:HG2	1:I:311:ARG:HH11	1.77	0.50
1:I:365:ARG:CD	1:I:383:LEU:HD22	2.42	0.50
1:K:237:LEU:CB	1:K:240:ILE:HD11	2.41	0.50
1:L:211:TYR:CD1	1:L:211:TYR:N	2.78	0.50
1:L:303:ILE:O	1:L:303:ILE:HG22	2.12	0.50
1:L:334:LYS:HD2	1:L:336:VAL:CG2	2.42	0.50
1:N:149:ILE:O	1:N:153:ILE:HG12	2.11	0.50
1:M:299:ARG:CD	1:N:357:ARG:HH21	2.24	0.50
1:C:194:LEU:CD2	1:C:194:LEU:N	2.68	0.50
1:C:262:ARG:O	1:C:263:LEU:C	2.48	0.50
1:D:146:MET:HA	1:D:146:MET:HE3	1.93	0.50
1:E:280:ASN:OD1	1:E:280:ASN:O	2.30	0.50
1:E:378:GLY:O	1:E:381:SER:OG	2.15	0.50
1:H:164:LEU:HD21	1:H:283:ILE:CD1	2.41	0.50
1:H:292:PHE:HE2	1:H:296:LEU:HB3	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:153:ILE:HD12	1:J:180:ILE:HG12	1.93	0.50
1:L:362:VAL:O	1:L:365:ARG:HB3	2.12	0.50
1:M:359:LEU:O	1:M:360:LYS:C	2.50	0.50
1:N:325:LEU:O	1:N:329:SER:HB2	2.12	0.50
1:A:189:GLU:HG2	1:A:232:GLY:O	2.12	0.50
1:C:243:LEU:CD1	1:C:251:LEU:HD12	2.41	0.50
1:D:250:LYS:O	1:D:254:VAL:HG23	2.12	0.50
1:F:309:PRO:O	1:F:313:ARG:HD3	2.12	0.50
1:I:296:LEU:HD21	1:I:300:LEU:HD12	1.94	0.50
1:L:319:PRO:O	1:L:322:ASN:HB2	2.11	0.50
1:L:324:PHE:CE2	1:L:360:LYS:HE2	2.47	0.50
1:N:194:LEU:HD21	1:N:237:LEU:HD23	1.93	0.50
1:N:245:LEU:HB2	1:N:246:GLU:OE2	2.12	0.50
1:A:339:PHE:H	1:A:339:PHE:HD1	1.55	0.50
1:A:375:ILE:HG22	1:A:380:LEU:HD23	1.93	0.50
1:C:284:LYS:HG3	1:C:285:GLU:N	2.26	0.50
1:C:325:LEU:HD23	1:C:326:LYS:N	2.26	0.50
1:D:240:ILE:HG13	1:D:277:ALA:CB	2.29	0.50
1:D:166:THR:HG22	1:D:279:THR:HG22	1.94	0.50
1:D:381:SER:HA	1:D:384:VAL:O	2.12	0.50
1:F:195:ASN:HB3	1:F:198:SER:OG	2.11	0.50
1:H:156:ILE:HG22	1:H:274:ARG:HH22	1.76	0.50
1:K:161:CYS:N	1:K:274:ARG:HH12	2.10	0.50
1:L:181:HIS:O	1:L:184:SER:OG	2.27	0.50
1:L:164:LEU:CD1	1:L:278:ALA:HA	2.41	0.50
1:N:146:MET:HE1	1:N:307:ILE:HG23	1.88	0.50
1:N:157:SER:HB3	1:N:184:SER:CA	2.41	0.50
1:C:179:LEU:O	1:C:179:LEU:HD23	2.12	0.49
1:E:150:LEU:O	1:E:154:LYS:HG3	2.12	0.49
1:E:179:LEU:C	1:E:181:HIS:H	2.16	0.49
1:G:148:GLU:O	1:G:150:LEU:N	2.45	0.49
1:G:233:GLY:O	1:G:273:VAL:HG13	2.11	0.49
1:I:253:ARG:CD	1:J:198:SER:HB2	2.42	0.49
1:K:267:LYS:HD2	1:K:267:LYS:N	2.26	0.49
1:K:230:ALA:O	1:K:273:VAL:HG22	2.12	0.49
1:M:347:LEU:HD21	1:M:380:LEU:CD1	2.42	0.49
1:N:340:THR:O	1:N:344:GLN:N	2.34	0.49
1:B:206:ALA:O	1:B:210:GLY:N	2.44	0.49
1:D:239:GLU:HA	1:D:279:THR:HA	1.94	0.49
1:D:275:ILE:O	1:D:276:LEU:HD23	2.12	0.49
1:D:365:ARG:HD2	1:D:383:LEU:HD22	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:LEU:O	1:D:384:VAL:N	2.43	0.49
1:E:159:ALA:O	1:E:274:ARG:NH1	2.45	0.49
1:F:138:GLU:HG3	1:F:139:TYR:H	1.76	0.49
1:H:171:VAL:HB	1:H:307:ILE:HG22	1.94	0.49
1:H:322:ASN:O	1:H:326:LYS:HG3	2.12	0.49
1:I:208:LEU:C	1:I:208:LEU:CD2	2.81	0.49
1:K:156:ILE:O	1:K:159:ALA:N	2.41	0.49
1:K:359:LEU:HD23	1:K:363:ILE:HG13	1.94	0.49
1:L:140:VAL:CG1	1:L:140:VAL:O	2.56	0.49
1:M:212:GLU:CB	1:M:264:GLY:HA3	2.42	0.49
1:M:342:SER:O	1:M:377:ARG:HD2	2.12	0.49
1:D:171:VAL:HG23	1:D:172:GLY:N	2.27	0.49
1:F:314:LYS:HA	1:F:317:ILE:CG1	2.41	0.49
1:F:327:LYS:O	1:F:330:ARG:N	2.46	0.49
1:G:299:ARG:O	1:G:302:VAL:HG23	2.12	0.49
1:G:365:ARG:HH11	1:G:383:LEU:HD22	1.77	0.49
1:G:381:SER:C	1:G:383:LEU:H	2.15	0.49
1:H:178:ARG:HH11	1:H:178:ARG:HG3	1.77	0.49
1:H:328:PHE:HB3	1:H:367:VAL:HG21	1.93	0.49
1:K:144:PRO:C	1:K:146:MET:H	2.16	0.49
1:L:236:PHE:HA	1:L:276:LEU:O	2.12	0.49
1:A:365:ARG:NH2	1:G:302:VAL:O	2.44	0.49
1:F:172:GLY:HA2	2:F:4:ADP:O1A	2.11	0.49
1:G:153:ILE:HG23	1:G:180:ILE:CG1	2.42	0.49
1:G:194:LEU:CD2	1:G:237:LEU:HD22	2.42	0.49
1:H:142:GLU:HB3	1:H:146:MET:CB	2.43	0.49
1:H:237:LEU:HB2	1:H:240:ILE:HD11	1.93	0.49
1:H:320:LEU:O	1:H:324:PHE:CD1	2.65	0.49
1:I:156:ILE:HG22	1:I:157:SER:N	2.28	0.49
1:K:255:ILE:HD11	1:K:300:LEU:HD21	1.93	0.49
1:L:164:LEU:HA	1:L:277:ALA:O	2.12	0.49
1:M:212:GLU:HB3	1:M:264:GLY:HA3	1.94	0.49
1:M:234:THR:HG22	1:M:235:LEU:N	2.28	0.49
1:M:252:LEU:CD1	1:M:299:ARG:HG3	2.42	0.49
1:M:227:PHE:HE2	1:M:273:VAL:HG21	1.71	0.49
1:N:181:HIS:HD2	1:N:234:THR:HB	1.76	0.49
1:B:142:GLU:O	1:B:143:SER:HB3	2.12	0.49
1:B:266:ARG:HB3	1:C:229:LEU:HD23	1.95	0.49
1:B:177:ALA:HB1	1:B:276:LEU:HD13	1.93	0.49
1:C:175:VAL:HG23	2:C:1:ADP:O1A	2.13	0.49
1:E:324:PHE:O	1:E:325:LEU:C	2.51	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ILE:O	1:E:366:ALA:HB3	2.12	0.49
1:F:366:ALA:O	1:F:369:PHE:N	2.45	0.49
1:G:324:PHE:CE1	1:G:360:LYS:HA	2.48	0.49
1:H:320:LEU:O	1:H:324:PHE:HD1	1.94	0.49
1:I:249:ALA:CB	1:I:293:ARG:NH1	2.75	0.49
1:I:251:LEU:O	1:I:254:VAL:N	2.45	0.49
1:L:158:CYS:O	1:L:158:CYS:SG	2.71	0.49
1:L:161:CYS:O	1:L:274:ARG:NE	2.45	0.49
1:L:379:GLU:C	1:L:381:SER:H	2.14	0.49
1:N:316:ASP:O	1:N:320:LEU:HG	2.12	0.49
1:A:192:VAL:HG21	1:A:229:LEU:HD12	1.94	0.49
1:B:157:SER:HB3	1:B:183:LEU:C	2.32	0.49
1:B:216:PHE:O	1:B:217:THR:C	2.50	0.49
1:C:341:LYS:O	1:C:345:GLU:HG3	2.12	0.49
1:D:262:ARG:O	1:D:263:LEU:C	2.51	0.49
1:F:225:GLY:O	1:F:226:PHE:C	2.51	0.49
1:J:324:PHE:O	1:J:327:LYS:HB3	2.13	0.49
1:L:208:LEU:C	1:L:208:LEU:HD23	2.33	0.49
1:L:320:LEU:O	1:L:321:ALA:C	2.50	0.49
1:L:347:LEU:N	1:L:347:LEU:HD23	2.28	0.49
1:M:173:LYS:HB2	2:M:12:ADP:O2B	2.12	0.49
1:M:207:GLU:O	1:M:226:PHE:CD1	2.56	0.49
1:M:265:GLY:HA2	1:N:203:ILE:HD11	1.94	0.49
1:M:359:LEU:O	1:M:363:ILE:HD13	2.12	0.49
1:N:200:PRO:O	1:N:202:ASP:N	2.46	0.49
1:N:239:GLU:O	1:N:240:ILE:C	2.51	0.49
1:A:143:SER:HA	1:A:315:GLU:HB2	1.93	0.49
1:A:168:GLU:O	1:A:171:VAL:HG22	2.13	0.49
1:A:244:SER:C	1:A:246:GLU:N	2.62	0.49
1:B:177:ALA:HA	1:B:180:ILE:HD12	1.93	0.49
1:B:328:PHE:CE1	1:B:364:GLU:HB2	2.47	0.49
1:C:171:VAL:HG21	1:C:307:ILE:HB	1.94	0.49
1:E:138:GLU:HB2	1:E:323:HIS:CD2	2.48	0.49
1:F:357:ARG:CG	1:F:357:ARG:NH1	2.75	0.49
1:G:192:VAL:O	1:G:235:LEU:HD12	2.13	0.49
1:G:248:GLN:OE1	1:G:292:PHE:HA	2.12	0.49
1:G:327:LYS:O	1:G:330:ARG:HB3	2.12	0.49
1:H:227:PHE:CE2	1:H:254:VAL:HG21	2.45	0.49
1:L:352:TRP:CZ3	1:L:362:VAL:HG21	2.47	0.49
1:M:171:VAL:HG12	1:M:309:PRO:HA	1.93	0.49
1:M:252:LEU:HD22	1:M:295:ASP:OD1	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:157:SER:HB3	1:N:183:LEU:C	2.32	0.49
1:C:321:ALA:HA	1:C:363:ILE:HD12	1.95	0.49
1:E:176:VAL:O	1:E:180:ILE:CG1	2.61	0.49
1:F:144:PRO:HG2	1:F:145:LYS:H	1.78	0.49
1:E:250:LYS:HG3	1:F:198:SER:O	2.12	0.49
1:F:310:LEU:HB2	1:F:355:ASN:HB3	1.94	0.49
1:H:143:SER:CA	1:H:147:LYS:HE3	2.38	0.49
1:H:198:SER:HB2	1:N:250:LYS:CG	2.43	0.49
1:J:149:ILE:O	1:J:153:ILE:HG12	2.13	0.49
1:J:157:SER:HB3	1:J:184:SER:HA	1.95	0.49
1:J:382:CYS:HB2	1:J:383:LEU:HD23	1.94	0.49
1:K:283:ILE:HG21	1:K:297:TYR:CD1	2.48	0.49
1:A:176:VAL:O	1:A:180:ILE:HG13	2.13	0.49
1:A:265:GLY:O	1:A:266:ARG:NE	2.43	0.49
1:A:377:ARG:HH21	1:L:285:GLU:CD	2.15	0.49
1:D:145:LYS:O	1:D:149:ILE:HG13	2.13	0.49
1:D:209:PHE:HE2	1:D:227:PHE:HE1	1.60	0.49
1:E:141:PHE:CG	1:E:150:LEU:HD22	2.48	0.49
1:E:156:ILE:HG13	1:E:303:ILE:HG21	1.95	0.49
1:G:191:PHE:CD2	1:G:191:PHE:C	2.86	0.49
1:G:267:LYS:HD3	1:G:267:LYS:O	2.12	0.49
1:H:244:SER:C	1:H:246:GLU:H	2.15	0.49
1:H:163:VAL:HB	1:H:276:LEU:HD23	1.94	0.49
1:I:194:LEU:HD21	1:I:235:LEU:HD11	1.94	0.49
1:I:310:LEU:O	1:I:312:GLU:N	2.46	0.49
1:K:298:TYR:O	1:K:300:LEU:N	2.45	0.49
1:L:194:LEU:HD21	1:L:237:LEU:CD2	2.40	0.49
1:L:225:GLY:O	1:L:228:GLU:N	2.30	0.49
1:L:283:ILE:HB	1:L:297:TYR:CE1	2.47	0.49
1:L:240:ILE:CG2	1:L:292:PHE:HE1	2.26	0.49
1:M:146:MET:CE	1:M:149:ILE:HD12	2.42	0.49
1:A:220:VAL:O	1:A:221:SER:CB	2.60	0.49
1:C:181:HIS:NE2	1:C:191:PHE:HB2	2.26	0.49
1:C:350:TYR:CG	1:C:351:PRO:HD2	2.47	0.49
1:D:230:ALA:O	1:D:231:ASP:C	2.51	0.49
1:E:309:PRO:HD2	1:E:312:GLU:OE1	2.13	0.49
1:G:163:VAL:HB	1:G:276:LEU:HD22	1.94	0.49
1:G:282:ASN:HD22	1:G:285:GLU:HB2	1.75	0.49
1:G:161:CYS:HB2	1:G:302:VAL:HG11	1.95	0.49
1:H:215:ALA:CB	1:I:223:LYS:NZ	2.76	0.49
1:K:213:LYS:NZ	1:K:220:VAL:HG13	2.28	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:365:ARG:HD2	1:K:383:LEU:CD2	2.42	0.49
1:L:164:LEU:HD12	1:L:165:ILE:H	1.77	0.49
1:L:272:ASN:C	1:L:272:ASN:HD22	2.16	0.49
1:L:144:PRO:HD3	1:L:315:GLU:OE2	2.13	0.49
1:A:178:ARG:HE	1:A:191:PHE:HE2	1.58	0.48
1:B:157:SER:OG	1:B:183:LEU:HB2	2.13	0.48
1:B:362:VAL:HG13	1:B:384:VAL:CG2	2.32	0.48
1:C:256:GLU:HG2	1:C:299:ARG:NH2	2.28	0.48
1:C:311:ARG:NH2	1:C:353:TYR:HD2	2.11	0.48
1:E:146:MET:HA	1:E:146:MET:HE3	1.95	0.48
1:H:240:ILE:HG22	1:H:292:PHE:HE1	1.78	0.48
1:I:269:ILE:HD12	1:I:269:ILE:H	1.77	0.48
1:L:192:VAL:HG21	1:L:230:ALA:HB2	1.95	0.48
1:L:254:VAL:HG22	1:L:260:PHE:HB3	1.95	0.48
1:M:162:PRO:HG2	1:M:302:VAL:CG2	2.42	0.48
1:N:168:GLU:OE1	1:N:311:ARG:NH2	2.45	0.48
1:N:352:TRP:CZ3	1:N:358:GLU:HG2	2.48	0.48
1:N:357:ARG:HH12	1:N:361:ASN:HD21	1.60	0.48
1:B:235:LEU:HG	1:B:237:LEU:CD2	2.43	0.48
1:B:256:GLU:HG2	1:B:299:ARG:HD3	1.95	0.48
1:C:179:LEU:HD23	1:C:183:LEU:HG	1.95	0.48
1:C:186:ARG:NH1	1:C:232:GLY:O	2.46	0.48
1:E:157:SER:HB3	1:E:183:LEU:C	2.32	0.48
1:F:217:THR:HG22	1:F:218:GLY:N	2.28	0.48
1:F:253:ARG:HH11	1:F:253:ARG:HG3	1.78	0.48
1:F:299:ARG:HE	1:F:299:ARG:CA	2.25	0.48
1:F:324:PHE:HB2	1:F:363:ILE:HD12	1.95	0.48
1:J:328:PHE:CD2	1:J:364:GLU:HG3	2.48	0.48
1:L:171:VAL:CG2	1:L:307:ILE:CG2	2.90	0.48
1:M:304:GLU:HA	1:M:304:GLU:OE2	2.13	0.48
1:M:310:LEU:HD12	1:M:355:ASN:HA	1.96	0.48
1:N:140:VAL:HG11	1:N:320:LEU:CD2	2.41	0.48
1:N:359:LEU:HD23	1:N:363:ILE:CD1	2.43	0.48
1:C:177:ALA:O	1:C:180:ILE:HB	2.13	0.48
1:D:262:ARG:HH11	1:D:262:ARG:CG	1.98	0.48
1:E:149:ILE:O	1:E:151:GLU:N	2.46	0.48
1:E:153:ILE:HD11	1:E:176:VAL:HG13	1.96	0.48
1:E:346:LEU:HA	1:E:349:SER:OG	2.13	0.48
1:G:376:ASP:O	1:G:378:GLY:N	2.46	0.48
1:H:181:HIS:O	1:H:187:SER:HB3	2.13	0.48
1:H:239:GLU:N	1:H:278:ALA:O	2.46	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:262:ARG:HG3	1:H:269:ILE:HD12	1.95	0.48
1:K:206:ALA:HB1	1:K:211:TYR:HD1	1.78	0.48
1:L:266:ARG:C	1:L:267:LYS:HG2	2.34	0.48
1:A:240:ILE:O	1:A:242:GLU:N	2.46	0.48
1:A:331:LYS:HD3	1:A:332:TYR:CZ	2.48	0.48
1:B:216:PHE:CD1	1:B:217:THR:HG22	2.49	0.48
1:B:334:LYS:HG3	1:B:367:VAL:O	2.13	0.48
1:C:149:ILE:O	1:C:153:ILE:HG12	2.12	0.48
1:C:244:SER:O	1:C:248:GLN:CG	2.60	0.48
1:C:326:LYS:HE2	1:C:330:ARG:NH2	2.28	0.48
1:E:253:ARG:HG3	1:E:253:ARG:NH1	2.27	0.48
1:E:234:THR:HG23	1:E:274:ARG:O	2.13	0.48
1:G:310:LEU:HD11	1:G:359:LEU:HD12	1.96	0.48
1:H:209:PHE:O	1:H:262:ARG:HG2	2.13	0.48
1:I:284:LYS:HE2	1:I:297:TYR:HH	1.74	0.48
1:I:146:MET:SD	1:I:313:ARG:NE	2.86	0.48
1:J:281:ARG:NH1	1:J:281:ARG:HG2	2.28	0.48
1:L:165:ILE:O	1:L:165:ILE:HG22	2.13	0.48
1:M:283:ILE:HG22	1:M:284:LYS:N	2.28	0.48
1:M:324:PHE:CE2	1:M:360:LYS:HG3	2.47	0.48
1:N:296:LEU:O	1:N:300:LEU:HG	2.13	0.48
1:A:204:PHE:CE2	1:A:243:LEU:HD21	2.45	0.48
1:D:294:GLU:O	1:D:297:TYR:HB3	2.12	0.48
1:E:173:LYS:HB2	2:E:3:ADP:O1B	2.13	0.48
1:E:230:ALA:O	1:E:273:VAL:HG22	2.12	0.48
1:F:149:ILE:O	1:F:153:ILE:HG12	2.13	0.48
1:G:145:LYS:O	1:G:149:ILE:HG13	2.13	0.48
1:I:328:PHE:HZ	1:I:360:LYS:HG3	1.78	0.48
1:K:240:ILE:HG13	1:K:277:ALA:CB	2.42	0.48
1:N:209:PHE:CE1	1:N:250:LYS:HD3	2.48	0.48
1:B:318:ILE:O	1:B:322:ASN:ND2	2.46	0.48
1:D:212:GLU:HA	1:D:222:SER:HB2	1.94	0.48
1:D:252:LEU:HD11	1:D:299:ARG:HG3	1.96	0.48
1:E:380:LEU:O	1:E:384:VAL:HB	2.13	0.48
1:F:156:ILE:O	1:F:159:ALA:N	2.46	0.48
1:F:254:VAL:HG22	1:F:260:PHE:HB3	1.96	0.48
1:F:380:LEU:N	1:F:380:LEU:CD2	2.77	0.48
1:G:148:GLU:O	1:G:151:GLU:N	2.46	0.48
1:G:235:LEU:HB2	1:G:273:VAL:HG11	1.96	0.48
1:G:234:THR:HG21	1:G:276:LEU:HD12	1.95	0.48
1:G:310:LEU:HG	1:G:356:VAL:CG2	2.44	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:168:GLU:CG	1:H:311:ARG:HH22	2.20	0.48
1:K:177:ALA:HB1	1:K:276:LEU:CD1	2.44	0.48
1:L:143:SER:O	1:L:147:LYS:HB2	2.13	0.48
1:L:210:GLY:O	1:L:263:LEU:HB2	2.13	0.48
1:N:157:SER:OG	1:N:183:LEU:HB2	2.13	0.48
1:N:245:LEU:CD2	1:N:293:ARG:HG3	2.38	0.48
1:A:171:VAL:HB	1:A:307:ILE:CG2	2.43	0.48
1:A:311:ARG:HB3	1:A:351:PRO:O	2.13	0.48
1:A:376:ASP:O	1:A:377:ARG:C	2.51	0.48
1:B:162:PRO:HB2	1:B:300:LEU:HD23	1.96	0.48
1:D:236:PHE:O	1:D:236:PHE:CD1	2.67	0.48
1:F:179:LEU:HD23	1:F:179:LEU:O	2.14	0.48
1:F:193:ALA:HB1	1:F:236:PHE:HD2	1.78	0.48
1:F:206:ALA:O	1:F:210:GLY:CA	2.62	0.48
1:F:283:ILE:HG21	1:F:297:TYR:CD1	2.49	0.48
1:G:181:HIS:ND1	1:G:181:HIS:C	2.66	0.48
1:G:240:ILE:HG13	1:G:277:ALA:CB	2.33	0.48
1:K:252:LEU:HD11	1:K:299:ARG:HG3	1.96	0.48
1:K:313:ARG:O	1:K:315:GLU:N	2.47	0.48
1:L:211:TYR:HD1	1:L:211:TYR:N	2.12	0.48
1:L:289:GLU:HG2	1:L:289:GLU:O	2.14	0.48
1:L:329:SER:HA	1:L:334:LYS:CE	2.26	0.48
1:L:324:PHE:HE2	1:L:360:LYS:HE2	1.79	0.48
1:M:194:LEU:HD23	1:M:194:LEU:H	1.78	0.48
1:M:209:PHE:HE2	1:M:227:PHE:CE1	2.32	0.48
1:M:248:GLN:H	1:M:248:GLN:NE2	2.11	0.48
1:N:173:LYS:HB2	2:N:13:ADP:O2B	2.14	0.48
1:A:256:GLU:OE2	1:B:357:ARG:NH1	2.47	0.48
1:B:314:LYS:N	1:B:314:LYS:CD	2.74	0.48
1:B:335:GLU:O	1:B:373:LYS:HA	2.13	0.48
1:C:282:ASN:O	1:C:284:LYS:N	2.47	0.48
1:D:308:PRO:O	1:D:313:ARG:CD	2.62	0.48
1:D:328:PHE:CD2	1:D:364:GLU:HG3	2.48	0.48
1:D:362:VAL:O	1:D:362:VAL:CG1	2.59	0.48
1:E:170:GLY:O	1:E:355:ASN:HB2	2.14	0.48
1:E:299:ARG:HE	1:E:299:ARG:HA	1.79	0.48
1:F:244:SER:O	1:F:248:GLN:HG3	2.14	0.48
1:G:167:GLY:N	1:G:173:LYS:HD3	2.29	0.48
1:G:191:PHE:CE2	1:G:236:PHE:HB3	2.45	0.48
1:G:251:LEU:HD22	1:G:255:ILE:HD11	1.95	0.48
1:G:261:TYR:CD2	1:G:263:LEU:O	2.67	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:SER:C	1:H:246:GLU:N	2.67	0.48
1:I:365:ARG:HD2	1:I:383:LEU:HD22	1.96	0.48
1:K:325:LEU:HD23	1:K:325:LEU:O	2.12	0.48
1:M:259:LYS:HD2	1:M:268:GLU:OE2	2.12	0.48
1:N:294:GLU:O	1:N:297:TYR:N	2.47	0.48
1:D:275:ILE:HG22	1:D:276:LEU:N	2.29	0.48
1:E:174:GLU:O	1:E:175:VAL:C	2.51	0.48
1:I:143:SER:O	1:I:147:LYS:HG3	2.13	0.48
1:I:319:PRO:O	1:I:320:LEU:C	2.51	0.48
1:K:283:ILE:O	1:K:287:VAL:HG23	2.13	0.48
1:L:269:ILE:N	1:L:269:ILE:HD12	2.28	0.48
1:M:302:VAL:O	1:M:303:ILE:HD13	2.13	0.48
1:N:227:PHE:CE2	1:N:235:LEU:HD23	2.47	0.48
1:N:231:ASP:OD1	1:N:271:VAL:HB	2.14	0.48
1:N:296:LEU:O	1:N:296:LEU:HD13	2.14	0.48
1:A:176:VAL:HG21	1:A:307:ILE:CD1	2.44	0.48
1:A:194:LEU:N	1:A:194:LEU:CD2	2.76	0.48
1:A:377:ARG:NH2	1:L:285:GLU:HG2	2.26	0.48
1:E:177:ALA:HB1	1:E:276:LEU:CD1	2.43	0.48
1:E:227:PHE:O	1:E:228:GLU:C	2.52	0.48
1:E:336:VAL:HG21	1:E:370:SER:CB	2.44	0.48
1:F:224:GLU:O	1:F:225:GLY:O	2.31	0.48
1:F:249:ALA:HB2	1:F:293:ARG:HH11	1.79	0.48
1:G:164:LEU:C	1:G:164:LEU:HD12	2.35	0.48
1:H:329:SER:N	1:H:367:VAL:HG11	2.29	0.48
1:L:164:LEU:HD12	1:L:165:ILE:N	2.29	0.48
1:N:240:ILE:HA	1:N:243:LEU:HD12	1.96	0.48
1:N:283:ILE:O	1:N:284:LYS:C	2.52	0.48
1:N:352:TRP:HZ3	1:N:358:GLU:HG2	1.78	0.48
1:A:199:ILE:HG22	1:A:200:PRO:O	2.14	0.47
1:A:227:PHE:HD2	1:A:273:VAL:HG21	1.79	0.47
1:C:283:ILE:O	1:C:286:LEU:N	2.34	0.47
1:C:309:PRO:HG3	1:C:311:ARG:HH11	1.79	0.47
1:C:330:ARG:O	1:C:333:ALA:N	2.43	0.47
1:D:292:PHE:HD2	1:D:293:ARG:O	1.97	0.47
1:D:321:ALA:HA	1:D:363:ILE:HD12	1.96	0.47
1:D:344:GLN:O	1:D:347:LEU:HB2	2.14	0.47
1:F:224:GLU:O	1:F:228:GLU:HB2	2.13	0.47
1:F:358:GLU:O	1:F:362:VAL:HG23	2.14	0.47
1:H:141:PHE:O	1:H:142:GLU:HG3	2.14	0.47
1:H:346:LEU:HD12	1:H:377:ARG:NE	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:165:ILE:HB	1:I:278:ALA:CB	2.42	0.47
1:K:149:ILE:HD13	1:K:307:ILE:HD13	1.96	0.47
1:L:165:ILE:H	1:L:278:ALA:CB	2.19	0.47
1:M:316:ASP:O	1:M:319:PRO:HD2	2.14	0.47
1:N:282:ASN:ND2	1:N:284:LYS:HB2	2.29	0.47
1:A:208:LEU:HD22	1:A:209:PHE:CZ	2.49	0.47
1:B:186:ARG:O	1:B:188:LYS:N	2.47	0.47
1:B:181:HIS:CE1	1:B:191:PHE:HB2	2.49	0.47
1:B:235:LEU:CD2	1:B:237:LEU:HD21	2.43	0.47
1:E:350:TYR:CE2	1:E:352:TRP:HA	2.49	0.47
1:F:242:GLU:CD	1:F:281:ARG:HH22	2.18	0.47
1:G:155:LYS:O	1:G:157:SER:N	2.47	0.47
1:G:234:THR:HG22	1:G:235:LEU:N	2.28	0.47
1:H:332:TYR:CG	1:H:332:TYR:O	2.68	0.47
1:I:165:ILE:CG2	1:I:173:LYS:HG2	2.41	0.47
1:I:208:LEU:O	1:I:226:PHE:N	2.47	0.47
1:J:263:LEU:HD23	1:J:264:GLY:N	2.29	0.47
1:J:325:LEU:O	1:J:327:LYS:N	2.47	0.47
1:L:150:LEU:O	1:L:150:LEU:HD22	2.14	0.47
1:L:300:LEU:O	1:L:302:VAL:N	2.47	0.47
1:M:316:ASP:C	1:M:319:PRO:HD2	2.34	0.47
1:N:179:LEU:HD23	1:N:183:LEU:HG	1.96	0.47
1:N:272:ASN:CG	1:N:272:ASN:O	2.51	0.47
1:A:172:GLY:O	1:A:174:GLU:N	2.47	0.47
1:A:379:GLU:H	1:A:379:GLU:CD	2.17	0.47
1:F:193:ALA:CB	1:F:236:PHE:HB3	2.44	0.47
1:G:181:HIS:HD2	1:G:234:THR:OG1	1.97	0.47
1:H:248:GLN:O	1:H:250:LYS:N	2.47	0.47
1:H:316:ASP:O	1:H:320:LEU:HG	2.14	0.47
1:D:271:VAL:CG2	1:D:273:VAL:HG23	2.43	0.47
1:F:196:VAL:HG22	1:F:204:PHE:HZ	1.79	0.47
1:F:354:GLY:O	1:F:355:ASN:C	2.53	0.47
1:I:296:LEU:C	1:I:296:LEU:HD23	2.34	0.47
1:L:362:VAL:HA	1:L:365:ARG:HH21	1.79	0.47
1:N:192:VAL:O	1:N:235:LEU:HD12	2.15	0.47
1:A:236:PHE:HE1	1:A:278:ALA:HB3	1.78	0.47
1:B:174:GLU:HG2	1:B:178:ARG:HD3	1.96	0.47
1:B:229:LEU:C	1:B:229:LEU:CD1	2.83	0.47
1:C:213:LYS:HG2	1:C:214:GLY:N	2.29	0.47
1:C:156:ILE:CD1	1:C:303:ILE:HG21	2.45	0.47
1:E:227:PHE:O	1:E:230:ALA:N	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:311:ARG:HG2	1:E:351:PRO:O	2.14	0.47
1:F:149:ILE:HD13	1:F:307:ILE:CD1	2.42	0.47
1:G:209:PHE:CZ	1:G:250:LYS:HB3	2.50	0.47
1:H:369:PHE:CD1	1:H:369:PHE:N	2.82	0.47
1:K:160:GLU:OE1	1:K:160:GLU:O	2.32	0.47
1:K:343:ALA:O	1:K:347:LEU:HG	2.14	0.47
1:L:203:ILE:O	1:L:206:ALA:HB3	2.15	0.47
1:L:305:ILE:HG22	1:L:305:ILE:O	2.15	0.47
1:M:234:THR:CG2	1:M:276:LEU:HD23	2.45	0.47
1:C:240:ILE:CD1	1:C:243:LEU:HD12	2.44	0.47
1:C:314:LYS:HA	1:C:317:ILE:CD1	2.45	0.47
1:C:318:ILE:HG12	1:C:318:ILE:H	1.43	0.47
1:D:292:PHE:C	1:D:292:PHE:HD2	2.18	0.47
1:F:239:GLU:HA	1:F:278:ALA:O	2.14	0.47
1:F:328:PHE:CE1	1:F:364:GLU:HB2	2.50	0.47
1:H:325:LEU:HD23	1:H:363:ILE:HG23	1.97	0.47
1:N:372:GLY:O	1:N:374:PHE:N	2.47	0.47
1:A:350:TYR:HD2	1:A:352:TRP:CD2	2.33	0.47
1:B:384:VAL:O	1:B:384:VAL:HG12	2.14	0.47
1:C:177:ALA:O	1:C:180:ILE:N	2.47	0.47
1:E:205:GLU:CB	1:E:263:LEU:HD11	2.45	0.47
1:G:262:ARG:O	1:G:263:LEU:HB3	2.15	0.47
1:H:204:PHE:O	1:H:206:ALA:N	2.48	0.47
1:H:207:GLU:CD	1:N:266:ARG:HH22	2.17	0.47
1:I:152:LYS:O	1:I:153:ILE:C	2.53	0.47
1:I:258:GLY:O	1:I:270:GLU:HG3	2.14	0.47
1:J:296:LEU:HD13	1:J:296:LEU:C	2.35	0.47
1:K:306:GLU:O	1:K:308:PRO:HD3	2.15	0.47
1:K:321:ALA:HB1	1:K:339:PHE:CZ	2.49	0.47
1:K:321:ALA:HA	1:K:363:ILE:HD12	1.95	0.47
1:L:300:LEU:C	1:L:302:VAL:H	2.18	0.47
1:N:251:LEU:HD21	1:N:255:ILE:HD11	1.95	0.47
1:B:181:HIS:ND1	1:B:191:PHE:HB2	2.30	0.47
1:B:336:VAL:HG13	1:B:373:LYS:O	2.15	0.47
1:C:202:ASP:C	1:C:203:ILE:HD13	2.35	0.47
1:C:212:GLU:O	1:C:215:ALA:HB2	2.13	0.47
1:C:300:LEU:HD23	1:C:300:LEU:N	2.30	0.47
1:D:251:LEU:HD13	1:D:296:LEU:HD21	1.96	0.47
1:E:298:TYR:CE1	1:F:354:GLY:HA2	2.50	0.47
1:H:196:VAL:HG22	1:H:204:PHE:CZ	2.50	0.47
1:H:356:VAL:O	1:H:357:ARG:C	2.52	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:214:GLY:HA2	1:K:219:ALA:O	2.15	0.47
1:L:149:ILE:HG22	1:L:150:LEU:N	2.28	0.47
1:L:299:ARG:O	1:L:302:VAL:HG23	2.15	0.47
1:M:209:PHE:CE1	1:M:250:LYS:HB3	2.50	0.47
1:A:328:PHE:HB2	1:A:367:VAL:HG21	1.97	0.47
1:B:339:PHE:CE2	1:B:347:LEU:HD11	2.50	0.47
1:C:296:LEU:O	1:C:297:TYR:C	2.53	0.47
1:E:157:SER:OG	1:E:183:LEU:HB2	2.15	0.47
1:E:301:GLY:HA2	1:E:304:GLU:HG2	1.96	0.47
1:E:320:LEU:O	1:E:323:HIS:N	2.48	0.47
1:H:194:LEU:HD21	1:H:237:LEU:CD2	2.34	0.47
1:H:328:PHE:HB3	1:H:367:VAL:HG11	1.96	0.47
1:J:211:TYR:OH	1:J:223:LYS:HD3	2.14	0.47
1:J:280:ASN:OD1	1:J:281:ARG:HD3	2.15	0.47
1:K:178:ARG:NE	1:K:191:PHE:HE2	2.13	0.47
1:K:213:LYS:CD	1:K:220:VAL:O	2.52	0.47
1:N:244:SER:O	1:N:245:LEU:C	2.51	0.47
1:B:144:PRO:HD3	1:B:315:GLU:CD	2.35	0.47
1:C:181:HIS:HD2	1:C:191:PHE:CG	2.31	0.47
1:C:211:TYR:HD1	1:C:211:TYR:C	2.18	0.47
1:D:157:SER:C	1:D:159:ALA:N	2.68	0.47
1:D:157:SER:O	1:D:159:ALA:N	2.47	0.47
1:D:292:PHE:C	1:D:292:PHE:CD2	2.88	0.47
1:E:251:LEU:O	1:E:255:ILE:HG13	2.14	0.47
1:E:316:ASP:O	1:E:317:ILE:C	2.53	0.47
1:E:325:LEU:HD13	1:E:338:GLY:HA2	1.96	0.47
1:F:383:LEU:HB2	1:F:384:VAL:H	1.59	0.47
1:G:211:TYR:HB2	1:G:223:LYS:HB2	1.96	0.47
1:H:224:GLU:HG3	1:H:262:ARG:NH2	2.30	0.47
1:H:328:PHE:O	1:H:332:TYR:HB3	2.15	0.47
1:I:166:THR:HB	1:I:306:GLU:OE2	2.15	0.47
1:J:227:PHE:CE2	1:J:254:VAL:HG11	2.50	0.47
1:K:200:PRO:HG2	1:K:203:ILE:HG13	1.97	0.47
1:M:275:ILE:HD12	1:M:275:ILE:H	1.80	0.47
1:A:180:ILE:O	1:A:180:ILE:CG2	2.63	0.47
1:B:149:ILE:O	1:B:153:ILE:HG12	2.15	0.47
1:D:237:LEU:N	1:D:237:LEU:HD23	2.30	0.47
1:C:303:ILE:CD1	1:D:365:ARG:HG3	2.45	0.47
1:E:243:LEU:HB3	1:E:248:GLN:HG3	1.97	0.47
1:F:174:GLU:OE2	1:F:178:ARG:NH1	2.35	0.47
1:F:380:LEU:HD23	1:F:380:LEU:H	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:224:GLU:HA	1:G:262:ARG:NH1	2.30	0.47
1:G:240:ILE:O	1:G:242:GLU:N	2.48	0.47
1:G:244:SER:O	1:G:248:GLN:HG3	2.15	0.47
1:H:196:VAL:HG12	1:H:242:GLU:HB3	1.97	0.47
1:I:192:VAL:HG21	1:I:230:ALA:HB2	1.96	0.47
1:I:283:ILE:HG21	1:I:297:TYR:HD1	1.80	0.47
1:J:365:ARG:HD2	1:J:383:LEU:HD13	1.96	0.47
1:K:176:VAL:HG21	1:K:307:ILE:CD1	2.45	0.47
1:K:209:PHE:CZ	1:K:250:LYS:HB3	2.50	0.47
1:M:206:ALA:HB2	1:M:216:PHE:HZ	1.80	0.47
1:M:252:LEU:O	1:M:253:ARG:C	2.53	0.47
1:A:377:ARG:NE	1:L:285:GLU:OE1	2.48	0.46
1:B:150:LEU:O	1:B:154:LYS:HG3	2.15	0.46
1:B:204:PHE:O	1:B:207:GLU:N	2.47	0.46
1:B:283:ILE:HG21	1:B:297:TYR:CD1	2.50	0.46
1:B:328:PHE:HD1	1:B:363:ILE:HG22	1.81	0.46
1:C:165:ILE:O	1:C:278:ALA:HB1	2.16	0.46
1:C:194:LEU:HD22	1:C:235:LEU:HD11	1.97	0.46
1:C:284:LYS:HG3	1:C:285:GLU:H	1.80	0.46
1:C:288:LYS:C	1:C:290:GLY:H	2.18	0.46
1:C:381:SER:C	1:C:383:LEU:H	2.18	0.46
1:D:235:LEU:CD1	1:D:237:LEU:HD23	2.38	0.46
1:D:252:LEU:HA	1:D:255:ILE:HD12	1.96	0.46
1:G:181:HIS:ND1	1:G:181:HIS:O	2.47	0.46
1:G:251:LEU:HD22	1:G:255:ILE:HG13	1.96	0.46
1:G:318:ILE:CB	1:G:319:PRO:HD3	2.44	0.46
1:G:352:TRP:CZ3	1:G:359:LEU:HA	2.49	0.46
1:H:216:PHE:CD2	1:H:216:PHE:O	2.68	0.46
1:L:334:LYS:HZ3	1:L:367:VAL:HG11	1.76	0.46
1:M:251:LEU:O	1:M:252:LEU:C	2.54	0.46
1:M:353:TYR:O	1:M:355:ASN:ND2	2.48	0.46
1:N:194:LEU:HD22	1:N:235:LEU:HD11	1.97	0.46
1:N:218:GLY:O	1:N:219:ALA:C	2.52	0.46
1:E:226:PHE:O	1:E:229:LEU:HB3	2.16	0.46
1:E:325:LEU:HD23	1:E:325:LEU:C	2.35	0.46
1:H:309:PRO:CB	1:H:311:ARG:HD2	2.45	0.46
1:K:303:ILE:HD11	1:L:368:LEU:CD1	2.44	0.46
1:L:161:CYS:HB2	1:L:162:PRO:HD2	1.97	0.46
1:L:244:SER:O	1:L:246:GLU:N	2.48	0.46
1:L:340:THR:O	1:L:344:GLN:HB2	2.16	0.46
1:M:156:ILE:HD11	1:M:303:ILE:HD12	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:314:LYS:HA	1:M:317:ILE:HG13	1.98	0.46
1:N:283:ILE:HG21	1:N:297:TYR:CD1	2.51	0.46
1:A:152:LYS:O	1:A:156:ILE:HG12	2.15	0.46
1:B:267:LYS:HD2	1:B:267:LYS:N	2.31	0.46
1:C:163:VAL:HG22	1:C:303:ILE:HB	1.97	0.46
1:C:293:ARG:HE	1:C:293:ARG:HB3	1.39	0.46
1:E:179:LEU:C	1:E:181:HIS:N	2.67	0.46
1:F:138:GLU:CG	1:F:139:TYR:N	2.78	0.46
1:H:227:PHE:HD1	1:H:235:LEU:CD1	2.28	0.46
1:I:208:LEU:O	1:I:208:LEU:HD23	2.15	0.46
1:I:252:LEU:CD2	1:I:295:ASP:HB2	2.45	0.46
1:J:269:ILE:CD1	1:J:269:ILE:H	2.28	0.46
1:J:279:THR:HG21	1:J:283:ILE:HD11	1.97	0.46
1:J:318:ILE:CG1	1:J:319:PRO:HD3	2.36	0.46
1:L:240:ILE:CD1	1:L:300:LEU:HD13	2.45	0.46
1:L:302:VAL:O	1:L:303:ILE:HD12	2.16	0.46
1:M:324:PHE:CD1	1:M:360:LYS:HA	2.50	0.46
1:N:189:GLU:HB3	1:N:233:GLY:HA2	1.97	0.46
1:A:260:PHE:C	1:A:260:PHE:CD1	2.88	0.46
1:A:325:LEU:CD1	1:A:339:PHE:CE1	2.99	0.46
1:C:204:PHE:O	1:C:207:GLU:N	2.49	0.46
1:C:256:GLU:HG2	1:C:299:ARG:CZ	2.45	0.46
1:C:273:VAL:O	1:C:275:ILE:HD12	2.16	0.46
1:D:324:PHE:O	1:D:325:LEU:C	2.54	0.46
1:E:213:LYS:HE3	1:E:221:SER:HA	1.98	0.46
1:F:225:GLY:O	1:F:227:PHE:N	2.49	0.46
1:F:250:LYS:O	1:F:254:VAL:HG23	2.14	0.46
1:G:242:GLU:HG2	1:G:281:ARG:HH21	1.80	0.46
1:G:171:VAL:HG12	1:G:313:ARG:NH1	2.31	0.46
1:H:260:PHE:C	1:H:260:PHE:CD1	2.88	0.46
1:I:220:VAL:CG1	1:I:221:SER:N	2.57	0.46
1:J:143:SER:HB3	1:J:316:ASP:OD2	2.15	0.46
1:K:248:GLN:O	1:K:251:LEU:N	2.49	0.46
1:K:336:VAL:HA	1:K:373:LYS:O	2.15	0.46
1:A:313:ARG:O	1:A:316:ASP:N	2.39	0.46
1:B:229:LEU:HD13	1:B:229:LEU:O	2.15	0.46
1:C:184:SER:O	1:C:186:ARG:N	2.48	0.46
1:C:211:TYR:CD1	1:C:211:TYR:C	2.89	0.46
1:C:342:SER:OG	1:C:377:ARG:HB2	2.16	0.46
1:C:358:GLU:O	1:C:362:VAL:HG23	2.16	0.46
1:E:153:ILE:HD12	1:E:180:ILE:HG13	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:ARG:NH2	1:J:203:ILE:HD11	2.31	0.46
1:K:209:PHE:CE2	1:K:250:LYS:HB3	2.51	0.46
1:K:349:SER:O	1:K:350:TYR:C	2.54	0.46
1:L:281:ARG:HH21	1:L:285:GLU:HG2	1.80	0.46
1:L:318:ILE:HG13	1:L:319:PRO:CD	2.46	0.46
1:L:346:LEU:O	1:L:347:LEU:O	2.33	0.46
1:L:352:TRP:HZ3	1:L:358:GLU:HG2	1.79	0.46
1:M:359:LEU:HG	1:M:363:ILE:HD13	1.97	0.46
1:M:365:ARG:HG2	1:M:383:LEU:HD22	1.98	0.46
1:N:145:LYS:O	1:N:149:ILE:HG13	2.16	0.46
1:N:235:LEU:HD12	1:N:236:PHE:H	1.81	0.46
1:A:299:ARG:NH2	1:A:302:VAL:HG21	2.29	0.46
1:A:356:VAL:HG11	2:A:6:ADP:C8	2.50	0.46
1:B:225:GLY:O	1:B:226:PHE:C	2.54	0.46
1:B:382:CYS:HB3	1:B:383:LEU:HD22	1.98	0.46
1:C:165:ILE:HB	1:C:278:ALA:CB	2.44	0.46
1:D:226:PHE:O	1:D:230:ALA:N	2.38	0.46
1:D:361:ASN:O	1:D:364:GLU:N	2.49	0.46
1:E:171:VAL:HG23	1:E:307:ILE:HG21	1.97	0.46
1:F:310:LEU:HA	1:F:310:LEU:HD23	1.64	0.46
1:G:205:GLU:HG2	1:G:247:ALA:HB2	1.97	0.46
1:I:300:LEU:C	1:I:302:VAL:N	2.69	0.46
1:K:139:TYR:HB3	1:K:140:VAL:H	1.44	0.46
1:L:246:GLU:O	1:L:249:ALA:N	2.49	0.46
1:M:157:SER:C	1:M:159:ALA:N	2.69	0.46
1:M:189:GLU:CG	1:M:190:PRO:HD2	2.42	0.46
1:M:247:ALA:O	1:M:248:GLN:C	2.52	0.46
1:N:254:VAL:HG22	1:N:260:PHE:HB3	1.97	0.46
1:A:178:ARG:NE	1:A:191:PHE:CE2	2.82	0.46
1:A:308:PRO:HG2	1:A:313:ARG:HD2	1.98	0.46
1:D:365:ARG:HD2	1:D:383:LEU:CD1	2.45	0.46
1:E:182:LYS:C	1:E:183:LEU:HD23	2.36	0.46
1:E:259:LYS:HD3	1:E:268:GLU:OE1	2.15	0.46
1:E:171:VAL:CG2	1:E:307:ILE:CG2	2.94	0.46
1:E:336:VAL:HG21	1:E:370:SER:HB2	1.98	0.46
1:G:251:LEU:HD22	1:G:255:ILE:CG1	2.45	0.46
1:G:334:LYS:HB3	1:G:336:VAL:HG23	1.97	0.46
1:I:212:GLU:HG3	1:I:265:GLY:HA3	1.98	0.46
1:K:223:LYS:HD3	1:K:223:LYS:HA	1.82	0.46
1:L:208:LEU:HD22	1:L:209:PHE:CG	2.51	0.46
1:L:226:PHE:O	1:L:227:PHE:C	2.52	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:149:ILE:HD13	1:M:307:ILE:HD13	1.97	0.46
1:N:152:LYS:CA	1:N:152:LYS:HE3	2.44	0.46
1:H:198:SER:CB	1:N:250:LYS:HB2	2.37	0.46
1:C:244:SER:OG	1:C:247:ALA:HB2	2.16	0.46
1:E:156:ILE:C	1:E:158:CYS:H	2.19	0.46
1:E:302:VAL:O	1:E:303:ILE:HD13	2.16	0.46
1:E:380:LEU:HD23	1:E:380:LEU:N	2.29	0.46
1:F:350:TYR:CD1	1:F:351:PRO:HD2	2.50	0.46
1:F:367:VAL:O	1:F:367:VAL:HG12	2.14	0.46
1:G:250:LYS:O	1:G:254:VAL:HG23	2.16	0.46
1:G:352:TRP:HB3	1:G:355:ASN:HA	1.97	0.46
1:H:299:ARG:HH11	1:H:302:VAL:HG21	1.81	0.46
1:K:325:LEU:HD21	1:K:336:VAL:CG1	2.46	0.46
1:K:325:LEU:HD12	1:K:339:PHE:CZ	2.50	0.46
1:K:365:ARG:HD2	1:K:383:LEU:HG	1.97	0.46
1:K:365:ARG:HH11	1:K:383:LEU:HG	1.81	0.46
1:M:231:ASP:OD1	1:M:271:VAL:HG23	2.16	0.46
1:M:312:GLU:C	1:M:314:LYS:H	2.20	0.46
1:A:165:ILE:HG21	1:A:173:LYS:HA	1.97	0.46
1:B:177:ALA:O	1:B:178:ARG:C	2.54	0.46
1:D:240:ILE:C	1:D:242:GLU:H	2.18	0.46
1:E:145:LYS:O	1:E:149:ILE:HG13	2.16	0.46
1:E:177:ALA:CA	1:E:180:ILE:CD1	2.60	0.46
1:E:350:TYR:CE1	1:E:384:VAL:HG13	2.51	0.46
1:F:153:ILE:HG22	1:F:183:LEU:HD12	1.96	0.46
1:F:205:GLU:OE1	1:F:250:LYS:HD2	2.16	0.46
1:F:363:ILE:O	1:F:366:ALA:HB3	2.16	0.46
1:G:196:VAL:O	1:G:196:VAL:HG12	2.14	0.46
1:G:204:PHE:C	1:G:206:ALA:H	2.17	0.46
1:G:192:VAL:HB	1:G:230:ALA:HB2	1.98	0.46
1:G:275:ILE:H	1:G:275:ILE:CD1	2.29	0.46
1:G:307:ILE:HG12	1:G:307:ILE:H	1.62	0.46
1:H:318:ILE:HG23	1:H:339:PHE:CZ	2.51	0.46
1:H:317:ILE:HG21	1:H:348:LEU:HD23	1.97	0.46
1:I:331:LYS:HE2	1:I:332:TYR:HE2	1.81	0.46
1:J:322:ASN:O	1:J:325:LEU:N	2.49	0.46
1:K:244:SER:C	1:K:246:GLU:N	2.70	0.46
1:K:302:VAL:CG1	1:K:302:VAL:O	2.64	0.46
1:M:325:LEU:HD23	1:M:325:LEU:C	2.36	0.46
1:N:294:GLU:O	1:N:295:ASP:C	2.53	0.46
1:E:252:LEU:O	1:E:255:ILE:HB	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:SER:C	1:E:259:LYS:H	2.19	0.46
1:H:270:GLU:O	1:H:271:VAL:CG2	2.62	0.46
1:H:368:LEU:C	1:H:370:SER:H	2.17	0.46
1:I:325:LEU:HB2	1:I:339:PHE:CZ	2.51	0.46
1:J:162:PRO:HA	1:J:275:ILE:O	2.16	0.46
1:K:275:ILE:N	1:K:275:ILE:CD1	2.76	0.46
1:K:249:ALA:HB2	1:K:293:ARG:HD2	1.96	0.46
1:L:274:ARG:NH1	1:L:276:LEU:HD21	2.31	0.46
1:M:227:PHE:CD2	1:M:273:VAL:HG21	2.50	0.46
1:N:181:HIS:CD2	1:N:234:THR:CB	2.98	0.46
1:B:178:ARG:NH1	1:B:191:PHE:HD2	2.14	0.45
1:D:249:ALA:O	1:D:252:LEU:N	2.49	0.45
1:D:328:PHE:C	1:D:330:ARG:N	2.69	0.45
1:E:280:ASN:O	1:E:280:ASN:CG	2.53	0.45
1:E:325:LEU:HD11	1:E:375:ILE:HD12	1.97	0.45
1:F:196:VAL:HG22	1:F:204:PHE:CZ	2.52	0.45
1:G:340:THR:OG1	1:G:376:ASP:HA	2.16	0.45
1:H:299:ARG:NH1	1:H:302:VAL:HG21	2.31	0.45
1:I:192:VAL:O	1:I:235:LEU:HD12	2.16	0.45
1:J:301:GLY:O	1:J:302:VAL:C	2.54	0.45
1:J:384:VAL:O	1:J:384:VAL:HG23	2.16	0.45
1:K:149:ILE:HA	1:K:152:LYS:CE	2.46	0.45
1:K:295:ASP:OD1	1:K:296:LEU:N	2.50	0.45
1:K:310:LEU:HD21	1:K:317:ILE:HG12	1.97	0.45
1:L:211:TYR:HB3	1:L:263:LEU:HB3	1.98	0.45
1:M:343:ALA:O	1:M:346:LEU:N	2.49	0.45
1:A:239:GLU:HA	1:A:279:THR:HA	1.98	0.45
1:A:250:LYS:O	1:A:254:VAL:HG23	2.16	0.45
1:A:312:GLU:O	1:A:313:ARG:HG3	2.16	0.45
1:C:153:ILE:CG2	1:C:179:LEU:HD22	2.42	0.45
1:E:194:LEU:H	1:E:194:LEU:HD23	1.80	0.45
1:E:309:PRO:CB	1:E:311:ARG:HD3	2.40	0.45
1:E:340:THR:HG21	1:E:376:ASP:HB3	1.98	0.45
1:F:191:PHE:CZ	1:F:236:PHE:HB2	2.51	0.45
1:F:140:VAL:HG23	1:F:323:HIS:HD2	1.82	0.45
1:G:156:ILE:HG22	1:G:156:ILE:O	2.16	0.45
1:G:276:LEU:HA	1:G:276:LEU:HD23	1.66	0.45
1:I:282:ASN:HD22	1:I:285:GLU:HB2	1.81	0.45
1:I:293:ARG:NH2	1:I:295:ASP:OD2	2.43	0.45
1:J:163:VAL:HG22	1:J:303:ILE:HB	1.98	0.45
1:J:196:VAL:HB	1:J:239:GLU:O	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:172:GLY:HA2	2:K:10:ADP:O1A	2.15	0.45
1:L:209:PHE:CE1	1:L:250:LYS:HB3	2.50	0.45
1:L:211:TYR:HE1	1:L:223:LYS:HB2	1.81	0.45
1:L:341:LYS:HA	1:L:344:GLN:HB2	1.97	0.45
1:M:167:GLY:HA3	1:M:171:VAL:HG21	1.97	0.45
1:M:335:GLU:O	1:M:336:VAL:CG2	2.65	0.45
1:N:165:ILE:HB	1:N:278:ALA:CB	2.41	0.45
1:N:325:LEU:CD2	1:N:325:LEU:C	2.80	0.45
1:B:179:LEU:O	1:B:182:LYS:N	2.50	0.45
1:D:181:HIS:CE1	1:D:187:SER:HA	2.52	0.45
1:E:164:LEU:CG	1:E:164:LEU:O	2.64	0.45
1:F:328:PHE:CE2	1:F:364:GLU:OE2	2.70	0.45
1:G:328:PHE:CD2	1:G:364:GLU:HG3	2.52	0.45
1:H:208:LEU:HD23	1:H:209:PHE:HE1	1.76	0.45
1:H:229:LEU:O	1:H:229:LEU:HD22	2.15	0.45
1:I:219:ALA:O	1:I:220:VAL:HB	2.16	0.45
1:F:349:SER:HB2	1:I:351:PRO:HG3	1.98	0.45
1:J:283:ILE:O	1:J:287:VAL:HG23	2.16	0.45
1:N:242:GLU:OE2	1:N:281:ARG:NH2	2.49	0.45
1:N:282:ASN:ND2	1:N:285:GLU:H	2.13	0.45
1:A:151:GLU:O	1:A:153:ILE:N	2.49	0.45
1:B:186:ARG:HH22	1:B:272:ASN:CG	2.20	0.45
1:C:266:ARG:NH2	1:D:203:ILE:HD11	2.32	0.45
1:D:354:GLY:HA3	1:D:358:GLU:HB2	1.99	0.45
1:E:363:ILE:O	1:E:367:VAL:CG2	2.51	0.45
1:E:363:ILE:C	1:E:367:VAL:HG23	2.35	0.45
1:F:332:TYR:CE1	1:F:368:LEU:HD11	2.52	0.45
1:H:204:PHE:O	1:H:205:GLU:C	2.55	0.45
1:H:309:PRO:HG3	1:H:311:ARG:NH1	2.31	0.45
1:I:194:LEU:HD23	1:I:236:PHE:O	2.15	0.45
1:K:208:LEU:HD13	1:K:209:PHE:HE1	1.81	0.45
1:A:167:GLY:O	1:A:280:ASN:HA	2.16	0.45
1:D:211:TYR:CE2	1:D:216:PHE:CZ	3.04	0.45
1:D:317:ILE:O	1:D:318:ILE:C	2.54	0.45
1:E:149:ILE:C	1:E:151:GLU:N	2.69	0.45
1:E:239:GLU:C	1:E:241:GLY:N	2.69	0.45
1:E:234:THR:CG2	1:E:274:ARG:O	2.65	0.45
1:E:317:ILE:HG21	1:E:347:LEU:O	2.16	0.45
1:F:205:GLU:OE2	1:F:246:GLU:HB2	2.17	0.45
1:H:162:PRO:HB2	1:H:300:LEU:CD2	2.46	0.45
1:H:310:LEU:CD1	1:H:356:VAL:H	2.29	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:331:LYS:HE2	1:I:332:TYR:CE2	2.51	0.45
1:I:324:PHE:HB2	1:I:363:ILE:HD12	1.99	0.45
1:K:189:GLU:CG	1:K:232:GLY:O	2.64	0.45
1:L:152:LYS:O	1:L:153:ILE:C	2.55	0.45
1:L:320:LEU:HB3	1:L:324:PHE:HE1	1.81	0.45
1:L:379:GLU:C	1:L:381:SER:N	2.70	0.45
1:M:253:ARG:CZ	1:M:257:SER:OG	2.64	0.45
1:M:324:PHE:CD2	1:M:360:LYS:HG3	2.52	0.45
1:N:227:PHE:HE2	1:N:275:ILE:HD11	1.82	0.45
1:N:350:TYR:O	1:N:352:TRP:CD1	2.69	0.45
1:C:149:ILE:O	1:C:152:LYS:HB2	2.16	0.45
1:C:349:SER:OG	1:C:350:TYR:N	2.49	0.45
1:D:211:TYR:CE2	1:D:216:PHE:HZ	2.34	0.45
1:E:146:MET:HA	1:E:146:MET:CE	2.47	0.45
1:E:236:PHE:CD1	1:E:276:LEU:O	2.60	0.45
1:E:317:ILE:CG2	1:E:347:LEU:O	2.65	0.45
1:G:365:ARG:O	1:G:367:VAL:N	2.50	0.45
1:H:215:ALA:H	1:I:223:LYS:HZ1	1.60	0.45
1:H:227:PHE:CE1	1:H:235:LEU:HD13	2.52	0.45
1:H:247:ALA:O	1:H:250:LYS:N	2.49	0.45
1:H:156:ILE:CG2	1:H:274:ARG:HH22	2.30	0.45
1:H:318:ILE:N	1:H:319:PRO:HD2	2.32	0.45
1:H:341:LYS:O	1:H:345:GLU:HG3	2.17	0.45
1:I:241:GLY:O	1:I:243:LEU:N	2.50	0.45
1:I:382:CYS:O	1:I:383:LEU:HD23	2.17	0.45
1:K:346:LEU:HD13	1:K:380:LEU:HB3	1.99	0.45
1:L:350:TYR:CD2	1:L:350:TYR:C	2.90	0.45
1:L:376:ASP:O	1:L:377:ARG:C	2.54	0.45
1:M:195:ASN:C	1:M:197:ALA:N	2.68	0.45
1:M:281:ARG:HD3	1:M:282:ASN:H	1.81	0.45
1:M:332:TYR:CE1	1:M:368:LEU:HD23	2.52	0.45
1:N:349:SER:O	1:N:350:TYR:C	2.55	0.45
1:B:235:LEU:HD21	1:B:237:LEU:HD21	1.99	0.45
1:B:274:ARG:HH11	1:B:274:ARG:HG2	1.82	0.45
1:D:365:ARG:NH1	1:D:383:LEU:HD22	2.31	0.45
1:E:146:MET:SD	1:E:149:ILE:HD12	2.57	0.45
1:E:244:SER:O	1:E:247:ALA:N	2.49	0.45
1:E:325:LEU:CD1	1:E:375:ILE:HD12	2.46	0.45
1:F:327:LYS:O	1:F:329:SER:N	2.49	0.45
1:F:380:LEU:HB3	1:F:384:VAL:CG2	2.46	0.45
1:G:259:LYS:HD3	1:G:267:LYS:HD2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:352:TRP:CZ2	1:G:359:LEU:HG	2.51	0.45
1:J:146:MET:O	1:J:149:ILE:N	2.50	0.45
1:J:344:GLN:O	1:J:347:LEU:N	2.50	0.45
1:K:199:ILE:HD13	1:K:207:GLU:HG2	1.98	0.45
1:K:309:PRO:HB2	1:K:311:ARG:HG2	1.99	0.45
1:L:189:GLU:CG	1:L:190:PRO:HD2	2.37	0.45
1:M:164:LEU:HD12	1:M:165:ILE:H	1.82	0.45
1:M:275:ILE:O	1:M:276:LEU:HD22	2.17	0.45
1:A:380:LEU:HD12	1:A:384:VAL:HG21	1.98	0.45
1:B:325:LEU:HD21	1:B:336:VAL:HG12	1.99	0.45
1:B:330:ARG:NH1	1:B:330:ARG:O	2.50	0.45
1:B:302:VAL:HG22	1:C:361:ASN:HB3	1.99	0.45
1:D:159:ALA:HB2	1:E:368:LEU:HD21	1.99	0.45
1:D:234:THR:HG21	1:D:276:LEU:HD12	1.99	0.45
1:D:287:VAL:HG13	1:D:292:PHE:O	2.17	0.45
1:E:171:VAL:HG23	1:E:307:ILE:CG2	2.47	0.45
1:F:170:GLY:C	1:F:172:GLY:N	2.67	0.45
1:F:267:LYS:O	1:F:269:ILE:HD12	2.17	0.45
1:F:215:ALA:O	1:G:216:PHE:HE1	2.00	0.45
1:H:239:GLU:HA	1:H:279:THR:HA	1.98	0.45
1:I:322:ASN:O	1:I:323:HIS:C	2.55	0.45
1:L:143:SER:N	1:L:316:ASP:OD1	2.49	0.45
1:L:210:GLY:C	1:L:262:ARG:HG2	2.37	0.45
1:M:139:TYR:HB3	2:M:12:ADP:C2	2.50	0.45
1:M:309:PRO:HG2	1:M:311:ARG:HD2	1.98	0.45
1:M:329:SER:O	1:M:330:ARG:HD3	2.16	0.45
1:A:339:PHE:HZ	1:A:363:ILE:HD13	1.81	0.45
1:B:375:ILE:HG22	1:B:380:LEU:HD23	1.99	0.45
1:C:240:ILE:O	1:C:243:LEU:HB2	2.16	0.45
1:D:141:PHE:CE1	1:D:179:LEU:HD12	2.50	0.45
1:E:204:PHE:O	1:E:206:ALA:N	2.49	0.45
1:G:204:PHE:CE2	1:G:243:LEU:HD21	2.52	0.45
1:G:352:TRP:HE3	1:G:358:GLU:HB3	1.82	0.45
1:K:298:TYR:C	1:K:300:LEU:N	2.69	0.45
1:L:227:PHE:CD2	1:L:254:VAL:HG11	2.48	0.45
1:M:206:ALA:CB	1:M:216:PHE:CE1	3.00	0.45
1:M:356:VAL:O	1:M:357:ARG:C	2.54	0.45
1:N:181:HIS:HD2	1:N:234:THR:OG1	2.00	0.45
1:B:157:SER:C	1:B:159:ALA:H	2.21	0.45
1:C:366:ALA:C	1:C:368:LEU:N	2.70	0.45
1:D:143:SER:O	1:D:147:LYS:HB2	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LYS:N	1:D:267:LYS:HD2	2.31	0.45
1:F:314:LYS:O	1:F:316:ASP:N	2.50	0.45
1:H:176:VAL:O	1:H:180:ILE:HG13	2.17	0.45
1:H:231:ASP:HA	1:H:273:VAL:CG2	2.46	0.45
1:H:244:SER:O	1:H:248:GLN:HG3	2.17	0.45
1:H:236:PHE:CD1	1:H:276:LEU:O	2.68	0.45
1:H:355:ASN:O	1:H:356:VAL:C	2.56	0.45
1:I:153:ILE:CD1	1:I:176:VAL:HG13	2.45	0.45
1:J:182:LYS:O	1:J:183:LEU:HD23	2.16	0.45
1:J:259:LYS:HD3	1:J:268:GLU:OE1	2.17	0.45
1:K:345:GLU:O	1:K:348:LEU:N	2.50	0.45
1:N:224:GLU:HA	1:N:262:ARG:NH2	2.32	0.45
1:B:159:ALA:O	1:B:160:GLU:HG2	2.17	0.44
1:C:288:LYS:C	1:C:290:GLY:N	2.71	0.44
1:C:140:VAL:HG21	1:C:320:LEU:HD23	1.99	0.44
1:D:189:GLU:HG2	1:D:232:GLY:O	2.17	0.44
1:D:168:GLU:OE1	1:D:311:ARG:NH1	2.50	0.44
1:D:318:ILE:HG23	1:D:348:LEU:HD21	1.99	0.44
1:D:352:TRP:CZ3	1:D:359:LEU:HA	2.52	0.44
1:E:182:LYS:O	1:E:183:LEU:HD23	2.17	0.44
1:E:361:ASN:ND2	1:E:361:ASN:H	2.14	0.44
1:F:232:GLY:N	1:F:272:ASN:O	2.46	0.44
1:F:365:ARG:HB3	1:F:383:LEU:HD11	2.00	0.44
1:H:303:ILE:O	1:H:303:ILE:HG22	2.16	0.44
1:I:325:LEU:HD12	1:I:339:PHE:CZ	2.53	0.44
1:J:332:TYR:CD1	1:J:368:LEU:HD21	2.52	0.44
1:L:281:ARG:HH21	1:L:285:GLU:CG	2.30	0.44
1:M:140:VAL:O	2:M:12:ADP:N6	2.48	0.44
1:M:308:PRO:O	1:M:313:ARG:HD2	2.16	0.44
1:N:192:VAL:CB	1:N:230:ALA:HB2	2.46	0.44
1:B:296:LEU:O	1:B:296:LEU:HD13	2.17	0.44
1:D:223:LYS:HG3	1:D:224:GLU:N	2.31	0.44
1:F:249:ALA:CB	1:F:293:ARG:HH11	2.30	0.44
1:G:151:GLU:O	1:G:152:LYS:C	2.52	0.44
1:G:207:GLU:HG2	1:G:226:PHE:HE1	1.80	0.44
1:H:175:VAL:HG21	2:H:14:ADP:C8	2.52	0.44
1:I:191:PHE:CE2	1:I:193:ALA:HB2	2.52	0.44
1:I:173:LYS:H	2:I:8:ADP:PB	2.40	0.44
1:K:242:GLU:OE2	1:K:281:ARG:NH2	2.50	0.44
1:K:269:ILE:N	1:K:269:ILE:CD1	2.78	0.44
1:K:342:SER:OG	1:K:377:ARG:HD3	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:306:GLU:O	1:L:307:ILE:HD13	2.17	0.44
1:M:353:TYR:C	1:M:355:ASN:N	2.71	0.44
1:A:143:SER:CB	1:A:144:PRO:CD	2.93	0.44
1:A:170:GLY:O	1:A:356:VAL:HG23	2.17	0.44
1:A:179:LEU:O	1:A:181:HIS:N	2.50	0.44
1:A:182:LYS:O	1:A:187:SER:HB3	2.17	0.44
1:A:352:TRP:HZ3	1:A:362:VAL:HG21	1.82	0.44
1:B:242:GLU:OE1	1:B:242:GLU:HA	2.18	0.44
1:B:260:PHE:HD1	1:B:261:TYR:N	2.15	0.44
1:C:254:VAL:O	1:C:258:GLY:HA2	2.17	0.44
1:F:311:ARG:NH1	1:F:311:ARG:CG	2.78	0.44
1:F:345:GLU:O	1:F:346:LEU:C	2.56	0.44
1:G:239:GLU:N	1:G:278:ALA:O	2.50	0.44
1:H:257:SER:O	1:H:259:LYS:HG3	2.17	0.44
1:I:253:ARG:CZ	1:J:198:SER:CB	2.95	0.44
1:I:284:LYS:HE2	1:I:297:TYR:CZ	2.53	0.44
1:J:313:ARG:O	1:J:314:LYS:C	2.55	0.44
1:J:326:LYS:O	1:J:326:LYS:HG2	2.16	0.44
1:L:143:SER:CB	1:L:144:PRO:CD	2.75	0.44
1:L:340:THR:OG1	1:L:376:ASP:HB3	2.16	0.44
1:M:141:PHE:O	1:M:143:SER:N	2.51	0.44
1:A:296:LEU:HD13	1:A:296:LEU:O	2.17	0.44
1:A:365:ARG:NH2	1:G:301:GLY:O	2.50	0.44
1:B:284:LYS:O	1:B:288:LYS:HG2	2.18	0.44
1:C:191:PHE:HE2	1:C:193:ALA:HB2	1.78	0.44
1:C:341:LYS:HA	1:C:344:GLN:HB2	2.00	0.44
1:D:153:ILE:HG23	1:D:180:ILE:HG12	2.00	0.44
1:E:324:PHE:C	1:E:326:LYS:N	2.70	0.44
1:E:335:GLU:O	1:E:373:LYS:HA	2.17	0.44
1:F:211:TYR:O	1:F:212:GLU:HG2	2.18	0.44
1:H:211:TYR:O	1:H:222:SER:HA	2.18	0.44
1:J:146:MET:HG3	1:J:313:ARG:NH2	2.33	0.44
1:J:181:HIS:HD2	1:J:234:THR:HB	1.83	0.44
1:J:346:LEU:HD21	1:J:384:VAL:HG23	1.98	0.44
1:K:277:ALA:O	1:K:278:ALA:HB2	2.18	0.44
1:M:201:ARG:NH2	1:M:242:GLU:O	2.51	0.44
1:M:206:ALA:HB2	1:M:216:PHE:CE1	2.53	0.44
1:M:238:ASP:O	1:M:239:GLU:CB	2.65	0.44
1:N:257:SER:C	1:N:259:LYS:H	2.20	0.44
1:B:240:ILE:CG1	1:B:277:ALA:HB1	2.39	0.44
1:D:343:ALA:O	1:D:344:GLN:C	2.56	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:ARG:HH11	1:D:383:LEU:HD22	1.82	0.44
1:E:178:ARG:HE	1:E:191:PHE:HD2	1.66	0.44
1:E:321:ALA:O	1:E:339:PHE:CE1	2.71	0.44
1:F:214:GLY:O	1:F:215:ALA:CB	2.65	0.44
1:F:343:ALA:HB2	1:F:377:ARG:N	2.33	0.44
1:H:223:LYS:NZ	1:N:215:ALA:HB2	2.32	0.44
1:H:244:SER:O	1:H:246:GLU:N	2.50	0.44
1:H:346:LEU:HD12	1:H:377:ARG:CG	2.48	0.44
1:I:216:PHE:O	1:I:218:GLY:N	2.49	0.44
1:I:234:THR:HG21	1:I:276:LEU:HD12	1.99	0.44
1:I:248:GLN:O	1:I:251:LEU:HB3	2.18	0.44
1:J:157:SER:HB3	1:J:184:SER:CA	2.47	0.44
1:J:190:PRO:O	1:J:233:GLY:HA3	2.17	0.44
1:J:249:ALA:CB	1:J:293:ARG:HH11	2.31	0.44
1:J:259:LYS:HA	1:J:269:ILE:O	2.18	0.44
1:J:359:LEU:O	1:J:362:VAL:HB	2.18	0.44
1:K:140:VAL:HG11	1:K:320:LEU:HD23	1.99	0.44
1:L:288:LYS:C	1:L:290:GLY:N	2.71	0.44
1:L:310:LEU:HD12	1:L:352:TRP:HB3	1.99	0.44
1:L:380:LEU:O	1:L:381:SER:C	2.56	0.44
1:M:139:TYR:HD1	1:M:139:TYR:H	1.64	0.44
1:M:236:PHE:CE2	1:M:238:ASP:HB2	2.53	0.44
1:M:340:THR:C	1:M:342:SER:N	2.71	0.44
1:B:285:GLU:O	1:B:286:LEU:C	2.56	0.44
1:B:283:ILE:HD13	1:B:286:LEU:CD1	2.47	0.44
1:B:328:PHE:CB	1:B:367:VAL:HG21	2.47	0.44
1:C:275:ILE:CD1	1:C:275:ILE:N	2.81	0.44
1:C:311:ARG:NH2	1:C:353:TYR:CD2	2.79	0.44
1:D:156:ILE:O	1:D:159:ALA:N	2.50	0.44
1:D:216:PHE:CD1	1:D:216:PHE:C	2.90	0.44
1:E:350:TYR:HE2	1:E:352:TRP:HA	1.82	0.44
1:F:174:GLU:O	1:F:175:VAL:C	2.55	0.44
1:F:363:ILE:O	1:F:364:GLU:C	2.55	0.44
1:F:380:LEU:O	1:F:383:LEU:N	2.50	0.44
1:G:181:HIS:CD2	1:G:234:THR:OG1	2.70	0.44
1:G:236:PHE:HE1	1:G:278:ALA:HB2	1.82	0.44
1:H:349:SER:HB2	1:H:350:TYR:HD1	1.83	0.44
1:H:373:LYS:O	1:H:374:PHE:HB2	2.17	0.44
1:J:157:SER:C	1:J:184:SER:HA	2.38	0.44
1:K:349:SER:HG	1:K:350:TYR:H	1.64	0.44
1:L:193:ALA:CB	1:L:236:PHE:HB3	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:239:GLU:C	1:L:241:GLY:N	2.63	0.44
1:L:334:LYS:HZ2	1:L:367:VAL:CB	2.30	0.44
1:L:355:ASN:O	1:L:357:ARG:N	2.50	0.44
1:L:379:GLU:O	1:L:381:SER:N	2.50	0.44
1:M:245:LEU:HA	1:M:248:GLN:NE2	2.32	0.44
1:M:253:ARG:O	1:M:256:GLU:N	2.39	0.44
1:C:177:ALA:HA	1:C:180:ILE:HD12	2.00	0.44
1:C:191:PHE:O	1:C:191:PHE:HD2	2.00	0.44
1:C:165:ILE:O	1:C:278:ALA:HA	2.17	0.44
1:C:340:THR:OG1	1:C:342:SER:HB3	2.18	0.44
1:D:361:ASN:C	1:D:363:ILE:H	2.21	0.44
1:E:282:ASN:O	1:E:283:ILE:C	2.56	0.44
1:G:310:LEU:HD12	1:G:356:VAL:N	2.30	0.44
1:G:328:PHE:C	1:G:330:ARG:N	2.70	0.44
1:G:355:ASN:HD22	1:G:355:ASN:N	2.15	0.44
1:G:380:LEU:O	1:G:384:VAL:HG22	2.18	0.44
1:H:332:TYR:O	1:H:333:ALA:CB	2.66	0.44
1:J:220:VAL:O	1:J:221:SER:OG	2.29	0.44
1:J:282:ASN:O	1:J:286:LEU:HG	2.16	0.44
1:N:186:ARG:O	1:N:189:GLU:N	2.51	0.44
1:N:254:VAL:C	1:N:256:GLU:N	2.70	0.44
1:A:196:VAL:HG12	1:A:196:VAL:O	2.17	0.44
1:A:356:VAL:HG11	2:A:6:ADP:C5	2.52	0.44
1:B:299:ARG:O	1:B:302:VAL:HG23	2.17	0.44
1:C:217:THR:O	1:C:217:THR:CG2	2.66	0.44
1:C:240:ILE:HD13	1:C:240:ILE:HA	1.77	0.44
1:C:296:LEU:O	1:C:299:ARG:HB2	2.17	0.44
1:E:204:PHE:O	1:E:205:GLU:C	2.55	0.44
1:F:354:GLY:HA3	1:F:358:GLU:HB2	2.00	0.44
1:F:366:ALA:C	1:F:368:LEU:N	2.71	0.44
1:G:155:LYS:C	1:G:157:SER:N	2.70	0.44
1:G:355:ASN:C	1:G:357:ARG:H	2.21	0.44
1:K:236:PHE:HD1	1:K:276:LEU:O	2.00	0.44
1:K:244:SER:C	1:K:246:GLU:H	2.19	0.44
1:K:329:SER:N	1:K:367:VAL:HG11	2.32	0.44
1:L:211:TYR:CE1	1:L:223:LYS:HB2	2.53	0.44
1:L:171:VAL:HG21	1:L:307:ILE:HB	2.00	0.44
1:L:324:PHE:O	1:L:328:PHE:CD1	2.64	0.44
1:M:181:HIS:C	1:M:183:LEU:N	2.72	0.44
1:M:253:ARG:O	1:M:256:GLU:O	2.35	0.44
1:M:296:LEU:HD11	1:M:300:LEU:CD1	2.47	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:139:TYR:HB3	1:N:141:PHE:CE1	2.52	0.44
1:N:178:ARG:HG3	1:N:178:ARG:NH1	2.33	0.44
1:N:244:SER:O	1:N:247:ALA:HB3	2.17	0.44
1:A:382:CYS:C	1:A:383:LEU:HD23	2.38	0.44
1:C:318:ILE:HG12	1:C:348:LEU:HD21	1.99	0.44
1:D:178:ARG:HH11	1:D:178:ARG:CG	2.31	0.44
1:D:299:ARG:O	1:D:302:VAL:HG23	2.18	0.44
1:E:313:ARG:C	1:E:315:GLU:N	2.70	0.44
1:H:203:ILE:O	1:H:206:ALA:HB3	2.18	0.44
1:H:293:ARG:CG	1:H:293:ARG:NH1	2.69	0.44
1:I:252:LEU:CD1	1:I:296:LEU:HA	2.40	0.44
1:L:172:GLY:HA2	2:L:11:ADP:PA	2.57	0.44
1:L:208:LEU:HD21	1:L:227:PHE:HD1	1.82	0.44
1:N:340:THR:H	1:N:343:ALA:HB3	1.83	0.44
1:A:158:CYS:HA	1:A:185:ASP:CG	2.39	0.43
1:A:240:ILE:HD11	1:A:277:ALA:HA	2.00	0.43
1:C:239:GLU:N	1:C:278:ALA:O	2.42	0.43
1:C:325:LEU:HD13	1:C:339:PHE:CE1	2.53	0.43
1:D:168:GLU:O	1:D:171:VAL:HG13	2.18	0.43
1:D:224:GLU:HG3	1:D:224:GLU:O	2.18	0.43
1:D:246:GLU:OE2	1:D:246:GLU:N	2.50	0.43
1:D:252:LEU:HD13	1:D:296:LEU:HA	1.99	0.43
1:H:286:LEU:HD22	1:H:291:LYS:CD	2.48	0.43
1:I:180:ILE:O	1:I:184:SER:HB3	2.18	0.43
1:J:324:PHE:CE1	1:J:359:LEU:HD12	2.53	0.43
1:K:302:VAL:C	1:K:303:ILE:HG12	2.38	0.43
1:K:363:ILE:O	1:K:367:VAL:HG23	2.18	0.43
1:L:261:TYR:C	1:L:262:ARG:O	2.56	0.43
1:L:277:ALA:O	1:L:278:ALA:HB2	2.17	0.43
1:M:335:GLU:O	1:M:336:VAL:HG23	2.18	0.43
1:N:203:ILE:O	1:N:205:GLU:N	2.45	0.43
1:N:259:LYS:HA	1:N:269:ILE:O	2.18	0.43
1:A:204:PHE:CZ	1:A:208:LEU:HD12	2.53	0.43
1:B:156:ILE:O	1:B:157:SER:C	2.57	0.43
1:C:328:PHE:CZ	1:C:364:GLU:HB2	2.53	0.43
1:E:313:ARG:C	1:E:315:GLU:H	2.20	0.43
1:F:314:LYS:HA	1:F:317:ILE:CD1	2.49	0.43
1:G:252:LEU:HD22	1:G:295:ASP:OD1	2.18	0.43
1:J:352:TRP:CZ3	1:J:362:VAL:HG21	2.52	0.43
1:K:283:ILE:O	1:K:286:LEU:N	2.52	0.43
1:K:311:ARG:HG3	1:K:312:GLU:HG3	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:343:ALA:HB2	1:K:376:ASP:HA	2.00	0.43
1:L:204:PHE:CZ	1:L:208:LEU:HD12	2.53	0.43
1:L:220:VAL:HG12	1:L:220:VAL:O	2.18	0.43
1:L:228:GLU:OE2	1:L:262:ARG:NH2	2.51	0.43
1:L:279:THR:OG1	1:L:280:ASN:N	2.51	0.43
1:M:275:ILE:HD12	1:M:275:ILE:N	2.33	0.43
1:M:328:PHE:CD2	1:M:364:GLU:HG3	2.53	0.43
1:N:259:LYS:HA	1:N:270:GLU:HA	2.00	0.43
1:N:305:ILE:HG22	1:N:307:ILE:CD1	2.47	0.43
1:C:328:PHE:CD2	1:C:364:GLU:HG3	2.54	0.43
1:C:349:SER:O	1:C:350:TYR:C	2.56	0.43
1:C:266:ARG:CZ	1:D:203:ILE:HD12	2.48	0.43
1:D:296:LEU:O	1:D:296:LEU:HD13	2.19	0.43
1:D:368:LEU:C	1:D:370:SER:N	2.70	0.43
1:F:359:LEU:O	1:F:360:LYS:C	2.56	0.43
1:G:216:PHE:O	1:G:216:PHE:CG	2.71	0.43
1:G:252:LEU:HD22	1:G:293:ARG:NH1	2.29	0.43
1:G:325:LEU:HD21	1:G:336:VAL:HG12	2.00	0.43
1:J:200:PRO:C	1:J:202:ASP:N	2.71	0.43
1:K:254:VAL:HG22	1:K:260:PHE:HB3	2.01	0.43
1:L:178:ARG:CG	1:L:178:ARG:HH11	2.28	0.43
1:L:244:SER:C	1:L:246:GLU:N	2.72	0.43
1:L:283:ILE:HG22	1:L:287:VAL:CG2	2.47	0.43
1:M:144:PRO:HG3	1:M:315:GLU:OE2	2.18	0.43
1:N:227:PHE:CE2	1:N:275:ILE:HD11	2.53	0.43
1:A:310:LEU:O	1:A:312:GLU:N	2.52	0.43
1:C:196:VAL:HG13	1:C:204:PHE:CE1	2.54	0.43
1:D:201:ARG:NH2	1:D:242:GLU:O	2.51	0.43
1:E:161:CYS:O	1:E:274:ARG:NH1	2.51	0.43
1:G:237:LEU:HB2	1:G:240:ILE:HD11	2.01	0.43
1:H:146:MET:O	1:H:149:ILE:HB	2.18	0.43
1:H:166:THR:O	1:H:173:LYS:HD3	2.19	0.43
1:H:192:VAL:HG21	1:H:230:ALA:CB	2.39	0.43
1:L:165:ILE:O	1:L:173:LYS:HD2	2.18	0.43
1:L:335:GLU:O	1:L:335:GLU:HG3	2.17	0.43
1:M:178:ARG:CG	1:M:178:ARG:HH11	2.27	0.43
1:M:235:LEU:HD12	1:M:236:PHE:H	1.83	0.43
1:M:369:PHE:O	1:M:370:SER:O	2.37	0.43
1:N:145:LYS:CB	1:N:148:GLU:HG2	2.48	0.43
1:N:339:PHE:CD1	1:N:339:PHE:N	2.86	0.43
1:A:139:TYR:HD2	1:A:175:VAL:CG1	2.29	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HD22	1:A:247:ALA:HB1	2.00	0.43
1:A:236:PHE:HE1	1:A:278:ALA:CB	2.31	0.43
1:B:153:ILE:HG23	1:B:180:ILE:HG12	1.99	0.43
1:B:346:LEU:O	1:B:346:LEU:HD23	2.19	0.43
1:E:174:GLU:O	1:E:177:ALA:N	2.51	0.43
1:E:208:LEU:HB3	1:E:209:PHE:HD1	1.84	0.43
1:F:161:CYS:SG	1:F:303:ILE:HG12	2.58	0.43
1:G:173:LYS:C	1:G:175:VAL:N	2.72	0.43
1:H:213:LYS:HA	1:H:219:ALA:HB1	2.01	0.43
1:I:149:ILE:O	1:I:153:ILE:HG13	2.19	0.43
1:I:288:LYS:C	1:I:290:GLY:H	2.21	0.43
1:L:145:LYS:O	1:L:148:GLU:N	2.47	0.43
1:L:193:ALA:HB2	1:L:236:PHE:HB3	1.99	0.43
1:L:325:LEU:HD13	1:L:339:PHE:CZ	2.54	0.43
1:M:206:ALA:CB	1:M:216:PHE:HE1	2.31	0.43
1:M:234:THR:HG23	1:M:274:ARG:O	2.18	0.43
1:M:284:LYS:HE3	1:M:297:TYR:HE2	1.83	0.43
1:M:253:ARG:HG2	1:N:198:SER:HB3	2.01	0.43
1:N:146:MET:HG3	1:N:313:ARG:NE	2.33	0.43
1:B:179:LEU:C	1:B:179:LEU:HD23	2.39	0.43
1:B:275:ILE:N	1:B:275:ILE:CD1	2.61	0.43
1:B:358:GLU:O	1:B:361:ASN:HB2	2.19	0.43
1:B:337:GLU:CG	1:B:373:LYS:HB3	2.46	0.43
1:C:297:TYR:C	1:C:299:ARG:H	2.22	0.43
1:C:146:MET:HG3	1:C:313:ARG:HH21	1.83	0.43
1:D:259:LYS:HB3	1:D:268:GLU:HG2	2.00	0.43
1:E:292:PHE:HD2	1:E:293:ARG:O	2.01	0.43
1:E:171:VAL:CB	1:E:307:ILE:HG22	2.46	0.43
1:F:242:GLU:HG2	1:F:281:ARG:NH2	2.28	0.43
1:G:340:THR:HG1	1:G:376:ASP:HA	1.83	0.43
1:H:141:PHE:CB	1:H:320:LEU:HD23	2.48	0.43
1:H:309:PRO:HG3	1:H:311:ARG:HH11	1.84	0.43
1:K:181:HIS:O	1:K:184:SER:OG	2.34	0.43
1:K:356:VAL:O	1:K:357:ARG:C	2.57	0.43
1:L:169:SER:OG	1:L:169:SER:O	2.32	0.43
1:L:299:ARG:HH21	1:L:302:VAL:HG21	1.84	0.43
1:L:310:LEU:O	1:L:311:ARG:C	2.56	0.43
1:N:292:PHE:CD2	1:N:292:PHE:C	2.91	0.43
1:N:365:ARG:CD	1:N:383:LEU:HD13	2.49	0.43
1:A:367:VAL:O	1:A:370:SER:OG	2.29	0.43
1:C:208:LEU:HD23	1:C:209:PHE:CZ	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:PHE:CD2	1:D:293:ARG:O	2.71	0.43
1:E:161:CYS:SG	1:E:303:ILE:HG13	2.59	0.43
1:E:196:VAL:HG11	1:E:243:LEU:CD2	2.48	0.43
1:E:206:ALA:CB	1:E:211:TYR:CE1	3.02	0.43
1:E:241:GLY:HA3	1:E:281:ARG:HH21	1.82	0.43
1:G:376:ASP:C	1:G:378:GLY:N	2.72	0.43
1:H:142:GLU:HG2	1:H:146:MET:SD	2.59	0.43
1:H:145:LYS:O	1:H:149:ILE:HG13	2.17	0.43
1:J:249:ALA:O	1:J:252:LEU:HB3	2.19	0.43
1:K:332:TYR:CD1	1:K:368:LEU:HG	2.53	0.43
1:L:244:SER:O	1:L:247:ALA:N	2.52	0.43
1:N:317:ILE:O	1:N:319:PRO:N	2.51	0.43
1:A:158:CYS:SG	1:A:158:CYS:O	2.76	0.43
1:A:325:LEU:HB2	1:A:339:PHE:CZ	2.54	0.43
1:B:144:PRO:HD3	1:B:315:GLU:OE2	2.18	0.43
1:B:160:GLU:HA	1:B:274:ARG:HH12	1.83	0.43
1:B:328:PHE:C	1:B:367:VAL:HG11	2.39	0.43
1:C:146:MET:HG3	1:C:313:ARG:HE	1.83	0.43
1:D:252:LEU:O	1:D:255:ILE:N	2.52	0.43
1:D:267:LYS:H	1:D:267:LYS:HD2	1.83	0.43
1:D:292:PHE:CZ	1:D:296:LEU:HD12	2.54	0.43
1:D:339:PHE:N	1:D:339:PHE:CD1	2.86	0.43
1:E:242:GLU:HA	1:E:242:GLU:OE1	2.19	0.43
1:E:247:ALA:O	1:E:251:LEU:N	2.50	0.43
1:F:156:ILE:O	1:F:157:SER:C	2.56	0.43
1:G:350:TYR:HD2	1:G:352:TRP:CD2	2.37	0.43
1:I:149:ILE:HD13	1:I:307:ILE:HD13	2.00	0.43
1:J:322:ASN:O	1:J:323:HIS:C	2.56	0.43
1:J:352:TRP:HH2	1:J:362:VAL:HG11	1.83	0.43
1:J:364:GLU:O	1:J:365:ARG:C	2.57	0.43
1:K:244:SER:O	1:K:248:GLN:HG3	2.18	0.43
1:K:248:GLN:OE1	1:K:292:PHE:CD2	2.72	0.43
1:K:325:LEU:HD23	1:K:325:LEU:C	2.39	0.43
1:L:138:GLU:O	1:L:139:TYR:CB	2.66	0.43
1:L:181:HIS:CD2	1:L:234:THR:HB	2.52	0.43
1:L:146:MET:CG	1:L:313:ARG:HE	2.31	0.43
1:M:149:ILE:CD1	1:M:307:ILE:HD13	2.48	0.43
1:M:162:PRO:HG3	1:M:299:ARG:O	2.18	0.43
1:M:247:ALA:C	1:M:249:ALA:N	2.69	0.43
1:M:355:ASN:O	1:M:358:GLU:N	2.51	0.43
1:N:252:LEU:O	1:N:253:ARG:C	2.57	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLY:N	1:A:272:ASN:O	2.51	0.43
1:B:179:LEU:O	1:B:180:ILE:C	2.57	0.43
1:C:283:ILE:HG22	1:C:284:LYS:N	2.33	0.43
1:D:262:ARG:HB2	1:D:269:ILE:HD13	2.01	0.43
1:D:175:VAL:HG21	2:D:2:ADP:C8	2.54	0.43
1:E:181:HIS:O	1:E:184:SER:OG	2.35	0.43
1:E:194:LEU:O	1:E:194:LEU:HD23	2.19	0.43
1:E:244:SER:C	1:E:246:GLU:N	2.71	0.43
1:E:356:VAL:HG11	2:E:3:ADP:C4	2.54	0.43
1:G:284:LYS:O	1:G:287:VAL:HB	2.19	0.43
1:H:178:ARG:HH11	1:H:178:ARG:CG	2.31	0.43
1:H:322:ASN:HB3	1:H:326:LYS:HE3	2.01	0.43
1:J:325:LEU:C	1:J:325:LEU:HD23	2.39	0.43
1:K:179:LEU:O	1:K:181:HIS:N	2.52	0.43
1:M:299:ARG:NH1	1:N:357:ARG:HH21	2.17	0.43
1:C:253:ARG:NH1	1:C:253:ARG:CG	2.81	0.43
1:C:263:LEU:HD22	1:C:264:GLY:N	2.33	0.43
1:C:240:ILE:CG1	1:C:277:ALA:HB1	2.38	0.43
1:C:299:ARG:HD3	1:C:299:ARG:HA	1.95	0.43
1:C:346:LEU:O	1:C:346:LEU:HD23	2.19	0.43
1:D:310:LEU:HD11	1:D:320:LEU:HD13	2.01	0.43
1:E:144:PRO:HD2	1:E:315:GLU:OE2	2.19	0.43
1:F:157:SER:HB3	1:F:183:LEU:O	2.19	0.43
1:F:211:TYR:C	1:F:212:GLU:HG2	2.39	0.43
1:F:325:LEU:HD11	1:F:336:VAL:CG1	2.49	0.43
1:H:157:SER:HB3	1:H:183:LEU:C	2.39	0.43
1:H:215:ALA:CB	1:H:264:GLY:HA3	2.48	0.43
1:H:215:ALA:HB2	1:I:223:LYS:HZ1	1.84	0.43
1:H:317:ILE:CG2	1:H:348:LEU:HD23	2.49	0.43
1:I:229:LEU:C	1:I:231:ASP:H	2.23	0.43
1:I:297:TYR:CD2	1:I:298:TYR:CD1	2.96	0.43
1:J:250:LYS:O	1:J:254:VAL:HG23	2.18	0.43
1:J:336:VAL:HG11	1:J:375:ILE:HD11	1.99	0.43
1:K:168:GLU:O	1:K:171:VAL:HG13	2.18	0.43
1:L:173:LYS:HZ3	2:L:11:ADP:PB	2.42	0.43
1:L:283:ILE:O	1:L:285:GLU:N	2.52	0.43
1:N:244:SER:O	1:N:247:ALA:N	2.52	0.43
1:C:194:LEU:HD21	1:C:235:LEU:HD11	2.00	0.42
1:C:376:ASP:C	1:C:378:GLY:N	2.72	0.42
1:F:267:LYS:CD	1:F:267:LYS:N	2.79	0.42
1:G:155:LYS:C	1:G:157:SER:H	2.22	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:LEU:HA	1:G:243:LEU:HD23	1.79	0.42
1:J:324:PHE:CE1	1:J:360:LYS:HA	2.53	0.42
1:J:376:ASP:O	1:J:378:GLY:N	2.51	0.42
1:K:195:ASN:O	1:K:197:ALA:N	2.52	0.42
1:L:318:ILE:O	1:L:319:PRO:C	2.56	0.42
1:M:325:LEU:HD12	1:M:339:PHE:CE1	2.54	0.42
1:N:148:GLU:O	1:N:152:LYS:HD2	2.19	0.42
1:N:350:TYR:CE1	1:N:384:VAL:HG21	2.54	0.42
1:A:332:TYR:OH	1:A:364:GLU:OE1	2.37	0.42
1:B:162:PRO:HD2	1:B:299:ARG:NH2	2.34	0.42
1:C:162:PRO:HG2	1:C:302:VAL:HG21	1.99	0.42
1:C:296:LEU:O	1:C:299:ARG:N	2.38	0.42
1:D:240:ILE:HD13	1:D:243:LEU:HD11	2.01	0.42
1:D:170:GLY:N	2:D:2:ADP:O3B	2.52	0.42
1:D:325:LEU:HD11	1:D:336:VAL:HG12	2.01	0.42
1:D:343:ALA:O	1:D:346:LEU:N	2.51	0.42
1:E:350:TYR:CD1	1:E:384:VAL:CG1	3.00	0.42
1:F:323:HIS:ND1	1:F:323:HIS:C	2.72	0.42
1:F:348:LEU:HD23	1:F:348:LEU:N	2.33	0.42
1:G:381:SER:C	1:G:383:LEU:N	2.73	0.42
1:H:289:GLU:HG2	1:H:289:GLU:O	2.19	0.42
1:I:292:PHE:CE2	1:I:296:LEU:HD22	2.54	0.42
1:I:316:ASP:C	1:I:319:PRO:HD2	2.39	0.42
1:J:325:LEU:C	1:J:327:LYS:N	2.72	0.42
1:J:346:LEU:C	1:J:346:LEU:CD2	2.88	0.42
1:K:260:PHE:C	1:K:260:PHE:CD1	2.93	0.42
1:L:309:PRO:HB2	1:L:355:ASN:OD1	2.20	0.42
1:L:316:ASP:O	1:L:320:LEU:HB2	2.19	0.42
1:L:342:SER:HB2	1:L:377:ARG:HB2	2.00	0.42
1:M:283:ILE:CA	1:M:286:LEU:HD12	2.40	0.42
1:M:359:LEU:O	1:M:362:VAL:N	2.52	0.42
1:M:365:ARG:HH22	1:M:384:VAL:HA	1.84	0.42
1:N:254:VAL:O	1:N:256:GLU:N	2.52	0.42
1:B:259:LYS:HB3	1:B:268:GLU:HG2	2.00	0.42
1:B:263:LEU:HD23	1:B:264:GLY:N	2.34	0.42
1:D:263:LEU:C	1:D:263:LEU:HD23	2.39	0.42
1:D:294:GLU:O	1:D:297:TYR:N	2.53	0.42
1:E:189:GLU:OE1	1:E:189:GLU:HA	2.14	0.42
1:F:164:LEU:HA	1:F:277:ALA:O	2.19	0.42
1:F:314:LYS:O	1:F:317:ILE:N	2.50	0.42
1:F:328:PHE:HZ	1:F:360:LYS:HG3	1.83	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:162:PRO:HB3	1:G:275:ILE:HB	2.00	0.42
1:H:228:GLU:OE2	1:H:269:ILE:HD13	2.19	0.42
1:I:259:LYS:HA	1:I:269:ILE:O	2.19	0.42
1:I:156:ILE:HG22	1:I:274:ARG:HH22	1.84	0.42
1:I:240:ILE:CG1	1:I:277:ALA:HB1	2.48	0.42
1:J:200:PRO:O	1:J:202:ASP:N	2.53	0.42
1:K:199:ILE:O	1:K:199:ILE:HG22	2.19	0.42
1:K:208:LEU:HB3	1:K:209:PHE:HD1	1.83	0.42
1:K:140:VAL:HG11	1:K:320:LEU:CD2	2.49	0.42
1:K:324:PHE:O	1:K:325:LEU:C	2.57	0.42
1:L:165:ILE:HG22	1:L:173:LYS:CG	2.48	0.42
1:L:318:ILE:HG13	1:L:319:PRO:HD2	2.02	0.42
1:M:140:VAL:C	1:M:141:PHE:CD1	2.90	0.42
1:M:227:PHE:C	1:M:229:LEU:N	2.69	0.42
1:M:245:LEU:HA	1:M:245:LEU:HD23	1.91	0.42
1:N:199:ILE:HA	1:N:200:PRO:HD2	1.75	0.42
1:N:378:GLY:C	1:N:380:LEU:H	2.22	0.42
1:A:178:ARG:O	1:A:181:HIS:HB3	2.18	0.42
1:A:213:LYS:HE2	1:A:220:VAL:HG12	2.00	0.42
1:C:191:PHE:O	1:C:191:PHE:CD2	2.72	0.42
1:C:340:THR:CG2	1:C:376:ASP:HB3	2.50	0.42
1:D:212:GLU:HA	1:D:222:SER:CB	2.49	0.42
1:D:359:LEU:HD23	1:D:359:LEU:O	2.19	0.42
1:E:195:ASN:HB3	1:E:198:SER:OG	2.19	0.42
1:E:208:LEU:O	1:E:226:PHE:N	2.52	0.42
1:E:244:SER:HB2	1:E:246:GLU:HG2	2.02	0.42
1:E:324:PHE:CD1	1:E:360:LYS:HA	2.55	0.42
1:F:159:ALA:C	1:F:160:GLU:HG3	2.40	0.42
1:F:181:HIS:CD2	1:F:191:PHE:HB2	2.55	0.42
1:F:259:LYS:HD3	1:F:268:GLU:OE2	2.20	0.42
1:G:200:PRO:O	1:G:202:ASP:N	2.53	0.42
1:G:259:LYS:HD3	1:G:267:LYS:HE3	2.01	0.42
1:G:294:GLU:OE1	1:G:298:TYR:HE1	2.01	0.42
1:H:212:GLU:HA	1:H:212:GLU:OE2	2.19	0.42
1:H:369:PHE:N	1:H:369:PHE:HD1	2.18	0.42
1:I:204:PHE:CE2	1:I:208:LEU:HB2	2.54	0.42
1:I:251:LEU:O	1:I:252:LEU:C	2.58	0.42
1:I:296:LEU:HD21	1:I:300:LEU:CD1	2.49	0.42
1:I:373:LYS:HB3	1:I:374:PHE:CD1	2.54	0.42
1:K:178:ARG:NE	1:K:191:PHE:CD2	2.83	0.42
1:K:248:GLN:C	1:K:250:LYS:N	2.73	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:293:ARG:HH21	1:L:295:ASP:CG	2.23	0.42
1:M:140:VAL:HB	1:M:320:LEU:HD23	2.00	0.42
1:A:153:ILE:HG23	1:A:180:ILE:HG12	2.01	0.42
1:A:253:ARG:NH2	1:A:268:GLU:OE2	2.53	0.42
1:B:211:TYR:CE1	1:B:223:LYS:HB2	2.54	0.42
1:C:309:PRO:CG	1:C:311:ARG:HH11	2.32	0.42
1:C:332:TYR:CD2	1:C:332:TYR:N	2.87	0.42
1:C:354:GLY:O	1:C:355:ASN:O	2.38	0.42
1:E:321:ALA:HB1	1:E:339:PHE:CE1	2.54	0.42
1:E:328:PHE:CD1	1:E:364:GLU:HA	2.55	0.42
1:I:311:ARG:NH1	1:I:311:ARG:HG2	2.35	0.42
1:I:328:PHE:CE2	1:I:364:GLU:HB2	2.55	0.42
1:K:250:LYS:HG3	1:L:198:SER:HB2	2.01	0.42
1:K:256:GLU:HG2	1:K:299:ARG:HD3	2.00	0.42
1:K:302:VAL:O	1:K:303:ILE:HD13	2.19	0.42
1:L:145:LYS:O	1:L:146:MET:C	2.58	0.42
1:L:204:PHE:O	1:L:205:GLU:C	2.56	0.42
1:M:141:PHE:O	1:M:316:ASP:OD1	2.38	0.42
1:A:151:GLU:O	1:A:154:LYS:N	2.53	0.42
1:A:179:LEU:HD23	1:A:179:LEU:HA	1.81	0.42
1:B:229:LEU:HD13	1:B:229:LEU:C	2.40	0.42
1:D:168:GLU:CD	1:D:311:ARG:HH12	2.23	0.42
1:E:138:GLU:HG2	1:E:138:GLU:H	1.63	0.42
1:E:213:LYS:O	1:E:215:ALA:N	2.53	0.42
1:E:262:ARG:O	1:E:263:LEU:C	2.58	0.42
1:F:179:LEU:C	1:F:179:LEU:HD23	2.40	0.42
1:G:173:LYS:C	1:G:175:VAL:H	2.23	0.42
1:H:359:LEU:HD23	1:H:359:LEU:C	2.40	0.42
1:I:253:ARG:CZ	1:J:198:SER:HB3	2.49	0.42
1:I:319:PRO:O	1:I:322:ASN:N	2.52	0.42
1:K:252:LEU:HD13	1:K:296:LEU:HA	2.00	0.42
1:M:177:ALA:O	1:M:180:ILE:HB	2.19	0.42
1:M:292:PHE:CZ	1:M:296:LEU:HD12	2.54	0.42
1:M:353:TYR:O	1:M:355:ASN:N	2.53	0.42
1:N:249:ALA:O	1:N:252:LEU:HB3	2.19	0.42
1:N:318:ILE:CG1	1:N:348:LEU:HD21	2.48	0.42
1:A:256:GLU:HG2	1:A:299:ARG:HD3	2.02	0.42
1:B:208:LEU:CD2	1:B:209:PHE:CE1	3.01	0.42
1:B:211:TYR:HA	1:B:263:LEU:O	2.19	0.42
1:B:160:GLU:CA	1:B:274:ARG:NH1	2.82	0.42
1:C:310:LEU:O	1:C:312:GLU:N	2.53	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:GLY:HA2	2:D:2:ADP:PB	2.60	0.42
1:D:314:LYS:HE3	1:D:348:LEU:O	2.19	0.42
1:E:208:LEU:HD23	1:E:209:PHE:CE1	2.55	0.42
1:E:307:ILE:HA	1:E:308:PRO:HD3	1.61	0.42
1:F:285:GLU:O	1:F:288:LYS:HB2	2.20	0.42
1:G:143:SER:HB2	1:G:144:PRO:HD2	2.00	0.42
1:G:161:CYS:O	1:G:274:ARG:NH1	2.53	0.42
1:H:199:ILE:HD13	1:H:207:GLU:HG3	2.02	0.42
1:H:210:GLY:O	1:H:263:LEU:N	2.47	0.42
1:H:246:GLU:O	1:H:247:ALA:C	2.57	0.42
1:K:206:ALA:HB1	1:K:211:TYR:CD1	2.54	0.42
1:K:298:TYR:C	1:K:300:LEU:H	2.23	0.42
1:L:214:GLY:HA3	1:M:223:LYS:HE2	2.01	0.42
1:L:229:LEU:HD13	1:L:230:ALA:N	2.34	0.42
1:M:271:VAL:HG22	1:M:273:VAL:HG13	2.02	0.42
1:M:313:ARG:O	1:M:315:GLU:N	2.52	0.42
1:M:339:PHE:HE2	1:M:380:LEU:HD21	1.84	0.42
1:N:245:LEU:O	1:N:246:GLU:C	2.58	0.42
1:B:171:VAL:HG23	1:B:172:GLY:N	2.35	0.42
1:B:324:PHE:HB2	1:B:363:ILE:HD13	2.01	0.42
1:E:240:ILE:HD11	1:E:277:ALA:CA	2.45	0.42
1:F:140:VAL:HG21	1:F:320:LEU:HD23	2.01	0.42
1:G:365:ARG:O	1:G:368:LEU:N	2.53	0.42
1:H:231:ASP:OD2	1:H:271:VAL:HG22	2.20	0.42
1:J:194:LEU:N	1:J:194:LEU:HD23	2.33	0.42
1:J:211:TYR:CZ	1:J:223:LYS:HB3	2.55	0.42
1:L:214:GLY:H	1:M:223:LYS:HE2	1.85	0.42
1:L:159:ALA:HB2	1:M:368:LEU:HD21	2.01	0.42
1:N:313:ARG:C	1:N:315:GLU:N	2.70	0.42
1:A:275:ILE:HG22	1:A:276:LEU:N	2.35	0.42
1:B:208:LEU:HD23	1:B:209:PHE:HE1	1.84	0.42
1:B:310:LEU:HD11	1:B:359:LEU:HD12	2.02	0.42
1:C:173:LYS:HE2	1:C:173:LYS:HB2	1.94	0.42
1:C:283:ILE:HG21	1:C:297:TYR:HD1	1.82	0.42
1:C:375:ILE:HG22	1:C:380:LEU:HD23	2.01	0.42
1:D:142:GLU:HA	1:D:147:LYS:HE2	2.01	0.42
1:D:198:SER:O	1:D:199:ILE:HG13	2.20	0.42
1:D:213:LYS:C	1:D:215:ALA:H	2.23	0.42
1:D:175:VAL:HG23	2:D:2:ADP:O1A	2.20	0.42
1:D:332:TYR:CE1	1:D:368:LEU:HD21	2.54	0.42
1:E:164:LEU:HD12	1:E:164:LEU:C	2.40	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ALA:O	1:F:233:GLY:N	2.49	0.42
1:F:376:ASP:C	1:F:378:GLY:N	2.73	0.42
1:H:292:PHE:CE2	1:H:296:LEU:HB3	2.55	0.42
1:J:203:ILE:HG22	1:J:207:GLU:HG2	2.00	0.42
1:J:236:PHE:CE2	1:J:238:ASP:HB2	2.55	0.42
1:L:208:LEU:HD22	1:L:209:PHE:CE1	2.54	0.42
1:L:347:LEU:HD21	1:L:380:LEU:CD1	2.48	0.42
1:N:265:GLY:C	1:N:266:ARG:HE	2.23	0.42
1:N:292:PHE:HE2	1:N:296:LEU:HB3	1.85	0.42
1:A:194:LEU:HD23	1:A:236:PHE:O	2.20	0.42
1:C:160:GLU:CA	1:C:274:ARG:NH1	2.80	0.42
1:D:184:SER:C	1:D:186:ARG:H	2.23	0.42
1:D:209:PHE:CE2	1:D:227:PHE:CE1	3.08	0.42
1:E:320:LEU:C	1:E:322:ASN:H	2.22	0.42
1:F:174:GLU:HG2	1:F:178:ARG:HH12	1.83	0.42
1:H:178:ARG:NE	1:H:191:PHE:CE2	2.88	0.42
1:H:293:ARG:NH1	1:H:295:ASP:OD1	2.53	0.42
1:I:141:PHE:CG	1:I:150:LEU:HD21	2.53	0.42
1:I:288:LYS:C	1:I:290:GLY:N	2.71	0.42
1:J:164:LEU:HA	1:J:277:ALA:HB3	2.01	0.42
1:K:226:PHE:O	1:K:227:PHE:C	2.58	0.42
1:K:236:PHE:O	1:K:236:PHE:CG	2.73	0.42
1:K:288:LYS:O	1:K:289:GLU:C	2.59	0.42
1:L:156:ILE:O	1:L:157:SER:C	2.58	0.42
1:L:355:ASN:O	1:L:356:VAL:C	2.58	0.42
1:M:246:GLU:C	1:M:249:ALA:HB3	2.38	0.42
1:N:194:LEU:N	1:N:194:LEU:HD23	2.34	0.42
1:N:292:PHE:O	1:N:293:ARG:C	2.58	0.42
1:N:372:GLY:O	1:N:373:LYS:C	2.58	0.42
1:B:239:GLU:C	1:B:241:GLY:N	2.74	0.41
1:B:283:ILE:HA	1:B:286:LEU:CD1	2.17	0.41
1:C:186:ARG:CD	1:C:233:GLY:O	2.67	0.41
1:C:320:LEU:CD1	1:C:356:VAL:HG13	2.50	0.41
1:C:322:ASN:O	1:C:324:PHE:N	2.53	0.41
1:C:350:TYR:CD1	1:C:351:PRO:HD2	2.55	0.41
1:C:376:ASP:OD2	1:C:376:ASP:C	2.58	0.41
1:D:245:LEU:HA	1:D:248:GLN:HE21	1.85	0.41
1:D:299:ARG:HE	1:D:299:ARG:C	2.23	0.41
1:D:339:PHE:HZ	1:D:363:ILE:HD13	1.85	0.41
1:F:328:PHE:CZ	1:F:364:GLU:HB2	2.55	0.41
1:G:310:LEU:H	1:G:355:ASN:CB	2.33	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:CYS:SG	1:H:303:ILE:HD11	2.60	0.41
1:H:318:ILE:CD1	1:H:344:GLN:HE21	2.31	0.41
1:H:357:ARG:O	1:H:360:LYS:N	2.53	0.41
1:I:207:GLU:O	1:I:225:GLY:HA2	2.20	0.41
1:I:314:LYS:HG2	1:I:317:ILE:HD11	2.02	0.41
1:J:208:LEU:HD11	1:J:235:LEU:HD21	2.01	0.41
1:J:249:ALA:HB2	1:J:293:ARG:HH11	1.84	0.41
1:J:380:LEU:O	1:J:383:LEU:HG	2.20	0.41
1:K:381:SER:C	1:K:383:LEU:H	2.22	0.41
1:L:195:ASN:C	1:L:197:ALA:N	2.73	0.41
1:L:328:PHE:HD2	1:L:332:TYR:HE1	1.67	0.41
1:L:350:TYR:CD2	1:L:351:PRO:N	2.88	0.41
1:B:212:GLU:OE1	1:B:212:GLU:HA	2.20	0.41
1:D:139:TYR:N	1:D:139:TYR:CD1	2.86	0.41
1:D:156:ILE:O	1:D:157:SER:C	2.59	0.41
1:D:212:GLU:OE1	1:D:262:ARG:NH1	2.52	0.41
1:D:314:LYS:HA	1:D:317:ILE:CD1	2.51	0.41
1:E:150:LEU:C	1:E:150:LEU:HD12	2.37	0.41
1:E:359:LEU:HD22	1:E:363:ILE:HG12	2.01	0.41
1:F:196:VAL:HA	1:F:204:PHE:CZ	2.55	0.41
1:F:343:ALA:HB2	1:F:376:ASP:CA	2.46	0.41
1:H:287:VAL:HG12	1:H:294:GLU:HG2	2.01	0.41
1:H:310:LEU:HG	1:H:355:ASN:HB3	2.01	0.41
1:I:356:VAL:HG11	2:I:8:ADP:C8	2.55	0.41
1:J:302:VAL:C	1:J:303:ILE:HD13	2.40	0.41
1:I:302:VAL:O	1:J:365:ARG:CZ	2.68	0.41
1:K:359:LEU:HD23	1:K:359:LEU:O	2.20	0.41
1:L:318:ILE:N	1:L:319:PRO:HD2	2.34	0.41
1:M:324:PHE:CE1	1:M:359:LEU:HD23	2.55	0.41
1:N:145:LYS:O	1:N:149:ILE:N	2.54	0.41
1:N:181:HIS:O	1:N:183:LEU:N	2.53	0.41
1:A:350:TYR:CD1	1:A:384:VAL:HG12	2.56	0.41
1:A:379:GLU:O	1:A:382:CYS:HB2	2.20	0.41
1:C:181:HIS:CD2	1:C:191:PHE:CB	2.79	0.41
1:C:157:SER:HB2	1:C:183:LEU:O	2.19	0.41
1:D:212:GLU:O	1:D:213:LYS:O	2.39	0.41
1:D:224:GLU:O	1:D:224:GLU:CG	2.67	0.41
1:D:283:ILE:O	1:D:287:VAL:HG23	2.20	0.41
1:D:327:LYS:O	1:D:330:ARG:N	2.39	0.41
1:E:173:LYS:CB	1:E:173:LYS:NZ	2.79	0.41
1:F:174:GLU:CD	1:F:178:ARG:HH12	2.18	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:LEU:HD22	1:F:255:ILE:HG13	2.02	0.41
1:F:265:GLY:O	1:F:266:ARG:NE	2.53	0.41
1:A:223:LYS:HZ1	1:G:266:ARG:HD2	1.85	0.41
1:I:374:PHE:N	1:I:374:PHE:CD1	2.89	0.41
1:K:199:ILE:O	1:K:200:PRO:C	2.57	0.41
1:K:208:LEU:HD21	1:K:227:PHE:HE1	1.86	0.41
1:K:238:ASP:C	1:K:238:ASP:OD1	2.59	0.41
1:K:243:LEU:N	1:K:243:LEU:HD23	2.35	0.41
1:L:141:PHE:HD1	1:L:150:LEU:HG	1.80	0.41
1:M:253:ARG:CG	1:N:198:SER:HB3	2.51	0.41
1:M:369:PHE:O	1:M:370:SER:C	2.59	0.41
1:N:174:GLU:HB3	2:N:13:ADP:O1A	2.20	0.41
1:N:252:LEU:O	1:N:254:VAL:N	2.54	0.41
1:N:261:TYR:CD1	1:N:261:TYR:N	2.89	0.41
1:A:376:ASP:C	1:A:378:GLY:N	2.73	0.41
1:B:266:ARG:CD	1:C:229:LEU:HD23	2.50	0.41
1:B:308:PRO:HG2	1:B:313:ARG:HD3	2.02	0.41
1:D:166:THR:HG22	1:D:279:THR:CG2	2.51	0.41
1:F:171:VAL:HG23	1:F:307:ILE:HG21	2.02	0.41
1:I:368:LEU:HA	1:I:368:LEU:HD23	1.92	0.41
1:J:339:PHE:CZ	1:J:363:ILE:HD13	2.56	0.41
1:J:365:ARG:NE	1:J:383:LEU:HD13	2.35	0.41
1:L:146:MET:CE	1:L:313:ARG:NE	2.81	0.41
1:M:314:LYS:HA	1:M:317:ILE:CG1	2.49	0.41
1:L:298:TYR:HE1	1:M:354:GLY:HA3	1.81	0.41
1:N:143:SER:OG	1:N:146:MET:HB2	2.20	0.41
1:N:365:ARG:HD2	1:N:383:LEU:HD13	2.02	0.41
1:A:248:GLN:O	1:A:249:ALA:C	2.58	0.41
1:B:244:SER:C	1:B:246:GLU:H	2.24	0.41
1:D:203:ILE:HA	1:D:203:ILE:HD13	1.89	0.41
1:D:227:PHE:CE2	1:D:235:LEU:HD23	2.55	0.41
1:D:276:LEU:HA	1:D:276:LEU:HD23	1.64	0.41
1:D:299:ARG:HE	1:D:299:ARG:CA	2.33	0.41
1:E:141:PHE:N	1:E:141:PHE:CD1	2.88	0.41
1:E:253:ARG:NH2	1:E:268:GLU:OE2	2.45	0.41
1:F:174:GLU:CG	1:F:178:ARG:HH12	2.34	0.41
1:F:318:ILE:N	1:F:319:PRO:CD	2.84	0.41
1:G:215:ALA:CB	1:G:263:LEU:HD13	2.51	0.41
1:H:247:ALA:O	1:H:248:GLN:O	2.38	0.41
1:I:143:SER:HB3	1:I:316:ASP:OD1	2.19	0.41
1:I:269:ILE:N	1:I:269:ILE:CD1	2.80	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:310:LEU:O	1:I:313:ARG:N	2.39	0.41
1:I:325:LEU:O	1:I:325:LEU:HD23	2.21	0.41
1:K:179:LEU:C	1:K:181:HIS:N	2.73	0.41
1:K:238:ASP:O	1:K:239:GLU:HB3	2.20	0.41
1:M:288:LYS:C	1:M:290:GLY:H	2.24	0.41
1:N:235:LEU:HD12	1:N:235:LEU:C	2.40	0.41
1:N:311:ARG:C	1:N:312:GLU:HG2	2.41	0.41
1:A:156:ILE:O	1:A:157:SER:C	2.59	0.41
1:A:161:CYS:SG	1:A:303:ILE:HG12	2.61	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD23	1.87	0.41
1:A:320:LEU:O	1:A:321:ALA:C	2.59	0.41
1:C:368:LEU:HA	1:C:368:LEU:HD23	1.78	0.41
1:D:159:ALA:CA	1:E:332:TYR:HE2	2.34	0.41
1:D:210:GLY:CA	1:D:225:GLY:N	2.79	0.41
1:D:313:ARG:HB3	1:D:316:ASP:OD2	2.20	0.41
1:F:152:LYS:O	1:F:156:ILE:HG12	2.21	0.41
1:G:259:LYS:HD3	1:G:267:LYS:CE	2.51	0.41
1:G:162:PRO:HA	1:G:275:ILE:O	2.21	0.41
1:H:279:THR:OG1	1:H:280:ASN:N	2.51	0.41
1:K:177:ALA:HB1	1:K:276:LEU:HD12	2.03	0.41
1:L:359:LEU:C	1:L:359:LEU:HD23	2.41	0.41
1:M:380:LEU:O	1:M:384:VAL:HB	2.21	0.41
1:N:253:ARG:HH11	1:N:253:ARG:HG3	1.86	0.41
1:N:359:LEU:HD23	1:N:363:ILE:HD11	2.03	0.41
1:B:313:ARG:HB3	1:B:316:ASP:OD2	2.21	0.41
1:C:156:ILE:HG13	1:D:369:PHE:HE1	1.85	0.41
1:C:140:VAL:HG21	1:C:320:LEU:CD2	2.51	0.41
1:D:299:ARG:HH21	1:D:302:VAL:HG21	1.84	0.41
1:D:324:PHE:CE1	1:D:360:LYS:HA	2.56	0.41
1:E:350:TYR:HD2	1:E:352:TRP:CD2	2.39	0.41
1:G:213:LYS:O	1:G:214:GLY:C	2.59	0.41
1:J:365:ARG:CD	1:J:383:LEU:HD13	2.51	0.41
1:L:298:TYR:CE1	1:M:354:GLY:CA	2.99	0.41
1:M:143:SER:OG	1:M:146:MET:HB2	2.21	0.41
1:M:289:GLU:O	1:M:291:LYS:HG3	2.20	0.41
1:M:312:GLU:HG2	1:M:312:GLU:H	1.72	0.41
1:N:328:PHE:CD1	1:N:364:GLU:HA	2.56	0.41
1:A:315:GLU:N	1:A:315:GLU:OE1	2.53	0.41
1:B:153:ILE:HG22	1:B:183:LEU:HD12	2.03	0.41
1:B:321:ALA:O	1:B:363:ILE:HD13	2.21	0.41
1:C:194:LEU:O	1:C:194:LEU:HD23	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:GLU:C	1:E:263:LEU:HD11	2.41	0.41
1:F:141:PHE:CD2	1:F:150:LEU:HB2	2.56	0.41
1:F:252:LEU:HD11	1:F:299:ARG:HG3	2.02	0.41
1:G:284:LYS:O	1:G:285:GLU:C	2.57	0.41
1:H:255:ILE:CD1	1:H:300:LEU:HD21	2.50	0.41
1:J:316:ASP:O	1:J:317:ILE:C	2.59	0.41
1:K:168:GLU:O	1:K:171:VAL:HG22	2.20	0.41
1:L:261:TYR:O	1:L:262:ARG:O	2.39	0.41
1:M:168:GLU:O	1:M:171:VAL:HG22	2.21	0.41
1:M:281:ARG:CG	1:M:282:ASN:H	2.33	0.41
1:H:223:LYS:HZ2	1:N:264:GLY:HA3	1.86	0.41
1:N:343:ALA:O	1:N:346:LEU:N	2.50	0.41
1:A:269:ILE:HD12	1:A:269:ILE:N	2.36	0.41
1:A:227:PHE:CD2	1:A:273:VAL:HG21	2.56	0.41
1:B:297:TYR:O	1:B:300:LEU:N	2.52	0.41
1:D:168:GLU:HB2	1:D:355:ASN:HD21	1.85	0.41
1:D:260:PHE:CD1	1:D:260:PHE:C	2.94	0.41
1:D:283:ILE:HD12	1:D:292:PHE:HE1	1.86	0.41
1:F:192:VAL:HG21	1:F:230:ALA:HB2	2.03	0.41
1:F:240:ILE:C	1:F:242:GLU:N	2.69	0.41
1:F:205:GLU:HG2	1:F:250:LYS:HD3	2.03	0.41
1:G:220:VAL:O	1:G:220:VAL:HG12	2.19	0.41
1:I:266:ARG:NH2	1:J:203:ILE:CD1	2.83	0.41
1:K:204:PHE:O	1:K:205:GLU:C	2.58	0.41
1:K:310:LEU:HD22	1:K:317:ILE:CG1	2.49	0.41
1:L:260:PHE:CG	1:L:260:PHE:O	2.74	0.41
1:L:339:PHE:O	1:L:344:GLN:HG3	2.21	0.41
1:L:328:PHE:CE2	1:L:364:GLU:OE2	2.74	0.41
1:L:335:GLU:O	1:L:373:LYS:HA	2.21	0.41
1:M:168:GLU:OE1	1:M:309:PRO:CB	2.64	0.41
1:M:165:ILE:HG22	1:M:173:LYS:HG2	2.03	0.41
1:M:186:ARG:NH1	1:M:232:GLY:O	2.53	0.41
1:N:245:LEU:O	1:N:248:GLN:N	2.53	0.41
1:A:175:VAL:O	1:A:178:ARG:HB2	2.21	0.41
1:A:292:PHE:HZ	1:A:296:LEU:HD12	1.83	0.41
1:B:208:LEU:HA	1:B:226:PHE:HB2	2.02	0.41
1:B:266:ARG:HH11	1:B:266:ARG:CG	2.33	0.41
1:B:284:LYS:HD3	1:B:284:LYS:N	2.32	0.41
1:B:343:ALA:O	1:B:347:LEU:HG	2.21	0.41
1:E:224:GLU:HG2	1:E:228:GLU:HB2	2.03	0.41
1:F:149:ILE:C	1:F:151:GLU:N	2.74	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:GLY:HA3	2:F:4:ADP:C8	2.55	0.41
1:I:261:TYR:CE2	1:I:268:GLU:HB2	2.56	0.41
1:I:288:LYS:O	1:I:290:GLY:N	2.54	0.41
1:I:314:LYS:O	1:I:317:ILE:HG13	2.20	0.41
1:J:190:PRO:HG2	1:J:233:GLY:HA3	2.02	0.41
1:J:308:PRO:O	1:J:313:ARG:HD2	2.21	0.41
1:J:173:LYS:HG3	2:J:9:ADP:O1B	2.21	0.41
1:K:209:PHE:HD1	1:K:209:PHE:H	1.69	0.41
1:K:189:GLU:HG2	1:K:232:GLY:O	2.20	0.41
1:L:296:LEU:O	1:L:297:TYR:C	2.59	0.41
1:M:245:LEU:C	1:M:247:ALA:N	2.72	0.41
1:M:362:VAL:O	1:M:364:GLU:N	2.54	0.41
1:M:367:VAL:O	1:M:367:VAL:HG12	2.20	0.41
1:A:313:ARG:C	1:A:315:GLU:N	2.72	0.41
1:B:162:PRO:CG	1:B:299:ARG:HH21	2.34	0.41
1:B:266:ARG:HG2	1:B:266:ARG:NH1	2.36	0.41
1:C:152:LYS:O	1:C:154:LYS:N	2.54	0.41
1:C:266:ARG:NH2	1:D:203:ILE:CD1	2.84	0.41
1:C:295:ASP:N	1:C:295:ASP:OD1	2.54	0.41
1:C:318:ILE:CD1	1:C:348:LEU:HD21	2.51	0.41
1:D:174:GLU:HG2	1:D:178:ARG:NH1	2.36	0.41
1:D:317:ILE:O	1:D:319:PRO:N	2.54	0.41
1:D:376:ASP:O	1:D:377:ARG:C	2.60	0.41
1:E:204:PHE:C	1:E:206:ALA:N	2.73	0.41
1:E:223:LYS:HZ3	1:E:223:LYS:HG2	1.66	0.41
1:E:359:LEU:CD2	1:E:363:ILE:HD11	2.51	0.41
1:E:365:ARG:HG2	1:E:369:PHE:CD2	2.56	0.41
1:F:230:ALA:O	1:F:231:ASP:C	2.59	0.41
1:H:153:ILE:HG23	1:H:180:ILE:HG12	2.03	0.41
1:H:288:LYS:C	1:H:290:GLY:N	2.72	0.41
1:H:317:ILE:HB	1:H:348:LEU:CD2	2.51	0.41
1:I:314:LYS:CA	1:I:317:ILE:HG13	2.49	0.41
1:I:340:THR:OG1	1:I:376:ASP:CB	2.69	0.41
1:L:143:SER:HB3	1:L:316:ASP:CG	2.41	0.41
1:L:328:PHE:CZ	1:L:364:GLU:HB2	2.55	0.41
1:N:186:ARG:O	1:N:189:GLU:HB2	2.20	0.41
1:N:208:LEU:HD23	1:N:209:PHE:CE2	2.56	0.41
1:N:320:LEU:CD1	1:N:356:VAL:HG13	2.50	0.41
1:N:332:TYR:O	1:N:333:ALA:C	2.58	0.41
1:A:203:ILE:HD11	1:G:264:GLY:HA2	2.03	0.40
1:A:274:ARG:HG2	1:A:274:ARG:HH11	1.86	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:C	1:A:325:LEU:CD2	2.90	0.40
1:B:216:PHE:HD1	1:B:217:THR:HG22	1.86	0.40
1:B:228:GLU:O	1:B:229:LEU:C	2.59	0.40
1:B:260:PHE:CE1	1:B:269:ILE:HB	2.56	0.40
1:B:305:ILE:HG22	1:B:305:ILE:O	2.21	0.40
1:C:143:SER:HB2	1:C:316:ASP:OD1	2.22	0.40
1:D:200:PRO:O	1:D:201:ARG:C	2.59	0.40
1:E:137:GLU:CG	1:E:138:GLU:N	2.83	0.40
1:E:194:LEU:H	1:E:194:LEU:CD2	2.34	0.40
1:E:275:ILE:HD12	1:E:275:ILE:N	2.36	0.40
1:E:321:ALA:HB1	1:E:339:PHE:CZ	2.56	0.40
1:F:359:LEU:C	1:F:361:ASN:N	2.74	0.40
1:F:366:ALA:C	1:F:368:LEU:H	2.24	0.40
1:G:251:LEU:HD22	1:G:255:ILE:CD1	2.51	0.40
1:G:324:PHE:O	1:G:325:LEU:C	2.59	0.40
1:G:379:GLU:O	1:G:383:LEU:HD12	2.21	0.40
1:H:157:SER:C	1:H:159:ALA:H	2.24	0.40
1:I:266:ARG:HH21	1:J:203:ILE:CD1	2.34	0.40
1:L:186:ARG:HD3	1:L:232:GLY:O	2.21	0.40
1:L:194:LEU:CD2	1:L:194:LEU:H	2.30	0.40
1:L:208:LEU:CD2	1:L:227:PHE:HD1	2.33	0.40
1:M:142:GLU:O	1:M:142:GLU:HG3	2.21	0.40
1:N:355:ASN:O	1:N:356:VAL:C	2.60	0.40
1:A:157:SER:C	1:A:159:ALA:H	2.24	0.40
1:A:283:ILE:O	1:A:286:LEU:N	2.54	0.40
1:B:244:SER:C	1:B:246:GLU:N	2.74	0.40
1:B:368:LEU:C	1:B:370:SER:H	2.25	0.40
1:C:195:ASN:O	1:C:196:VAL:C	2.58	0.40
1:C:240:ILE:HG22	1:C:241:GLY:N	2.35	0.40
1:C:251:LEU:HD22	1:C:255:ILE:CD1	2.39	0.40
1:C:281:ARG:N	1:C:281:ARG:HD3	2.36	0.40
1:C:255:ILE:HD13	1:C:300:LEU:CD2	2.51	0.40
1:C:310:LEU:C	1:C:312:GLU:H	2.24	0.40
1:D:138:GLU:O	1:D:139:TYR:C	2.60	0.40
1:D:194:LEU:C	1:D:194:LEU:HD23	2.42	0.40
1:D:235:LEU:HD12	1:D:236:PHE:CA	2.40	0.40
1:E:171:VAL:CG2	1:E:307:ILE:HG22	2.52	0.40
1:E:189:GLU:HB3	1:E:233:GLY:HA2	2.02	0.40
1:E:211:TYR:CE2	1:E:263:LEU:HB2	2.55	0.40
1:G:235:LEU:HG	1:G:237:LEU:HD23	2.02	0.40
1:G:254:VAL:HG12	1:G:254:VAL:O	2.21	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:175:VAL:O	1:I:176:VAL:C	2.59	0.40
1:I:171:VAL:CG1	1:I:307:ILE:CG2	2.95	0.40
1:J:339:PHE:N	1:J:339:PHE:CD1	2.89	0.40
1:J:350:TYR:HD2	1:J:352:TRP:CE3	2.39	0.40
1:L:318:ILE:CG1	1:L:319:PRO:CD	2.99	0.40
1:M:166:THR:HA	1:M:279:THR:O	2.21	0.40
1:N:179:LEU:C	1:N:181:HIS:N	2.73	0.40
1:A:144:PRO:C	1:A:146:MET:H	2.25	0.40
1:A:236:PHE:HD1	1:A:276:LEU:O	2.04	0.40
1:C:165:ILE:O	1:C:278:ALA:CB	2.69	0.40
1:D:324:PHE:O	1:D:327:LYS:HB3	2.21	0.40
1:D:369:PHE:CD1	1:D:369:PHE:N	2.87	0.40
1:E:252:LEU:O	1:E:253:ARG:C	2.60	0.40
1:F:213:LYS:HD3	1:G:220:VAL:CG1	2.46	0.40
1:G:146:MET:C	1:G:148:GLU:N	2.68	0.40
1:G:275:ILE:HG21	1:G:300:LEU:CD2	2.52	0.40
1:G:161:CYS:CB	1:G:302:VAL:HG11	2.50	0.40
1:G:308:PRO:O	1:G:313:ARG:CD	2.69	0.40
1:G:361:ASN:O	1:G:362:VAL:C	2.60	0.40
1:H:180:ILE:O	1:H:184:SER:HB3	2.21	0.40
1:H:367:VAL:O	1:H:367:VAL:HG12	2.19	0.40
1:J:196:VAL:HG12	1:J:242:GLU:HB2	2.03	0.40
1:J:262:ARG:HH11	1:J:262:ARG:CG	2.31	0.40
1:J:361:ASN:O	1:J:362:VAL:C	2.59	0.40
1:L:269:ILE:N	1:L:269:ILE:CD1	2.85	0.40
1:L:341:LYS:O	1:L:345:GLU:HG3	2.21	0.40
1:L:350:TYR:HD2	1:L:350:TYR:C	2.25	0.40
1:L:365:ARG:NH2	1:L:383:LEU:HD22	2.36	0.40
1:M:163:VAL:HG22	1:M:303:ILE:HB	2.02	0.40
1:A:383:LEU:HD23	1:A:383:LEU:N	2.36	0.40
1:B:195:ASN:O	1:B:196:VAL:C	2.60	0.40
1:A:256:GLU:OE1	1:B:357:ARG:NH1	2.55	0.40
1:E:349:SER:HG	1:E:349:SER:H	1.61	0.40
1:F:196:VAL:HG12	1:F:242:GLU:HB2	2.03	0.40
1:F:358:GLU:O	1:F:359:LEU:O	2.38	0.40
1:G:156:ILE:O	1:G:157:SER:C	2.59	0.40
1:H:211:TYR:HB3	1:H:263:LEU:CB	2.51	0.40
1:I:336:VAL:HG11	1:I:375:ILE:CD1	2.52	0.40
1:K:263:LEU:HD23	1:K:264:GLY:N	2.36	0.40
1:M:248:GLN:O	1:M:249:ALA:O	2.40	0.40
1:M:252:LEU:HD13	1:M:296:LEU:HA	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLU:HG2	1:A:246:GLU:H	1.72	0.40
1:C:195:ASN:O	1:C:198:SER:N	2.46	0.40
1:C:204:PHE:CE2	1:C:243:LEU:HD21	2.56	0.40
1:C:301:GLY:O	1:C:302:VAL:C	2.59	0.40
1:D:216:PHE:O	1:D:216:PHE:CD1	2.75	0.40
1:D:296:LEU:HD13	1:D:300:LEU:HD11	2.00	0.40
1:D:375:ILE:HG23	1:D:379:GLU:HB2	2.03	0.40
1:E:165:ILE:HG22	1:E:173:LYS:HG2	2.03	0.40
1:E:240:ILE:HG13	1:E:240:ILE:H	1.64	0.40
1:E:382:CYS:O	1:E:383:LEU:HD23	2.21	0.40
1:F:204:PHE:O	1:F:205:GLU:C	2.60	0.40
1:F:242:GLU:OE1	1:F:242:GLU:HA	2.21	0.40
1:G:165:ILE:O	1:G:278:ALA:HA	2.22	0.40
1:G:308:PRO:HG2	1:G:313:ARG:CD	2.47	0.40
1:G:325:LEU:HD13	1:G:338:GLY:HA2	2.04	0.40
1:H:212:GLU:HA	1:H:222:SER:CB	2.52	0.40
1:H:280:ASN:CG	1:H:280:ASN:O	2.60	0.40
1:I:240:ILE:O	1:I:241:GLY:C	2.58	0.40
1:L:236:PHE:CD1	1:L:276:LEU:O	2.74	0.40
1:L:322:ASN:O	1:L:325:LEU:HB3	2.22	0.40
1:L:334:LYS:HZ2	1:L:367:VAL:HG22	1.86	0.40
1:M:152:LYS:O	1:M:153:ILE:C	2.60	0.40
1:N:211:TYR:CE2	1:N:223:LYS:HB2	2.56	0.40
1:N:320:LEU:HD23	1:N:320:LEU:N	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	245/267 (92%)	192 (78%)	39 (16%)	14 (6%)	<b>1</b> <b>10</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	241/267 (90%)	155 (64%)	64 (27%)	22 (9%)	1	4
1	C	246/267 (92%)	180 (73%)	49 (20%)	17 (7%)	1	7
1	D	245/267 (92%)	165 (67%)	55 (22%)	25 (10%)	0	3
1	E	246/267 (92%)	165 (67%)	56 (23%)	25 (10%)	0	3
1	F	246/267 (92%)	179 (73%)	39 (16%)	28 (11%)	0	2
1	G	246/267 (92%)	177 (72%)	49 (20%)	20 (8%)	1	5
1	H	243/267 (91%)	171 (70%)	55 (23%)	17 (7%)	1	7
1	I	245/267 (92%)	174 (71%)	48 (20%)	23 (9%)	0	3
1	J	245/267 (92%)	182 (74%)	48 (20%)	15 (6%)	1	9
1	K	246/267 (92%)	173 (70%)	53 (22%)	20 (8%)	1	5
1	L	244/267 (91%)	158 (65%)	53 (22%)	33 (14%)	0	1
1	M	245/267 (92%)	164 (67%)	57 (23%)	24 (10%)	0	3
1	N	245/267 (92%)	169 (69%)	57 (23%)	19 (8%)	1	5
All	All	3428/3738 (92%)	2404 (70%)	722 (21%)	302 (9%)	1	4

All (302) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	PRO
1	A	221	SER
1	B	157	SER
1	B	217	THR
1	B	381	SER
1	B	382	CYS
1	C	220	VAL
1	C	221	SER
1	C	283	ILE
1	C	301	GLY
1	C	317	ILE
1	D	144	PRO
1	D	157	SER
1	D	213	LYS
1	D	302	VAL
1	D	317	ILE
1	D	327	LYS
1	D	355	ASN
1	D	362	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	157	SER
1	E	196	VAL
1	E	314	LYS
1	F	157	SER
1	F	168	GLU
1	F	171	VAL
1	F	215	ALA
1	F	224	GLU
1	F	225	GLY
1	F	226	PHE
1	F	241	GLY
1	F	314	LYS
1	F	327	LYS
1	F	344	GLN
1	F	377	ARG
1	G	213	LYS
1	G	224	GLU
1	H	143	SER
1	H	144	PRO
1	H	217	THR
1	H	248	GLN
1	H	334	LYS
1	H	356	VAL
1	I	156	ILE
1	I	157	SER
1	I	213	LYS
1	I	220	VAL
1	I	356	VAL
1	J	224	GLU
1	J	241	GLY
1	K	140	VAL
1	K	189	GLU
1	K	217	THR
1	K	356	VAL
1	L	139	TYR
1	L	157	SER
1	L	240	ILE
1	L	262	ARG
1	L	287	VAL
1	L	344	GLN
1	L	347	LEU
1	L	348	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	377	ARG
1	M	142	GLU
1	M	144	PRO
1	M	283	ILE
1	M	355	ASN
1	M	370	SER
1	N	144	PRO
1	N	229	LEU
1	N	240	ILE
1	N	268	GLU
1	N	317	ILE
1	A	173	LYS
1	A	241	GLY
1	A	377	ARG
1	A	378	GLY
1	B	180	ILE
1	B	187	SER
1	B	206	ALA
1	B	207	GLU
1	C	311	ARG
1	C	355	ASN
1	C	377	ARG
1	D	158	CYS
1	D	214	GLY
1	D	225	GLY
1	D	241	GLY
1	E	168	GLU
1	E	173	LYS
1	E	245	LEU
1	E	317	ILE
1	E	321	ALA
1	E	325	LEU
1	E	347	LEU
1	E	352	TRP
1	E	382	CYS
1	F	196	VAL
1	F	218	GLY
1	F	311	ARG
1	F	315	GLU
1	F	360	LYS
1	F	367	VAL
1	G	149	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	158	CYS
1	G	173	LYS
1	G	174	GLU
1	G	201	ARG
1	G	263	LEU
1	G	366	ALA
1	G	377	ARG
1	H	335	GLU
1	I	221	SER
1	I	222	SER
1	I	242	GLU
1	I	252	LEU
1	I	301	GLY
1	I	311	ARG
1	I	367	VAL
1	I	377	ARG
1	J	311	ARG
1	J	317	ILE
1	J	356	VAL
1	J	372	GLY
1	J	377	ARG
1	K	196	VAL
1	K	214	GLY
1	K	249	ALA
1	K	309	PRO
1	L	185	ASP
1	L	196	VAL
1	L	215	ALA
1	L	219	ALA
1	L	311	ARG
1	L	356	VAL
1	L	372	GLY
1	M	156	ILE
1	M	157	SER
1	M	158	CYS
1	M	217	THR
1	M	249	ALA
1	M	267	LYS
1	M	359	LEU
1	N	182	LYS
1	N	201	ARG
1	N	314	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	373	LYS
1	A	152	LYS
1	B	203	ILE
1	B	205	GLU
1	B	208	LEU
1	B	222	SER
1	B	227	PHE
1	B	360	LYS
1	C	185	ASP
1	C	298	TYR
1	D	231	ASP
1	D	249	ALA
1	D	348	LEU
1	E	150	LEU
1	E	206	ALA
1	E	302	VAL
1	F	221	SER
1	F	328	PHE
1	F	359	LEU
1	G	214	GLY
1	G	311	ARG
1	G	355	ASN
1	G	356	VAL
1	H	289	GLU
1	H	309	PRO
1	H	381	SER
1	I	230	ALA
1	I	333	ALA
1	I	359	LEU
1	J	144	PRO
1	K	239	GLU
1	K	248	GLN
1	K	278	ALA
1	K	299	ARG
1	K	314	LYS
1	L	171	VAL
1	L	267	LYS
1	L	291	LYS
1	L	340	THR
1	L	380	LEU
1	M	196	VAL
1	M	257	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	314	LYS
1	M	333	ALA
1	M	372	GLY
1	N	157	SER
1	N	278	ALA
1	A	218	GLY
1	A	311	ARG
1	B	251	LEU
1	B	372	GLY
1	B	383	LEU
1	C	162	PRO
1	C	239	GLU
1	C	322	ASN
1	D	215	ALA
1	E	138	GLU
1	E	182	LYS
1	E	204	PHE
1	E	227	PHE
1	F	138	GLU
1	F	294	GLU
1	F	295	ASP
1	G	156	ILE
1	G	157	SER
1	H	205	GLU
1	H	219	ALA
1	H	249	ALA
1	H	314	LYS
1	I	168	GLU
1	I	204	PHE
1	I	219	ALA
1	I	355	ASN
1	J	314	LYS
1	J	326	LYS
1	K	141	PHE
1	K	319	PRO
1	K	326	LYS
1	L	170	GLY
1	L	255	ILE
1	L	284	LYS
1	L	355	ASN
1	L	359	LEU
1	L	360	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	M	247	ALA
1	M	281	ARG
1	N	204	PHE
1	N	219	ALA
1	N	253	ARG
1	N	355	ASN
1	A	158	CYS
1	A	205	GLU
1	B	289	GLU
1	B	309	PRO
1	D	141	PHE
1	D	253	ARG
1	D	314	LYS
1	D	347	LEU
1	D	377	ARG
1	E	214	GLY
1	E	309	PRO
1	E	327	LYS
1	G	286	LEU
1	G	341	LYS
1	G	352	TRP
1	H	245	LEU
1	H	333	ALA
1	I	239	GLU
1	J	201	ARG
1	J	221	SER
1	J	278	ALA
1	J	344	GLN
1	J	355	ASN
1	K	190	PRO
1	L	153	ILE
1	L	204	PHE
1	L	295	ASP
1	L	381	SER
1	M	253	ARG
1	M	289	GLU
1	N	356	VAL
1	A	145	LYS
1	B	252	LEU
1	C	323	HIS
1	F	175	VAL
1	I	319	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	200	PRO
1	K	355	ASN
1	L	301	GLY
1	L	363	ILE
1	M	239	GLU
1	M	363	ILE
1	A	240	ILE
1	B	196	VAL
1	B	210	GLY
1	F	144	PRO
1	F	356	VAL
1	M	264	GLY
1	N	318	ILE
1	C	140	VAL
1	D	192	VAL
1	D	372	GLY
1	E	303	ILE
1	F	240	ILE
1	K	303	ILE
1	N	255	ILE
1	A	180	ILE
1	D	156	ILE
1	D	200	PRO
1	E	144	PRO
1	E	175	VAL
1	G	241	GLY
1	N	175	VAL
1	C	196	VAL
1	C	153	ILE
1	H	180	ILE
1	I	153	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	212/232 (91%)	187 (88%)	25 (12%)	5 21
1	B	208/232 (90%)	185 (89%)	23 (11%)	6 24
1	C	213/232 (92%)	188 (88%)	25 (12%)	5 22
1	D	212/232 (91%)	180 (85%)	32 (15%)	3 12
1	E	213/232 (92%)	176 (83%)	37 (17%)	2 9
1	F	213/232 (92%)	175 (82%)	38 (18%)	2 8
1	G	213/232 (92%)	188 (88%)	25 (12%)	5 22
1	H	208/232 (90%)	187 (90%)	21 (10%)	7 28
1	I	209/232 (90%)	187 (90%)	22 (10%)	7 26
1	J	211/232 (91%)	193 (92%)	18 (8%)	10 37
1	K	213/232 (92%)	188 (88%)	25 (12%)	5 22
1	L	211/232 (91%)	171 (81%)	40 (19%)	1 6
1	M	212/232 (91%)	186 (88%)	26 (12%)	4 19
1	N	212/232 (91%)	185 (87%)	27 (13%)	4 18
All	All	2960/3248 (91%)	2576 (87%)	384 (13%)	4 18

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
1	A	179	LEU
1	A	194	LEU
1	A	201	ARG
1	A	202	ASP
1	A	211	TYR
1	A	216	PHE
1	A	222	SER
1	A	227	PHE
1	A	244	SER
1	A	246	GLU
1	A	251	LEU
1	A	262	ARG
1	A	263	LEU
1	A	274	ARG
1	A	285	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	299	ARG
1	A	310	LEU
1	A	318	ILE
1	A	322	ASN
1	A	339	PHE
1	A	342	SER
1	A	357	ARG
1	A	359	LEU
1	A	383	LEU
1	B	166	THR
1	B	178	ARG
1	B	189	GLU
1	B	200	PRO
1	B	202	ASP
1	B	226	PHE
1	B	227	PHE
1	B	229	LEU
1	B	239	GLU
1	B	251	LEU
1	B	260	PHE
1	B	262	ARG
1	B	266	ARG
1	B	272	ASN
1	B	274	ARG
1	B	275	ILE
1	B	281	ARG
1	B	284	LYS
1	B	285	GLU
1	B	299	ARG
1	B	314	LYS
1	B	318	ILE
1	B	377	ARG
1	C	139	TYR
1	C	178	ARG
1	C	181	HIS
1	C	194	LEU
1	C	203	ILE
1	C	211	TYR
1	C	217	THR
1	C	223	LYS
1	C	227	PHE
1	C	229	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	240	ILE
1	C	246	GLU
1	C	253	ARG
1	C	262	ARG
1	C	263	LEU
1	C	274	ARG
1	C	281	ARG
1	C	284	LYS
1	C	299	ARG
1	C	310	LEU
1	C	318	ILE
1	C	320	LEU
1	C	357	ARG
1	C	359	LEU
1	C	371	GLU
1	D	138	GLU
1	D	139	TYR
1	D	160	GLU
1	D	164	LEU
1	D	178	ARG
1	D	179	LEU
1	D	185	ASP
1	D	189	GLU
1	D	194	LEU
1	D	213	LYS
1	D	216	PHE
1	D	220	VAL
1	D	227	PHE
1	D	228	GLU
1	D	229	LEU
1	D	235	LEU
1	D	236	PHE
1	D	237	LEU
1	D	246	GLU
1	D	251	LEU
1	D	262	ARG
1	D	274	ARG
1	D	280	ASN
1	D	281	ARG
1	D	285	GLU
1	D	292	PHE
1	D	295	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	299	ARG
1	D	304	GLU
1	D	310	LEU
1	D	318	ILE
1	D	346	LEU
1	E	139	TYR
1	E	142	GLU
1	E	143	SER
1	E	150	LEU
1	E	156	ILE
1	E	158	CYS
1	E	164	LEU
1	E	173	LYS
1	E	175	VAL
1	E	179	LEU
1	E	184	SER
1	E	189	GLU
1	E	194	LEU
1	E	201	ARG
1	E	202	ASP
1	E	209	PHE
1	E	211	TYR
1	E	213	LYS
1	E	216	PHE
1	E	222	SER
1	E	234	THR
1	E	243	LEU
1	E	246	GLU
1	E	251	LEU
1	E	274	ARG
1	E	280	ASN
1	E	281	ARG
1	E	285	GLU
1	E	295	ASP
1	E	299	ARG
1	E	311	ARG
1	E	318	ILE
1	E	319	PRO
1	E	329	SER
1	E	355	ASN
1	E	359	LEU
1	E	361	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	138	GLU
1	F	142	GLU
1	F	166	THR
1	F	171	VAL
1	F	178	ARG
1	F	185	ASP
1	F	194	LEU
1	F	201	ARG
1	F	204	PHE
1	F	211	TYR
1	F	224	GLU
1	F	229	LEU
1	F	246	GLU
1	F	251	LEU
1	F	262	ARG
1	F	263	LEU
1	F	274	ARG
1	F	275	ILE
1	F	285	GLU
1	F	291	LYS
1	F	296	LEU
1	F	299	ARG
1	F	310	LEU
1	F	311	ARG
1	F	318	ILE
1	F	323	HIS
1	F	325	LEU
1	F	339	PHE
1	F	346	LEU
1	F	348	LEU
1	F	355	ASN
1	F	357	ARG
1	F	359	LEU
1	F	361	ASN
1	F	370	SER
1	F	380	LEU
1	F	383	LEU
1	F	384	VAL
1	G	139	TYR
1	G	161	CYS
1	G	178	ARG
1	G	179	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	191	PHE
1	G	194	LEU
1	G	195	ASN
1	G	201	ARG
1	G	211	TYR
1	G	221	SER
1	G	227	PHE
1	G	251	LEU
1	G	261	TYR
1	G	262	ARG
1	G	263	LEU
1	G	274	ARG
1	G	281	ARG
1	G	285	GLU
1	G	295	ASP
1	G	299	ARG
1	G	307	ILE
1	G	310	LEU
1	G	318	ILE
1	G	355	ASN
1	G	359	LEU
1	H	178	ARG
1	H	189	GLU
1	H	194	LEU
1	H	202	ASP
1	H	216	PHE
1	H	227	PHE
1	H	229	LEU
1	H	242	GLU
1	H	251	LEU
1	H	252	LEU
1	H	263	LEU
1	H	274	ARG
1	H	279	THR
1	H	280	ASN
1	H	293	ARG
1	H	299	ARG
1	H	311	ARG
1	H	323	HIS
1	H	328	PHE
1	H	339	PHE
1	H	369	PHE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	I	158	CYS
1	I	178	ARG
1	I	195	ASN
1	I	202	ASP
1	I	227	PHE
1	I	229	LEU
1	I	242	GLU
1	I	246	GLU
1	I	251	LEU
1	I	262	ARG
1	I	274	ARG
1	I	281	ARG
1	I	285	GLU
1	I	295	ASP
1	I	299	ARG
1	I	311	ARG
1	I	318	ILE
1	I	346	LEU
1	I	357	ARG
1	I	359	LEU
1	I	365	ARG
1	I	373	LYS
1	J	141	PHE
1	J	143	SER
1	J	201	ARG
1	J	202	ASP
1	J	204	PHE
1	J	216	PHE
1	J	229	LEU
1	J	262	ARG
1	J	274	ARG
1	J	281	ARG
1	J	285	GLU
1	J	299	ARG
1	J	318	ILE
1	J	341	LYS
1	J	349	SER
1	J	363	ILE
1	J	376	ASP
1	J	383	LEU
1	K	141	PHE
1	K	147	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	K	160	GLU
1	K	179	LEU
1	K	189	GLU
1	K	190	PRO
1	K	201	ARG
1	K	209	PHE
1	K	216	PHE
1	K	221	SER
1	K	229	LEU
1	K	237	LEU
1	K	238	ASP
1	K	242	GLU
1	K	251	LEU
1	K	262	ARG
1	K	274	ARG
1	K	281	ARG
1	K	285	GLU
1	K	292	PHE
1	K	299	ARG
1	K	310	LEU
1	K	318	ILE
1	K	359	LEU
1	K	361	ASN
1	L	141	PHE
1	L	147	LYS
1	L	150	LEU
1	L	151	GLU
1	L	166	THR
1	L	178	ARG
1	L	189	GLU
1	L	211	TYR
1	L	217	THR
1	L	227	PHE
1	L	229	LEU
1	L	238	ASP
1	L	242	GLU
1	L	245	LEU
1	L	251	LEU
1	L	253	ARG
1	L	259	LYS
1	L	262	ARG
1	L	263	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	L	266	ARG
1	L	272	ASN
1	L	273	VAL
1	L	274	ARG
1	L	279	THR
1	L	296	LEU
1	L	297	TYR
1	L	299	ARG
1	L	305	ILE
1	L	315	GLU
1	L	318	ILE
1	L	325	LEU
1	L	334	LYS
1	L	335	GLU
1	L	337	GLU
1	L	344	GLN
1	L	348	LEU
1	L	350	TYR
1	L	369	PHE
1	L	370	SER
1	L	383	LEU
1	M	139	TYR
1	M	145	LYS
1	M	146	MET
1	M	161	CYS
1	M	178	ARG
1	M	179	LEU
1	M	191	PHE
1	M	198	SER
1	M	201	ARG
1	M	211	TYR
1	M	213	LYS
1	M	227	PHE
1	M	229	LEU
1	M	248	GLN
1	M	251	LEU
1	M	253	ARG
1	M	274	ARG
1	M	276	LEU
1	M	294	GLU
1	M	311	ARG
1	M	322	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	M	352	TRP
1	M	359	LEU
1	M	361	ASN
1	M	368	LEU
1	M	374	PHE
1	N	138	GLU
1	N	148	GLU
1	N	152	LYS
1	N	189	GLU
1	N	194	LEU
1	N	201	ARG
1	N	205	GLU
1	N	207	GLU
1	N	212	GLU
1	N	227	PHE
1	N	229	LEU
1	N	239	GLU
1	N	262	ARG
1	N	263	LEU
1	N	266	ARG
1	N	281	ARG
1	N	292	PHE
1	N	295	ASP
1	N	296	LEU
1	N	299	ARG
1	N	314	LYS
1	N	318	ILE
1	N	320	LEU
1	N	339	PHE
1	N	346	LEU
1	N	350	TYR
1	N	356	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	272	ASN
1	A	282	ASN
1	A	355	ASN
1	A	361	ASN
1	B	272	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	322	ASN
1	B	355	ASN
1	B	361	ASN
1	C	181	HIS
1	C	361	ASN
1	D	181	HIS
1	D	248	GLN
1	D	282	ASN
1	D	355	ASN
1	D	361	ASN
1	E	181	HIS
1	E	272	ASN
1	E	361	ASN
1	F	181	HIS
1	F	195	ASN
1	F	282	ASN
1	G	181	HIS
1	G	282	ASN
1	G	361	ASN
1	H	344	GLN
1	I	195	ASN
1	I	282	ASN
1	I	361	ASN
1	J	181	HIS
1	J	282	ASN
1	K	181	HIS
1	K	272	ASN
1	K	282	ASN
1	K	361	ASN
1	L	181	HIS
1	L	272	ASN
1	L	361	ASN
1	M	181	HIS
1	M	248	GLN
1	M	282	ASN
1	M	361	ASN
1	N	181	HIS
1	N	248	GLN
1	N	282	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	C	1	-	24,29,29	1.47	3 (12%)	29,45,45	1.55	1 (3%)
2	ADP	B	7	-	24,29,29	1.52	5 (20%)	29,45,45	1.65	3 (10%)
2	ADP	J	9	-	24,29,29	1.49	6 (25%)	29,45,45	1.61	3 (10%)
2	ADP	D	2	-	24,29,29	1.48	5 (20%)	29,45,45	1.67	4 (13%)
2	ADP	G	5	-	24,29,29	1.48	3 (12%)	29,45,45	1.73	4 (13%)
2	ADP	F	4	-	24,29,29	1.45	3 (12%)	29,45,45	1.59	3 (10%)
2	ADP	L	11	-	24,29,29	1.56	6 (25%)	29,45,45	1.56	2 (6%)
2	ADP	I	8	-	24,29,29	1.49	4 (16%)	29,45,45	1.59	3 (10%)
2	ADP	M	12	-	24,29,29	1.39	3 (12%)	29,45,45	1.57	3 (10%)
2	ADP	K	10	-	24,29,29	1.55	5 (20%)	29,45,45	1.63	3 (10%)
2	ADP	A	6	-	24,29,29	1.59	5 (20%)	29,45,45	1.67	3 (10%)
2	ADP	N	13	-	24,29,29	1.49	5 (20%)	29,45,45	1.55	2 (6%)
2	ADP	E	3	-	24,29,29	1.52	5 (20%)	29,45,45	1.61	1 (3%)
2	ADP	H	14	-	24,29,29	1.53	5 (20%)	29,45,45	1.56	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	1	-	-	6/12/32/32	0/3/3/3
2	ADP	B	7	-	-	6/12/32/32	0/3/3/3
2	ADP	J	9	-	-	7/12/32/32	0/3/3/3
2	ADP	D	2	-	-	8/12/32/32	0/3/3/3
2	ADP	G	5	-	-	5/12/32/32	0/3/3/3
2	ADP	F	4	-	-	6/12/32/32	0/3/3/3
2	ADP	L	11	-	-	8/12/32/32	0/3/3/3
2	ADP	I	8	-	-	6/12/32/32	0/3/3/3
2	ADP	M	12	-	-	5/12/32/32	0/3/3/3
2	ADP	K	10	-	-	8/12/32/32	0/3/3/3
2	ADP	A	6	-	-	8/12/32/32	0/3/3/3
2	ADP	N	13	-	-	7/12/32/32	0/3/3/3
2	ADP	E	3	-	-	6/12/32/32	0/3/3/3
2	ADP	H	14	-	-	6/12/32/32	0/3/3/3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	ADP	O4'-C1'	3.53	1.46	1.41
2	L	11	ADP	C2-N3	3.49	1.37	1.32
2	H	14	ADP	O4'-C1'	3.40	1.45	1.41
2	H	14	ADP	C2-N3	3.31	1.37	1.32
2	C	1	ADP	C2-N3	3.25	1.37	1.32
2	K	10	ADP	C2-N3	3.19	1.37	1.32
2	N	13	ADP	O4'-C1'	3.18	1.45	1.41
2	B	7	ADP	C2-N3	3.17	1.37	1.32
2	F	4	ADP	O4'-C1'	3.17	1.45	1.41
2	K	10	ADP	O4'-C1'	3.17	1.45	1.41
2	D	2	ADP	C2-N3	3.14	1.37	1.32
2	N	13	ADP	C2-N3	3.13	1.37	1.32
2	F	4	ADP	C2-N3	3.10	1.37	1.32
2	J	9	ADP	O4'-C1'	3.09	1.45	1.41
2	I	8	ADP	O4'-C1'	3.09	1.45	1.41
2	J	9	ADP	C2-N3	3.08	1.37	1.32
2	A	6	ADP	O4'-C1'	2.99	1.45	1.41
2	E	3	ADP	C2-N3	2.94	1.36	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	ADP	O4'-C1'	2.93	1.45	1.41
2	A	6	ADP	C2-N3	2.88	1.36	1.32
2	G	5	ADP	C2-N3	2.86	1.36	1.32
2	A	6	ADP	C5-N7	-2.82	1.29	1.39
2	I	8	ADP	C2-N3	2.77	1.36	1.32
2	D	2	ADP	O4'-C1'	2.67	1.44	1.41
2	M	12	ADP	C2-N3	2.67	1.36	1.32
2	C	1	ADP	C5-N7	-2.66	1.30	1.39
2	L	11	ADP	O4'-C1'	2.65	1.44	1.41
2	M	12	ADP	C5-N7	-2.62	1.30	1.39
2	E	3	ADP	O4'-C1'	2.61	1.44	1.41
2	E	3	ADP	C5-N7	-2.54	1.30	1.39
2	L	11	ADP	C5-N7	-2.53	1.30	1.39
2	K	10	ADP	C5-N7	-2.48	1.30	1.39
2	G	5	ADP	C5-N7	-2.46	1.30	1.39
2	I	8	ADP	C5-N7	-2.44	1.30	1.39
2	H	14	ADP	C4-N3	2.40	1.39	1.35
2	F	4	ADP	C5-N7	-2.39	1.31	1.39
2	B	7	ADP	C5-N7	-2.36	1.31	1.39
2	H	14	ADP	C5-N7	-2.36	1.31	1.39
2	A	6	ADP	C8-N7	-2.34	1.30	1.34
2	D	2	ADP	C4-N3	2.31	1.38	1.35
2	N	13	ADP	C5-N7	-2.28	1.31	1.39
2	J	9	ADP	C5-N7	-2.28	1.31	1.39
2	G	5	ADP	O4'-C1'	2.24	1.44	1.41
2	E	3	ADP	PA-O2A	-2.21	1.45	1.55
2	K	10	ADP	C4-N3	2.20	1.38	1.35
2	K	10	ADP	C5'-C4'	2.20	1.58	1.51
2	D	2	ADP	C5-N7	-2.18	1.31	1.39
2	L	11	ADP	C2-N1	2.16	1.37	1.33
2	N	13	ADP	C4-N3	2.15	1.38	1.35
2	M	12	ADP	C2'-C1'	-2.15	1.50	1.53
2	B	7	ADP	C4-N3	2.14	1.38	1.35
2	J	9	ADP	C4-N3	2.14	1.38	1.35
2	I	8	ADP	C5'-C4'	2.13	1.58	1.51
2	L	11	ADP	C4-N3	2.13	1.38	1.35
2	A	6	ADP	C2-N1	2.12	1.37	1.33
2	L	11	ADP	C8-N7	-2.11	1.30	1.34
2	J	9	ADP	C5'-C4'	2.11	1.58	1.51
2	E	3	ADP	C4-N3	2.09	1.38	1.35
2	D	2	ADP	PA-O2A	-2.08	1.45	1.55
2	N	13	ADP	C5'-C4'	2.08	1.58	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	14	ADP	C5'-C4'	2.06	1.58	1.51
2	B	7	ADP	C5'-C4'	2.03	1.57	1.51
2	J	9	ADP	C2-N1	2.02	1.37	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	ADP	N3-C2-N1	-7.02	117.70	128.68
2	K	10	ADP	N3-C2-N1	-6.82	118.01	128.68
2	G	5	ADP	N3-C2-N1	-6.80	118.05	128.68
2	D	2	ADP	N3-C2-N1	-6.75	118.12	128.68
2	J	9	ADP	N3-C2-N1	-6.72	118.17	128.68
2	H	14	ADP	N3-C2-N1	-6.72	118.17	128.68
2	A	6	ADP	N3-C2-N1	-6.69	118.22	128.68
2	L	11	ADP	N3-C2-N1	-6.66	118.27	128.68
2	B	7	ADP	N3-C2-N1	-6.64	118.29	128.68
2	N	13	ADP	N3-C2-N1	-6.64	118.30	128.68
2	M	12	ADP	N3-C2-N1	-6.61	118.35	128.68
2	I	8	ADP	N3-C2-N1	-6.61	118.35	128.68
2	F	4	ADP	N3-C2-N1	-6.54	118.45	128.68
2	C	1	ADP	N3-C2-N1	-6.42	118.64	128.68
2	B	7	ADP	C2'-C3'-C4'	2.85	108.19	102.64
2	A	6	ADP	C2'-C3'-C4'	2.69	107.87	102.64
2	K	10	ADP	C2'-C3'-C4'	2.66	107.81	102.64
2	G	5	ADP	C2'-C3'-C4'	2.60	107.69	102.64
2	G	5	ADP	O3B-PB-O3A	2.54	113.15	104.64
2	D	2	ADP	C2'-C3'-C4'	2.50	107.50	102.64
2	F	4	ADP	O4'-C4'-C5'	-2.42	101.40	109.37
2	B	7	ADP	C3'-C2'-C1'	2.39	104.57	100.98
2	A	6	ADP	C3'-C2'-C1'	2.34	104.49	100.98
2	J	9	ADP	C2'-C3'-C4'	2.31	107.14	102.64
2	L	11	ADP	O4'-C4'-C5'	-2.29	101.83	109.37
2	K	10	ADP	C3'-C2'-C1'	2.24	104.35	100.98
2	D	2	ADP	C3'-C2'-C1'	2.22	104.31	100.98
2	G	5	ADP	O4'-C1'-C2'	2.19	110.13	106.93
2	I	8	ADP	O5'-C5'-C4'	-2.15	101.58	108.99
2	H	14	ADP	C2'-C3'-C4'	2.14	106.79	102.64
2	M	12	ADP	C2-N1-C6	2.08	122.32	118.75
2	I	8	ADP	PA-O5'-C5'	2.08	133.89	121.68
2	F	4	ADP	C4-C5-N7	-2.08	107.24	109.40
2	D	2	ADP	C4-C5-N7	-2.06	107.25	109.40
2	N	13	ADP	C2'-C3'-C4'	2.06	106.64	102.64

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	12	ADP	C2'-C3'-C4'	2.02	106.57	102.64
2	J	9	ADP	C3'-C2'-C1'	2.00	104.00	100.98

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	ADP	C5'-O5'-PA-O1A
2	C	1	ADP	C5'-O5'-PA-O2A
2	C	1	ADP	C5'-O5'-PA-O3A
2	B	7	ADP	C5'-O5'-PA-O1A
2	B	7	ADP	C5'-O5'-PA-O2A
2	B	7	ADP	C5'-O5'-PA-O3A
2	J	9	ADP	PA-O3A-PB-O2B
2	J	9	ADP	C5'-O5'-PA-O1A
2	J	9	ADP	C5'-O5'-PA-O2A
2	J	9	ADP	C5'-O5'-PA-O3A
2	D	2	ADP	PA-O3A-PB-O2B
2	D	2	ADP	C5'-O5'-PA-O1A
2	D	2	ADP	C5'-O5'-PA-O2A
2	D	2	ADP	C5'-O5'-PA-O3A
2	G	5	ADP	C5'-O5'-PA-O1A
2	G	5	ADP	C5'-O5'-PA-O2A
2	G	5	ADP	C5'-O5'-PA-O3A
2	F	4	ADP	C5'-O5'-PA-O1A
2	F	4	ADP	C5'-O5'-PA-O2A
2	F	4	ADP	C5'-O5'-PA-O3A
2	L	11	ADP	PA-O3A-PB-O2B
2	L	11	ADP	C5'-O5'-PA-O1A
2	L	11	ADP	C5'-O5'-PA-O2A
2	L	11	ADP	C5'-O5'-PA-O3A
2	I	8	ADP	C5'-O5'-PA-O1A
2	I	8	ADP	C5'-O5'-PA-O2A
2	I	8	ADP	C5'-O5'-PA-O3A
2	M	12	ADP	C5'-O5'-PA-O1A
2	M	12	ADP	C5'-O5'-PA-O2A
2	M	12	ADP	C5'-O5'-PA-O3A
2	K	10	ADP	PA-O3A-PB-O2B
2	K	10	ADP	C5'-O5'-PA-O1A
2	K	10	ADP	C5'-O5'-PA-O2A
2	K	10	ADP	C5'-O5'-PA-O3A
2	A	6	ADP	PA-O3A-PB-O2B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	A	6	ADP	C5'-O5'-PA-O1A
2	A	6	ADP	C5'-O5'-PA-O2A
2	A	6	ADP	C5'-O5'-PA-O3A
2	A	6	ADP	O4'-C4'-C5'-O5'
2	N	13	ADP	PA-O3A-PB-O2B
2	N	13	ADP	C5'-O5'-PA-O1A
2	N	13	ADP	C5'-O5'-PA-O2A
2	N	13	ADP	C5'-O5'-PA-O3A
2	E	3	ADP	PA-O3A-PB-O2B
2	E	3	ADP	C5'-O5'-PA-O1A
2	E	3	ADP	C5'-O5'-PA-O2A
2	E	3	ADP	C5'-O5'-PA-O3A
2	H	14	ADP	C5'-O5'-PA-O1A
2	H	14	ADP	C5'-O5'-PA-O2A
2	H	14	ADP	C5'-O5'-PA-O3A
2	H	14	ADP	O4'-C4'-C5'-O5'
2	B	7	ADP	O4'-C4'-C5'-O5'
2	H	14	ADP	C3'-C4'-C5'-O5'
2	C	1	ADP	O4'-C4'-C5'-O5'
2	C	1	ADP	C3'-C4'-C5'-O5'
2	J	9	ADP	O4'-C4'-C5'-O5'
2	J	9	ADP	C3'-C4'-C5'-O5'
2	D	2	ADP	O4'-C4'-C5'-O5'
2	D	2	ADP	C3'-C4'-C5'-O5'
2	F	4	ADP	O4'-C4'-C5'-O5'
2	F	4	ADP	C3'-C4'-C5'-O5'
2	L	11	ADP	O4'-C4'-C5'-O5'
2	L	11	ADP	C3'-C4'-C5'-O5'
2	I	8	ADP	O4'-C4'-C5'-O5'
2	I	8	ADP	C3'-C4'-C5'-O5'
2	K	10	ADP	O4'-C4'-C5'-O5'
2	K	10	ADP	C3'-C4'-C5'-O5'
2	A	6	ADP	C3'-C4'-C5'-O5'
2	N	13	ADP	O4'-C4'-C5'-O5'
2	N	13	ADP	C3'-C4'-C5'-O5'
2	E	3	ADP	C3'-C4'-C5'-O5'
2	G	5	ADP	O4'-C4'-C5'-O5'
2	G	5	ADP	C3'-C4'-C5'-O5'
2	M	12	ADP	O4'-C4'-C5'-O5'
2	E	3	ADP	O4'-C4'-C5'-O5'
2	M	12	ADP	C3'-C4'-C5'-O5'
2	C	1	ADP	PA-O3A-PB-O1B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	F	4	ADP	PA-O3A-PB-O1B
2	I	8	ADP	PA-O3A-PB-O1B
2	H	14	ADP	PA-O3A-PB-O1B
2	B	7	ADP	C3'-C4'-C5'-O5'
2	D	2	ADP	PA-O3A-PB-O3B
2	B	7	ADP	PB-O3A-PA-O2A
2	K	10	ADP	PA-O3A-PB-O1B
2	A	6	ADP	PA-O3A-PB-O1B
2	L	11	ADP	PA-O3A-PB-O3B
2	K	10	ADP	PA-O3A-PB-O3B
2	A	6	ADP	PA-O3A-PB-O3B
2	N	13	ADP	PA-O3A-PB-O3B
2	J	9	ADP	PA-O3A-PB-O1B
2	D	2	ADP	PA-O3A-PB-O1B
2	L	11	ADP	PA-O3A-PB-O1B

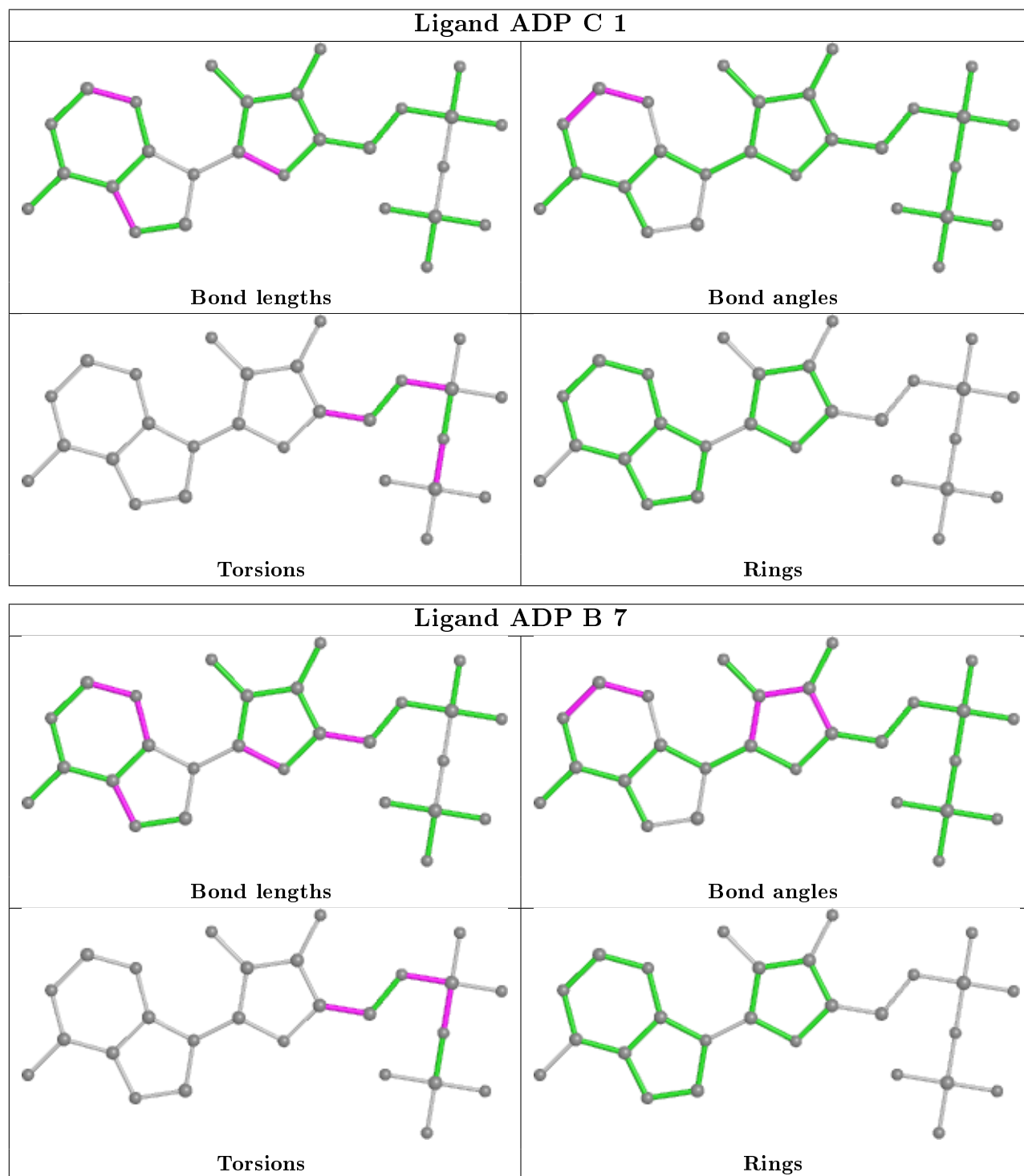
There are no ring outliers.

13 monomers are involved in 47 short contacts:

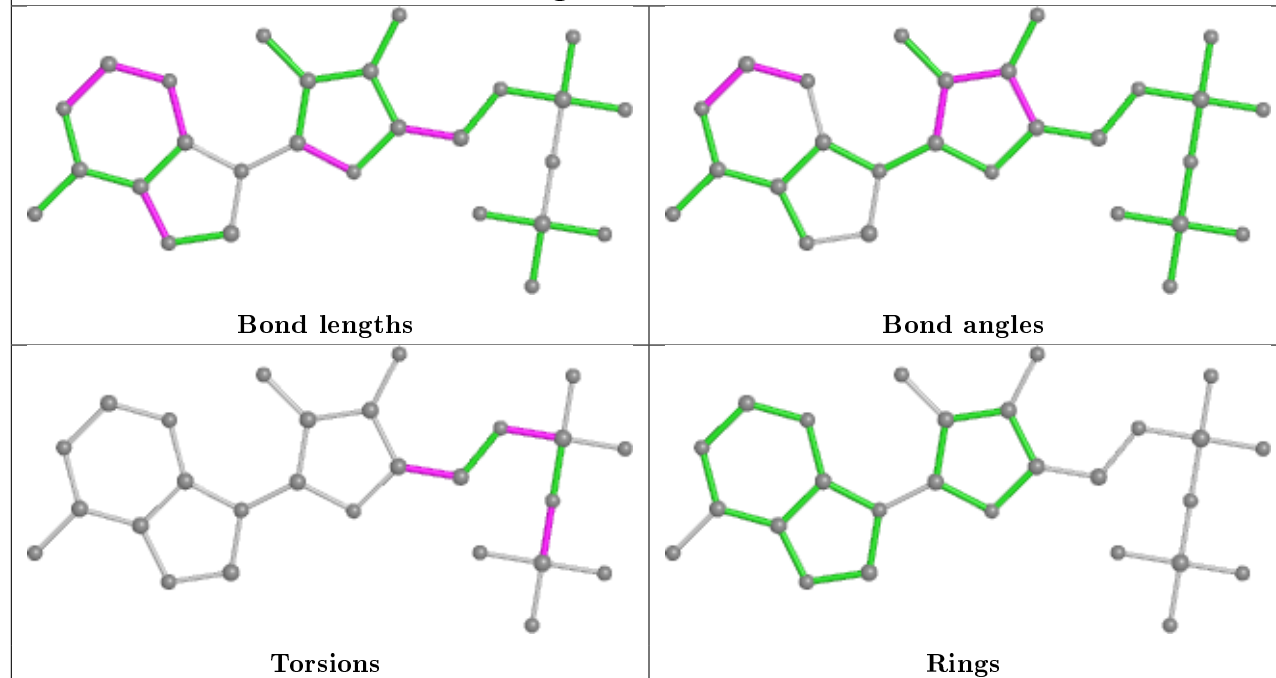
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	ADP	4	0
2	B	7	ADP	1	0
2	J	9	ADP	1	0
2	D	2	ADP	6	0
2	F	4	ADP	7	0
2	L	11	ADP	6	0
2	I	8	ADP	5	0
2	M	12	ADP	6	0
2	K	10	ADP	1	0
2	A	6	ADP	2	0
2	N	13	ADP	2	0
2	E	3	ADP	3	0
2	H	14	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

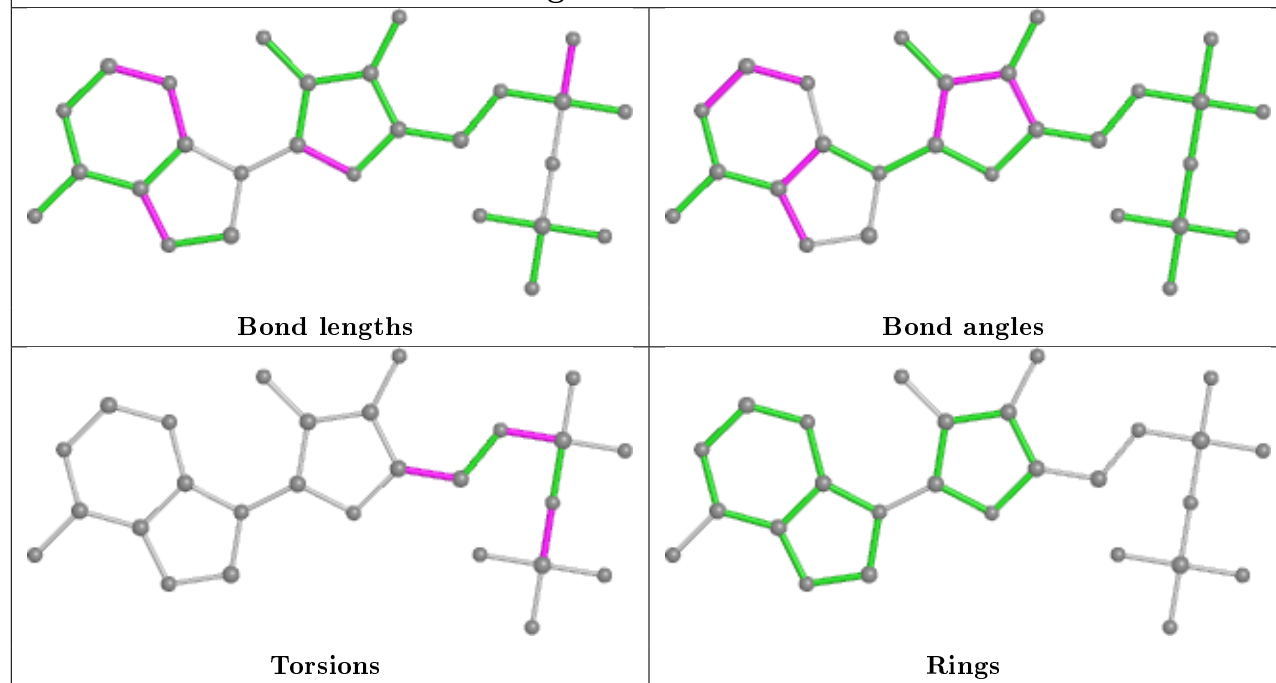
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



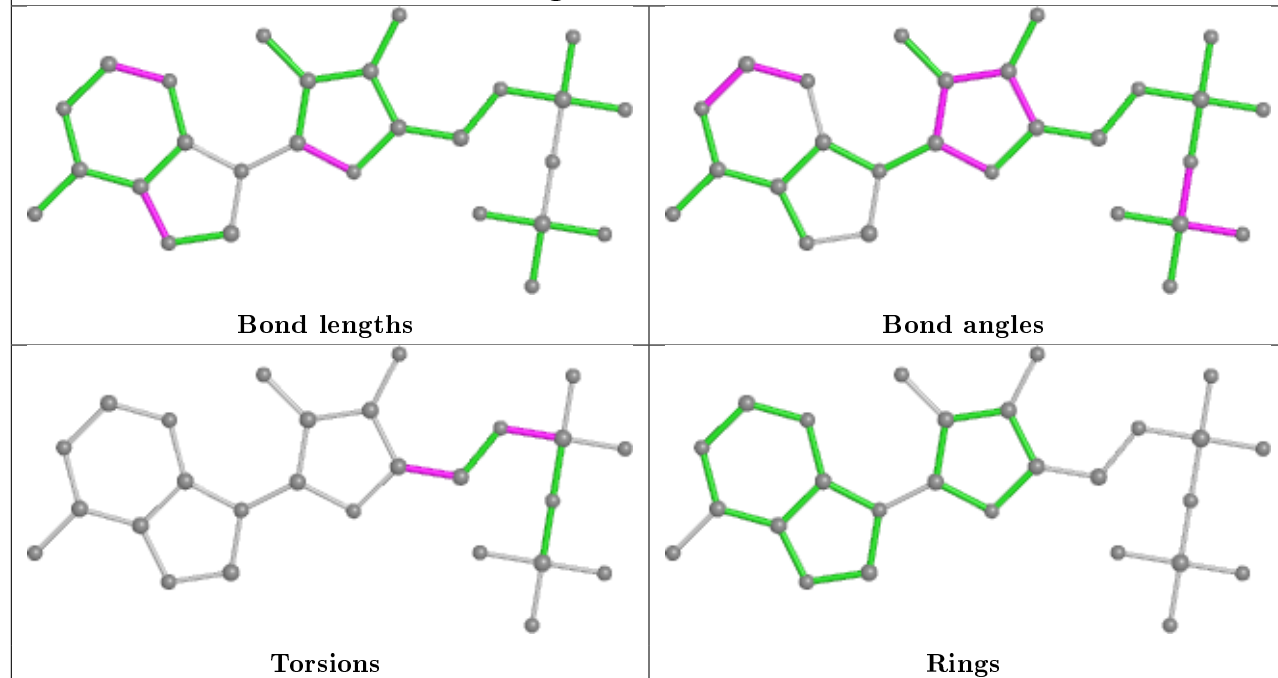
## Ligand ADP J 9



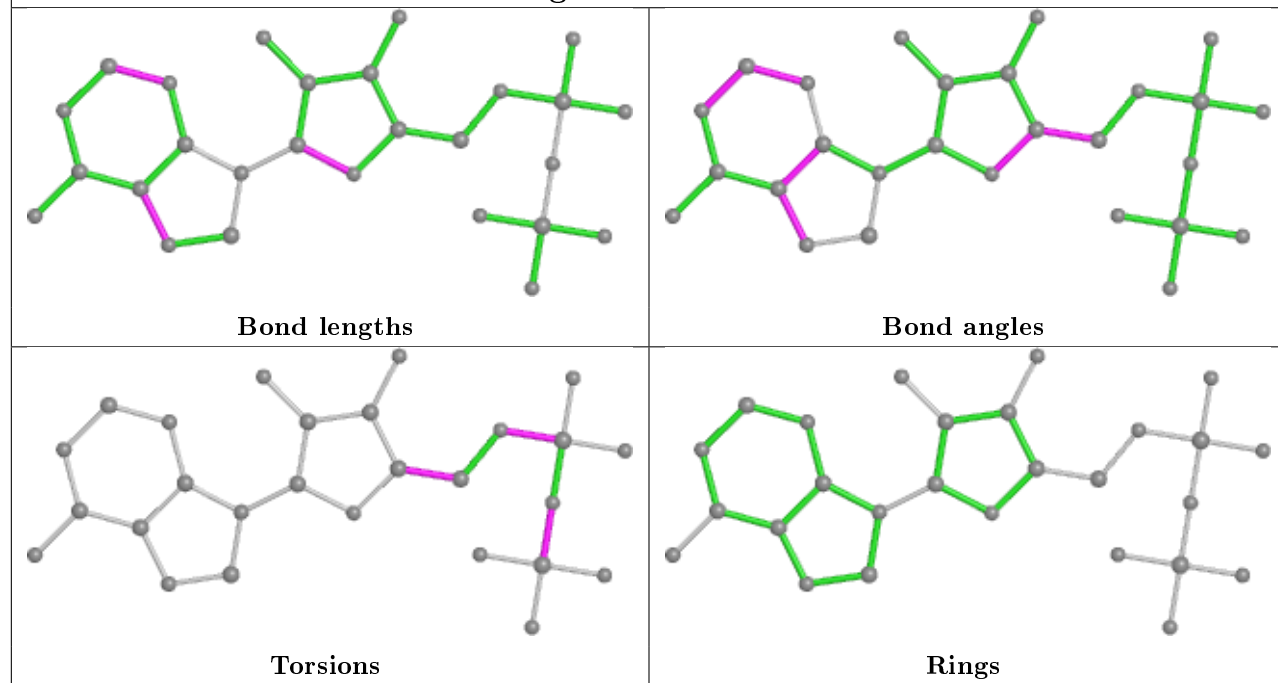
## Ligand ADP D 2



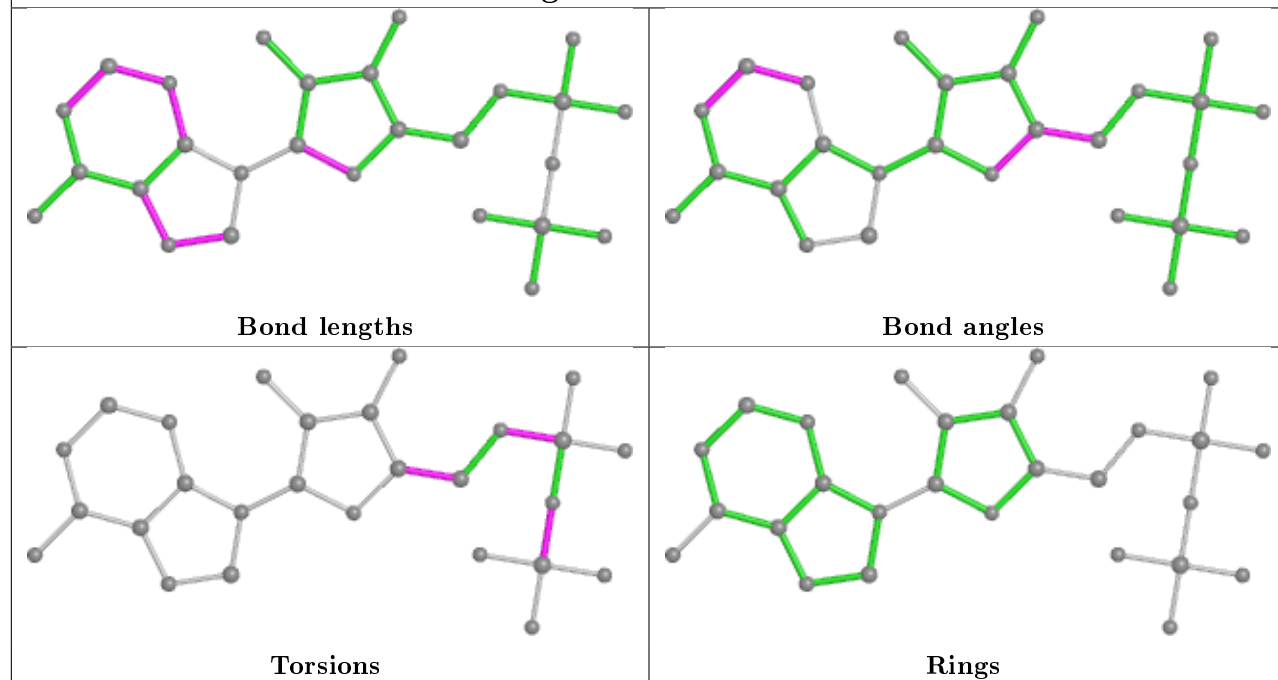
## Ligand ADP G 5



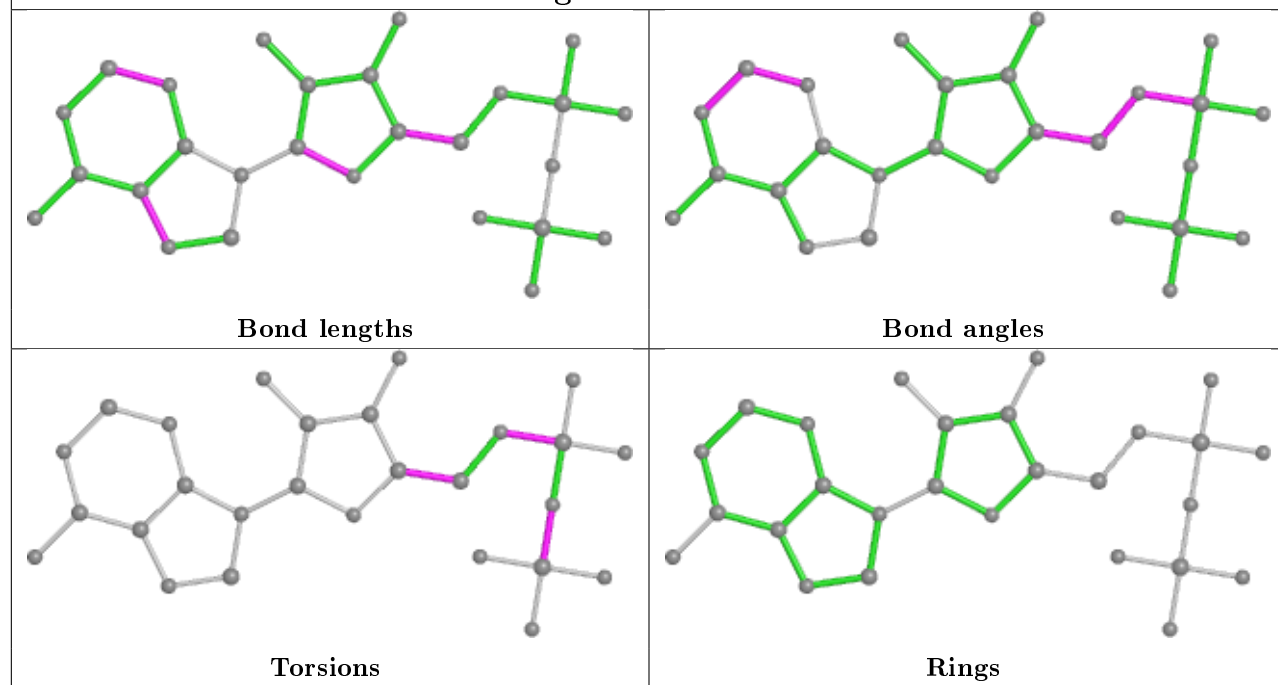
## Ligand ADP F 4



## Ligand ADP L 11

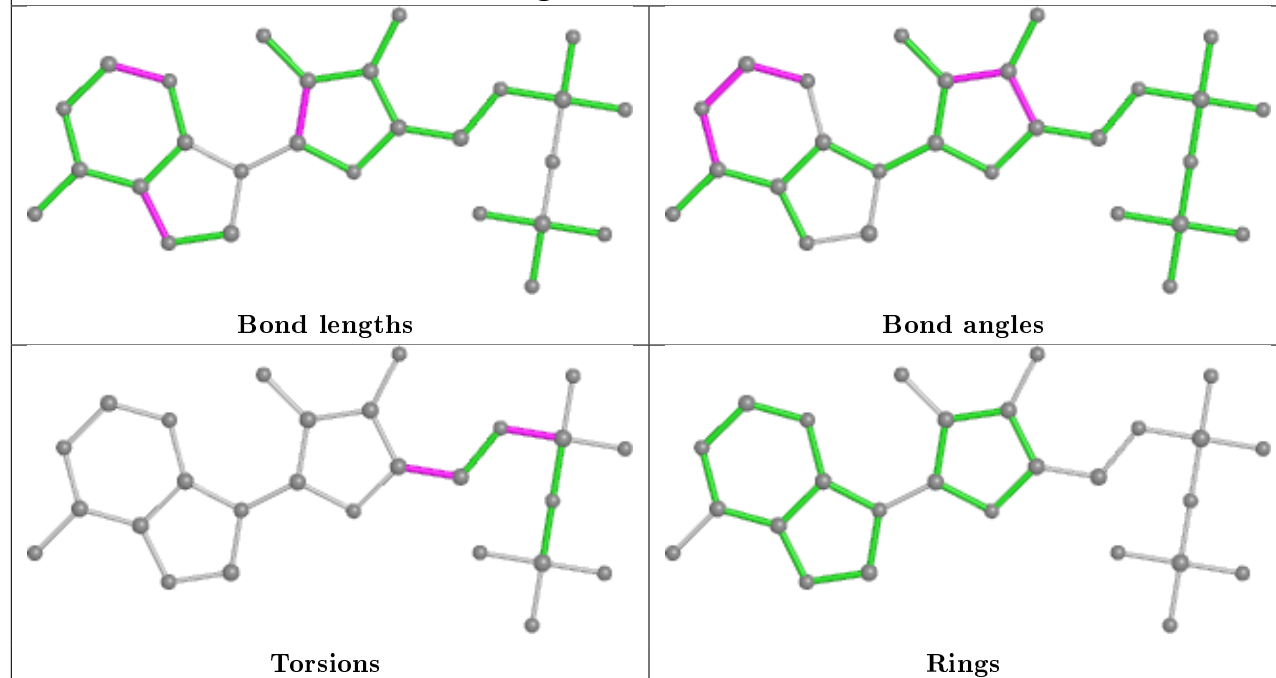


## Ligand ADP I 8

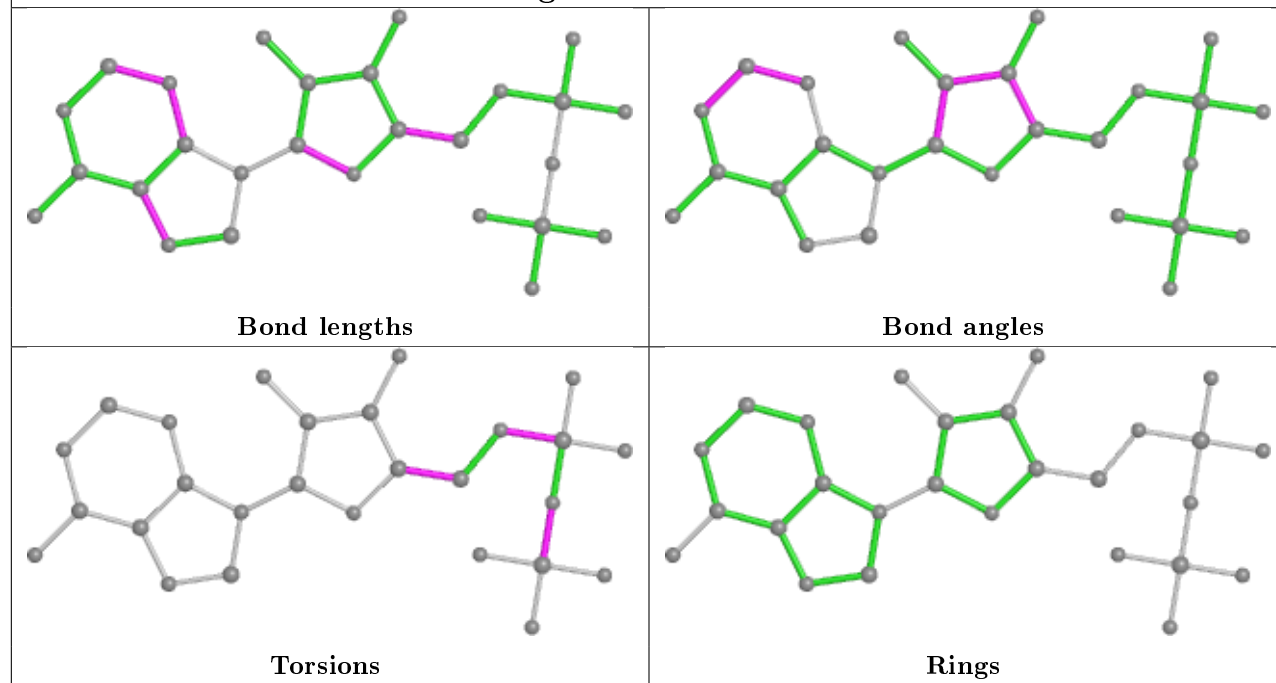




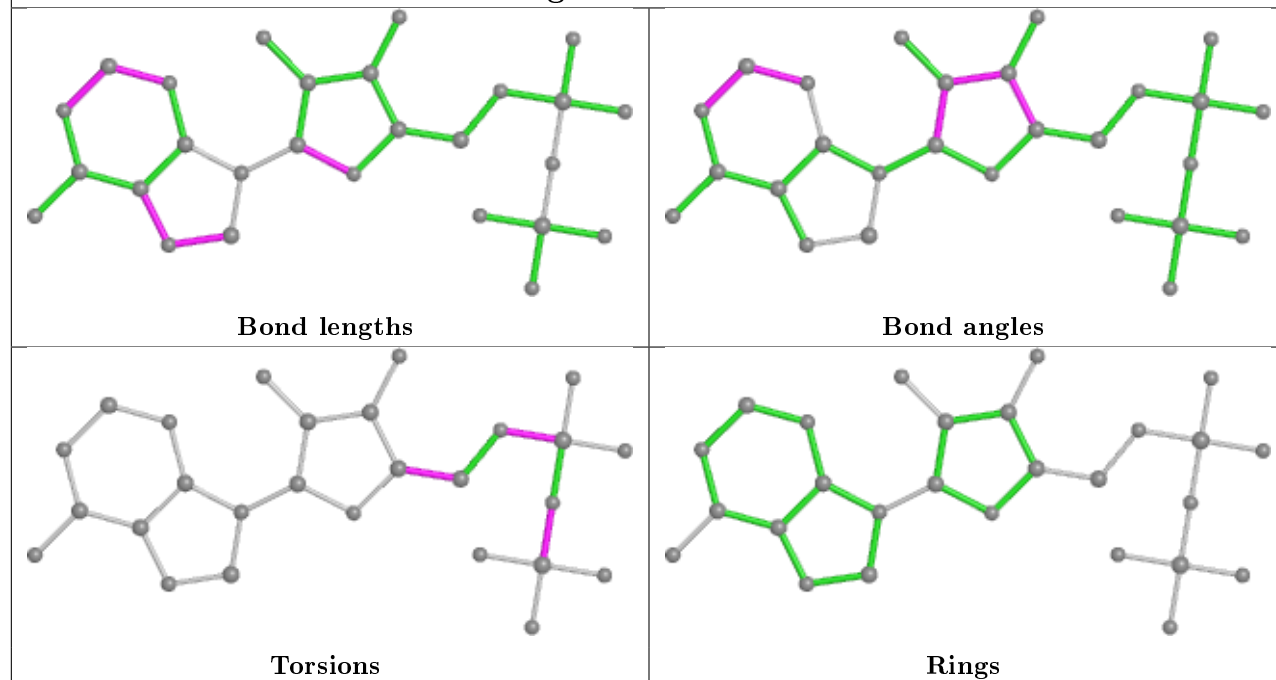
## Ligand ADP M 12



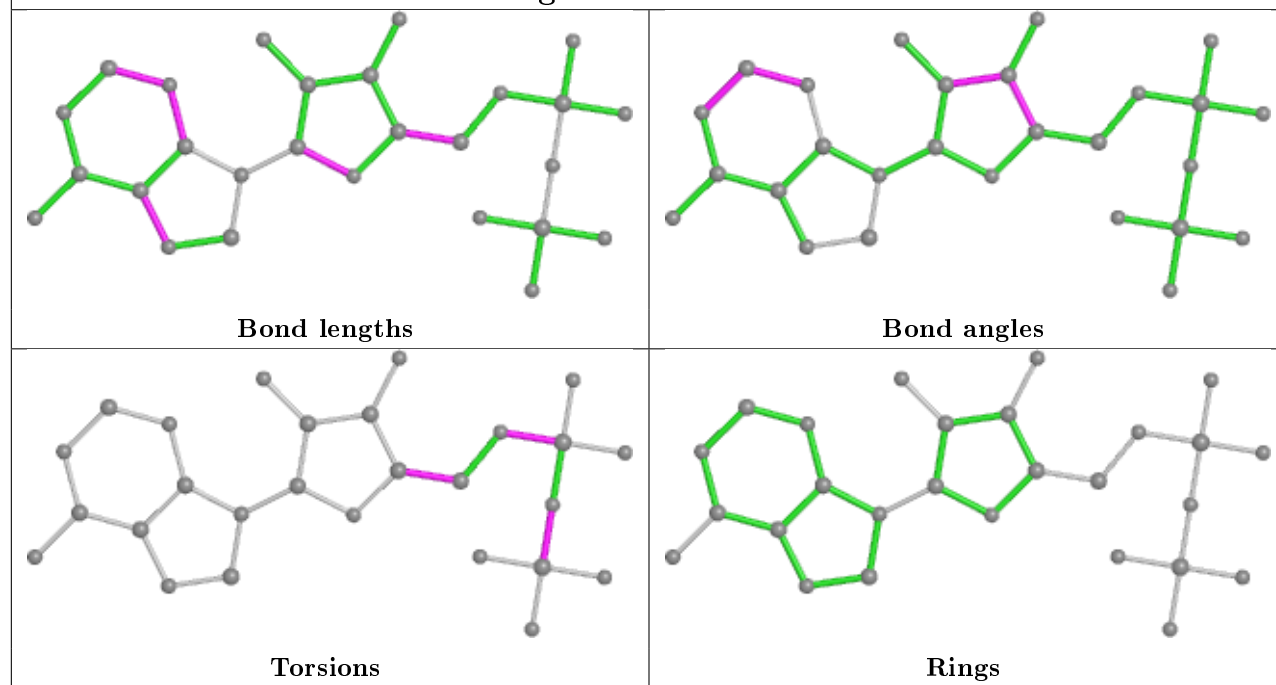
## Ligand ADP K 10

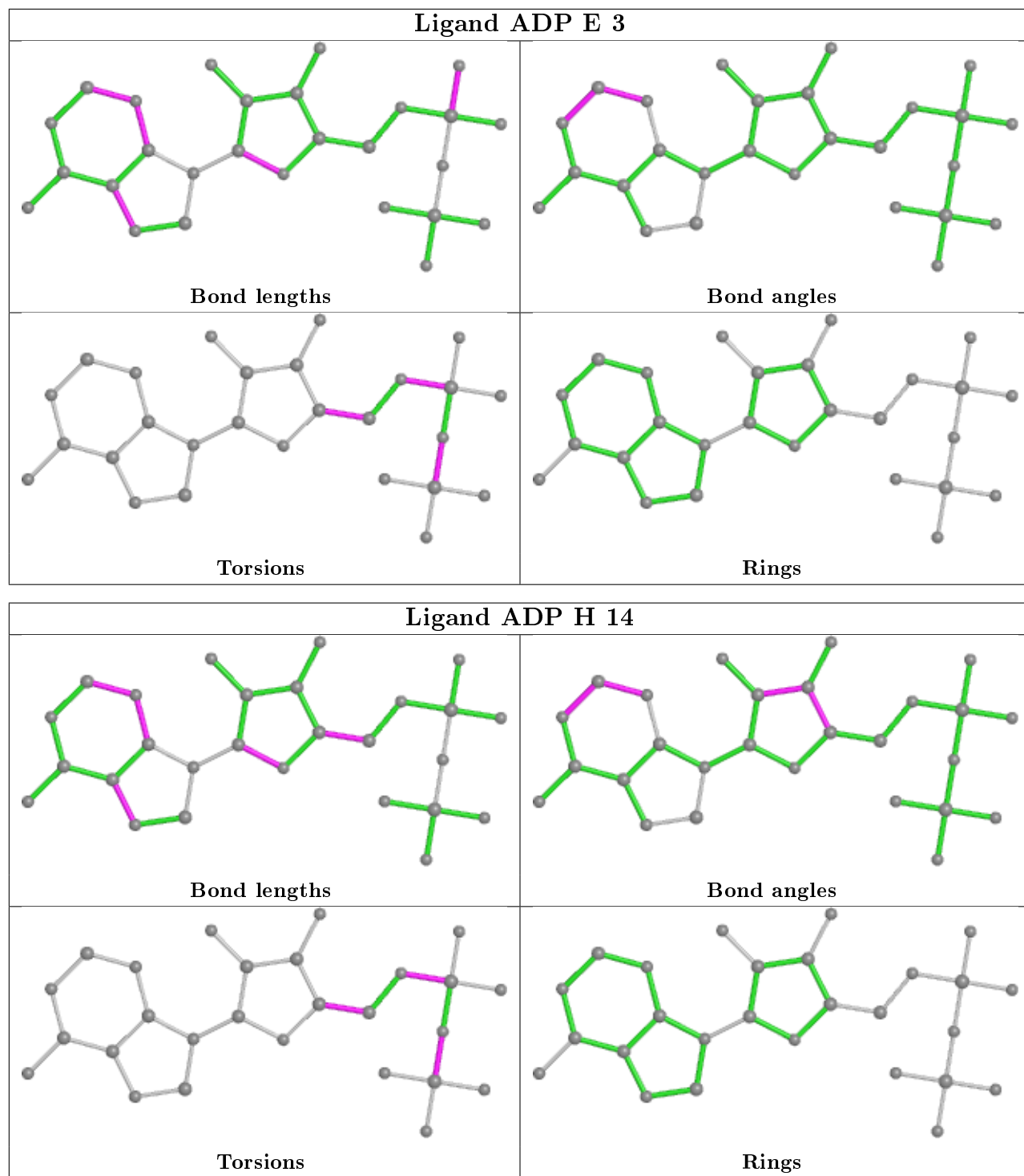


## Ligand ADP A 6



## Ligand ADP N 13





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	247/267 (92%)	-0.04	5 (2%) 65 44	29, 107, 142, 151	0
1	B	243/267 (91%)	0.05	7 (2%) 51 28	18, 101, 150, 151	0
1	C	248/267 (92%)	-0.13	0 100 100	43, 85, 128, 142	0
1	D	247/267 (92%)	-0.15	0 100 100	43, 90, 136, 148	0
1	E	248/267 (92%)	-0.09	7 (2%) 53 30	18, 83, 140, 151	0
1	F	248/267 (92%)	-0.03	8 (3%) 47 25	44, 106, 146, 150	0
1	G	248/267 (92%)	0.07	7 (2%) 53 30	64, 114, 150, 151	0
1	H	245/267 (91%)	0.25	13 (5%) 26 12	77, 129, 151, 151	0
1	I	247/267 (92%)	-0.09	5 (2%) 65 44	65, 103, 147, 151	0
1	J	247/267 (92%)	0.19	15 (6%) 21 9	71, 119, 147, 151	0
1	K	248/267 (92%)	0.03	6 (2%) 59 37	57, 104, 137, 148	0
1	L	246/267 (92%)	-0.11	2 (0%) 86 72	27, 80, 126, 150	0
1	M	247/267 (92%)	-0.07	2 (0%) 86 72	25, 100, 139, 146	0
1	N	247/267 (92%)	-0.10	3 (1%) 79 61	67, 106, 138, 151	0
All	All	3456/3738 (92%)	-0.02	80 (2%) 60 39	18, 102, 148, 151	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	382	CYS	6.9
1	E	264	GLY	6.0
1	F	276	LEU	5.4
1	J	305	ILE	5.0
1	E	211	TYR	4.6
1	B	339	PHE	4.6
1	E	263	LEU	4.4
1	J	255	ILE	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	4.2
1	H	347	LEU	4.0
1	H	357	ARG	3.8
1	H	339	PHE	3.7
1	A	300	LEU	3.3
1	F	275	ILE	3.2
1	H	333	ALA	3.2
1	H	380	LEU	3.1
1	I	347	LEU	3.1
1	J	237	LEU	3.1
1	G	270	GLU	3.0
1	N	141	PHE	3.0
1	H	366	ALA	3.0
1	M	380	LEU	2.9
1	J	204	PHE	2.9
1	I	300	LEU	2.9
1	G	251	LEU	2.9
1	E	266	ARG	2.8
1	E	209	PHE	2.8
1	K	139	TYR	2.8
1	A	302	VAL	2.8
1	H	350	TYR	2.7
1	I	380	LEU	2.7
1	J	163	VAL	2.7
1	J	273	VAL	2.7
1	J	303	ILE	2.6
1	H	364	GLU	2.5
1	G	204	PHE	2.5
1	K	259	LYS	2.5
1	E	139	TYR	2.5
1	B	320	LEU	2.4
1	K	277	ALA	2.4
1	J	275	ILE	2.3
1	F	299	ARG	2.3
1	G	255	ILE	2.3
1	K	303	ILE	2.3
1	B	237	LEU	2.3
1	J	251	LEU	2.3
1	A	223	LYS	2.3
1	H	168	GLU	2.3
1	E	261	TYR	2.3
1	N	277	ALA	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	163	VAL	2.2
1	I	260	PHE	2.2
1	F	191	PHE	2.2
1	G	369	PHE	2.2
1	K	380	LEU	2.1
1	H	310	LEU	2.1
1	L	139	TYR	2.1
1	J	208	LEU	2.1
1	B	240	ILE	2.1
1	N	216	PHE	2.1
1	A	180	ILE	2.1
1	J	153	ILE	2.1
1	B	332	TYR	2.1
1	L	298	TYR	2.1
1	J	381	SER	2.1
1	H	276	LEU	2.1
1	F	165	ILE	2.1
1	I	221	SER	2.1
1	M	266	ARG	2.1
1	H	328	PHE	2.1
1	G	269	ILE	2.1
1	F	227	PHE	2.0
1	F	213	LYS	2.0
1	J	227	PHE	2.0
1	B	382	CYS	2.0
1	A	183	LEU	2.0
1	J	375	ILE	2.0
1	F	237	LEU	2.0
1	J	339	PHE	2.0
1	K	305	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

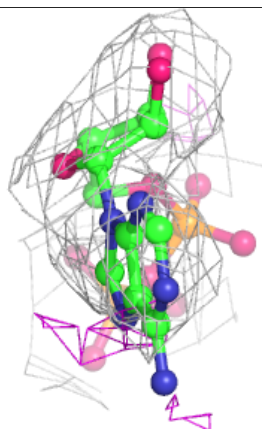
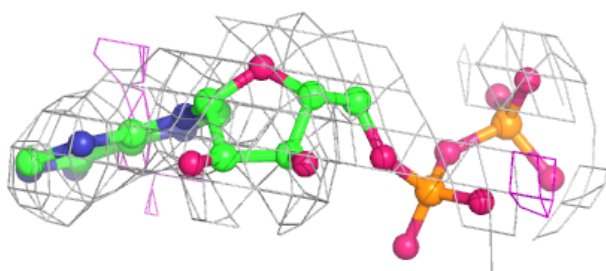
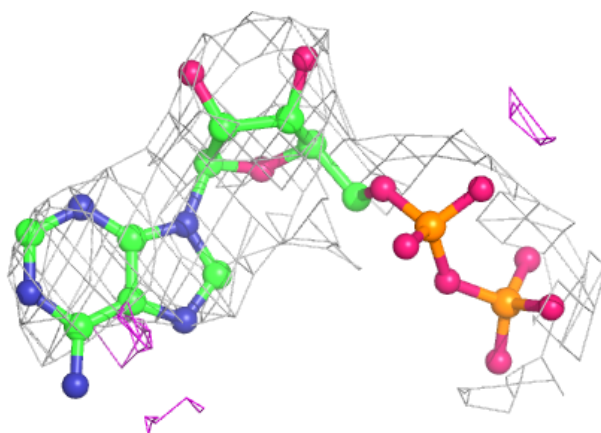
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	B	7	27/27	0.91	0.21	96,111,114,114	0
2	ADP	K	10	27/27	0.91	0.21	99,103,108,110	0
2	ADP	N	13	27/27	0.91	0.18	100,106,110,111	0
2	ADP	J	9	27/27	0.92	0.16	92,95,102,104	0
2	ADP	D	2	27/27	0.92	0.22	71,82,91,93	0
2	ADP	H	14	27/27	0.92	0.24	125,141,143,143	0
2	ADP	A	6	27/27	0.93	0.20	84,88,92,96	0
2	ADP	M	12	27/27	0.93	0.18	51,67,86,87	0
2	ADP	G	5	27/27	0.93	0.19	52,65,75,80	0
2	ADP	L	11	27/27	0.94	0.20	48,60,84,93	0
2	ADP	F	4	27/27	0.94	0.17	62,66,84,87	0
2	ADP	I	8	27/27	0.96	0.18	66,81,87,90	0
2	ADP	E	3	27/27	0.96	0.18	51,64,70,79	0
2	ADP	C	1	27/27	0.96	0.19	54,70,77,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

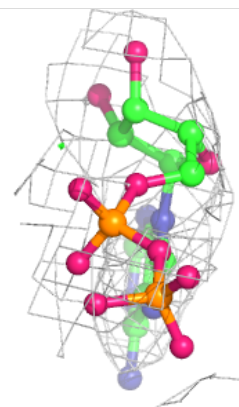
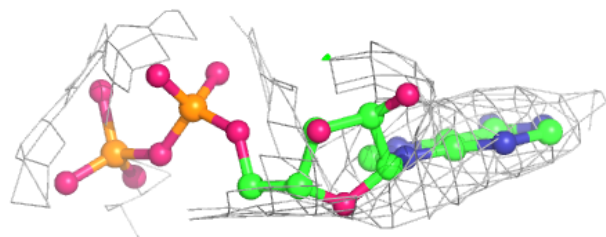
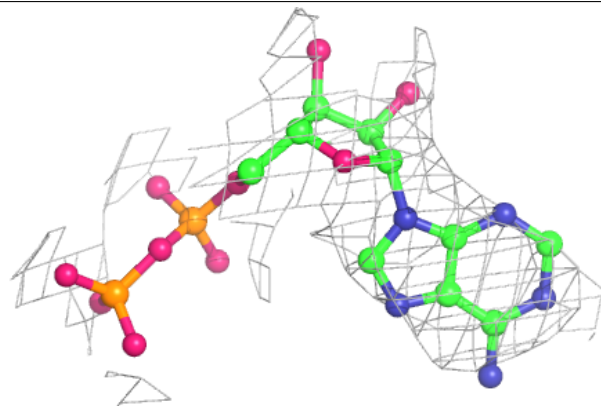


**Electron density around ADP B 7:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

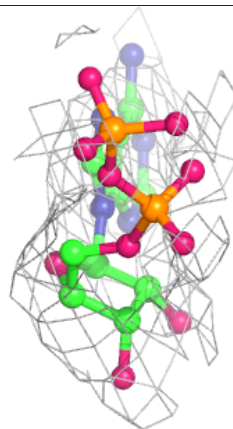
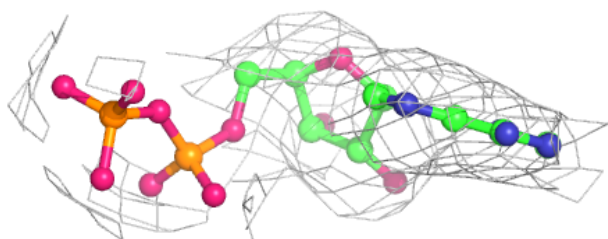
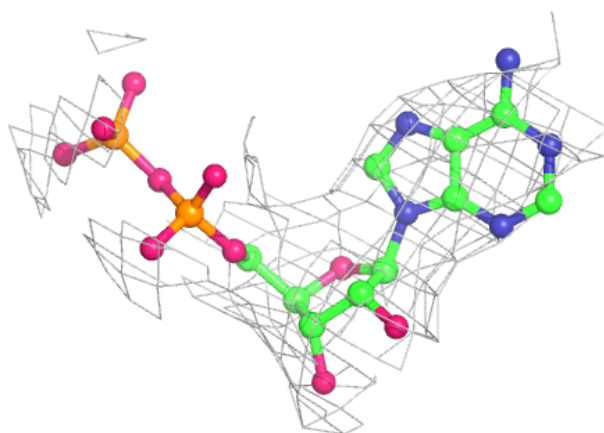
**Electron density around ADP K 10:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



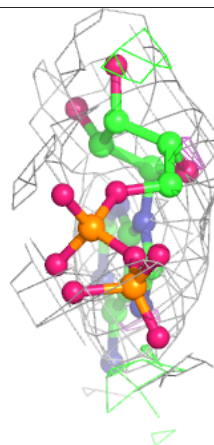
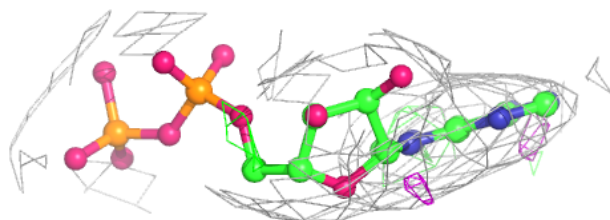
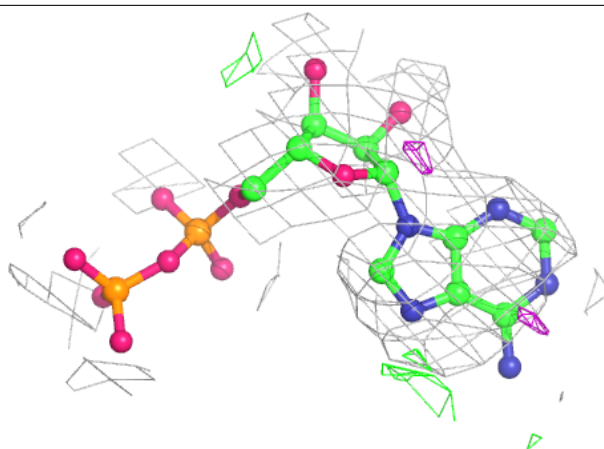
**Electron density around ADP N 13:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

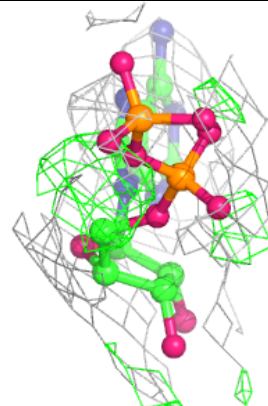
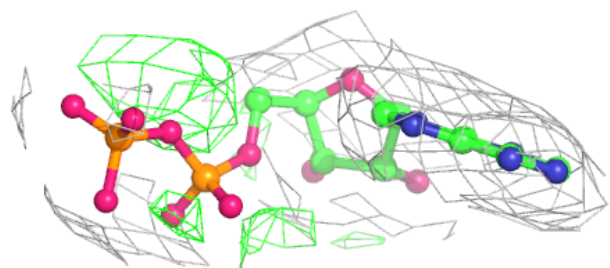
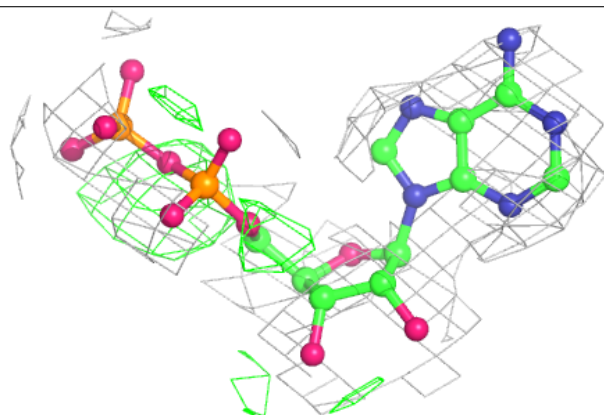


**Electron density around ADP J 9:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

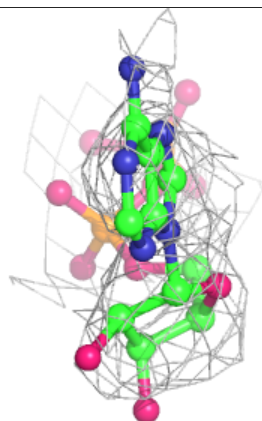
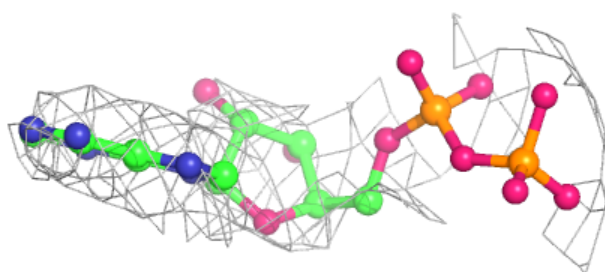
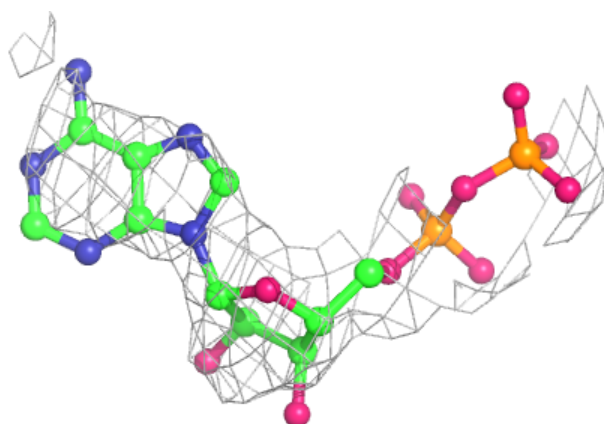
**Electron density around ADP D 2:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

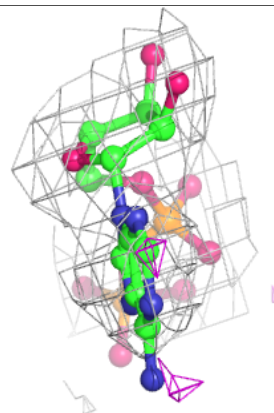
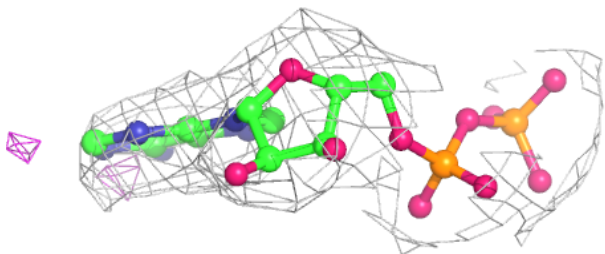
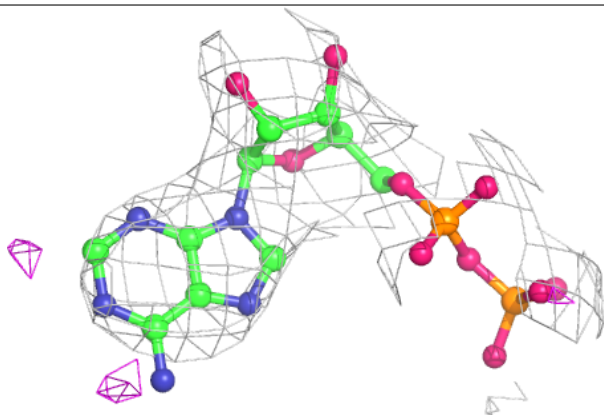


**Electron density around ADP H 14:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

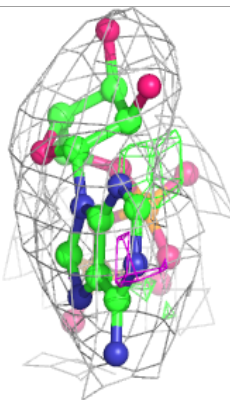
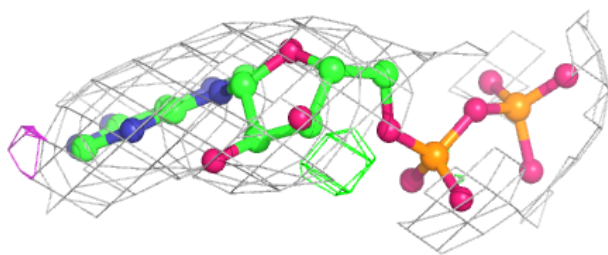
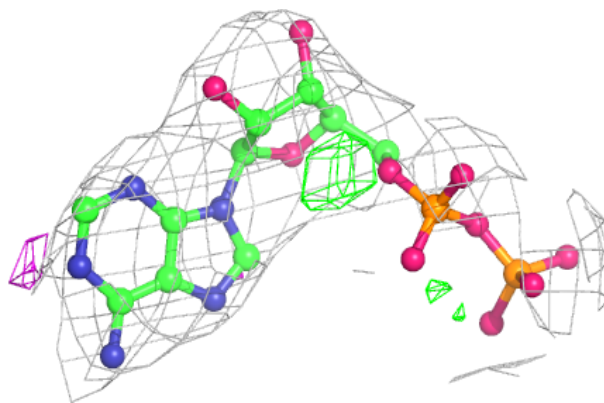
**Electron density around ADP A 6:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

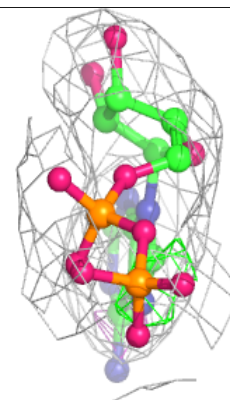
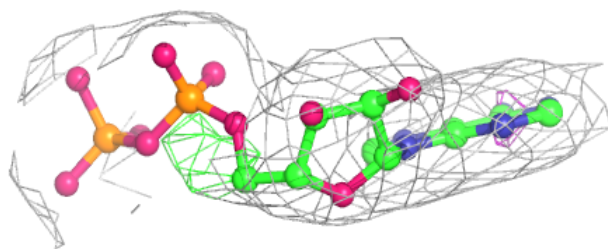
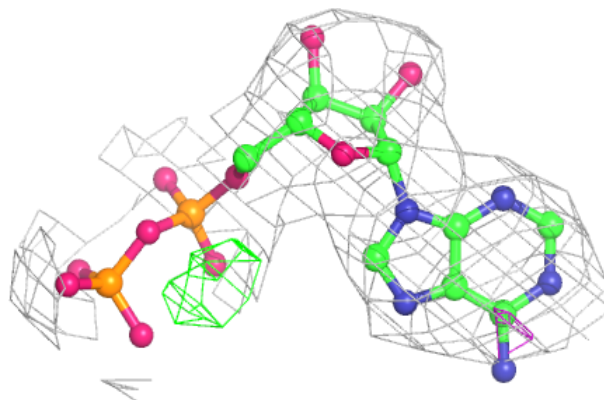


**Electron density around ADP M 12:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP G 5:**

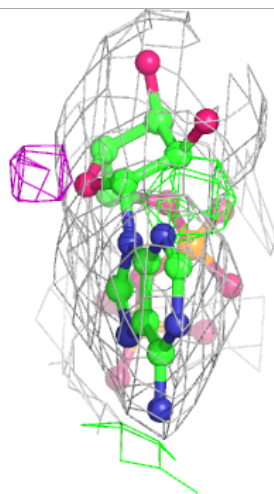
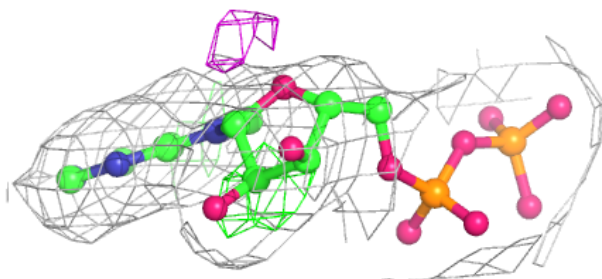
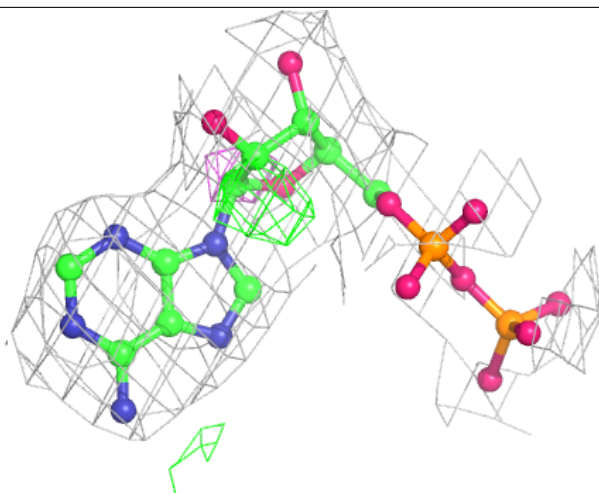
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





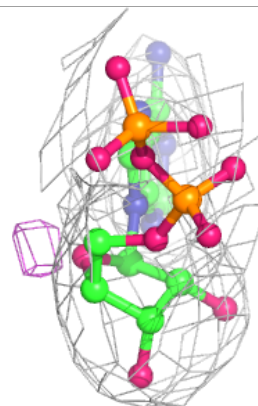
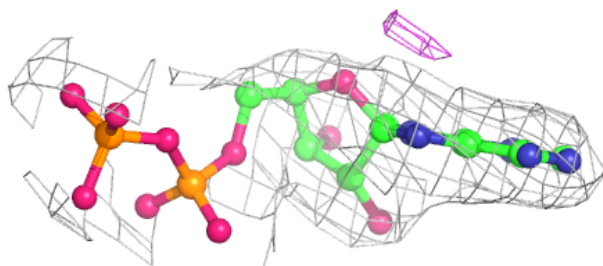
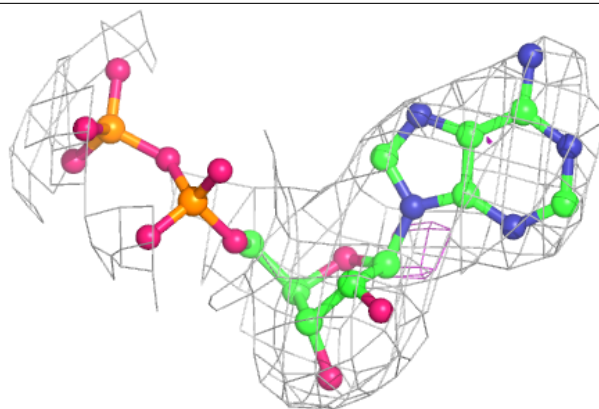
**Electron density around ADP L 11:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

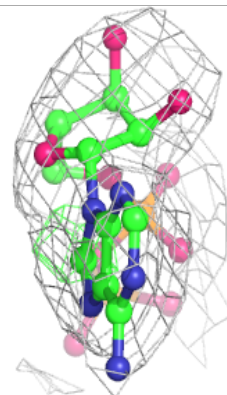
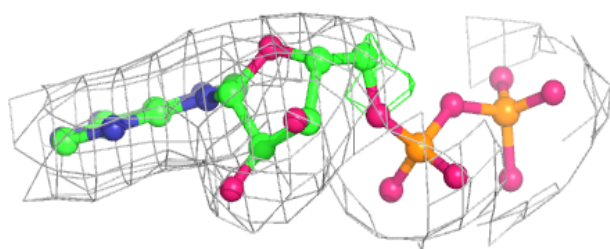
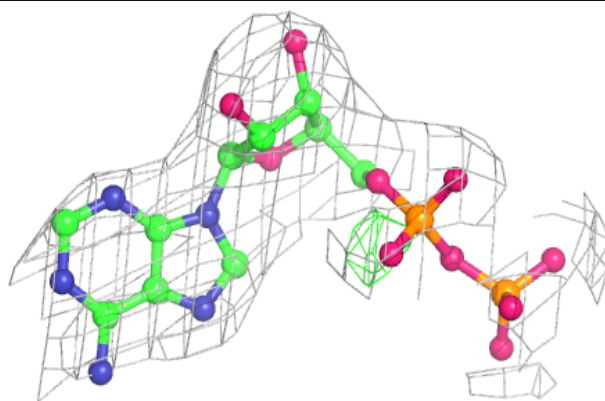


**Electron density around ADP F 4:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

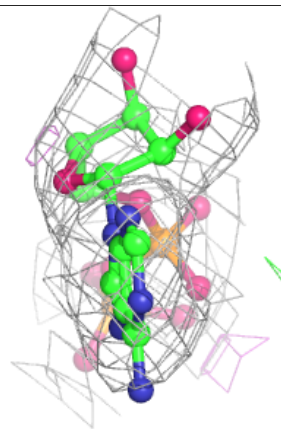
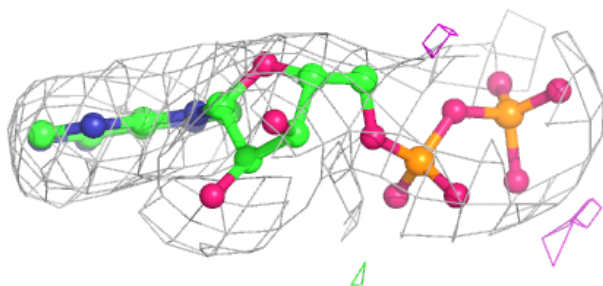
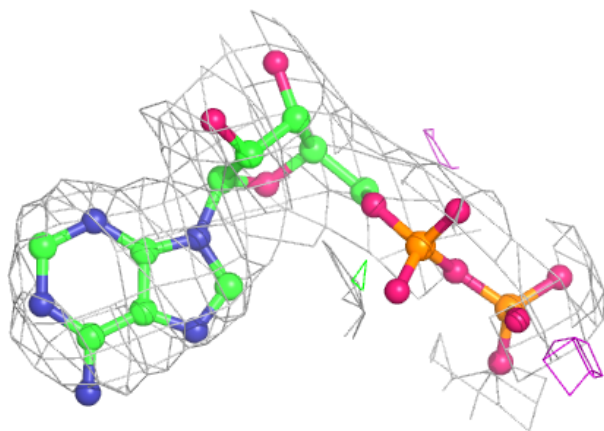
**Electron density around ADP I 8:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

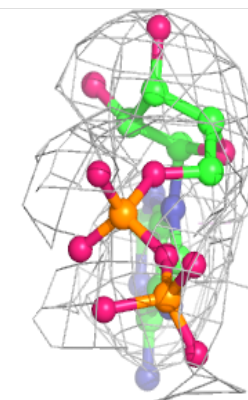
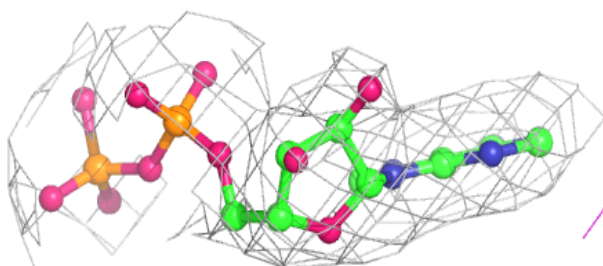
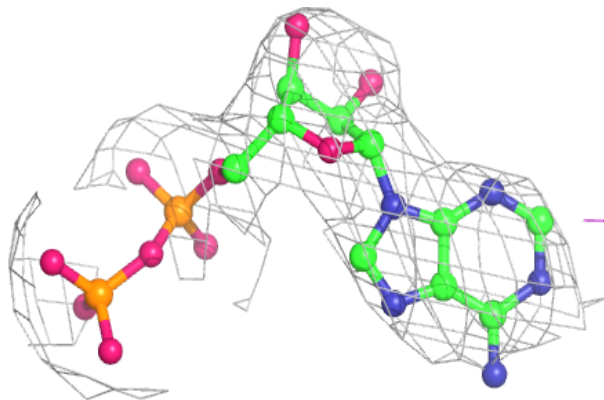


**Electron density around ADP E 3:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ADP C 1:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers

There are no such residues in this entry.