



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:42 am BST

PDB ID : 1E7P  
Title : QUINOL:FUMARATE REDUCTASE FROM WOLINELLA SUCCINO-  
GENES  
Authors : Lancaster, C.R.D.; Kroeger, A.  
Deposited on : 2000-09-01  
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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

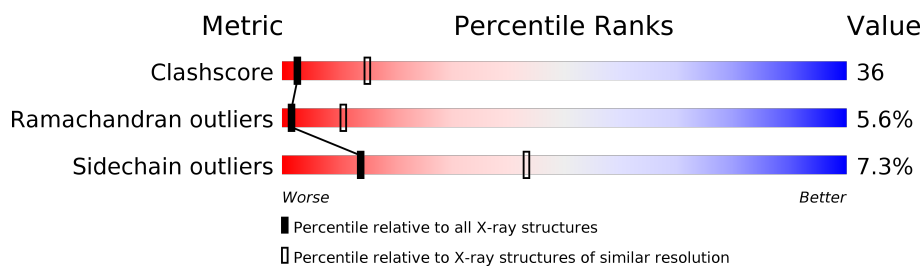
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)


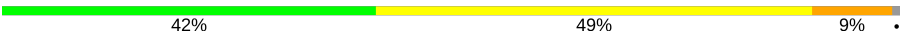
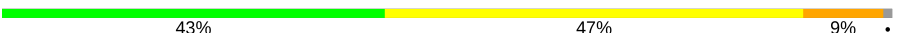

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	656	
1	D	656	
1	G	656	
1	J	656	
2	B	239	
2	E	239	
2	H	239	
2	K	239	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	C	256	
3	F	256	
3	I	256	
3	L	256	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MLA	A	702	-	-	X	-
5	MLA	D	702	-	-	X	-
5	MLA	G	702	-	-	X	-
5	MLA	J	702	-	-	X	-
8	F3S	B	302	-	-	X	-
8	F3S	E	302	-	-	X	-
8	F3S	H	302	-	-	X	-
8	F3S	K	302	-	-	X	-

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 37072 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			
1	D	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			
1	G	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			
1	J	655	Total	C	N	O	S	33	0	0
			5093	3190	910	961	32			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			
2	E	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			
2	H	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			
2	K	239	Total	C	N	O	S	0	0	0
			1894	1194	322	355	23			

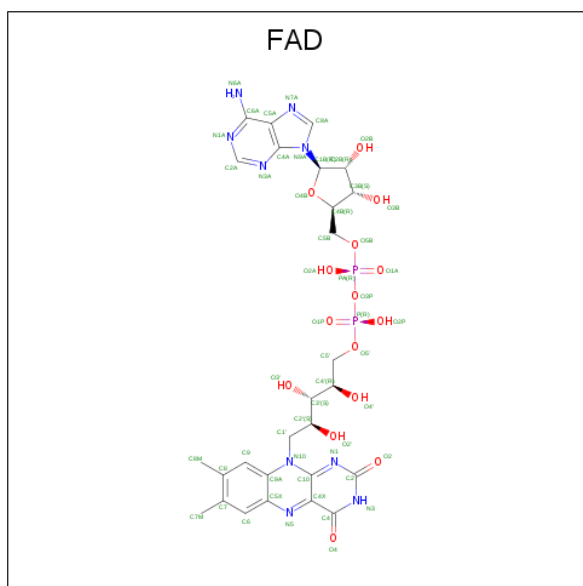
- Molecule 3 is a protein called Fumarate reductase cytochrome b subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			
3	F	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			
3	I	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			
3	L	254	Total	C	N	O	S	24	0	0
			2080	1388	334	344	14			

There are 4 discrepancies between the modelled and reference sequences:

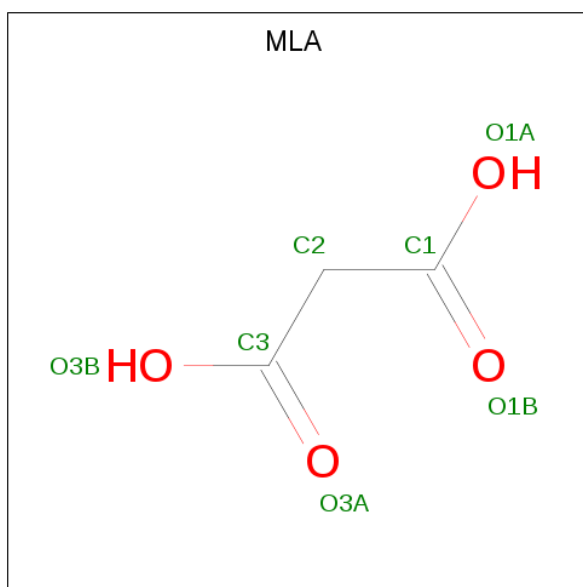
Chain	Residue	Modelled	Actual	Comment	Reference
C	66	GLN	GLU	engineered mutation	UNP P17413
F	66	GLN	GLU	engineered mutation	UNP P17413
I	66	GLN	GLU	engineered mutation	UNP P17413
L	66	GLN	GLU	engineered mutation	UNP P17413

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	G	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	J	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is MALONIC ACID (three-letter code: MLA) (formula:  $C_3H_4O_4$ ).

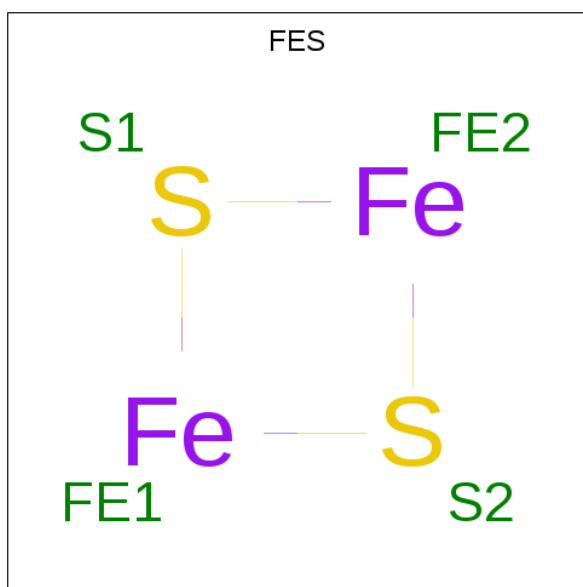


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	3	4		
5	D	1	Total	C	O	0	0
			7	3	4		
5	G	1	Total	C	O	0	0
			7	3	4		
5	J	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

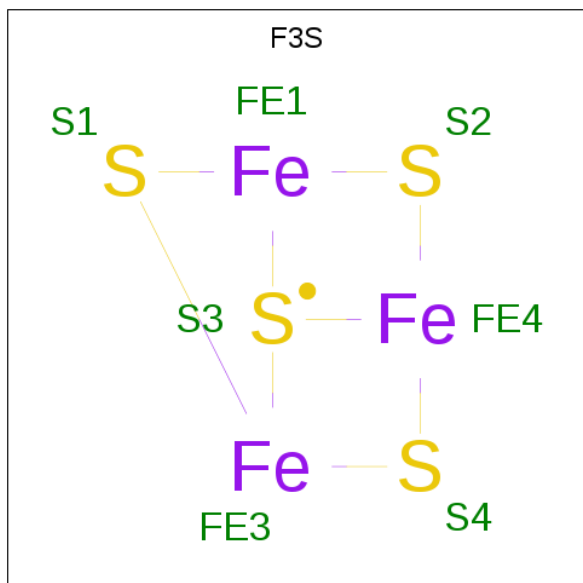
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Na	0	0
			1	1		
6	J	1	Total	Na	0	0
			1	1		
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



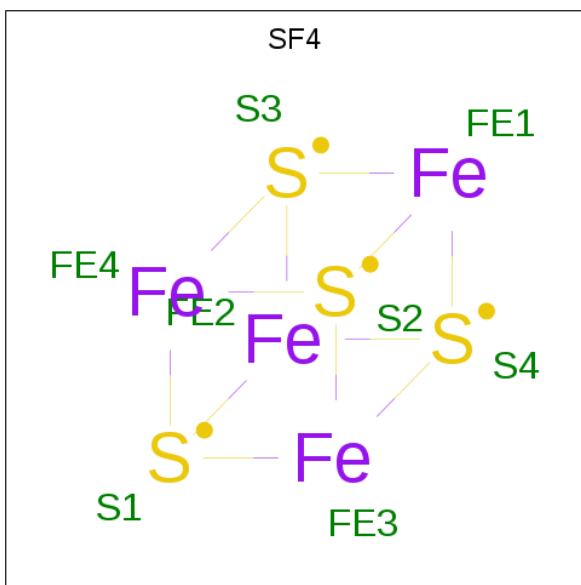
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	E	1	Total	Fe	S	0	0
			4	2	2		
7	H	1	Total	Fe	S	0	0
			4	2	2		
7	K	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	E	1	Total	Fe	S	0	0
			7	3	4		
8	H	1	Total	Fe	S	0	0
			7	3	4		
8	K	1	Total	Fe	S	0	0
			7	3	4		

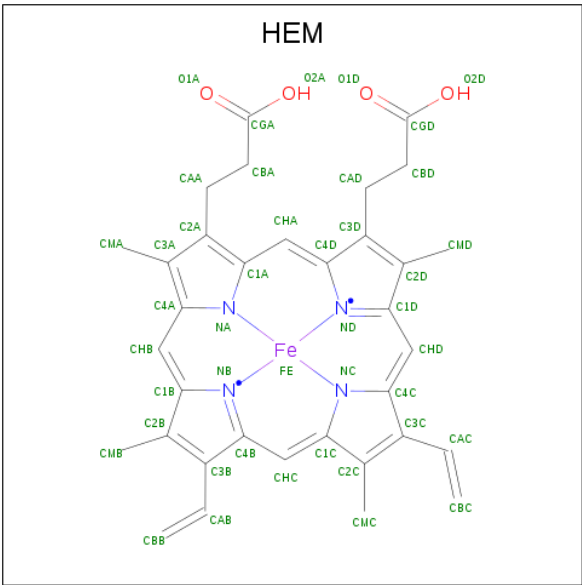
- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	E	1	Total	Fe	S	0	0
			8	4	4		
9	H	1	Total	Fe	S	0	0
			8	4	4		
9	K	1	Total	Fe	S	0	0
			8	4	4		

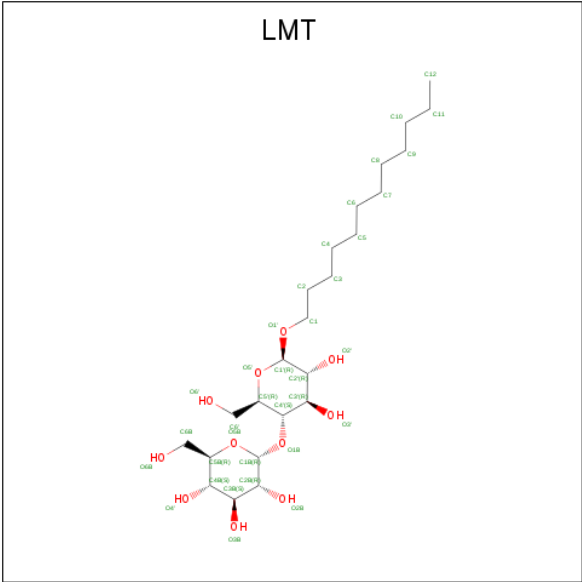
- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 11 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



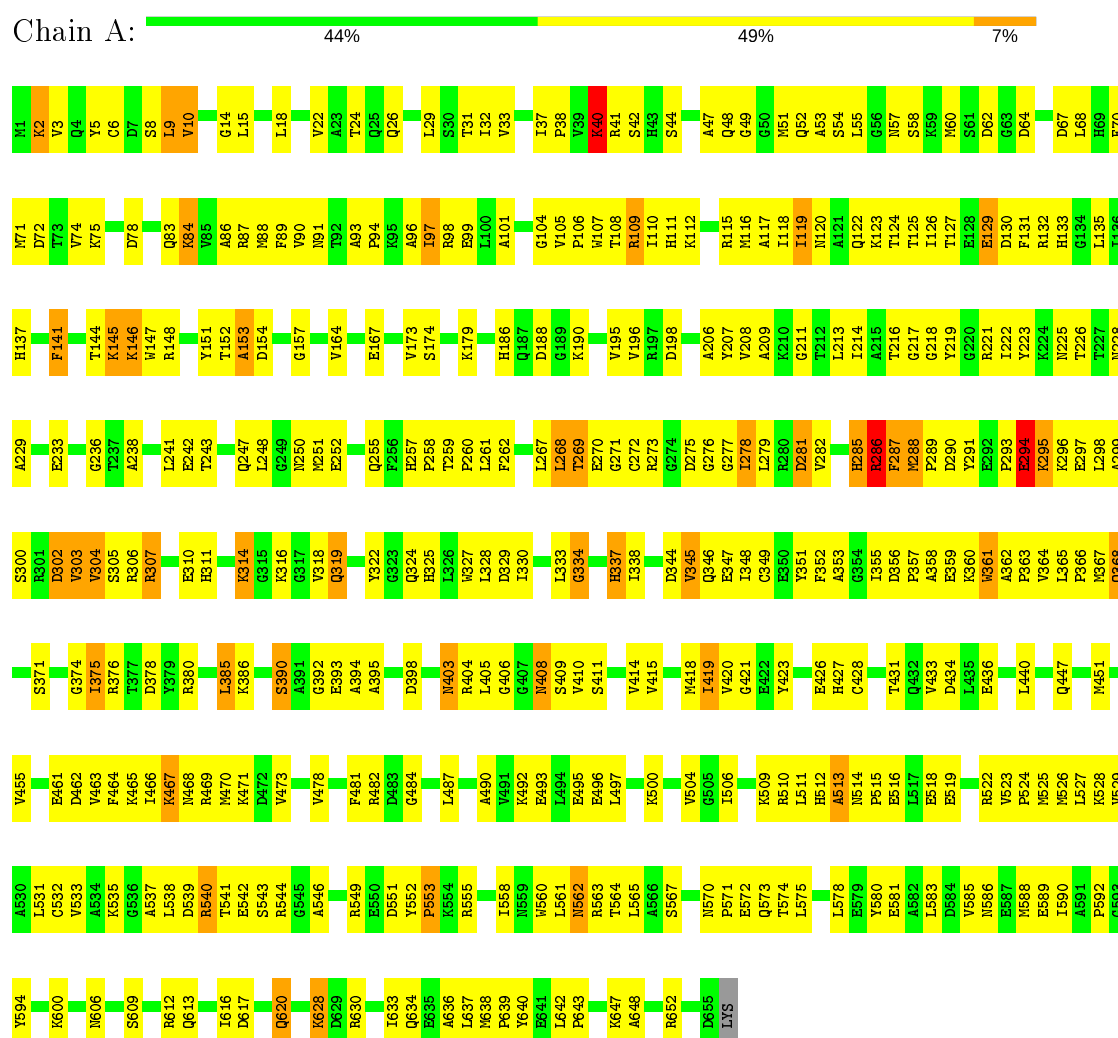
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	17	0
			35	24	11		
11	F	1	Total	C	O	17	0
			35	24	11		
11	I	1	Total	C	O	17	0
			35	24	11		
11	L	1	Total	C	O	17	0
			35	24	11		

### 3 Residue-property plots

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

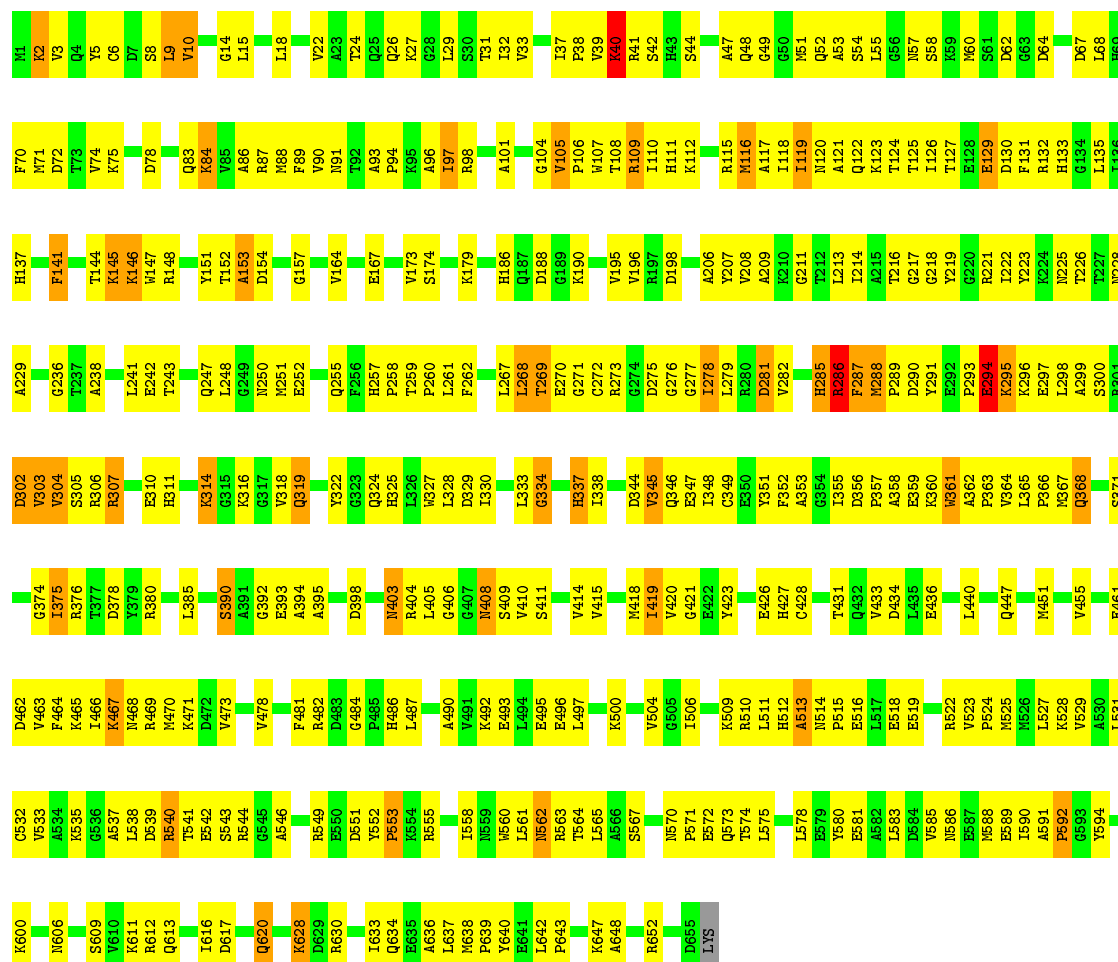
Note EDS was not executed.

#### • Molecule 1: Fumarate reductase flavoprotein subunit



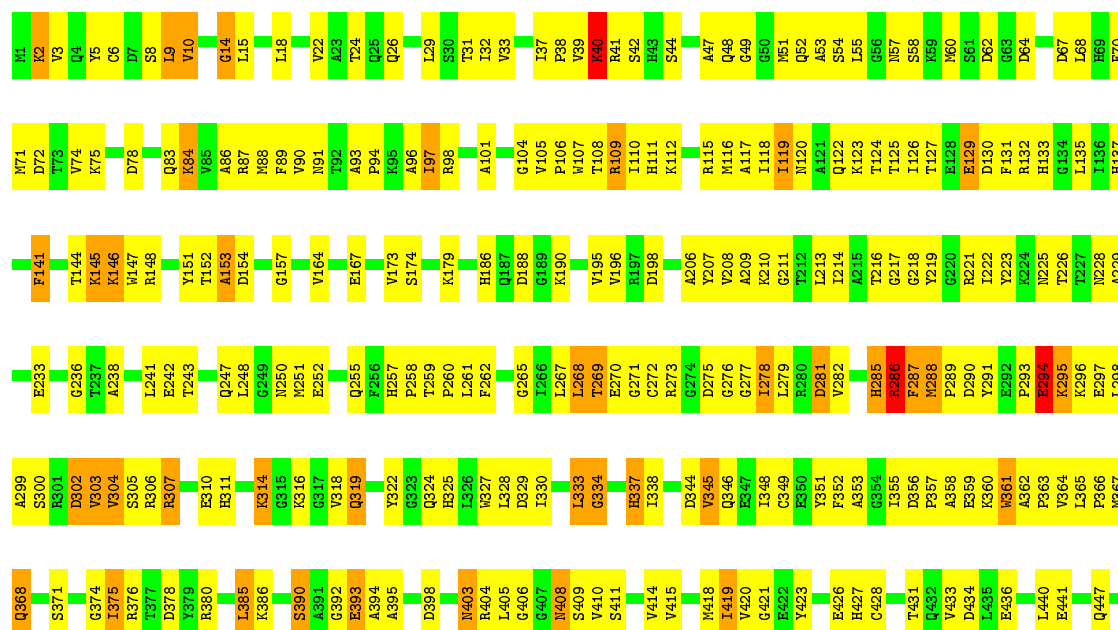
#### • Molecule 1: Fumarate reductase flavoprotein subunit

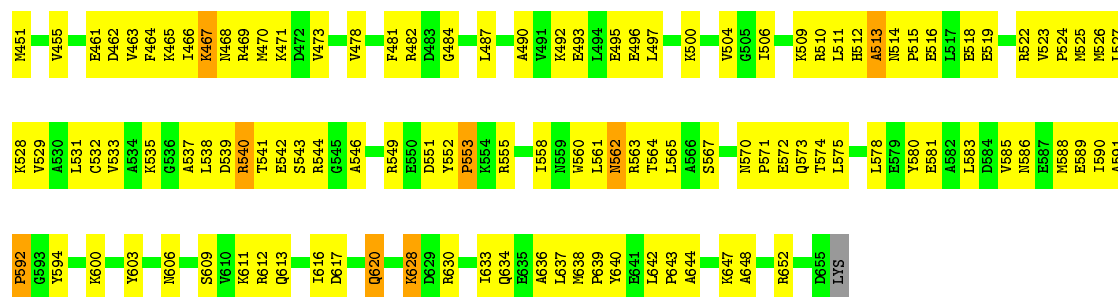




• Molecule 1: Fumarate reductase flavoprotein subunit

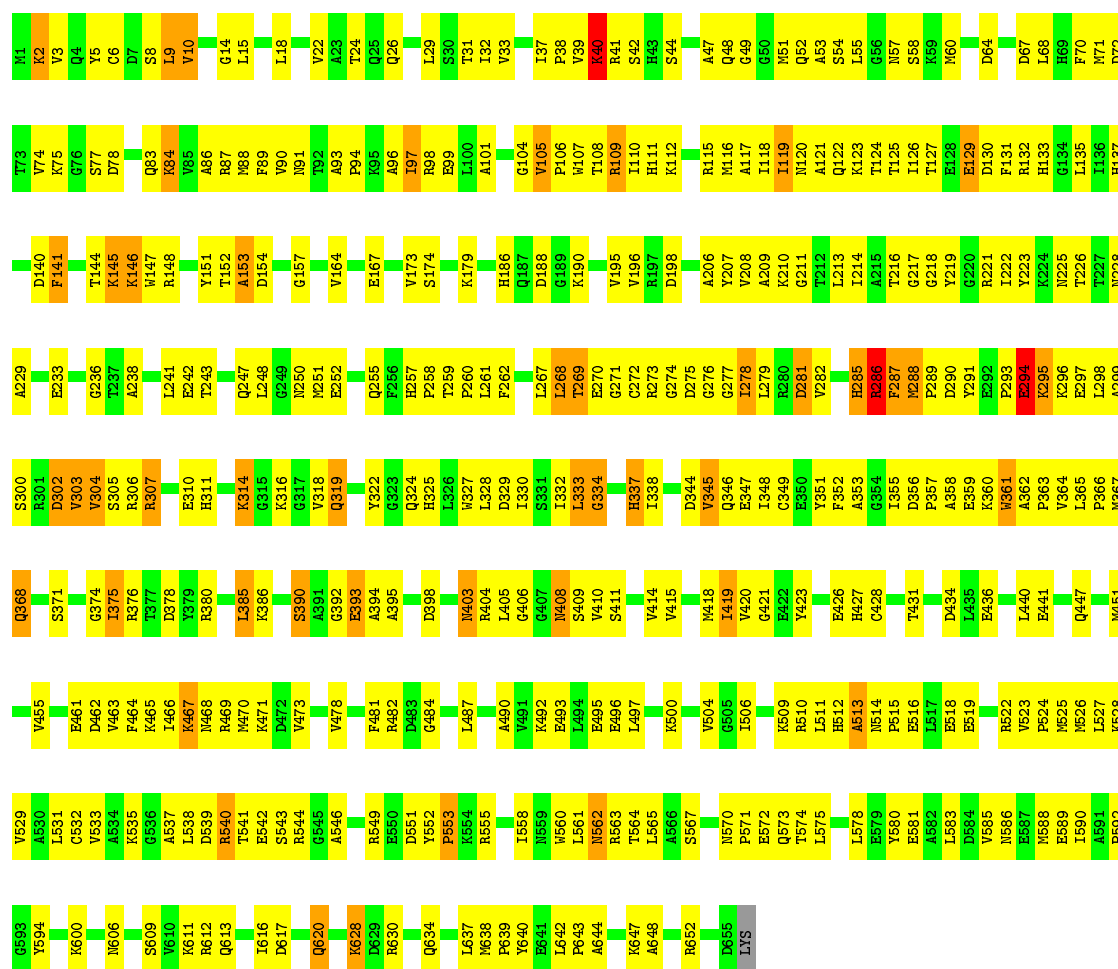
Chain G: 43% 49% 7%





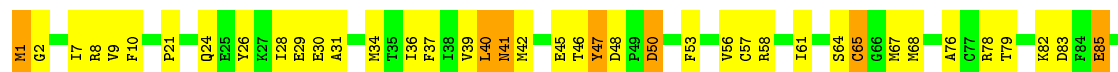
• Molecule 1: Fumarate reductase flavoprotein subunit

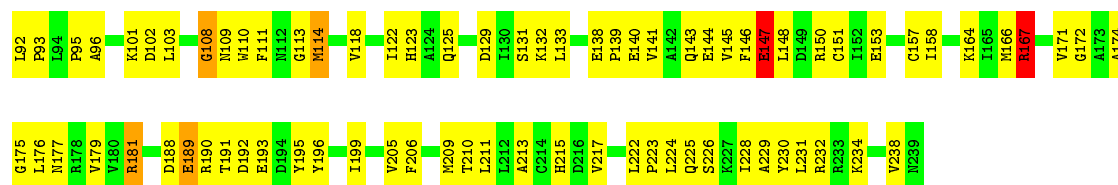
Chain J: 43% 50% 7%



• Molecule 2: Fumarate reductase iron-sulfur subunit

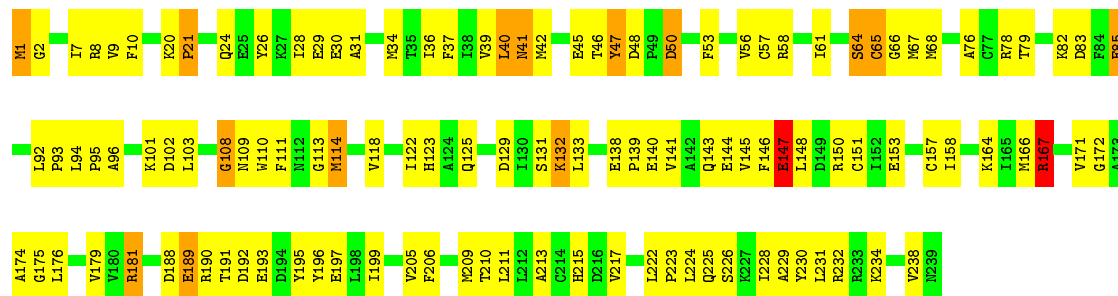
Chain B: 51% 43% 5%





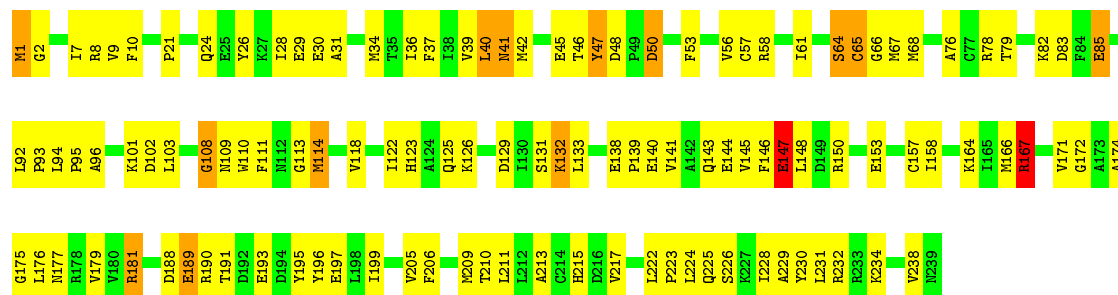
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain E: 50% 43% 6%



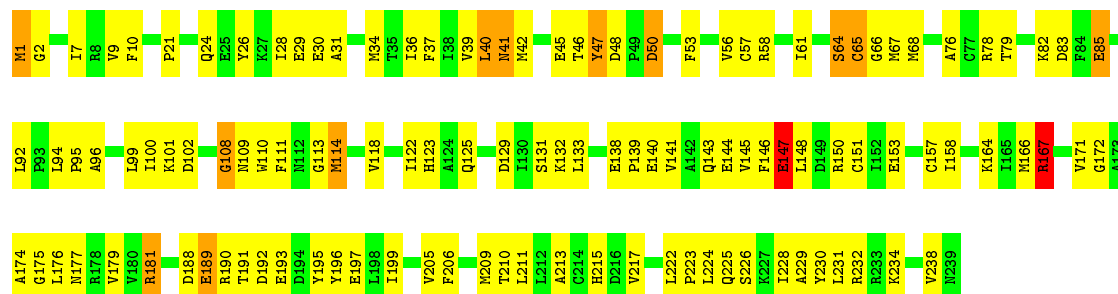
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain H: 51% 43% 5%



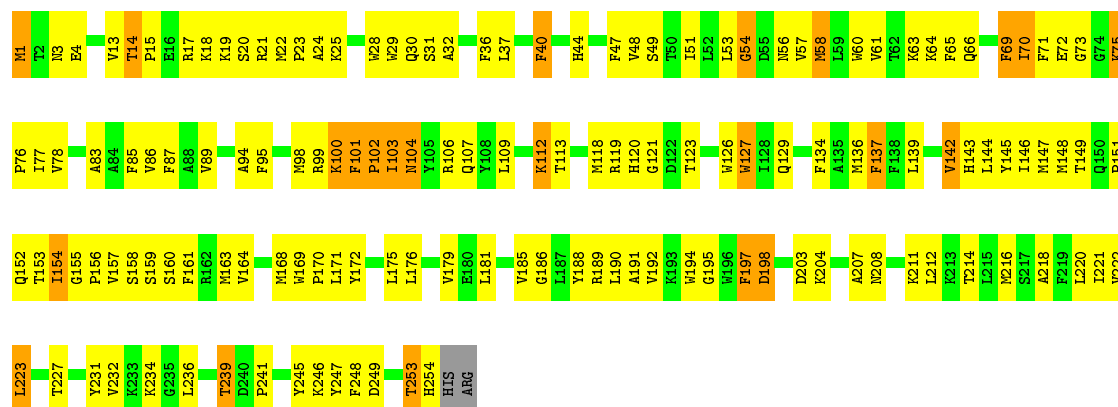
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain K: 51% 44% 5%



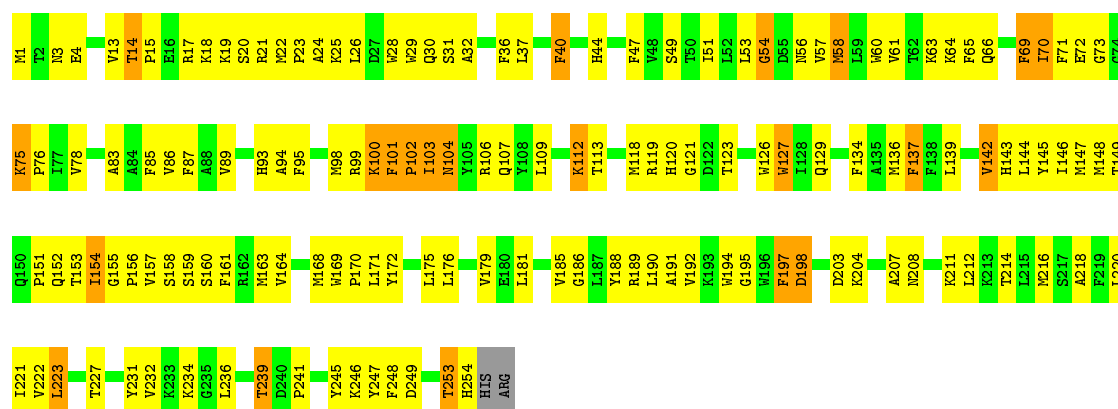
• Molecule 3: Fumarate reductase cytochrome b subunit

Chain C: 42% 48% 9%



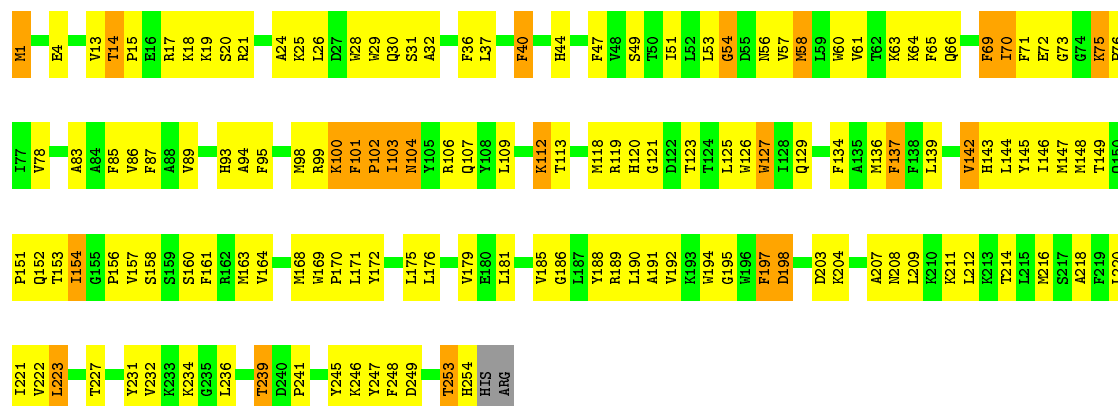
• Molecule 3: Fumarate reductase cytochrome b subunit

Chain F: 42% 49% 9% .



• Molecule 3: Fumarate reductase cytochrome b subunit

Chain I: 43% 47% 9% .



• Molecule 3: Fumarate reductase cytochrome b subunit

Chain L: 43% 48% 9% .





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.07 Å   290.24 Å   153.61 Å 90.00°   95.73°   90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	80.8 (30.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.283 , 0.291	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	37072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	84.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLA, NA, SF4, LMT, F3S, FES, HEM, FAD

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	0.57	0/5189	0.73	0/6996
1	D	0.58	0/5189	0.73	0/6996
1	G	0.58	0/5189	0.73	0/6996
1	J	0.58	0/5189	0.73	0/6996
2	B	0.47	0/1931	0.70	1/2604 (0.0%)
2	E	0.47	0/1931	0.70	1/2604 (0.0%)
2	H	0.47	0/1931	0.70	1/2604 (0.0%)
2	K	0.47	0/1931	0.70	1/2604 (0.0%)
3	C	0.60	0/2146	0.67	1/2904 (0.0%)
3	F	0.60	0/2146	0.67	1/2904 (0.0%)
3	I	0.60	0/2146	0.67	1/2904 (0.0%)
3	L	0.60	0/2146	0.67	1/2904 (0.0%)
All	All	0.56	0/37064	0.71	8/50016 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	102	PRO	N-CA-C	-5.31	98.30	112.10
3	F	102	PRO	N-CA-C	-5.30	98.31	112.10
3	C	102	PRO	N-CA-C	-5.30	98.32	112.10
3	I	102	PRO	N-CA-C	-5.30	98.32	112.10
2	H	167	ARG	N-CA-C	-5.14	97.13	111.00
2	E	167	ARG	N-CA-C	-5.13	97.15	111.00
2	K	167	ARG	N-CA-C	-5.13	97.15	111.00
2	B	167	ARG	N-CA-C	-5.12	97.16	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5093	0	5069	407	11
1	D	5093	0	5069	408	16
1	G	5093	0	5069	416	13
1	J	5093	0	5069	413	14
2	B	1894	0	1861	105	0
2	E	1894	0	1861	106	0
2	H	1894	0	1861	107	0
2	K	1894	0	1861	103	0
3	C	2080	0	2103	163	0
3	F	2080	0	2103	163	0
3	I	2080	0	2103	166	0
3	L	2080	0	2103	162	0
4	A	53	0	29	4	0
4	D	53	0	29	4	0
4	G	53	0	29	4	0
4	J	53	0	29	4	0
5	A	7	0	2	5	0
5	D	7	0	2	5	0
5	G	7	0	2	6	0
5	J	7	0	2	5	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	J	1	0	0	0	0
7	B	4	0	0	0	0
7	E	4	0	0	0	0
7	H	4	0	0	0	0
7	K	4	0	0	0	0
8	B	7	0	0	2	0
8	E	7	0	0	2	0
8	H	7	0	0	2	0
8	K	7	0	0	2	0
9	B	8	0	0	0	0
9	E	8	0	0	0	0
9	H	8	0	0	0	0
9	K	8	0	0	0	0
10	C	86	0	60	11	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	86	0	60	12	0
10	I	86	0	60	11	0
10	L	86	0	60	11	0
11	C	35	0	46	3	0
11	F	35	0	46	3	0
11	I	35	0	46	3	0
11	L	35	0	46	3	0
All	All	37072	0	36680	2632	27

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

All (2632) 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:216:THR:HG21	1:D:236:GLY:HA3	1.32	1.12
1:J:327:TRP:HB3	1:J:361:TRP:HB2	1.30	1.11
1:G:216:THR:HG21	1:G:236:GLY:HA3	1.32	1.09
3:L:152:GLN:HE21	3:L:153:THR:HG23	1.18	1.07
1:G:327:TRP:HB3	1:G:361:TRP:HB2	1.30	1.06
1:J:216:THR:HG21	1:J:236:GLY:HA3	1.32	1.06
1:D:327:TRP:HB3	1:D:361:TRP:HB2	1.30	1.06
3:C:152:GLN:HE21	3:C:153:THR:HG23	1.18	1.06
1:A:216:THR:HG21	1:A:236:GLY:HA3	1.32	1.05
1:A:327:TRP:HB3	1:A:361:TRP:HB2	1.30	1.05
3:I:152:GLN:HE21	3:I:153:THR:HG23	1.18	1.04
3:F:152:GLN:HE21	3:F:153:THR:HG23	1.18	1.04
3:L:30:GLN:HE22	3:L:100:LYS:HE3	1.26	1.01
3:C:30:GLN:HE22	3:C:100:LYS:HE3	1.26	1.00
3:F:30:GLN:HE22	3:F:100:LYS:HE3	1.26	0.99
3:I:30:GLN:HE22	3:I:100:LYS:HE3	1.26	0.99
1:J:281:ASP:HB2	1:J:285:HIS:CD2	2.01	0.96
3:F:142:VAL:HG21	3:F:171:LEU:HD11	1.48	0.95
1:A:281:ASP:HB2	1:A:285:HIS:CD2	2.01	0.95
1:A:269:THR:HG22	1:A:345:VAL:HG21	1.49	0.95
3:I:142:VAL:HG21	3:I:171:LEU:HD11	1.48	0.95
1:G:281:ASP:HB2	1:G:285:HIS:CD2	2.01	0.95
1:D:269:THR:HG22	1:D:345:VAL:HG21	1.49	0.95
1:D:281:ASP:HB2	1:D:285:HIS:CD2	2.01	0.94
3:L:142:VAL:HG21	3:L:171:LEU:HD11	1.48	0.94
1:G:269:THR:HG22	1:G:345:VAL:HG21	1.49	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:142:VAL:HG23	3:I:143:HIS:H	1.33	0.94
3:F:142:VAL:HG23	3:F:143:HIS:H	1.33	0.93
1:J:48:GLN:HG3	1:J:267:LEU:HD23	1.51	0.93
1:A:48:GLN:HG3	1:A:267:LEU:HD23	1.51	0.93
1:A:307:ARG:NH1	1:A:307:ARG:H	1.66	0.93
1:J:47:ALA:HB3	1:J:157:GLY:HA3	1.51	0.93
1:D:307:ARG:H	1:D:307:ARG:NH1	1.67	0.93
1:A:47:ALA:HB3	1:A:157:GLY:HA3	1.51	0.93
1:J:269:THR:HG22	1:J:345:VAL:HG21	1.49	0.93
1:D:288:MET:HB3	1:D:289:PRO:CD	1.99	0.92
3:C:142:VAL:HG21	3:C:171:LEU:HD11	1.48	0.92
1:A:286:ARG:HD2	1:A:288:MET:HE3	1.52	0.92
1:G:48:GLN:HG3	1:G:267:LEU:HD23	1.51	0.92
3:C:142:VAL:HG23	3:C:143:HIS:H	1.33	0.91
1:G:288:MET:HB3	1:G:289:PRO:CD	1.99	0.91
1:G:307:ARG:NH1	1:G:307:ARG:H	1.67	0.91
3:L:142:VAL:HG23	3:L:143:HIS:H	1.33	0.91
1:A:288:MET:HB3	1:A:289:PRO:CD	1.99	0.91
1:D:48:GLN:HG3	1:D:267:LEU:HD23	1.51	0.91
1:J:288:MET:HB3	1:J:289:PRO:CD	1.99	0.91
1:A:119:ILE:HG22	1:A:120:ASN:H	1.35	0.91
1:G:47:ALA:HB3	1:G:157:GLY:HA3	1.51	0.90
1:G:279:LEU:HD23	1:G:328:LEU:HD13	1.54	0.90
1:J:307:ARG:H	1:J:307:ARG:NH1	1.66	0.90
1:J:404:ARG:HE	1:J:409:SER:HB2	1.36	0.90
1:D:47:ALA:HB3	1:D:157:GLY:HA3	1.51	0.90
1:G:404:ARG:HE	1:G:409:SER:HB2	1.36	0.90
1:D:344:ASP:O	1:D:348:ILE:HG12	1.71	0.90
1:A:344:ASP:O	1:A:348:ILE:HG12	1.71	0.90
1:A:346:GLN:HA	1:A:357:PRO:HG2	1.54	0.90
1:D:119:ILE:HG22	1:D:120:ASN:H	1.35	0.90
1:D:346:GLN:HA	1:D:357:PRO:HG2	1.54	0.90
1:J:346:GLN:HA	1:J:357:PRO:HG2	1.54	0.90
1:A:107:TRP:HA	1:A:152:THR:HG22	1.53	0.90
1:A:404:ARG:HE	1:A:409:SER:HB2	1.36	0.90
1:A:279:LEU:HD23	1:A:328:LEU:HD13	1.54	0.90
1:J:307:ARG:N	1:J:307:ARG:HH11	1.70	0.90
1:J:258:PRO:HA	1:J:366:PRO:HG3	1.54	0.89
1:J:119:ILE:HG22	1:J:120:ASN:H	1.35	0.89
1:D:279:LEU:HD23	1:D:328:LEU:HD13	1.54	0.89
1:J:107:TRP:HA	1:J:152:THR:HG22	1.53	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:ARG:HH11	1:G:307:ARG:N	1.70	0.89
1:G:344:ASP:O	1:G:348:ILE:HG12	1.71	0.89
1:J:344:ASP:O	1:J:348:ILE:HG12	1.72	0.89
1:G:346:GLN:HA	1:G:357:PRO:HG2	1.54	0.89
1:D:258:PRO:HA	1:D:366:PRO:HG3	1.54	0.89
1:D:307:ARG:HH11	1:D:307:ARG:N	1.70	0.89
1:G:119:ILE:HG22	1:G:120:ASN:H	1.36	0.89
3:I:142:VAL:HG12	3:L:142:VAL:HA	1.52	0.89
1:D:107:TRP:HA	1:D:152:THR:HG22	1.53	0.88
1:A:258:PRO:HA	1:A:366:PRO:HG3	1.54	0.88
1:G:258:PRO:HA	1:G:366:PRO:HG3	1.54	0.88
3:I:142:VAL:HA	3:L:142:VAL:HG12	1.54	0.88
1:A:307:ARG:N	1:A:307:ARG:HH11	1.70	0.88
1:J:279:LEU:HD23	1:J:328:LEU:HD13	1.54	0.88
3:C:142:VAL:HG12	3:F:142:VAL:HA	1.53	0.88
1:D:404:ARG:HE	1:D:409:SER:HB2	1.36	0.88
1:G:107:TRP:HA	1:G:152:THR:HG22	1.53	0.88
3:C:142:VAL:HA	3:F:142:VAL:HG12	1.54	0.87
3:C:30:GLN:NE2	3:C:100:LYS:HE3	1.90	0.87
3:F:30:GLN:NE2	3:F:100:LYS:HE3	1.90	0.87
2:K:138:GLU:HB2	2:K:141:VAL:HG23	1.56	0.87
3:I:30:GLN:NE2	3:I:100:LYS:HE3	1.90	0.86
1:G:286:ARG:HD2	1:G:288:MET:HE3	1.58	0.86
1:J:286:ARG:HD2	1:J:288:MET:HE3	1.57	0.86
1:J:262:PHE:HB3	1:J:363:PRO:O	1.76	0.86
1:A:262:PHE:HB3	1:A:363:PRO:O	1.76	0.85
1:J:482:ARG:HB3	1:J:487:LEU:HD11	1.58	0.85
2:H:138:GLU:HB2	2:H:141:VAL:HG23	1.56	0.85
1:A:482:ARG:HB3	1:A:487:LEU:HD11	1.58	0.85
2:E:138:GLU:HB2	2:E:141:VAL:HG23	1.56	0.85
1:D:262:PHE:HB3	1:D:363:PRO:O	1.76	0.85
2:B:138:GLU:HB2	2:B:141:VAL:HG23	1.56	0.85
1:D:482:ARG:HB3	1:D:487:LEU:HD11	1.58	0.85
1:G:262:PHE:HB3	1:G:363:PRO:O	1.77	0.85
3:L:30:GLN:NE2	3:L:100:LYS:HE3	1.90	0.85
3:C:253:THR:HG22	3:C:254:HIS:H	1.42	0.84
1:D:287:PHE:CE1	1:D:291:TYR:HB2	2.13	0.84
1:G:287:PHE:CE1	1:G:291:TYR:HB2	2.13	0.84
1:J:287:PHE:HB3	1:J:296:LYS:HZ2	1.43	0.84
1:A:287:PHE:CE1	1:A:291:TYR:HB2	2.13	0.83
3:F:253:THR:HG22	3:F:254:HIS:H	1.41	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:482:ARG:HB3	1:G:487:LEU:HD11	1.58	0.83
3:L:253:THR:HG22	3:L:254:HIS:H	1.41	0.83
1:J:225:ASN:HB3	1:J:367:MET:HE2	1.61	0.83
3:F:100:LYS:HG2	10:F:302:HEM:O1A	1.79	0.83
1:J:287:PHE:CE1	1:J:291:TYR:HB2	2.13	0.83
3:I:66:GLN:HB3	3:I:75:LYS:H	1.44	0.82
3:C:100:LYS:HG2	10:C:301:HEM:O1A	1.79	0.82
3:F:66:GLN:HB3	3:F:75:LYS:H	1.45	0.82
1:D:286:ARG:HD2	1:D:288:MET:HE3	1.62	0.82
3:I:253:THR:HG22	3:I:254:HIS:H	1.41	0.82
1:A:87:ARG:HD2	1:A:640:TYR:CE2	2.15	0.81
1:D:87:ARG:HD2	1:D:640:TYR:CE2	2.15	0.81
1:G:87:ARG:HD2	1:G:640:TYR:CE2	2.15	0.81
1:J:87:ARG:HD2	1:J:640:TYR:CE2	2.15	0.81
1:G:252:GLU:HA	1:G:533:VAL:HG13	1.63	0.81
1:A:118:ILE:HD13	1:A:123:LYS:HE3	1.63	0.81
1:J:118:ILE:HD13	1:J:123:LYS:HE3	1.63	0.81
1:J:83:GLN:NE2	1:J:588:MET:HB3	1.95	0.81
1:D:83:GLN:NE2	1:D:588:MET:HB3	1.95	0.81
3:C:66:GLN:HB3	3:C:75:LYS:H	1.44	0.81
1:D:287:PHE:HB3	1:D:296:LYS:NZ	1.96	0.81
3:I:100:LYS:HG2	10:I:301:HEM:O1A	1.79	0.81
1:A:83:GLN:NE2	1:A:588:MET:HB3	1.95	0.80
3:L:100:LYS:HG2	10:L:302:HEM:O1A	1.79	0.80
3:F:142:VAL:HG23	3:F:143:HIS:N	1.96	0.80
1:G:83:GLN:NE2	1:G:588:MET:HB3	1.95	0.80
1:J:252:GLU:HA	1:J:533:VAL:HG13	1.63	0.80
3:I:142:VAL:HG23	3:I:143:HIS:N	1.96	0.80
1:D:118:ILE:HD13	1:D:123:LYS:HE3	1.63	0.80
1:J:87:ARG:HB3	1:J:640:TYR:CD2	2.17	0.80
1:A:287:PHE:HB3	1:A:296:LYS:NZ	1.96	0.80
3:L:66:GLN:HB3	3:L:75:LYS:H	1.45	0.80
1:A:225:ASN:HB3	1:A:367:MET:HE2	1.63	0.80
1:D:252:GLU:HA	1:D:533:VAL:HG13	1.63	0.80
1:J:287:PHE:HB3	1:J:296:LYS:NZ	1.96	0.80
3:L:142:VAL:HG23	3:L:143:HIS:N	1.96	0.80
1:G:87:ARG:HB3	1:G:640:TYR:CD2	2.17	0.79
1:A:252:GLU:HA	1:A:533:VAL:HG13	1.63	0.79
1:G:208:VAL:HG11	1:G:440:LEU:HD11	1.64	0.79
1:J:208:VAL:HG11	1:J:440:LEU:HD11	1.64	0.79
1:D:208:VAL:HG11	1:D:440:LEU:HD11	1.64	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:287:PHE:HB3	1:G:296:LYS:NZ	1.96	0.79
1:A:216:THR:CG2	1:A:236:GLY:HA3	2.13	0.79
3:C:142:VAL:HG23	3:C:143:HIS:N	1.96	0.79
1:D:87:ARG:HB3	1:D:640:TYR:CD2	2.17	0.79
1:A:208:VAL:HG11	1:A:440:LEU:HD11	1.64	0.78
1:G:118:ILE:HD13	1:G:123:LYS:HE3	1.63	0.78
1:A:83:GLN:HE21	1:A:588:MET:HB3	1.48	0.78
1:G:87:ARG:HD2	1:G:640:TYR:HE2	1.48	0.78
1:J:87:ARG:HD2	1:J:640:TYR:HE2	1.48	0.78
1:A:87:ARG:HB3	1:A:640:TYR:CD2	2.17	0.78
3:C:36:PHE:HD2	3:C:89:VAL:HG11	1.49	0.78
1:D:87:ARG:HD2	1:D:640:TYR:HE2	1.48	0.78
1:J:216:THR:CG2	1:J:236:GLY:HA3	2.13	0.77
1:J:83:GLN:HE21	1:J:588:MET:HB3	1.48	0.77
1:A:360:LYS:CG	1:A:361:TRP:H	1.97	0.77
1:D:360:LYS:CG	1:D:361:TRP:H	1.97	0.77
1:G:241:LEU:HB2	1:G:248:LEU:HD21	1.66	0.77
1:J:307:ARG:H	1:J:307:ARG:HH11	0.84	0.77
1:D:327:TRP:CB	1:D:361:TRP:HB2	2.14	0.77
2:K:179:VAL:HG21	2:K:199:ILE:HD13	1.67	0.77
1:G:360:LYS:CG	1:G:361:TRP:H	1.97	0.77
3:L:36:PHE:HD2	3:L:89:VAL:HG11	1.49	0.77
2:H:179:VAL:HG21	2:H:199:ILE:HD13	1.67	0.76
1:J:360:LYS:CG	1:J:361:TRP:H	1.97	0.76
1:A:612:ARG:O	1:A:616:ILE:HG13	1.86	0.76
1:A:241:LEU:HB2	1:A:248:LEU:HD21	1.66	0.76
2:B:179:VAL:HG21	2:B:199:ILE:HD13	1.67	0.76
1:G:83:GLN:HE21	1:G:588:MET:HB3	1.48	0.76
1:D:241:LEU:HB2	1:D:248:LEU:HD21	1.66	0.76
3:L:69:PHE:HD1	3:L:70:ILE:HG13	1.50	0.76
1:D:216:THR:CG2	1:D:236:GLY:HA3	2.13	0.76
1:J:241:LEU:HB2	1:J:248:LEU:HD21	1.66	0.76
1:J:612:ARG:O	1:J:616:ILE:HG13	1.86	0.76
1:D:83:GLN:HE21	1:D:588:MET:HB3	1.48	0.76
1:D:404:ARG:NE	1:D:409:SER:HB2	2.00	0.76
3:F:36:PHE:HD2	3:F:89:VAL:HG11	1.49	0.76
1:G:540:ARG:HH22	1:G:562:ASN:ND2	1.84	0.76
1:J:294:GLU:O	1:J:295:LYS:HG2	1.86	0.76
1:A:404:ARG:NE	1:A:409:SER:HB2	2.00	0.76
1:D:294:GLU:O	1:D:295:LYS:HG2	1.86	0.76
1:G:404:ARG:NE	1:G:409:SER:HB2	2.00	0.76

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:VAL:HG21	10:C:302:HEM:HAC	1.66	0.76
1:D:225:ASN:HB3	1:D:367:MET:HE2	1.66	0.76
3:F:69:PHE:HD1	3:F:70:ILE:HG13	1.50	0.76
1:G:294:GLU:O	1:G:295:LYS:HG2	1.86	0.76
1:J:404:ARG:NE	1:J:409:SER:HB2	2.00	0.76
1:G:612:ARG:O	1:G:616:ILE:HG13	1.86	0.76
3:I:179:VAL:HG21	10:I:302:HEM:HAC	1.66	0.76
3:C:29:TRP:HA	3:C:32:ALA:HB3	1.68	0.75
3:I:69:PHE:HD1	3:I:70:ILE:HG13	1.50	0.75
1:J:540:ARG:HH22	1:J:562:ASN:ND2	1.84	0.75
3:C:69:PHE:HD1	3:C:70:ILE:HG13	1.50	0.75
1:D:540:ARG:HH22	1:D:562:ASN:ND2	1.84	0.75
1:G:327:TRP:CB	1:G:361:TRP:HB2	2.14	0.75
3:I:36:PHE:HD2	3:I:89:VAL:HG11	1.49	0.75
1:J:286:ARG:HD2	1:J:288:MET:CE	2.17	0.75
3:F:179:VAL:HG21	10:F:303:HEM:HAC	1.66	0.75
3:L:179:VAL:HG21	10:L:303:HEM:HAC	1.66	0.75
1:A:294:GLU:O	1:A:295:LYS:HG2	1.86	0.75
1:A:87:ARG:HD2	1:A:640:TYR:HE2	1.48	0.75
1:D:286:ARG:HD2	1:D:288:MET:CE	2.17	0.75
1:A:286:ARG:HD2	1:A:288:MET:CE	2.17	0.74
1:A:540:ARG:HH22	1:A:562:ASN:ND2	1.84	0.74
3:F:134:PHE:O	3:F:137:PHE:HB2	1.87	0.74
1:G:225:ASN:HB3	1:G:367:MET:HE2	1.67	0.74
1:G:286:ARG:HD2	1:G:288:MET:CE	2.17	0.74
3:I:134:PHE:O	3:I:137:PHE:HB2	1.87	0.74
3:C:134:PHE:O	3:C:137:PHE:HB2	1.87	0.74
1:J:277:GLY:HA3	1:J:330:ILE:HG22	1.70	0.74
3:L:29:TRP:HA	3:L:32:ALA:HB3	1.68	0.74
1:A:327:TRP:CB	1:A:361:TRP:HB2	2.14	0.74
2:E:179:VAL:HG21	2:E:199:ILE:HD13	1.67	0.74
3:F:76:PRO:HB2	3:F:151:PRO:HG2	1.70	0.74
1:G:277:GLY:HA3	1:G:330:ILE:HG22	1.70	0.74
1:J:327:TRP:CB	1:J:361:TRP:HB2	2.14	0.74
1:D:612:ARG:O	1:D:616:ILE:HG13	1.86	0.74
1:G:216:THR:CG2	1:G:236:GLY:HA3	2.13	0.74
1:G:307:ARG:HH11	1:G:307:ARG:H	0.84	0.74
3:I:29:TRP:HA	3:I:32:ALA:HB3	1.68	0.74
3:F:152:GLN:NE2	3:F:153:THR:HG23	2.00	0.73
3:F:29:TRP:HA	3:F:32:ALA:HB3	1.68	0.73
3:L:134:PHE:O	3:L:137:PHE:HB2	1.87	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:76:PRO:HB2	3:L:151:PRO:HG2	1.70	0.73
3:C:76:PRO:HB2	3:C:151:PRO:HG2	1.70	0.73
1:G:282:VAL:HG21	1:G:316:LYS:O	1.89	0.73
3:L:152:GLN:NE2	3:L:153:THR:HG23	2.00	0.73
1:D:307:ARG:HH11	1:D:307:ARG:H	0.84	0.73
1:G:282:VAL:HG22	1:G:318:VAL:HG12	1.71	0.73
1:G:141:PHE:CZ	5:G:702:MLA:HC22	2.24	0.72
1:A:141:PHE:CZ	5:A:702:MLA:HC22	2.24	0.72
3:F:249:ASP:HA	3:F:254:HIS:HB3	1.71	0.72
3:L:249:ASP:HA	3:L:254:HIS:HB3	1.71	0.72
3:I:249:ASP:HA	3:I:254:HIS:HB3	1.71	0.72
1:J:141:PHE:CZ	5:J:702:MLA:HC22	2.24	0.72
1:J:282:VAL:HG21	1:J:316:LYS:O	1.89	0.72
1:A:282:VAL:HG22	1:A:318:VAL:HG12	1.71	0.72
3:C:249:ASP:HA	3:C:254:HIS:HB3	1.71	0.72
1:D:2:LYS:HB2	1:D:2:LYS:NZ	2.05	0.72
1:G:327:TRP:HA	1:G:362:ALA:O	1.90	0.72
1:D:282:VAL:HG21	1:D:316:LYS:O	1.88	0.72
1:D:277:GLY:HA3	1:D:330:ILE:HG22	1.70	0.72
1:D:282:VAL:HG22	1:D:318:VAL:HG12	1.71	0.72
3:F:142:VAL:HG21	3:F:171:LEU:CD1	2.20	0.72
3:F:36:PHE:CD2	3:F:89:VAL:HG11	2.25	0.72
1:J:48:GLN:CG	1:J:267:LEU:HD23	2.19	0.72
1:A:277:GLY:HA3	1:A:330:ILE:HG22	1.70	0.72
1:A:2:LYS:HB2	1:A:2:LYS:NZ	2.05	0.72
1:A:307:ARG:HH11	1:A:307:ARG:H	0.84	0.72
1:J:2:LYS:HB2	1:J:2:LYS:NZ	2.05	0.72
3:C:36:PHE:CD2	3:C:89:VAL:HG11	2.25	0.72
1:D:327:TRP:HA	1:D:362:ALA:O	1.90	0.72
3:I:36:PHE:CD2	3:I:89:VAL:HG11	2.25	0.72
1:A:282:VAL:HG21	1:A:316:LYS:O	1.89	0.71
2:B:58:ARG:HG2	2:B:58:ARG:O	1.89	0.71
1:D:48:GLN:CG	1:D:267:LEU:HD23	2.19	0.71
1:D:141:PHE:CZ	5:D:702:MLA:HC22	2.24	0.71
1:J:282:VAL:HG22	1:J:318:VAL:HG12	1.71	0.71
1:J:299:ALA:HB1	1:J:303:VAL:HG11	1.72	0.71
1:A:327:TRP:HA	1:A:362:ALA:O	1.90	0.71
1:G:469:ARG:O	1:G:473:VAL:HG23	1.90	0.71
3:L:36:PHE:CD2	3:L:89:VAL:HG11	2.25	0.71
3:I:142:VAL:HG21	3:I:171:LEU:CD1	2.20	0.71
1:A:52:GLN:HG3	1:A:148:ARG:HG3	1.73	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:LYS:HZ2	1:D:314:LYS:HB2	1.56	0.71
2:H:167:ARG:HH11	2:H:167:ARG:HG3	1.56	0.71
1:A:48:GLN:CG	1:A:267:LEU:HD23	2.19	0.71
1:A:252:GLU:HB2	1:A:537:ALA:HB2	1.72	0.71
1:D:287:PHE:HB3	1:D:296:LYS:HZ2	1.53	0.71
1:D:252:GLU:HB2	1:D:537:ALA:HB2	1.72	0.71
1:G:252:GLU:HB2	1:G:537:ALA:HB2	1.72	0.71
1:J:327:TRP:HA	1:J:362:ALA:O	1.90	0.71
1:A:299:ALA:HB1	1:A:303:VAL:HG11	1.72	0.71
1:D:469:ARG:O	1:D:473:VAL:HG23	1.90	0.71
2:E:58:ARG:HG2	2:E:58:ARG:O	1.89	0.71
1:G:48:GLN:CG	1:G:267:LEU:HD23	2.20	0.71
2:E:167:ARG:HG3	2:E:167:ARG:HH11	1.55	0.71
1:G:52:GLN:HG3	1:G:148:ARG:HG3	1.73	0.71
3:I:76:PRO:HB2	3:I:151:PRO:HG2	1.70	0.71
1:J:469:ARG:O	1:J:473:VAL:HG23	1.90	0.71
3:C:139:LEU:O	3:C:142:VAL:HG22	1.91	0.71
2:H:58:ARG:HG2	2:H:58:ARG:O	1.89	0.71
3:L:139:LEU:O	3:L:142:VAL:HG22	1.91	0.71
3:F:4:GLU:HB3	3:F:15:PRO:HG2	1.73	0.70
1:A:300:SER:O	1:A:304:VAL:HG23	1.91	0.70
2:B:167:ARG:HG3	2:B:167:ARG:HH11	1.56	0.70
1:D:558:ILE:HA	1:D:606:ASN:HD22	1.56	0.70
3:I:139:LEU:O	3:I:142:VAL:HG22	1.91	0.70
3:L:142:VAL:CG2	3:L:143:HIS:H	2.04	0.70
1:D:52:GLN:HE22	1:D:144:THR:HG21	1.56	0.70
1:G:2:LYS:HB2	1:G:2:LYS:NZ	2.05	0.70
1:G:299:ALA:HB3	1:G:304:VAL:HG22	1.74	0.70
1:J:9:LEU:HD23	1:J:10:VAL:H	1.56	0.70
1:J:558:ILE:HA	1:J:606:ASN:HD22	1.56	0.70
3:L:146:ILE:C	3:L:148:MET:H	1.95	0.70
1:A:9:LEU:HD23	1:A:10:VAL:H	1.56	0.70
3:F:189:ARG:HG3	3:F:189:ARG:HH11	1.57	0.70
3:F:18:LYS:HE3	3:F:21:ARG:HH12	1.57	0.70
1:J:414:VAL:O	1:J:418:MET:HG3	1.92	0.70
1:J:252:GLU:HB2	1:J:537:ALA:HB2	1.72	0.70
1:D:52:GLN:HG3	1:D:148:ARG:HG3	1.73	0.70
3:I:146:ILE:C	3:I:148:MET:H	1.95	0.70
1:J:299:ALA:HB3	1:J:304:VAL:HG22	1.74	0.70
3:C:146:ILE:C	3:C:148:MET:H	1.95	0.70
3:F:146:ILE:C	3:F:148:MET:H	1.95	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:562:ASN:H	1:J:562:ASN:HD22	1.40	0.70
3:C:4:GLU:HB3	3:C:15:PRO:HG2	1.73	0.70
3:F:139:LEU:O	3:F:142:VAL:HG22	1.91	0.70
2:K:167:ARG:HH11	2:K:167:ARG:HG3	1.56	0.70
1:D:300:SER:O	1:D:304:VAL:HG23	1.91	0.70
1:G:52:GLN:HE22	1:G:144:THR:HG21	1.56	0.70
1:J:52:GLN:HG3	1:J:148:ARG:HG3	1.73	0.70
1:D:414:VAL:O	1:D:418:MET:HG3	1.92	0.70
1:J:52:GLN:HE22	1:J:144:THR:HG21	1.56	0.70
1:J:300:SER:O	1:J:304:VAL:HG23	1.91	0.70
1:A:47:ALA:HB3	1:A:157:GLY:CA	2.22	0.70
3:C:152:GLN:NE2	3:C:153:THR:HG23	2.00	0.70
1:G:269:THR:CG2	1:G:345:VAL:HG21	2.22	0.70
3:I:4:GLU:HB3	3:I:15:PRO:HG2	1.73	0.70
3:I:189:ARG:HH11	3:I:189:ARG:HG3	1.57	0.70
2:K:58:ARG:HG2	2:K:58:ARG:O	1.89	0.70
1:A:414:VAL:O	1:A:418:MET:HG3	1.92	0.69
3:C:18:LYS:HE3	3:C:21:ARG:HH12	1.57	0.69
3:I:18:LYS:HE3	3:I:21:ARG:HH12	1.57	0.69
1:A:469:ARG:O	1:A:473:VAL:HG23	1.90	0.69
1:G:300:SER:O	1:G:304:VAL:HG23	1.91	0.69
2:E:1:MET:CE	2:E:31:ALA:HA	2.22	0.69
1:A:299:ALA:HB3	1:A:304:VAL:HG22	1.74	0.69
2:B:1:MET:CE	2:B:31:ALA:HA	2.22	0.69
3:F:175:LEU:HG	10:F:303:HEM:HMD3	1.75	0.69
1:G:562:ASN:H	1:G:562:ASN:HD22	1.39	0.69
2:H:1:MET:CE	2:H:31:ALA:HA	2.22	0.69
3:I:142:VAL:CG2	3:I:143:HIS:H	2.04	0.69
3:I:152:GLN:NE2	3:I:153:THR:HG23	2.00	0.69
1:A:558:ILE:HA	1:A:606:ASN:HD22	1.56	0.69
1:G:141:PHE:HZ	5:G:702:MLA:HC22	1.58	0.69
1:G:47:ALA:HB3	1:G:157:GLY:CA	2.22	0.69
1:G:558:ILE:HA	1:G:606:ASN:HD22	1.56	0.69
2:B:179:VAL:HG13	2:B:195:TYR:HD2	1.58	0.69
1:G:299:ALA:HB1	1:G:303:VAL:HG11	1.72	0.69
1:J:269:THR:CG2	1:J:345:VAL:HG21	2.22	0.69
1:A:52:GLN:HE22	1:A:144:THR:HG21	1.56	0.69
3:C:142:VAL:HG21	3:C:171:LEU:CD1	2.20	0.69
3:C:175:LEU:HG	10:C:302:HEM:HMD3	1.75	0.69
1:D:299:ALA:HB1	1:D:303:VAL:HG11	1.72	0.69
1:A:269:THR:CG2	1:A:345:VAL:HG21	2.21	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:142:VAL:CG2	3:F:143:HIS:H	2.04	0.69
3:C:189:ARG:HH11	3:C:189:ARG:HG3	1.57	0.69
1:D:9:LEU:HD23	1:D:10:VAL:H	1.56	0.69
1:G:52:GLN:NE2	1:G:144:THR:HG21	2.08	0.69
1:D:52:GLN:NE2	1:D:144:THR:HG21	2.08	0.68
1:D:47:ALA:HB3	1:D:157:GLY:CA	2.22	0.68
2:K:179:VAL:HG13	2:K:195:TYR:HD2	1.58	0.68
3:L:142:VAL:HG21	3:L:171:LEU:CD1	2.20	0.68
3:L:189:ARG:HG3	3:L:189:ARG:HH11	1.57	0.68
1:G:9:LEU:HD23	1:G:10:VAL:H	1.56	0.68
1:G:535:LYS:HG3	1:G:578:LEU:HD11	1.75	0.68
3:I:156:PRO:HD2	3:I:254:HIS:NE2	2.08	0.68
3:L:18:LYS:HE3	3:L:21:ARG:HH12	1.57	0.68
3:L:94:ALA:HB2	10:L:302:HEM:HAB	1.75	0.68
1:A:288:MET:HB3	1:A:289:PRO:HD3	1.76	0.68
3:C:126:TRP:O	3:C:129:GLN:N	2.27	0.68
1:D:299:ALA:HB3	1:D:304:VAL:HG22	1.74	0.68
1:D:325:HIS:HB2	1:D:364:VAL:O	1.93	0.68
1:D:540:ARG:NH2	1:D:562:ASN:ND2	2.42	0.68
1:G:414:VAL:O	1:G:418:MET:HG3	1.92	0.68
2:K:1:MET:CE	2:K:31:ALA:HA	2.22	0.68
1:D:141:PHE:HZ	5:D:702:MLA:HC22	1.58	0.68
2:E:68:MET:HB2	2:E:92:LEU:HB2	1.76	0.68
1:G:325:HIS:HB2	1:G:364:VAL:O	1.93	0.68
1:G:154:ASP:OD2	1:G:345:VAL:HG23	1.94	0.68
3:I:175:LEU:O	3:I:175:LEU:HD12	1.94	0.68
1:J:447:GLN:HA	1:J:447:GLN:OE1	1.94	0.68
1:A:314:LYS:HB2	1:A:314:LYS:NZ	2.09	0.68
1:G:288:MET:HB3	1:G:289:PRO:HD3	1.76	0.68
3:I:126:TRP:O	3:I:129:GLN:N	2.27	0.68
3:L:126:TRP:O	3:L:129:GLN:N	2.27	0.68
1:A:52:GLN:NE2	1:A:144:THR:HG21	2.08	0.68
1:D:24:THR:OG1	1:D:31:THR:HG21	1.94	0.68
1:D:360:LYS:HG3	1:D:361:TRP:H	1.58	0.68
2:E:179:VAL:HG13	2:E:195:TYR:HD2	1.58	0.68
3:F:156:PRO:HD2	3:F:254:HIS:NE2	2.09	0.68
1:J:52:GLN:NE2	1:J:144:THR:HG21	2.08	0.68
1:A:24:THR:OG1	1:A:31:THR:HG21	1.94	0.68
1:A:360:LYS:HG3	1:A:361:TRP:H	1.58	0.68
1:D:447:GLN:HA	1:D:447:GLN:OE1	1.94	0.68
1:G:314:LYS:HB2	1:G:314:LYS:NZ	2.09	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:325:HIS:HB2	1:J:364:VAL:O	1.93	0.68
3:L:4:GLU:HB3	3:L:15:PRO:HG2	1.73	0.68
1:A:535:LYS:HG3	1:A:578:LEU:HD11	1.75	0.68
3:C:94:ALA:HB2	10:C:301:HEM:HAB	1.75	0.68
3:F:94:ALA:HB2	10:F:302:HEM:HAB	1.75	0.68
1:J:141:PHE:HZ	5:J:702:MLA:HC22	1.58	0.68
1:J:314:LYS:NZ	1:J:314:LYS:HB2	2.09	0.68
1:A:540:ARG:NH2	1:A:562:ASN:ND2	2.42	0.68
1:D:314:LYS:NZ	1:D:314:LYS:HB2	2.09	0.68
1:G:540:ARG:NH2	1:G:562:ASN:ND2	2.42	0.68
2:H:2:GLY:HA2	2:H:29:GLU:OE2	1.94	0.68
2:K:68:MET:HB2	2:K:92:LEU:HB2	1.76	0.68
1:A:562:ASN:HD22	1:A:562:ASN:H	1.39	0.67
2:B:2:GLY:HA2	2:B:29:GLU:OE2	1.94	0.67
3:C:156:PRO:HD2	3:C:254:HIS:NE2	2.08	0.67
1:D:269:THR:CG2	1:D:345:VAL:HG21	2.22	0.67
3:F:175:LEU:HD12	3:F:175:LEU:O	1.94	0.67
2:H:179:VAL:HG13	2:H:195:TYR:HD2	1.58	0.67
2:H:68:MET:HB2	2:H:92:LEU:HB2	1.76	0.67
1:J:47:ALA:HB3	1:J:157:GLY:CA	2.22	0.67
1:J:303:VAL:HG12	1:J:304:VAL:N	2.09	0.67
1:J:154:ASP:OD2	1:J:345:VAL:HG23	1.94	0.67
1:A:303:VAL:HG12	1:A:304:VAL:N	2.09	0.67
2:B:179:VAL:HG13	2:B:195:TYR:CD2	2.30	0.67
1:D:574:THR:O	1:D:575:LEU:HD23	1.95	0.67
2:E:179:VAL:HG13	2:E:195:TYR:CD2	2.30	0.67
2:H:179:VAL:HG13	2:H:195:TYR:CD2	2.30	0.67
3:I:94:ALA:HB2	10:I:301:HEM:HAB	1.75	0.67
1:J:360:LYS:CG	1:J:361:TRP:N	2.57	0.67
3:L:156:PRO:HD2	3:L:254:HIS:NE2	2.08	0.67
3:L:175:LEU:HG	10:L:303:HEM:HMD3	1.75	0.67
1:A:141:PHE:HZ	5:A:702:MLA:HC22	1.58	0.67
1:D:535:LYS:HG3	1:D:578:LEU:HD11	1.75	0.67
1:G:273:ARG:HA	1:G:277:GLY:O	1.95	0.67
3:C:175:LEU:HD12	3:C:175:LEU:O	1.94	0.67
1:D:562:ASN:H	1:D:562:ASN:HD22	1.40	0.67
1:G:314:LYS:HB2	1:G:314:LYS:HZ2	1.58	0.67
1:J:574:THR:O	1:J:575:LEU:HD23	1.95	0.67
2:K:2:GLY:HA2	2:K:29:GLU:OE2	1.94	0.67
1:A:496:GLU:O	1:A:500:LYS:HG3	1.95	0.67
1:J:216:THR:HG21	1:J:236:GLY:CA	2.19	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:HIS:HB2	1:A:364:VAL:O	1.93	0.67
1:G:303:VAL:HG12	1:G:304:VAL:N	2.09	0.67
1:J:24:THR:OG1	1:J:31:THR:HG21	1.94	0.67
1:A:154:ASP:OD2	1:A:345:VAL:HG23	1.94	0.67
1:G:447:GLN:OE1	1:G:447:GLN:HA	1.94	0.67
1:J:540:ARG:NH2	1:J:562:ASN:ND2	2.42	0.67
3:L:175:LEU:HD12	3:L:175:LEU:O	1.94	0.67
1:A:574:THR:O	1:A:575:LEU:HD23	1.95	0.67
2:E:2:GLY:HA2	2:E:29:GLU:OE2	1.94	0.67
1:G:24:THR:OG1	1:G:31:THR:HG21	1.94	0.67
1:D:154:ASP:OD2	1:D:345:VAL:HG23	1.94	0.67
3:F:157:VAL:HB	3:F:254:HIS:HE1	1.60	0.67
2:K:179:VAL:HG13	2:K:195:TYR:CD2	2.30	0.67
3:F:126:TRP:O	3:F:129:GLN:N	2.27	0.67
1:J:535:LYS:HG3	1:J:578:LEU:HD11	1.75	0.67
1:A:447:GLN:HA	1:A:447:GLN:OE1	1.94	0.66
3:C:142:VAL:CG2	3:C:143:HIS:H	2.04	0.66
1:A:64:ASP:HA	1:A:68:LEU:HD12	1.78	0.66
1:D:303:VAL:HG12	1:D:304:VAL:N	2.09	0.66
1:G:289:PRO:HG3	1:G:295:LYS:HA	1.77	0.66
3:I:175:LEU:HG	10:I:302:HEM:HMD3	1.75	0.66
1:A:360:LYS:CG	1:A:361:TRP:N	2.57	0.66
2:B:68:MET:HB2	2:B:92:LEU:HB2	1.76	0.66
1:D:273:ARG:HA	1:D:277:GLY:O	1.95	0.66
1:D:289:PRO:HG3	1:D:295:LYS:HA	1.77	0.66
1:D:496:GLU:O	1:D:500:LYS:HG3	1.95	0.66
1:J:288:MET:HB3	1:J:289:PRO:HD3	1.76	0.66
1:A:279:LEU:N	1:A:288:MET:HE1	2.11	0.66
1:A:287:PHE:HB3	1:A:296:LYS:HZ2	1.56	0.66
1:D:360:LYS:CG	1:D:361:TRP:N	2.58	0.66
1:J:285:HIS:CD2	1:J:285:HIS:N	2.64	0.66
1:J:360:LYS:HG3	1:J:361:TRP:H	1.58	0.66
3:L:157:VAL:HB	3:L:254:HIS:HE1	1.60	0.66
1:A:289:PRO:HG3	1:A:295:LYS:HA	1.77	0.66
1:G:360:LYS:CG	1:G:361:TRP:N	2.57	0.66
1:J:289:PRO:HG3	1:J:295:LYS:HA	1.77	0.66
1:J:496:GLU:O	1:J:500:LYS:HG3	1.95	0.66
3:C:157:VAL:HB	3:C:254:HIS:HE1	1.60	0.66
1:D:463:VAL:HB	1:D:504:VAL:HG11	1.78	0.66
1:G:216:THR:HG21	1:G:236:GLY:CA	2.19	0.66
1:J:540:ARG:HH22	1:J:562:ASN:HD22	1.44	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:MET:HB3	1:D:289:PRO:HD3	1.76	0.66
1:D:286:ARG:C	1:D:288:MET:H	1.99	0.66
1:G:285:HIS:N	1:G:285:HIS:CD2	2.64	0.66
1:G:64:ASP:HA	1:G:68:LEU:HD12	1.78	0.66
1:A:289:PRO:HB3	1:A:293:PRO:HA	1.78	0.66
1:G:287:PHE:HB3	1:G:296:LYS:HZ2	1.59	0.66
1:G:360:LYS:HG3	1:G:361:TRP:H	1.58	0.66
1:G:496:GLU:O	1:G:500:LYS:HG3	1.95	0.66
1:G:574:THR:O	1:G:575:LEU:HD23	1.95	0.66
1:A:273:ARG:HA	1:A:277:GLY:O	1.95	0.66
2:B:125:GLN:HB2	2:B:189:GLU:OE1	1.96	0.66
2:H:125:GLN:HB2	2:H:189:GLU:OE1	1.96	0.66
1:J:273:ARG:HA	1:J:277:GLY:O	1.95	0.66
1:G:289:PRO:HB3	1:G:293:PRO:HA	1.78	0.66
3:L:83:ALA:HA	10:L:303:HEM:HBB1	1.78	0.66
2:E:125:GLN:HB2	2:E:189:GLU:OE1	1.96	0.65
3:C:175:LEU:HG	10:C:302:HEM:CMD	2.26	0.65
3:C:181:LEU:O	3:C:185:VAL:HG23	1.96	0.65
1:J:463:VAL:HB	1:J:504:VAL:HG11	1.77	0.65
3:F:40:PHE:CE1	3:F:86:VAL:HG21	2.32	0.65
1:A:195:VAL:HG11	1:A:447:GLN:HG3	1.78	0.65
3:C:40:PHE:CE1	3:C:86:VAL:HG21	2.31	0.65
3:F:13:VAL:HG22	3:F:18:LYS:N	2.12	0.65
3:L:40:PHE:CE1	3:L:86:VAL:HG21	2.32	0.65
1:J:289:PRO:HB3	1:J:293:PRO:HA	1.78	0.65
1:J:64:ASP:HA	1:J:68:LEU:HD12	1.78	0.65
3:L:181:LEU:O	3:L:185:VAL:HG23	1.96	0.65
3:I:157:VAL:HB	3:I:254:HIS:HE1	1.60	0.65
3:I:83:ALA:HA	10:I:302:HEM:HBB1	1.78	0.65
1:J:287:PHE:CD1	1:J:291:TYR:HB2	2.32	0.65
3:C:103:ILE:O	3:C:104:ASN:HB3	1.97	0.65
1:D:285:HIS:N	1:D:285:HIS:CD2	2.64	0.65
1:D:64:ASP:HA	1:D:68:LEU:HD12	1.78	0.65
3:F:175:LEU:HG	10:F:303:HEM:CMD	2.27	0.65
1:G:330:ILE:O	1:G:338:ILE:HD11	1.97	0.65
3:I:13:VAL:HG22	3:I:18:LYS:N	2.12	0.65
1:J:286:ARG:C	1:J:288:MET:H	2.00	0.65
1:A:285:HIS:N	1:A:285:HIS:CD2	2.64	0.65
3:I:103:ILE:O	3:I:104:ASN:HB3	1.97	0.65
1:D:287:PHE:CD1	1:D:291:TYR:HB2	2.32	0.65
3:F:181:LEU:O	3:F:185:VAL:HG23	1.96	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:40:PHE:CE1	3:I:86:VAL:HG21	2.32	0.65
1:J:330:ILE:O	1:J:338:ILE:HD11	1.97	0.65
1:A:241:LEU:HD12	1:A:248:LEU:CD2	2.27	0.64
3:F:103:ILE:O	3:F:104:ASN:HB3	1.97	0.64
1:G:241:LEU:HD12	1:G:248:LEU:CD2	2.28	0.64
1:G:286:ARG:C	1:G:288:MET:H	2.00	0.64
3:I:142:VAL:CG2	3:I:171:LEU:HD11	2.25	0.64
3:C:87:PHE:CD2	3:C:144:LEU:HD13	2.32	0.64
1:J:195:VAL:HG11	1:J:447:GLN:HG3	1.78	0.64
1:J:279:LEU:N	1:J:288:MET:HE1	2.12	0.64
1:A:287:PHE:CD1	1:A:291:TYR:HB2	2.32	0.64
3:L:175:LEU:HG	10:L:303:HEM:CMD	2.26	0.64
1:A:119:ILE:HG22	1:A:120:ASN:N	2.10	0.64
1:A:463:VAL:HB	1:A:504:VAL:HG11	1.77	0.64
3:C:13:VAL:HG22	3:C:18:LYS:N	2.12	0.64
1:D:289:PRO:HB3	1:D:293:PRO:HA	1.78	0.64
1:D:242:GLU:HG2	1:D:528:LYS:NZ	2.13	0.64
1:G:287:PHE:CD1	1:G:291:TYR:HB2	2.32	0.64
1:G:463:VAL:HB	1:G:504:VAL:HG11	1.78	0.64
3:I:181:LEU:O	3:I:185:VAL:HG23	1.96	0.64
1:A:330:ILE:O	1:A:338:ILE:HD11	1.97	0.64
1:D:195:VAL:HG11	1:D:447:GLN:HG3	1.78	0.64
1:D:288:MET:C	1:D:290:ASP:H	2.01	0.64
1:D:540:ARG:HH22	1:D:562:ASN:HD22	1.44	0.64
2:E:1:MET:HE3	2:E:31:ALA:HA	1.77	0.64
3:I:145:TYR:CE2	3:I:149:THR:HG21	2.33	0.64
1:A:242:GLU:HG2	1:A:528:LYS:NZ	2.13	0.64
3:C:145:TYR:CE2	3:C:149:THR:HG21	2.33	0.64
3:C:83:ALA:HA	10:C:302:HEM:HBB1	1.78	0.64
1:D:330:ILE:O	1:D:338:ILE:HD11	1.97	0.64
3:I:175:LEU:HG	10:I:302:HEM:CMD	2.26	0.64
3:L:103:ILE:O	3:L:103:ILE:HG12	1.98	0.64
1:G:287:PHE:C	1:G:290:ASP:HB3	2.18	0.64
1:G:540:ARG:HH22	1:G:562:ASN:HD22	1.44	0.64
1:J:287:PHE:C	1:J:290:ASP:HB3	2.18	0.64
1:A:288:MET:C	1:A:290:ASP:H	2.01	0.64
1:D:287:PHE:C	1:D:290:ASP:HB3	2.18	0.64
1:G:279:LEU:N	1:G:288:MET:HE1	2.12	0.64
2:K:125:GLN:HB2	2:K:189:GLU:OE1	1.96	0.64
3:L:13:VAL:HG22	3:L:18:LYS:N	2.12	0.64
1:D:241:LEU:HD12	1:D:248:LEU:CD2	2.27	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:142:VAL:CG2	3:F:171:LEU:HD11	2.25	0.64
1:G:195:VAL:HG11	1:G:447:GLN:HG3	1.78	0.64
1:A:287:PHE:C	1:A:290:ASP:HB3	2.18	0.64
1:G:242:GLU:HG2	1:G:528:LYS:NZ	2.13	0.64
1:J:241:LEU:HD12	1:J:248:LEU:CD2	2.28	0.64
3:L:145:TYR:CE2	3:L:149:THR:HG21	2.33	0.64
1:A:286:ARG:C	1:A:288:MET:H	2.00	0.63
1:A:540:ARG:HH22	1:A:562:ASN:HD22	1.44	0.63
3:F:83:ALA:HA	10:F:303:HEM:HBB1	1.78	0.63
2:K:1:MET:HE2	2:K:30:GLU:O	1.98	0.63
3:L:142:VAL:CG2	3:L:171:LEU:HD11	2.25	0.63
3:F:145:TYR:CE2	3:F:149:THR:HG21	2.33	0.63
3:I:87:PHE:CD2	3:I:144:LEU:HD13	2.32	0.63
3:L:87:PHE:CD2	3:L:144:LEU:HD13	2.32	0.63
1:G:288:MET:C	1:G:290:ASP:H	2.01	0.63
3:L:103:ILE:O	3:L:104:ASN:HB3	1.97	0.63
1:A:360:LYS:HG2	1:A:361:TRP:O	1.99	0.63
1:G:293:PRO:C	1:G:294:GLU:HG3	2.19	0.63
1:G:41:ARG:HH11	1:G:41:ARG:HG2	1.63	0.63
1:J:288:MET:C	1:J:290:ASP:H	2.01	0.63
1:D:293:PRO:C	1:D:294:GLU:HG3	2.19	0.63
1:D:41:ARG:HH11	1:D:41:ARG:HG2	1.63	0.63
2:E:1:MET:HE2	2:E:30:GLU:O	1.99	0.63
1:G:15:LEU:HB2	1:G:44:SER:OG	1.98	0.63
1:G:242:GLU:HG2	1:G:528:LYS:HZ1	1.64	0.63
2:H:1:MET:HE2	2:H:30:GLU:O	1.98	0.63
1:A:15:LEU:HB2	1:A:44:SER:OG	1.98	0.63
1:D:15:LEU:HB2	1:D:44:SER:OG	1.98	0.63
1:J:293:PRO:C	1:J:294:GLU:HG3	2.19	0.63
1:A:216:THR:HG21	1:A:236:GLY:CA	2.19	0.63
1:A:41:ARG:HH11	1:A:41:ARG:HG2	1.63	0.63
3:F:87:PHE:CD2	3:F:144:LEU:HD13	2.32	0.63
1:J:41:ARG:HH11	1:J:41:ARG:HG2	1.63	0.63
1:J:570:ASN:ND2	1:J:571:PRO:HD2	2.14	0.63
1:D:288:MET:CB	1:D:289:PRO:CD	2.76	0.62
2:B:205:VAL:HG13	2:B:206:PHE:CD2	2.34	0.62
2:B:1:MET:HE2	2:B:30:GLU:O	1.98	0.62
1:D:463:VAL:HG21	1:D:519:GLU:O	1.99	0.62
1:G:302:ASP:O	1:G:306:ARG:HD3	1.99	0.62
2:K:205:VAL:HG13	2:K:206:PHE:CD2	2.34	0.62
1:D:570:ASN:ND2	1:D:571:PRO:HD2	2.14	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:MET:CB	1:J:289:PRO:CD	2.76	0.62
1:J:242:GLU:HG2	1:J:528:LYS:NZ	2.13	0.62
1:A:316:LYS:HA	1:A:316:LYS:HE2	1.82	0.62
1:D:216:THR:HG21	1:D:236:GLY:CA	2.19	0.62
1:A:419:ILE:HG22	1:A:420:VAL:N	2.15	0.62
1:D:279:LEU:N	1:D:288:MET:HE1	2.14	0.62
1:D:360:LYS:HG2	1:D:361:TRP:O	1.99	0.62
2:E:205:VAL:HG13	2:E:206:PHE:CD2	2.34	0.62
2:H:205:VAL:HG13	2:H:206:PHE:CD2	2.34	0.62
1:J:119:ILE:HG22	1:J:120:ASN:N	2.10	0.62
1:G:570:ASN:ND2	1:G:571:PRO:HD2	2.14	0.62
1:J:15:LEU:HB2	1:J:44:SER:OG	1.98	0.62
1:D:316:LYS:HE2	1:D:316:LYS:HA	1.82	0.62
1:D:462:ASP:HB3	1:D:465:LYS:HG3	1.82	0.62
1:G:213:LEU:HD23	1:G:214:ILE:N	2.15	0.62
1:G:281:ASP:HB2	1:G:285:HIS:HD2	1.61	0.62
1:G:287:PHE:HB3	1:G:296:LYS:HZ3	1.64	0.62
2:B:210:THR:HA	8:B:302:F3S:S1	2.40	0.62
1:D:302:ASP:O	1:D:306:ARG:HD3	1.99	0.62
1:D:411:SER:O	1:D:415:VAL:HG23	2.00	0.62
1:G:411:SER:O	1:G:415:VAL:HG23	2.00	0.62
1:G:463:VAL:HG21	1:G:519:GLU:O	1.99	0.62
1:J:302:ASP:O	1:J:306:ARG:HD3	1.99	0.62
3:C:103:ILE:HG12	3:C:103:ILE:O	1.98	0.62
1:D:272:CYS:HB3	1:D:328:LEU:HD21	1.82	0.62
2:E:210:THR:HG22	2:E:210:THR:O	2.00	0.62
3:F:103:ILE:O	3:F:103:ILE:HG12	1.98	0.62
1:G:272:CYS:HB3	1:G:328:LEU:HD21	1.82	0.62
1:G:462:ASP:HB3	1:G:465:LYS:HG3	1.82	0.62
1:J:360:LYS:HG2	1:J:361:TRP:O	1.99	0.62
1:J:462:ASP:HB3	1:J:465:LYS:HG3	1.82	0.62
1:A:302:ASP:O	1:A:306:ARG:HD3	1.99	0.62
1:A:463:VAL:HG21	1:A:519:GLU:O	1.99	0.62
2:B:215:HIS:HA	2:B:224:LEU:HD12	1.82	0.62
2:H:1:MET:HE3	2:H:31:ALA:HA	1.82	0.62
2:H:210:THR:HA	8:H:302:F3S:S1	2.40	0.62
1:A:462:ASP:HB3	1:A:465:LYS:HG3	1.82	0.61
3:C:146:ILE:O	3:C:148:MET:N	2.33	0.61
1:G:360:LYS:HG2	1:G:361:TRP:O	1.99	0.61
3:I:57:VAL:O	3:I:60:TRP:HB3	2.00	0.61
1:J:271:GLY:O	1:J:275:ASP:HB2	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:146:ILE:O	3:L:148:MET:N	2.33	0.61
1:A:213:LEU:HD23	1:A:214:ILE:N	2.15	0.61
1:A:411:SER:O	1:A:415:VAL:HG23	2.00	0.61
3:C:142:VAL:CG2	3:C:171:LEU:HD11	2.25	0.61
1:J:463:VAL:HG21	1:J:519:GLU:O	1.99	0.61
3:L:57:VAL:O	3:L:60:TRP:HB3	2.00	0.61
1:A:570:ASN:ND2	1:A:571:PRO:HD2	2.14	0.61
1:D:145:LYS:O	1:D:146:LYS:HB2	2.00	0.61
1:D:271:GLY:O	1:D:275:ASP:HB2	2.01	0.61
1:J:411:SER:O	1:J:415:VAL:HG23	2.00	0.61
1:A:293:PRO:C	1:A:294:GLU:HG3	2.19	0.61
1:A:272:CYS:HB3	1:A:328:LEU:HD21	1.82	0.61
2:E:215:HIS:HA	2:E:224:LEU:HD12	1.82	0.61
2:E:210:THR:HA	8:E:302:F3S:S1	2.40	0.61
3:I:146:ILE:O	3:I:148:MET:N	2.33	0.61
1:J:288:MET:HG3	1:J:297:GLU:OE2	2.00	0.61
1:J:272:CYS:HB3	1:J:328:LEU:HD21	1.82	0.61
2:K:215:HIS:HA	2:K:224:LEU:HD12	1.82	0.61
1:G:119:ILE:HG22	1:G:120:ASN:N	2.10	0.61
3:I:103:ILE:HG12	3:I:103:ILE:O	1.98	0.61
2:K:210:THR:HA	8:K:302:F3S:S1	2.40	0.61
1:A:271:GLY:O	1:A:275:ASP:HB2	2.01	0.61
1:G:316:LYS:HA	1:G:316:LYS:HE2	1.82	0.61
1:D:119:ILE:HG22	1:D:120:ASN:N	2.10	0.61
1:D:213:LEU:HD23	1:D:214:ILE:N	2.15	0.61
1:D:565:LEU:HD11	1:D:581:GLU:OE2	2.01	0.61
3:F:146:ILE:O	3:F:148:MET:N	2.33	0.61
1:G:271:GLY:O	1:G:275:ASP:HB2	2.01	0.61
1:J:213:LEU:HD23	1:J:214:ILE:N	2.15	0.61
1:J:281:ASP:HB2	1:J:285:HIS:HD2	1.61	0.61
1:J:570:ASN:OD1	1:J:572:GLU:N	2.34	0.61
1:J:565:LEU:HD11	1:J:581:GLU:OE2	2.01	0.61
1:A:288:MET:HG3	1:A:297:GLU:OE2	2.00	0.61
3:C:57:VAL:O	3:C:60:TRP:HB3	2.00	0.61
3:F:57:VAL:O	3:F:60:TRP:HB3	2.00	0.61
1:G:285:HIS:O	1:G:286:ARG:HG2	2.01	0.61
1:J:217:GLY:H	1:J:394:ALA:HB2	1.66	0.61
1:J:285:HIS:O	1:J:286:ARG:HG2	2.01	0.61
1:J:289:PRO:O	1:J:293:PRO:HG3	2.01	0.61
1:J:493:GLU:O	1:J:497:LEU:HD13	2.01	0.61
1:G:117:ALA:O	1:G:123:LYS:HA	2.01	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ALA:O	1:A:123:LYS:HA	2.01	0.61
1:A:404:ARG:HE	1:A:409:SER:CB	2.13	0.61
1:D:281:ASP:HB2	1:D:285:HIS:HD2	1.61	0.61
1:D:288:MET:HA	1:D:296:LYS:CB	2.31	0.61
2:E:213:ALA:O	2:E:217:VAL:HG22	2.01	0.61
1:G:145:LYS:O	1:G:146:LYS:HB2	2.00	0.61
1:G:208:VAL:CG1	1:G:440:LEU:HD11	2.31	0.61
1:J:208:VAL:CG1	1:J:440:LEU:HD11	2.31	0.61
1:J:288:MET:HA	1:J:296:LYS:CB	2.31	0.61
1:J:288:MET:CB	1:J:289:PRO:HD3	2.31	0.61
2:B:213:ALA:O	2:B:217:VAL:HG22	2.01	0.60
1:D:288:MET:HG3	1:D:297:GLU:OE2	2.00	0.60
2:E:28:ILE:HD12	2:E:42:MET:HE2	1.83	0.60
1:G:419:ILE:HG22	1:G:420:VAL:N	2.15	0.60
1:J:117:ALA:O	1:J:123:LYS:HA	2.01	0.60
1:J:419:ILE:HG22	1:J:420:VAL:N	2.15	0.60
1:A:145:LYS:O	1:A:146:LYS:HB2	2.00	0.60
1:A:217:GLY:H	1:A:394:ALA:HB2	1.66	0.60
1:A:288:MET:CB	1:A:289:PRO:HD3	2.31	0.60
1:A:565:LEU:HD11	1:A:581:GLU:OE2	2.01	0.60
1:A:570:ASN:OD1	1:A:572:GLU:N	2.34	0.60
2:B:210:THR:HG22	2:B:210:THR:O	2.00	0.60
1:D:493:GLU:O	1:D:497:LEU:HD13	2.01	0.60
1:G:288:MET:HA	1:G:296:LYS:HB2	1.83	0.60
1:G:493:GLU:O	1:G:497:LEU:HD13	2.01	0.60
2:H:210:THR:O	2:H:210:THR:HG22	2.00	0.60
2:H:215:HIS:HA	2:H:224:LEU:HD12	1.82	0.60
1:A:288:MET:HA	1:A:296:LYS:HB2	1.83	0.60
1:D:561:LEU:O	1:D:583:LEU:HD13	2.01	0.60
1:G:67:ASP:OD2	1:G:630:ARG:HD2	2.02	0.60
1:J:561:LEU:O	1:J:583:LEU:HD13	2.01	0.60
1:J:87:ARG:HG3	1:J:638:MET:HE3	1.83	0.60
1:A:281:ASP:OD2	1:A:287:PHE:HB2	2.01	0.60
1:A:285:HIS:O	1:A:286:ARG:HG2	2.01	0.60
1:D:117:ALA:O	1:D:123:LYS:HA	2.01	0.60
1:D:288:MET:HA	1:D:296:LYS:HB2	1.83	0.60
1:D:510:ARG:HD2	1:D:512:HIS:O	2.02	0.60
1:G:288:MET:HA	1:G:296:LYS:CB	2.31	0.60
1:G:288:MET:CB	1:G:289:PRO:CD	2.76	0.60
1:G:565:LEU:HD11	1:G:581:GLU:OE2	2.01	0.60
1:G:652:ARG:HH11	1:G:652:ARG:HG3	1.67	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:210:THR:HG22	2:K:210:THR:O	2.00	0.60
2:K:213:ALA:O	2:K:217:VAL:HG22	2.01	0.60
1:A:288:MET:HA	1:A:296:LYS:CB	2.31	0.60
1:A:208:VAL:CG1	1:A:440:LEU:HD11	2.31	0.60
1:A:561:LEU:O	1:A:583:LEU:HD13	2.02	0.60
1:A:652:ARG:HH11	1:A:652:ARG:HG3	1.67	0.60
1:A:67:ASP:OD2	1:A:630:ARG:HD2	2.01	0.60
11:C:303:LMT:H101	11:C:303:LMT:H61	1.84	0.60
1:D:281:ASP:OD2	1:D:287:PHE:HB2	2.01	0.60
1:G:288:MET:HG3	1:G:297:GLU:OE2	2.00	0.60
1:J:316:LYS:HE2	1:J:316:LYS:HA	1.82	0.60
1:D:217:GLY:H	1:D:394:ALA:HB2	1.66	0.60
1:D:208:VAL:CG1	1:D:440:LEU:HD11	2.31	0.60
1:D:67:ASP:OD2	1:D:630:ARG:HD2	2.01	0.60
1:G:289:PRO:O	1:G:293:PRO:HG3	2.01	0.60
1:J:145:LYS:O	1:J:146:LYS:HB2	2.00	0.60
2:B:166:MET:HE1	3:C:102:PRO:HA	1.84	0.60
3:C:136:MET:HE1	3:C:179:VAL:HA	1.84	0.60
1:D:570:ASN:OD1	1:D:572:GLU:N	2.34	0.60
2:E:166:MET:HE1	3:F:102:PRO:HA	1.84	0.60
3:I:157:VAL:HB	3:I:254:HIS:CE1	2.37	0.60
1:J:186:HIS:HA	1:J:190:LYS:O	2.02	0.60
1:A:87:ARG:HG3	1:A:638:MET:HE3	1.83	0.60
3:C:75:LYS:HA	3:C:75:LYS:HE2	1.84	0.60
1:D:285:HIS:O	1:D:286:ARG:HG2	2.01	0.60
1:D:419:ILE:HG22	1:D:420:VAL:N	2.15	0.60
1:D:652:ARG:HG3	1:D:652:ARG:HH11	1.67	0.60
1:G:561:LEU:O	1:G:583:LEU:HD13	2.02	0.60
2:H:28:ILE:HD12	2:H:42:MET:HE2	1.83	0.60
1:J:67:ASP:OD2	1:J:630:ARG:HD2	2.01	0.60
3:L:157:VAL:HB	3:L:254:HIS:CE1	2.37	0.60
1:A:278:ILE:HD12	1:A:286:ARG:HH11	1.67	0.60
1:A:288:MET:CB	1:A:289:PRO:CD	2.76	0.60
1:D:289:PRO:O	1:D:293:PRO:HG3	2.01	0.60
11:F:301:LMT:H61	11:F:301:LMT:H101	1.84	0.60
3:I:75:LYS:HA	3:I:75:LYS:HE2	1.84	0.60
3:L:75:LYS:HE2	3:L:75:LYS:HA	1.84	0.60
1:A:289:PRO:O	1:A:293:PRO:HG3	2.01	0.59
1:G:186:HIS:HA	1:G:190:LYS:O	2.02	0.59
1:G:314:LYS:CB	1:G:314:LYS:NZ	2.65	0.59
2:H:213:ALA:O	2:H:217:VAL:HG22	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:MET:HA	1:J:296:LYS:HB2	1.83	0.59
1:J:652:ARG:HG3	1:J:652:ARG:HH11	1.67	0.59
1:A:186:HIS:HA	1:A:190:LYS:O	2.02	0.59
1:D:186:HIS:HA	1:D:190:LYS:O	2.02	0.59
1:D:288:MET:CB	1:D:289:PRO:HD3	2.31	0.59
2:E:46:THR:HG1	2:E:47:TYR:HD1	1.48	0.59
1:G:281:ASP:OD2	1:G:287:PHE:HB2	2.01	0.59
1:G:288:MET:CB	1:G:289:PRO:HD3	2.31	0.59
1:G:570:ASN:OD1	1:G:572:GLU:N	2.34	0.59
1:J:281:ASP:OD2	1:J:287:PHE:HB2	2.01	0.59
3:L:249:ASP:CA	3:L:254:HIS:HB3	2.32	0.59
1:A:493:GLU:O	1:A:497:LEU:HD13	2.01	0.59
1:G:404:ARG:HE	1:G:409:SER:CB	2.13	0.59
1:G:87:ARG:HG3	1:G:638:MET:HE3	1.85	0.59
1:J:214:ILE:HG23	1:J:216:THR:HG23	1.85	0.59
1:A:314:LYS:CB	1:A:314:LYS:NZ	2.65	0.59
1:A:539:ASP:O	1:A:541:THR:HG23	2.02	0.59
1:D:70:PHE:O	1:D:74:VAL:HG23	2.03	0.59
2:H:143:GLN:O	2:H:146:PHE:HB3	2.03	0.59
2:H:166:MET:HE1	3:I:102:PRO:HA	1.84	0.59
1:G:510:ARG:HD2	1:G:512:HIS:O	2.02	0.59
2:B:143:GLN:O	2:B:146:PHE:HB3	2.03	0.59
1:G:214:ILE:HG23	1:G:216:THR:HG23	1.85	0.59
11:I:303:LMT:H101	11:I:303:LMT:H61	1.84	0.59
1:J:404:ARG:HE	1:J:409:SER:CB	2.13	0.59
1:A:295:LYS:HD2	1:A:298:LEU:HD12	1.85	0.59
2:B:145:VAL:O	2:B:145:VAL:HG12	2.03	0.59
3:F:157:VAL:HB	3:F:254:HIS:CE1	2.37	0.59
3:F:75:LYS:HE2	3:F:75:LYS:HA	1.84	0.59
3:I:249:ASP:CA	3:I:254:HIS:HB3	2.32	0.59
2:K:1:MET:HE2	2:K:31:ALA:HA	1.84	0.59
1:A:510:ARG:HD2	1:A:512:HIS:O	2.02	0.59
2:B:28:ILE:HD12	2:B:42:MET:HE2	1.85	0.59
1:D:214:ILE:HG23	1:D:216:THR:HG23	1.85	0.59
1:D:539:ASP:O	1:D:541:THR:HG23	2.02	0.59
1:D:652:ARG:HG3	1:D:652:ARG:NH1	2.18	0.59
1:G:539:ASP:O	1:G:541:THR:HG23	2.03	0.59
1:J:392:GLY:O	1:J:394:ALA:N	2.36	0.59
3:L:208:ASN:HA	3:L:211:LYS:HG2	1.85	0.59
3:F:86:VAL:O	3:F:86:VAL:HG12	2.03	0.59
1:G:217:GLY:H	1:G:394:ALA:HB2	1.66	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:278:ILE:HD12	1:G:286:ARG:HH11	1.67	0.59
1:G:570:ASN:CG	1:G:571:PRO:HD2	2.24	0.59
1:J:70:PHE:O	1:J:74:VAL:HG23	2.03	0.59
1:A:392:GLY:O	1:A:394:ALA:N	2.36	0.59
1:D:461:GLU:O	1:D:504:VAL:HG13	2.03	0.59
1:J:510:ARG:HD2	1:J:512:HIS:O	2.02	0.59
1:J:570:ASN:CG	1:J:571:PRO:HD2	2.24	0.59
2:K:166:MET:HE1	3:L:102:PRO:HA	1.84	0.59
3:C:86:VAL:HG12	3:C:86:VAL:O	2.03	0.58
1:D:295:LYS:HD2	1:D:298:LEU:HD12	1.85	0.58
1:D:87:ARG:HG3	1:D:638:MET:HE3	1.84	0.58
1:D:93:ALA:HB3	1:D:94:PRO:HD3	1.85	0.58
2:E:171:VAL:HG12	2:E:175:GLY:HA3	1.85	0.58
1:J:461:GLU:O	1:J:504:VAL:HG13	2.03	0.58
1:J:98:ARG:NH2	2:K:133:LEU:HD12	2.18	0.58
1:A:2:LYS:HB2	1:A:2:LYS:HZ2	1.68	0.58
1:A:346:GLN:CA	1:A:357:PRO:HG2	2.31	0.58
2:B:1:MET:HE3	2:B:31:ALA:HA	1.84	0.58
1:D:98:ARG:NH2	2:E:133:LEU:HD12	2.18	0.58
1:A:98:ARG:NH2	2:B:133:LEU:HD12	2.18	0.58
1:G:392:GLY:O	1:G:394:ALA:N	2.36	0.58
1:J:179:LYS:HG3	1:J:196:VAL:HG11	1.85	0.58
3:C:208:ASN:HA	3:C:211:LYS:HG2	1.85	0.58
1:D:179:LYS:HG3	1:D:196:VAL:HG11	1.86	0.58
2:E:143:GLN:O	2:E:146:PHE:HB3	2.03	0.58
2:E:145:VAL:HG12	2:E:145:VAL:O	2.03	0.58
1:J:93:ALA:HB3	1:J:94:PRO:HD3	1.85	0.58
1:A:570:ASN:CG	1:A:571:PRO:HD2	2.24	0.58
1:A:652:ARG:NH1	1:A:652:ARG:HG3	2.17	0.58
1:D:52:GLN:HE22	1:D:144:THR:CG2	2.17	0.58
2:H:171:VAL:HG12	2:H:175:GLY:HA3	1.85	0.58
3:I:188:TYR:O	3:I:192:VAL:HG22	2.04	0.58
1:D:122:GLN:O	1:D:124:THR:HG23	2.04	0.58
1:D:570:ASN:CG	1:D:571:PRO:HD2	2.24	0.58
2:H:145:VAL:HG12	2:H:145:VAL:O	2.03	0.58
2:K:143:GLN:O	2:K:146:PHE:HB3	2.03	0.58
1:A:70:PHE:O	1:A:74:VAL:HG23	2.03	0.58
1:D:278:ILE:HD12	1:D:286:ARG:HH11	1.67	0.58
1:G:122:GLN:O	1:G:124:THR:HG23	2.04	0.58
1:G:652:ARG:NH1	1:G:652:ARG:HG3	2.18	0.58
1:J:652:ARG:NH1	1:J:652:ARG:HG3	2.18	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:145:VAL:HG12	2:K:145:VAL:O	2.03	0.58
1:A:93:ALA:HB3	1:A:94:PRO:HD3	1.84	0.58
1:G:98:ARG:NH2	2:H:133:LEU:HD12	2.18	0.58
2:H:46:THR:HG1	2:H:47:TYR:HD1	1.51	0.58
2:B:171:VAL:HG12	2:B:175:GLY:HA3	1.85	0.58
3:C:145:TYR:O	3:C:148:MET:HB3	2.04	0.58
1:D:314:LYS:CB	1:D:314:LYS:NZ	2.65	0.58
1:D:392:GLY:O	1:D:394:ALA:N	2.36	0.58
2:H:193:GLU:CD	2:H:193:GLU:H	2.07	0.58
1:J:278:ILE:HD12	1:J:286:ARG:HH11	1.67	0.58
1:J:314:LYS:NZ	1:J:314:LYS:CB	2.65	0.58
1:A:179:LYS:HG3	1:A:196:VAL:HG11	1.86	0.58
1:A:78:ASP:OD2	1:A:544:ARG:HG3	2.04	0.58
3:C:188:TYR:O	3:C:192:VAL:HG22	2.04	0.58
3:C:249:ASP:CA	3:C:254:HIS:HB3	2.32	0.58
3:C:157:VAL:HB	3:C:254:HIS:CE1	2.37	0.58
3:F:145:TYR:O	3:F:148:MET:HB3	2.04	0.58
1:G:78:ASP:OD2	1:G:544:ARG:HG3	2.04	0.58
1:G:93:ALA:HB3	1:G:94:PRO:HD3	1.85	0.58
1:A:410:VAL:HG22	4:A:701:FAD:O2	2.04	0.57
2:B:193:GLU:H	2:B:193:GLU:CD	2.07	0.57
2:E:108:GLY:O	2:E:110:TRP:N	2.37	0.57
3:F:249:ASP:CA	3:F:254:HIS:HB3	2.32	0.57
3:I:136:MET:HE1	3:I:179:VAL:HA	1.86	0.57
2:K:193:GLU:CD	2:K:193:GLU:H	2.07	0.57
11:L:301:LMT:H101	11:L:301:LMT:H61	1.84	0.57
1:A:287:PHE:HB3	1:A:296:LYS:HZ3	1.67	0.57
2:B:108:GLY:O	2:B:110:TRP:N	2.38	0.57
3:C:58:MET:O	3:C:61:VAL:HG22	2.04	0.57
3:I:145:TYR:O	3:I:148:MET:HB3	2.04	0.57
1:J:78:ASP:OD2	1:J:544:ARG:HG3	2.04	0.57
3:L:188:TYR:O	3:L:192:VAL:HG22	2.04	0.57
1:G:52:GLN:HE22	1:G:144:THR:CG2	2.17	0.57
1:J:346:GLN:CA	1:J:357:PRO:HG2	2.31	0.57
1:D:78:ASP:OD2	1:D:544:ARG:HG3	2.04	0.57
1:G:295:LYS:HD2	1:G:298:LEU:HD12	1.85	0.57
1:J:295:LYS:HD2	1:J:298:LEU:HD12	1.85	0.57
1:A:242:GLU:HG2	1:A:528:LYS:HZ1	1.69	0.57
3:F:188:TYR:O	3:F:192:VAL:HG22	2.04	0.57
1:G:461:GLU:O	1:G:504:VAL:HG13	2.03	0.57
2:H:138:GLU:HB2	2:H:141:VAL:CG2	2.33	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:GLN:O	1:J:124:THR:HG23	2.04	0.57
1:J:462:ASP:OD2	1:J:465:LYS:HG3	2.05	0.57
1:J:52:GLN:HE22	1:J:144:THR:CG2	2.17	0.57
1:J:539:ASP:O	1:J:541:THR:HG23	2.02	0.57
3:L:145:TYR:O	3:L:148:MET:HB3	2.04	0.57
3:L:86:VAL:O	3:L:86:VAL:HG12	2.03	0.57
1:A:461:GLU:O	1:A:504:VAL:HG13	2.03	0.57
3:F:208:ASN:HA	3:F:211:LYS:HG2	1.85	0.57
1:G:70:PHE:O	1:G:74:VAL:HG23	2.03	0.57
2:K:28:ILE:HD12	2:K:42:MET:HE2	1.86	0.57
1:D:93:ALA:O	1:D:96:ALA:HB3	2.05	0.57
1:A:214:ILE:HG23	1:A:216:THR:HG23	1.85	0.57
2:E:193:GLU:H	2:E:193:GLU:CD	2.07	0.57
3:F:58:MET:O	3:F:61:VAL:HG22	2.04	0.57
1:G:179:LYS:HG3	1:G:196:VAL:HG11	1.86	0.57
3:I:208:ASN:HA	3:I:211:LYS:HG2	1.85	0.57
3:I:86:VAL:HG12	3:I:86:VAL:O	2.03	0.57
2:K:171:VAL:HG12	2:K:175:GLY:HA3	1.85	0.57
1:A:122:GLN:O	1:A:124:THR:HG23	2.04	0.57
2:E:138:GLU:HB2	2:E:141:VAL:CG2	2.33	0.57
3:I:71:PHE:HB3	3:I:75:LYS:HG3	1.87	0.57
1:J:410:VAL:HG22	4:J:701:FAD:O2	2.04	0.57
1:D:337:HIS:ND1	1:D:337:HIS:N	2.53	0.57
1:G:410:VAL:HG22	4:G:701:FAD:O2	2.04	0.57
1:J:296:LYS:O	1:J:304:VAL:HG22	2.05	0.57
1:A:93:ALA:O	1:A:96:ALA:HB3	2.05	0.56
1:D:346:GLN:CA	1:D:357:PRO:HG2	2.31	0.56
1:D:462:ASP:OD2	1:D:465:LYS:HG3	2.05	0.56
1:D:410:VAL:HG22	4:D:701:FAD:O2	2.04	0.56
1:J:93:ALA:O	1:J:96:ALA:HB3	2.05	0.56
2:K:108:GLY:O	2:K:110:TRP:N	2.38	0.56
3:L:71:PHE:HB3	3:L:75:LYS:HG3	1.87	0.56
3:I:103:ILE:HG21	3:L:103:ILE:HD13	1.86	0.56
1:J:634:GLN:NE2	1:J:638:MET:O	2.37	0.56
1:A:296:LYS:O	1:A:304:VAL:HG22	2.05	0.56
1:D:287:PHE:HB3	1:D:296:LYS:HZ3	1.71	0.56
3:I:58:MET:O	3:I:61:VAL:HG22	2.04	0.56
2:K:147:GLU:HA	2:K:150:ARG:CD	2.36	0.56
1:D:296:LYS:O	1:D:304:VAL:HG22	2.05	0.56
2:H:108:GLY:O	2:H:110:TRP:N	2.37	0.56
2:H:123:HIS:CD2	2:H:190:ARG:CZ	2.89	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLN:HE22	1:A:144:THR:CG2	2.17	0.56
1:A:229:ALA:HB1	2:B:56:VAL:O	2.06	0.56
3:C:239:THR:O	3:C:241:PRO:HD3	2.06	0.56
2:E:123:HIS:CD2	2:E:190:ARG:CZ	2.89	0.56
1:J:281:ASP:HB2	1:J:285:HIS:NE2	2.21	0.56
1:A:462:ASP:OD2	1:A:465:LYS:HG3	2.05	0.56
1:A:634:GLN:NE2	1:A:638:MET:O	2.37	0.56
2:B:123:HIS:CD2	2:B:190:ARG:CZ	2.89	0.56
1:D:221:ARG:O	1:D:471:LYS:HE3	2.05	0.56
3:F:239:THR:O	3:F:241:PRO:HD3	2.06	0.56
1:G:93:ALA:O	1:G:96:ALA:HB3	2.05	0.56
2:K:123:HIS:CD2	2:K:190:ARG:CZ	2.89	0.56
3:L:239:THR:O	3:L:241:PRO:HD3	2.06	0.56
3:L:58:MET:O	3:L:61:VAL:HG22	2.04	0.56
1:A:179:LYS:HG3	1:A:196:VAL:CG1	2.36	0.56
3:F:89:VAL:HG12	3:F:89:VAL:O	2.06	0.56
1:G:296:LYS:O	1:G:304:VAL:HG22	2.05	0.56
1:G:32:ILE:HG22	1:G:33:VAL:N	2.21	0.56
1:G:221:ARG:O	1:G:471:LYS:HE3	2.05	0.56
1:J:337:HIS:ND1	1:J:337:HIS:N	2.53	0.56
2:B:147:GLU:HA	2:B:150:ARG:CD	2.36	0.56
1:G:462:ASP:OD2	1:G:465:LYS:HG3	2.05	0.56
1:J:380:ARG:HB2	1:J:423:TYR:CD1	2.41	0.56
1:D:179:LYS:HG3	1:D:196:VAL:CG1	2.36	0.56
1:D:404:ARG:HE	1:D:409:SER:CB	2.13	0.56
3:F:151:PRO:HA	3:F:154:ILE:HD11	1.88	0.56
2:H:147:GLU:HA	2:H:150:ARG:CD	2.36	0.56
1:J:179:LYS:HG3	1:J:196:VAL:CG1	2.36	0.56
2:H:234:LYS:O	2:H:238:VAL:HG23	2.07	0.56
3:I:103:ILE:HG13	3:L:99:ARG:HA	1.88	0.56
3:I:103:ILE:HD13	3:L:103:ILE:HG21	1.88	0.56
2:E:234:LYS:O	2:E:238:VAL:HG23	2.07	0.55
1:G:380:ARG:HB2	1:G:423:TYR:CD1	2.41	0.55
3:L:176:LEU:O	3:L:176:LEU:HD12	2.06	0.55
1:A:221:ARG:O	1:A:471:LYS:HE3	2.05	0.55
1:A:337:HIS:ND1	1:A:337:HIS:N	2.53	0.55
1:A:32:ILE:HG22	1:A:33:VAL:N	2.21	0.55
1:A:482:ARG:HB3	1:A:487:LEU:CD1	2.34	0.55
3:C:176:LEU:O	3:C:176:LEU:HD12	2.06	0.55
3:C:49:SER:HA	3:C:227:THR:CG2	2.36	0.55
1:D:32:ILE:HG22	1:D:33:VAL:N	2.21	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:HIS:O	1:D:366:PRO:HA	2.07	0.55
3:F:71:PHE:HB3	3:F:75:LYS:HG3	1.87	0.55
1:G:179:LYS:HG3	1:G:196:VAL:CG1	2.36	0.55
3:I:49:SER:HA	3:I:227:THR:CG2	2.36	0.55
1:J:221:ARG:O	1:J:471:LYS:HE3	2.06	0.55
3:C:71:PHE:HB3	3:C:75:LYS:HG3	1.87	0.55
3:C:89:VAL:HG12	3:C:89:VAL:O	2.06	0.55
3:F:136:MET:HE1	3:F:179:VAL:HA	1.88	0.55
1:G:270:GLU:N	5:G:702:MLA:O3B	2.40	0.55
3:I:151:PRO:HA	3:I:154:ILE:HD11	1.88	0.55
1:J:270:GLU:N	5:J:702:MLA:O3B	2.40	0.55
1:J:344:ASP:C	1:J:346:GLN:H	2.10	0.55
1:J:229:ALA:HB1	2:K:56:VAL:O	2.06	0.55
3:L:49:SER:HA	3:L:227:THR:CG2	2.37	0.55
3:L:89:VAL:HG12	3:L:89:VAL:O	2.06	0.55
1:D:344:ASP:C	1:D:346:GLN:H	2.10	0.55
3:F:49:SER:HA	3:F:227:THR:CG2	2.36	0.55
3:I:176:LEU:O	3:I:176:LEU:HD12	2.06	0.55
3:I:89:VAL:HG12	3:I:89:VAL:O	2.06	0.55
2:K:234:LYS:O	2:K:238:VAL:HG23	2.07	0.55
1:A:270:GLU:N	5:A:702:MLA:O3B	2.40	0.55
1:A:344:ASP:C	1:A:346:GLN:H	2.10	0.55
2:E:147:GLU:HA	2:E:150:ARG:CD	2.36	0.55
3:F:248:PHE:O	3:F:254:HIS:HB3	2.07	0.55
1:G:337:HIS:ND1	1:G:337:HIS:N	2.53	0.55
1:G:229:ALA:HB1	2:H:56:VAL:O	2.06	0.55
1:J:314:LYS:HZ2	1:J:314:LYS:HB2	1.71	0.55
1:A:241:LEU:HD12	1:A:248:LEU:HD21	1.88	0.55
1:A:278:ILE:HG21	1:A:286:ARG:NH1	2.22	0.55
2:B:234:LYS:O	2:B:238:VAL:HG23	2.07	0.55
1:D:270:GLU:N	5:D:702:MLA:O3B	2.40	0.55
1:D:229:ALA:HB1	2:E:56:VAL:O	2.06	0.55
1:G:281:ASP:HB2	1:G:285:HIS:NE2	2.21	0.55
2:H:8:ARG:HH12	3:L:3:ASN:HD21	1.54	0.55
1:J:32:ILE:HG22	1:J:33:VAL:N	2.21	0.55
1:A:281:ASP:HB2	1:A:285:HIS:NE2	2.21	0.55
1:A:380:ARG:HB2	1:A:423:TYR:CD1	2.41	0.55
3:C:191:ALA:O	3:C:195:GLY:HA2	2.07	0.55
1:D:380:ARG:HB2	1:D:423:TYR:CD1	2.41	0.55
3:L:248:PHE:O	3:L:254:HIS:HB3	2.07	0.55
1:D:281:ASP:HB2	1:D:285:HIS:NE2	2.21	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:176:LEU:HD12	3:F:176:LEU:O	2.06	0.55
1:G:48:GLN:HG3	1:G:267:LEU:CD2	2.32	0.55
3:I:239:THR:O	3:I:241:PRO:HD3	2.06	0.55
1:J:302:ASP:HB2	1:J:546:ALA:HA	1.89	0.55
3:C:223:LEU:HD23	3:C:223:LEU:O	2.07	0.55
1:D:88:MET:HA	1:D:642:LEU:HD21	1.88	0.55
1:G:241:LEU:HD12	1:G:248:LEU:HD21	1.88	0.55
1:G:88:MET:HA	1:G:642:LEU:HD21	1.89	0.55
2:K:138:GLU:HB2	2:K:141:VAL:CG2	2.33	0.55
3:C:53:LEU:O	3:C:57:VAL:HB	2.07	0.55
1:G:53:ALA:O	1:G:55:LEU:N	2.38	0.55
2:H:144:GLU:C	2:H:146:PHE:H	2.10	0.55
3:I:53:LEU:O	3:I:57:VAL:HB	2.07	0.55
1:J:106:PRO:O	1:J:152:THR:HG22	2.07	0.55
3:L:53:LEU:O	3:L:57:VAL:HB	2.07	0.55
1:D:106:PRO:O	1:D:152:THR:HG22	2.07	0.54
1:D:278:ILE:HG21	1:D:286:ARG:NH1	2.22	0.54
1:D:303:VAL:O	1:D:307:ARG:CZ	2.55	0.54
3:I:223:LEU:O	3:I:223:LEU:HD23	2.07	0.54
1:J:278:ILE:HG21	1:J:286:ARG:NH1	2.22	0.54
1:J:303:VAL:O	1:J:307:ARG:CZ	2.56	0.54
1:A:302:ASP:HB2	1:A:546:ALA:HA	1.89	0.54
1:A:257:HIS:O	1:A:366:PRO:HA	2.06	0.54
3:C:248:PHE:O	3:C:254:HIS:HB3	2.07	0.54
1:D:241:LEU:HD12	1:D:248:LEU:HD21	1.88	0.54
1:G:106:PRO:O	1:G:152:THR:HG22	2.07	0.54
1:G:344:ASP:C	1:G:346:GLN:H	2.10	0.54
1:J:88:MET:HA	1:J:642:LEU:HD21	1.89	0.54
3:L:246:LYS:HE3	3:L:247:TYR:CZ	2.43	0.54
1:A:288:MET:CG	1:A:297:GLU:OE2	2.56	0.54
3:F:191:ALA:O	3:F:195:GLY:HA2	2.07	0.54
3:F:223:LEU:HD23	3:F:223:LEU:O	2.07	0.54
1:G:278:ILE:HG21	1:G:286:ARG:NH1	2.22	0.54
1:G:257:HIS:O	1:G:366:PRO:HA	2.07	0.54
1:A:281:ASP:HB2	1:A:285:HIS:HD2	1.61	0.54
1:D:267:LEU:HD22	4:D:701:FAD:H6	1.90	0.54
2:B:8:ARG:HH12	3:F:3:ASN:HD21	1.55	0.54
1:J:288:MET:CG	1:J:297:GLU:OE2	2.56	0.54
3:L:136:MET:HE1	3:L:179:VAL:HA	1.88	0.54
3:L:191:ALA:O	3:L:195:GLY:HA2	2.07	0.54
1:A:267:LEU:HD22	4:A:701:FAD:H6	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:O	1:A:55:LEU:N	2.38	0.54
1:A:423:TYR:CE2	1:A:643:PRO:HG3	2.43	0.54
1:J:257:HIS:O	1:J:366:PRO:HA	2.06	0.54
3:L:151:PRO:HA	3:L:154:ILE:HD11	1.88	0.54
2:E:57:CYS:O	2:E:58:ARG:HB3	2.08	0.54
3:C:103:ILE:HG21	3:F:103:ILE:HD13	1.89	0.54
3:I:191:ALA:O	3:I:195:GLY:HA2	2.07	0.54
1:J:241:LEU:HD11	1:J:532:CYS:SG	2.48	0.54
1:J:423:TYR:CE2	1:J:643:PRO:HG3	2.43	0.54
1:J:53:ALA:O	1:J:55:LEU:N	2.38	0.54
1:A:106:PRO:O	1:A:152:THR:HG22	2.07	0.54
1:A:241:LEU:HD11	1:A:532:CYS:SG	2.48	0.54
2:B:196:TYR:OH	3:C:21:ARG:HA	2.08	0.54
3:C:146:ILE:C	3:C:148:MET:N	2.61	0.54
3:C:249:ASP:OD1	3:C:253:THR:HA	2.08	0.54
3:C:136:MET:HB2	10:C:301:HEM:HBB2	1.90	0.54
1:D:8:SER:OG	1:D:31:THR:HG22	2.08	0.54
1:D:32:ILE:CG2	1:D:33:VAL:N	2.71	0.54
3:F:53:LEU:O	3:F:57:VAL:HB	2.07	0.54
3:I:136:MET:HB2	10:I:301:HEM:HBB2	1.90	0.54
3:I:146:ILE:C	3:I:148:MET:N	2.61	0.54
3:I:249:ASP:OD1	3:I:253:THR:HA	2.08	0.54
1:J:272:CYS:CB	1:J:328:LEU:HD21	2.38	0.54
3:L:146:ILE:C	3:L:148:MET:N	2.61	0.54
3:L:223:LEU:HD23	3:L:223:LEU:O	2.07	0.54
3:L:249:ASP:OD1	3:L:253:THR:HA	2.08	0.54
1:A:259:THR:N	1:A:260:PRO:HD3	2.23	0.54
1:A:303:VAL:O	1:A:307:ARG:CZ	2.55	0.54
1:A:88:MET:HA	1:A:642:LEU:HD21	1.89	0.54
3:C:151:PRO:HA	3:C:154:ILE:HD11	1.88	0.54
1:G:303:VAL:O	1:G:307:ARG:CZ	2.55	0.54
1:G:302:ASP:HB2	1:G:546:ALA:HA	1.89	0.54
1:J:259:THR:N	1:J:260:PRO:HD3	2.23	0.54
1:J:436:GLU:O	1:J:440:LEU:HD23	2.08	0.54
1:A:378:ASP:OD1	1:A:380:ARG:HG2	2.08	0.54
1:D:634:GLN:NE2	1:D:638:MET:O	2.37	0.54
2:H:196:TYR:OH	3:I:21:ARG:HA	2.08	0.54
2:H:57:CYS:O	2:H:58:ARG:HB3	2.08	0.54
3:I:248:PHE:O	3:I:254:HIS:HB3	2.07	0.54
2:B:57:CYS:O	2:B:58:ARG:HB3	2.08	0.54
3:C:246:LYS:HE3	3:C:247:TYR:CZ	2.43	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:TRP:CE2	3:C:64:LYS:HD2	2.43	0.54
1:J:241:LEU:HD12	1:J:248:LEU:HD21	1.88	0.54
1:A:349:CYS:HB2	1:A:357:PRO:HG3	1.90	0.53
2:B:144:GLU:C	2:B:146:PHE:H	2.10	0.53
1:D:288:MET:CG	1:D:297:GLU:OE2	2.56	0.53
1:D:272:CYS:CB	1:D:328:LEU:HD21	2.38	0.53
1:G:32:ILE:CG2	1:G:33:VAL:N	2.71	0.53
3:I:60:TRP:CE2	3:I:64:LYS:HD2	2.44	0.53
1:A:272:CYS:CB	1:A:328:LEU:HD21	2.38	0.53
3:C:103:ILE:HG13	3:F:99:ARG:HA	1.89	0.53
1:D:436:GLU:O	1:D:440:LEU:HD23	2.08	0.53
1:D:302:ASP:HB2	1:D:546:ALA:HA	1.89	0.53
1:G:259:THR:N	1:G:260:PRO:HD3	2.23	0.53
1:G:288:MET:CG	1:G:297:GLU:OE2	2.56	0.53
1:G:8:SER:OG	1:G:31:THR:HG22	2.08	0.53
1:A:334:GLY:O	1:A:338:ILE:HG13	2.09	0.53
1:D:259:THR:N	1:D:260:PRO:HD3	2.23	0.53
3:C:103:ILE:HD13	3:F:103:ILE:HG21	1.89	0.53
1:D:251:MET:CE	1:D:529:VAL:HG13	2.39	0.53
3:F:223:LEU:C	3:F:223:LEU:HD23	2.29	0.53
1:G:272:CYS:CB	1:G:328:LEU:HD21	2.38	0.53
1:J:2:LYS:HB2	1:J:2:LYS:HZ2	1.71	0.53
3:L:60:TRP:CE2	3:L:64:LYS:HD2	2.44	0.53
1:A:32:ILE:CG2	1:A:33:VAL:N	2.71	0.53
1:D:241:LEU:HD11	1:D:532:CYS:SG	2.48	0.53
3:F:249:ASP:OD1	3:F:253:THR:HA	2.08	0.53
1:J:267:LEU:HD21	5:J:702:MLA:O3A	2.09	0.53
1:J:378:ASP:OD1	1:J:380:ARG:HG2	2.08	0.53
1:G:3:VAL:HB	1:J:5:TYR:CD2	2.42	0.53
3:C:223:LEU:HD23	3:C:223:LEU:C	2.29	0.53
2:E:167:ARG:HG3	2:E:167:ARG:NH1	2.23	0.53
2:E:196:TYR:OH	3:F:21:ARG:HA	2.08	0.53
3:I:246:LYS:HE3	3:I:247:TYR:CZ	2.43	0.53
3:L:136:MET:HB2	10:L:302:HEM:HBB2	1.90	0.53
1:D:390:SER:OG	1:D:395:ALA:HB2	2.09	0.53
1:G:423:TYR:CE2	1:G:643:PRO:HG3	2.43	0.53
1:J:349:CYS:HB2	1:J:357:PRO:HG3	1.91	0.53
1:J:8:SER:OG	1:J:31:THR:HG22	2.08	0.53
1:A:390:SER:OG	1:A:395:ALA:HB2	2.09	0.53
1:A:436:GLU:O	1:A:440:LEU:HD23	2.08	0.53
1:D:423:TYR:CE2	1:D:643:PRO:HG3	2.43	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:246:LYS:HE3	3:F:247:TYR:CZ	2.43	0.53
1:G:251:MET:CE	1:G:529:VAL:HG13	2.39	0.53
1:G:267:LEU:HD22	4:G:701:FAD:H6	1.90	0.53
1:G:319:GLN:HA	1:G:324:GLN:HA	1.91	0.53
2:H:10:PHE:HB2	2:H:92:LEU:HD23	1.91	0.53
3:I:223:LEU:C	3:I:223:LEU:HD23	2.29	0.53
2:K:167:ARG:HG3	2:K:167:ARG:NH1	2.23	0.53
2:K:196:TYR:OH	3:L:21:ARG:HA	2.08	0.53
3:L:246:LYS:HE3	3:L:247:TYR:CE2	2.44	0.53
3:L:36:PHE:CD2	3:L:37:LEU:HD23	2.44	0.53
1:A:542:GLU:HA	1:A:552:TYR:HB3	1.91	0.53
2:E:144:GLU:C	2:E:146:PHE:H	2.10	0.53
1:G:241:LEU:HD11	1:G:532:CYS:SG	2.48	0.53
1:G:461:GLU:HB2	1:G:504:VAL:HA	1.91	0.53
1:G:634:GLN:NE2	1:G:638:MET:O	2.37	0.53
1:A:251:MET:CE	1:A:529:VAL:HG13	2.39	0.53
1:A:314:LYS:HB2	1:A:314:LYS:HZ2	1.72	0.53
3:F:136:MET:HB2	10:F:302:HEM:HBB2	1.90	0.53
1:G:267:LEU:HD21	5:G:702:MLA:O3A	2.09	0.53
1:J:32:ILE:CG2	1:J:33:VAL:N	2.71	0.53
1:J:334:GLY:O	1:J:338:ILE:HG13	2.09	0.53
1:J:242:GLU:HG2	1:J:528:LYS:HZ1	1.73	0.53
1:J:267:LEU:HD22	4:J:701:FAD:H6	1.90	0.53
2:K:57:CYS:O	2:K:58:ARG:HB3	2.08	0.53
1:A:8:SER:OG	1:A:31:THR:HG22	2.08	0.52
1:D:378:ASP:OD1	1:D:380:ARG:HG2	2.08	0.52
3:F:60:TRP:CE2	3:F:64:LYS:HD2	2.44	0.52
1:A:84:LYS:O	1:A:88:MET:HG3	2.10	0.52
1:D:319:GLN:HA	1:D:324:GLN:HA	1.91	0.52
1:D:562:ASN:HD22	1:D:562:ASN:N	2.03	0.52
1:G:378:ASP:OD1	1:G:380:ARG:HG2	2.08	0.52
1:J:214:ILE:CG2	1:J:216:THR:HG23	2.39	0.52
3:L:223:LEU:HD23	3:L:223:LEU:C	2.29	0.52
1:A:267:LEU:HD21	5:A:702:MLA:O3A	2.09	0.52
1:D:349:CYS:HB2	1:D:357:PRO:HG3	1.90	0.52
1:G:390:SER:OG	1:G:395:ALA:HB2	2.09	0.52
1:G:436:GLU:O	1:G:440:LEU:HD23	2.08	0.52
2:K:144:GLU:C	2:K:146:PHE:H	2.10	0.52
1:A:286:ARG:C	1:A:288:MET:N	2.62	0.52
1:A:279:LEU:H	1:A:288:MET:HE1	1.73	0.52
1:D:214:ILE:CG2	1:D:216:THR:HG23	2.39	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ARG:C	1:D:288:MET:N	2.62	0.52
3:F:53:LEU:O	3:F:54:GLY:O	2.27	0.52
1:G:334:GLY:O	1:G:338:ILE:HG13	2.09	0.52
3:I:197:PHE:N	3:I:197:PHE:CD2	2.78	0.52
1:J:461:GLU:HB2	1:J:504:VAL:HA	1.91	0.52
1:J:586:ASN:HA	1:J:612:ARG:HD3	1.92	0.52
2:B:138:GLU:HB2	2:B:141:VAL:CG2	2.33	0.52
1:A:3:VAL:HB	1:D:5:TYR:CD2	2.45	0.52
1:D:267:LEU:HD21	5:D:702:MLA:O3A	2.09	0.52
1:D:84:LYS:O	1:D:88:MET:HG3	2.10	0.52
1:G:349:CYS:HB2	1:G:357:PRO:HG3	1.90	0.52
2:H:167:ARG:NH1	2:H:167:ARG:HG3	2.23	0.52
3:I:36:PHE:CD2	3:I:37:LEU:HD23	2.44	0.52
1:J:286:ARG:C	1:J:288:MET:N	2.62	0.52
1:J:390:SER:OG	1:J:395:ALA:HB2	2.09	0.52
3:C:71:PHE:CB	3:C:75:LYS:HG3	2.39	0.52
1:D:586:ASN:HA	1:D:612:ARG:HD3	1.92	0.52
2:E:111:PHE:C	2:E:113:GLY:N	2.63	0.52
3:F:71:PHE:CB	3:F:75:LYS:HG3	2.39	0.52
1:G:482:ARG:HB3	1:G:487:LEU:CD1	2.34	0.52
3:I:249:ASP:HA	3:I:254:HIS:CB	2.39	0.52
3:I:53:LEU:O	3:I:54:GLY:O	2.27	0.52
1:A:461:GLU:HB2	1:A:504:VAL:HA	1.91	0.52
1:D:334:GLY:O	1:D:338:ILE:HG13	2.09	0.52
3:F:249:ASP:HA	3:F:254:HIS:CB	2.40	0.52
1:G:286:ARG:C	1:G:288:MET:N	2.62	0.52
3:I:246:LYS:HE3	3:I:247:TYR:CE2	2.44	0.52
1:J:251:MET:CE	1:J:529:VAL:HG13	2.39	0.52
1:J:295:LYS:CD	1:J:298:LEU:HD12	2.40	0.52
1:J:84:LYS:O	1:J:88:MET:HG3	2.10	0.52
3:L:53:LEU:O	3:L:54:GLY:O	2.27	0.52
1:A:214:ILE:CG2	1:A:216:THR:HG23	2.39	0.52
1:D:278:ILE:HB	1:D:288:MET:HE3	1.91	0.52
1:G:214:ILE:CG2	1:G:216:THR:HG23	2.39	0.52
1:G:360:LYS:HG2	1:G:361:TRP:N	2.25	0.52
1:G:5:TYR:CD2	1:J:3:VAL:HB	2.45	0.52
1:G:84:LYS:O	1:G:88:MET:HG3	2.10	0.52
1:J:285:HIS:N	1:J:285:HIS:HD2	2.08	0.52
1:D:461:GLU:HB2	1:D:504:VAL:HA	1.91	0.52
1:G:346:GLN:CA	1:G:357:PRO:HG2	2.31	0.52
2:K:10:PHE:HB2	2:K:92:LEU:HD23	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:28:TRP:HE3	3:L:29:TRP:CD1	2.28	0.52
1:A:217:GLY:N	1:A:394:ALA:HB2	2.25	0.52
2:B:111:PHE:C	2:B:113:GLY:N	2.63	0.52
3:F:246:LYS:HE3	3:F:247:TYR:CE2	2.44	0.52
1:G:295:LYS:CD	1:G:298:LEU:HD12	2.40	0.52
1:G:542:GLU:HA	1:G:552:TYR:HB3	1.91	0.52
3:I:254:HIS:O	3:I:254:HIS:ND1	2.43	0.52
1:J:303:VAL:HG13	1:J:307:ARG:NH2	2.25	0.52
3:L:71:PHE:CB	3:L:75:LYS:HG3	2.39	0.52
3:C:28:TRP:HE3	3:C:29:TRP:CD1	2.28	0.51
3:C:36:PHE:CD2	3:C:37:LEU:HD23	2.44	0.51
1:D:329:ASP:CG	1:D:361:TRP:HD1	2.14	0.51
2:E:85:GLU:HA	2:E:85:GLU:OE2	2.10	0.51
1:G:285:HIS:N	1:G:285:HIS:HD2	2.08	0.51
3:L:249:ASP:HA	3:L:254:HIS:CB	2.40	0.51
1:A:132:ARG:HH11	1:A:132:ARG:HG2	1.76	0.51
1:A:295:LYS:CD	1:A:298:LEU:HD12	2.40	0.51
1:A:319:GLN:HA	1:A:324:GLN:HA	1.91	0.51
2:B:167:ARG:NH1	2:B:167:ARG:HG3	2.23	0.51
2:B:10:PHE:HB2	2:B:92:LEU:HD23	1.91	0.51
3:C:53:LEU:O	3:C:54:GLY:O	2.28	0.51
1:D:90:VAL:HG23	1:D:91:ASN:N	2.25	0.51
3:F:18:LYS:HE3	3:F:21:ARG:NH1	2.23	0.51
3:F:28:TRP:HE3	3:F:29:TRP:CD1	2.28	0.51
1:G:132:ARG:HH11	1:G:132:ARG:HG2	1.76	0.51
3:I:18:LYS:HE3	3:I:21:ARG:NH1	2.23	0.51
3:I:87:PHE:HD2	3:I:144:LEU:HD13	1.76	0.51
1:J:643:PRO:O	1:J:647:LYS:HG2	2.11	0.51
3:L:197:PHE:N	3:L:197:PHE:HD2	2.08	0.51
1:A:303:VAL:HG13	1:A:307:ARG:NH2	2.25	0.51
1:J:319:GLN:HA	1:J:324:GLN:HA	1.91	0.51
1:J:360:LYS:HG2	1:J:361:TRP:N	2.25	0.51
2:K:85:GLU:HA	2:K:85:GLU:OE2	2.10	0.51
1:A:360:LYS:HG2	1:A:361:TRP:N	2.25	0.51
1:A:543:SER:OG	1:A:553:PRO:HA	2.11	0.51
1:A:586:ASN:HA	1:A:612:ARG:HD3	1.92	0.51
2:B:37:PHE:O	2:B:41:ASN:HB2	2.11	0.51
1:D:295:LYS:HG3	1:D:298:LEU:HB2	1.93	0.51
1:D:37:ILE:HD12	1:D:37:ILE:O	2.11	0.51
3:F:197:PHE:CD2	3:F:197:PHE:N	2.78	0.51
3:F:254:HIS:O	3:F:254:HIS:ND1	2.43	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:36:PHE:CD2	3:F:37:LEU:HD23	2.44	0.51
1:G:217:GLY:N	1:G:394:ALA:HB2	2.25	0.51
1:G:344:ASP:C	1:G:348:ILE:HG12	2.31	0.51
1:G:329:ASP:CG	1:G:361:TRP:HD1	2.14	0.51
1:G:543:SER:OG	1:G:553:PRO:HA	2.11	0.51
2:H:37:PHE:O	2:H:41:ASN:HB2	2.11	0.51
3:I:71:PHE:CB	3:I:75:LYS:HG3	2.39	0.51
1:J:490:ALA:C	1:J:492:LYS:N	2.64	0.51
1:J:552:TYR:N	1:J:553:PRO:CD	2.73	0.51
2:K:111:PHE:C	2:K:113:GLY:N	2.63	0.51
2:K:37:PHE:O	2:K:41:ASN:HB2	2.11	0.51
1:A:552:TYR:N	1:A:553:PRO:CD	2.73	0.51
2:B:85:GLU:OE2	2:B:85:GLU:HA	2.10	0.51
3:C:246:LYS:HE3	3:C:247:TYR:CE2	2.44	0.51
1:D:217:GLY:N	1:D:394:ALA:HB2	2.25	0.51
1:D:542:GLU:HA	1:D:552:TYR:HB3	1.91	0.51
3:C:99:ARG:HA	3:F:103:ILE:HG13	1.92	0.51
1:G:643:PRO:O	1:G:647:LYS:HG2	2.11	0.51
1:J:217:GLY:N	1:J:394:ALA:HB2	2.25	0.51
1:J:279:LEU:H	1:J:288:MET:HE1	1.76	0.51
1:J:318:VAL:HG13	1:J:318:VAL:O	2.11	0.51
1:A:314:LYS:HZ3	1:A:314:LYS:CB	2.24	0.51
1:A:325:HIS:HE1	1:A:327:TRP:CZ2	2.29	0.51
1:A:37:ILE:O	1:A:37:ILE:HD12	2.11	0.51
1:A:462:ASP:HB3	1:A:465:LYS:CG	2.40	0.51
1:A:594:TYR:CZ	1:A:600:LYS:HG2	2.46	0.51
1:D:543:SER:OG	1:D:553:PRO:HA	2.11	0.51
1:D:53:ALA:O	1:D:55:LEU:N	2.38	0.51
3:F:197:PHE:N	3:F:197:PHE:HD2	2.08	0.51
1:G:318:VAL:HG13	1:G:318:VAL:O	2.11	0.51
1:G:392:GLY:C	1:G:394:ALA:N	2.64	0.51
1:G:594:TYR:CZ	1:G:600:LYS:HG2	2.46	0.51
2:H:146:PHE:O	2:H:148:LEU:N	2.44	0.51
1:J:132:ARG:HH11	1:J:132:ARG:HG2	1.76	0.51
1:J:462:ASP:HB3	1:J:465:LYS:CG	2.40	0.51
1:J:542:GLU:HA	1:J:552:TYR:HB3	1.91	0.51
2:K:215:HIS:CG	2:K:225:GLN:HB2	2.46	0.51
1:A:318:VAL:HG13	1:A:318:VAL:O	2.11	0.51
2:B:95:PRO:O	2:B:96:ALA:HB3	2.11	0.51
1:D:594:TYR:CZ	1:D:600:LYS:HG2	2.46	0.51
1:D:643:PRO:O	1:D:647:LYS:HG2	2.11	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:146:PHE:O	2:E:148:LEU:N	2.44	0.51
2:E:37:PHE:O	2:E:41:ASN:HB2	2.11	0.51
2:E:10:PHE:HB2	2:E:92:LEU:HD23	1.91	0.51
2:H:215:HIS:CG	2:H:225:GLN:HB2	2.46	0.51
2:H:85:GLU:OE2	2:H:85:GLU:HA	2.10	0.51
3:I:28:TRP:HE3	3:I:29:TRP:CD1	2.28	0.51
1:J:392:GLY:C	1:J:394:ALA:N	2.64	0.51
1:J:482:ARG:HB3	1:J:487:LEU:CD1	2.34	0.51
3:C:254:HIS:O	3:C:254:HIS:ND1	2.43	0.51
1:D:267:LEU:HG	1:D:268:LEU:N	2.26	0.51
1:D:392:GLY:C	1:D:394:ALA:N	2.64	0.51
1:D:86:ALA:O	1:D:90:VAL:HG13	2.11	0.51
1:G:295:LYS:HG3	1:G:298:LEU:HB2	1.93	0.51
1:G:441:GLU:OE2	1:J:210:LYS:NZ	2.43	0.51
1:G:462:ASP:HB3	1:G:465:LYS:CG	2.41	0.51
1:J:543:SER:OG	1:J:553:PRO:HA	2.11	0.51
1:A:295:LYS:HG3	1:A:298:LEU:HB2	1.93	0.51
1:A:60:MET:HB3	1:A:147:TRP:CG	2.46	0.51
1:A:643:PRO:O	1:A:647:LYS:HG2	2.11	0.51
1:D:295:LYS:CD	1:D:298:LEU:HD12	2.40	0.51
1:G:60:MET:HB3	1:G:147:TRP:CG	2.46	0.51
3:I:75:LYS:HA	3:I:75:LYS:CE	2.41	0.51
1:J:90:VAL:HG23	1:J:91:ASN:N	2.25	0.51
3:L:227:THR:HG22	3:L:231:TYR:HE1	1.76	0.51
3:L:63:LYS:O	3:L:66:GLN:HB2	2.11	0.51
1:A:329:ASP:CG	1:A:361:TRP:HD1	2.14	0.51
1:A:562:ASN:HD22	1:A:562:ASN:N	2.03	0.51
2:B:215:HIS:CG	2:B:225:GLN:HB2	2.46	0.51
3:C:197:PHE:N	3:C:197:PHE:HD2	2.08	0.51
1:D:303:VAL:HG13	1:D:307:ARG:NH2	2.25	0.51
1:D:325:HIS:HE1	1:D:327:TRP:CZ2	2.29	0.51
1:G:303:VAL:HG13	1:G:307:ARG:NH2	2.25	0.51
1:G:325:HIS:HE1	1:G:327:TRP:CZ2	2.29	0.51
1:G:37:ILE:HD12	1:G:37:ILE:O	2.11	0.51
1:G:552:TYR:N	1:G:553:PRO:CD	2.73	0.51
1:G:495:GLU:HG3	1:G:574:THR:HB	1.93	0.51
1:G:586:ASN:HA	1:G:612:ARG:HD3	1.92	0.51
1:A:5:TYR:CD2	1:D:3:VAL:HB	2.46	0.50
3:C:18:LYS:HE3	3:C:21:ARG:NH1	2.23	0.50
1:D:462:ASP:HB3	1:D:465:LYS:CG	2.41	0.50
1:D:48:GLN:HG3	1:D:267:LEU:CD2	2.32	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:TYR:N	1:D:553:PRO:CD	2.73	0.50
2:E:111:PHE:C	2:E:113:GLY:H	2.15	0.50
3:F:227:THR:HG22	3:F:231:TYR:HE1	1.76	0.50
3:F:63:LYS:O	3:F:66:GLN:HB2	2.11	0.50
1:G:90:VAL:HG23	1:G:91:ASN:N	2.25	0.50
2:H:111:PHE:C	2:H:113:GLY:N	2.63	0.50
3:I:169:TRP:CD1	3:I:170:PRO:HD3	2.46	0.50
1:J:295:LYS:HG3	1:J:298:LEU:HB2	1.93	0.50
1:J:37:ILE:HD12	1:J:37:ILE:O	2.11	0.50
3:L:75:LYS:CE	3:L:75:LYS:HA	2.41	0.50
1:A:214:ILE:HG23	1:A:216:THR:CG2	2.42	0.50
2:B:146:PHE:O	2:B:148:LEU:N	2.44	0.50
3:C:169:TRP:CD1	3:C:170:PRO:HD3	2.47	0.50
1:D:360:LYS:HG2	1:D:361:TRP:N	2.25	0.50
2:E:95:PRO:O	2:E:96:ALA:HB3	2.11	0.50
1:G:267:LEU:HG	1:G:268:LEU:N	2.26	0.50
3:I:99:ARG:HA	3:L:103:ILE:HG13	1.92	0.50
3:L:87:PHE:HD2	3:L:144:LEU:HD13	1.76	0.50
1:A:628:LYS:HE3	1:A:628:LYS:HA	1.94	0.50
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.76	0.50
2:E:215:HIS:CG	2:E:225:GLN:HB2	2.46	0.50
3:F:14:THR:O	3:F:17:ARG:N	2.43	0.50
1:G:270:GLU:HB2	5:G:702:MLA:O3B	2.12	0.50
1:G:490:ALA:C	1:G:492:LYS:N	2.64	0.50
1:J:329:ASP:CG	1:J:361:TRP:HD1	2.14	0.50
2:K:146:PHE:O	2:K:148:LEU:N	2.44	0.50
1:A:101:ALA:HB2	1:A:107:TRP:CD1	2.47	0.50
1:A:392:GLY:C	1:A:394:ALA:N	2.64	0.50
1:A:90:VAL:HG23	1:A:91:ASN:N	2.25	0.50
3:C:249:ASP:HA	3:C:254:HIS:CB	2.40	0.50
3:F:249:ASP:HA	3:F:254:HIS:N	2.27	0.50
3:F:75:LYS:HA	3:F:75:LYS:CE	2.41	0.50
1:J:270:GLU:HB2	5:J:702:MLA:O3B	2.12	0.50
1:J:495:GLU:HG3	1:J:574:THR:HB	1.93	0.50
2:K:1:MET:HE3	2:K:31:ALA:HA	1.93	0.50
3:L:197:PHE:N	3:L:197:PHE:CD2	2.78	0.50
3:L:254:HIS:O	3:L:254:HIS:ND1	2.43	0.50
3:L:31:SER:HB3	3:L:190:LEU:HD11	1.94	0.50
1:A:107:TRP:O	1:A:109:ARG:HD2	2.12	0.50
2:B:1:MET:HE2	2:B:31:ALA:HA	1.93	0.50
3:C:31:SER:HB3	3:C:190:LEU:HD11	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:227:THR:HG22	3:C:231:TYR:HE1	1.76	0.50
3:C:249:ASP:HA	3:C:254:HIS:N	2.27	0.50
1:D:270:GLU:HB2	5:D:702:MLA:O3B	2.12	0.50
1:D:60:MET:HB3	1:D:147:TRP:CG	2.46	0.50
2:H:111:PHE:C	2:H:113:GLY:H	2.15	0.50
3:C:63:LYS:O	3:C:66:GLN:HB2	2.11	0.50
1:D:288:MET:CG	1:D:289:PRO:HD3	2.42	0.50
1:D:242:GLU:HG2	1:D:528:LYS:HZ1	1.74	0.50
1:D:628:LYS:HE3	1:D:628:LYS:HA	1.94	0.50
1:G:107:TRP:O	1:G:109:ARG:HD2	2.12	0.50
1:G:86:ALA:O	1:G:90:VAL:HG13	2.11	0.50
2:H:46:THR:OG1	2:H:47:TYR:HD1	1.95	0.50
1:J:101:ALA:HB2	1:J:107:TRP:CD1	2.47	0.50
1:J:616:ILE:HG23	1:J:637:LEU:HD22	1.94	0.50
1:A:48:GLN:HG3	1:A:267:LEU:CD2	2.32	0.50
3:C:75:LYS:HA	3:C:75:LYS:CE	2.41	0.50
1:D:318:VAL:O	1:D:318:VAL:HG13	2.11	0.50
1:D:40:LYS:HD3	2:E:153:GLU:OE1	2.12	0.50
2:E:199:ILE:HD12	2:E:231:LEU:HD21	1.94	0.50
3:F:169:TRP:CD1	3:F:170:PRO:HD3	2.47	0.50
3:F:197:PHE:O	3:F:198:ASP:C	2.50	0.50
1:G:288:MET:CG	1:G:289:PRO:HD3	2.42	0.50
1:G:461:GLU:HB3	1:G:466:ILE:HD11	1.94	0.50
3:I:227:THR:HG22	3:I:231:TYR:HE1	1.76	0.50
1:J:325:HIS:HE1	1:J:327:TRP:CZ2	2.29	0.50
1:J:60:MET:HB3	1:J:147:TRP:CG	2.46	0.50
3:L:95:PHE:CE1	11:L:301:LMT:H82	2.47	0.50
1:A:288:MET:CG	1:A:289:PRO:HD3	2.42	0.50
1:A:344:ASP:C	1:A:348:ILE:HG12	2.31	0.50
3:C:197:PHE:N	3:C:197:PHE:CD2	2.78	0.50
1:D:251:MET:HE1	1:D:529:VAL:HG13	1.93	0.50
3:F:31:SER:HB3	3:F:190:LEU:HD11	1.94	0.50
1:G:40:LYS:HD3	2:H:153:GLU:OE1	2.12	0.50
1:J:241:LEU:HD12	1:J:248:LEU:HD23	1.94	0.50
1:J:40:LYS:HD3	2:K:153:GLU:OE1	2.12	0.50
1:J:48:GLN:HG3	1:J:267:LEU:CD2	2.32	0.50
3:L:40:PHE:C	3:L:40:PHE:CD2	2.85	0.50
1:A:267:LEU:HG	1:A:268:LEU:N	2.26	0.50
1:A:285:HIS:N	1:A:285:HIS:HD2	2.08	0.50
2:B:199:ILE:HD12	2:B:231:LEU:HD21	1.94	0.50
3:C:40:PHE:CD2	3:C:40:PHE:C	2.85	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:VAL:O	1:D:307:ARG:NH1	2.45	0.50
1:D:523:VAL:HB	1:D:524:PRO:HD3	1.94	0.50
2:H:95:PRO:O	2:H:96:ALA:HB3	2.11	0.50
3:I:197:PHE:O	3:I:198:ASP:C	2.50	0.50
3:I:63:LYS:O	3:I:66:GLN:HB2	2.11	0.50
1:J:86:ALA:O	1:J:90:VAL:HG13	2.11	0.50
1:A:52:GLN:CG	1:A:148:ARG:HG3	2.42	0.49
1:A:278:ILE:HG21	1:A:286:ARG:HH11	1.77	0.49
1:A:616:ILE:HG23	1:A:637:LEU:HD22	1.93	0.49
1:A:642:LEU:HB2	1:A:647:LYS:HE3	1.94	0.49
1:A:86:ALA:O	1:A:90:VAL:HG13	2.11	0.49
2:B:111:PHE:C	2:B:113:GLY:H	2.15	0.49
1:D:141:PHE:O	1:D:298:LEU:HD22	2.12	0.49
2:E:191:THR:O	2:E:195:TYR:HD1	1.95	0.49
1:G:101:ALA:HB2	1:G:107:TRP:CD1	2.47	0.49
1:G:141:PHE:O	1:G:298:LEU:HD22	2.12	0.49
1:G:214:ILE:HG23	1:G:216:THR:CG2	2.42	0.49
3:I:40:PHE:CD2	3:I:40:PHE:C	2.85	0.49
1:J:104:GLY:O	1:J:105:VAL:C	2.50	0.49
1:J:594:TYR:CZ	1:J:600:LYS:HG2	2.46	0.49
3:L:248:PHE:HB3	3:L:254:HIS:HD1	1.77	0.49
1:A:40:LYS:HD3	2:B:153:GLU:OE1	2.12	0.49
1:D:101:ALA:HB2	1:D:107:TRP:CD1	2.47	0.49
1:G:303:VAL:O	1:G:307:ARG:NH1	2.45	0.49
3:I:197:PHE:N	3:I:197:PHE:HD2	2.08	0.49
1:J:307:ARG:HA	1:J:310:GLU:HB2	1.94	0.49
1:J:628:LYS:HE3	1:J:628:LYS:HA	1.94	0.49
3:L:169:TRP:CD1	3:L:170:PRO:HD3	2.46	0.49
3:L:58:MET:HE3	3:L:156:PRO:HA	1.94	0.49
1:A:303:VAL:O	1:A:307:ARG:NH1	2.45	0.49
3:C:248:PHE:HB3	3:C:254:HIS:HD1	1.77	0.49
1:D:214:ILE:HG23	1:D:216:THR:CG2	2.42	0.49
3:F:40:PHE:CD2	3:F:40:PHE:C	2.85	0.49
3:I:31:SER:HB3	3:I:190:LEU:HD11	1.94	0.49
1:J:211:GLY:HA3	1:J:428:CYS:SG	2.53	0.49
1:J:214:ILE:HG23	1:J:216:THR:CG2	2.42	0.49
1:J:642:LEU:HB2	1:J:647:LYS:HE3	1.94	0.49
1:G:523:VAL:HB	1:G:524:PRO:HD3	1.94	0.49
1:J:303:VAL:O	1:J:307:ARG:NH1	2.45	0.49
2:K:95:PRO:O	2:K:96:ALA:HB3	2.11	0.49
3:L:249:ASP:HA	3:L:254:HIS:N	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ALA:C	1:A:492:LYS:N	2.64	0.49
1:G:585:VAL:HA	1:G:588:MET:HG3	1.95	0.49
1:G:616:ILE:HG23	1:G:637:LEU:HD22	1.93	0.49
3:I:189:ARG:NH1	3:I:189:ARG:HG3	2.26	0.49
3:I:249:ASP:HA	3:I:254:HIS:N	2.27	0.49
2:B:48:ASP:OD1	2:B:50:ASP:HB3	2.13	0.49
1:D:285:HIS:N	1:D:285:HIS:HD2	2.08	0.49
1:D:482:ARG:HB3	1:D:487:LEU:CD1	2.34	0.49
3:I:58:MET:HE3	3:I:156:PRO:HA	1.94	0.49
1:J:111:HIS:CD2	2:K:139:PRO:HG3	2.48	0.49
1:A:306:ARG:HB2	1:A:307:ARG:HH12	1.78	0.49
1:A:461:GLU:HB3	1:A:466:ILE:HD11	1.94	0.49
3:C:169:TRP:N	3:C:170:PRO:CD	2.76	0.49
3:C:197:PHE:O	3:C:198:ASP:C	2.50	0.49
1:D:211:GLY:HA3	1:D:428:CYS:SG	2.53	0.49
1:D:495:GLU:HG3	1:D:574:THR:HB	1.93	0.49
1:G:111:HIS:CD2	2:H:139:PRO:HG3	2.48	0.49
2:H:191:THR:O	2:H:195:TYR:HD1	1.95	0.49
2:H:215:HIS:CD2	2:H:225:GLN:HB2	2.48	0.49
2:H:36:ILE:HG22	2:H:76:ALA:HB1	1.95	0.49
1:J:267:LEU:HG	1:J:268:LEU:N	2.26	0.49
1:J:410:VAL:HG13	4:J:701:FAD:N1	2.28	0.49
1:A:523:VAL:HB	1:A:524:PRO:HD3	1.94	0.49
1:A:585:VAL:HA	1:A:588:MET:HG3	1.95	0.49
2:B:36:ILE:HG22	2:B:76:ALA:HB1	1.95	0.49
1:D:307:ARG:HA	1:D:310:GLU:HB2	1.94	0.49
3:F:126:TRP:O	3:F:127:TRP:C	2.51	0.49
11:F:301:LMT:C6	11:F:301:LMT:H101	2.43	0.49
1:G:241:LEU:HD12	1:G:248:LEU:HD23	1.93	0.49
1:G:278:ILE:HG21	1:G:286:ARG:HH11	1.77	0.49
1:G:2:LYS:HB2	1:G:2:LYS:HZ2	1.74	0.49
1:G:57:ASN:OD1	1:G:135:LEU:HB3	2.13	0.49
1:J:107:TRP:O	1:J:109:ARG:HD2	2.12	0.49
2:K:191:THR:O	2:K:195:TYR:HD1	1.95	0.49
2:K:46:THR:OG1	2:K:47:TYR:HD1	1.95	0.49
2:K:48:ASP:OD1	2:K:50:ASP:HB3	2.13	0.49
3:L:189:ARG:HG3	3:L:189:ARG:NH1	2.26	0.49
11:L:301:LMT:H101	11:L:301:LMT:C6	2.43	0.49
1:A:307:ARG:HA	1:A:310:GLU:HB2	1.94	0.49
1:A:51:MET:SD	1:A:97:ILE:HG13	2.53	0.49
1:D:642:LEU:HB2	1:D:647:LYS:HE3	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:ARG:HB2	1:G:307:ARG:HH12	1.78	0.49
1:G:307:ARG:HA	1:G:310:GLU:HB2	1.94	0.49
1:G:405:LEU:O	1:G:408:ASN:HB2	2.13	0.49
1:G:628:LYS:HA	1:G:628:LYS:HE3	1.94	0.49
1:J:141:PHE:O	1:J:298:LEU:HD22	2.13	0.49
3:L:169:TRP:N	3:L:170:PRO:CD	2.76	0.49
3:L:197:PHE:O	3:L:198:ASP:C	2.50	0.49
3:L:161:PHE:CE2	3:L:246:LYS:HB2	2.48	0.49
1:A:104:GLY:O	1:A:105:VAL:C	2.50	0.49
1:D:104:GLY:O	1:D:105:VAL:C	2.50	0.49
1:D:111:HIS:CD2	2:E:139:PRO:HG3	2.48	0.49
2:E:46:THR:OG1	2:E:47:TYR:HD1	1.95	0.49
2:E:48:ASP:OD1	2:E:50:ASP:HB3	2.13	0.49
2:E:36:ILE:HG22	2:E:76:ALA:HB1	1.95	0.49
1:G:118:ILE:CD1	1:G:123:LYS:HE3	2.41	0.49
1:G:211:GLY:HA3	1:G:428:CYS:SG	2.53	0.49
1:G:278:ILE:HB	1:G:288:MET:HE3	1.95	0.49
1:G:48:GLN:HA	1:G:154:ASP:O	2.13	0.49
1:G:410:VAL:HG13	4:G:701:FAD:N1	2.28	0.49
2:H:48:ASP:OD1	2:H:50:ASP:HB3	2.13	0.49
3:I:14:THR:O	3:I:17:ARG:N	2.42	0.49
1:J:288:MET:CG	1:J:289:PRO:HD3	2.42	0.49
2:K:111:PHE:C	2:K:113:GLY:H	2.15	0.49
3:L:18:LYS:HE3	3:L:21:ARG:NH1	2.23	0.49
1:A:141:PHE:O	1:A:298:LEU:HD22	2.12	0.48
1:D:241:LEU:HD12	1:D:248:LEU:HD23	1.94	0.48
1:D:57:ASN:OD1	1:D:135:LEU:HB3	2.13	0.48
2:E:215:HIS:CD2	2:E:225:GLN:HB2	2.48	0.48
3:F:169:TRP:N	3:F:170:PRO:CD	2.76	0.48
2:H:199:ILE:HD12	2:H:231:LEU:HD21	1.94	0.48
1:J:57:ASN:OD1	1:J:135:LEU:HB3	2.13	0.48
1:J:306:ARG:HB2	1:J:307:ARG:HH12	1.78	0.48
2:K:215:HIS:CD2	2:K:225:GLN:HB2	2.48	0.48
3:L:126:TRP:O	3:L:127:TRP:C	2.51	0.48
1:A:241:LEU:HD12	1:A:248:LEU:HD23	1.94	0.48
1:A:270:GLU:HB2	5:A:702:MLA:O3B	2.12	0.48
1:A:495:GLU:HG3	1:A:574:THR:HB	1.93	0.48
1:D:111:HIS:HD2	2:E:139:PRO:HG3	1.78	0.48
1:D:112:LYS:HG3	1:D:133:HIS:HB2	1.95	0.48
1:D:303:VAL:O	1:D:305:SER:N	2.46	0.48
1:D:461:GLU:HB3	1:D:466:ILE:HD11	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:GLN:HG2	1:G:567:SER:HB3	1.95	0.48
1:J:48:GLN:NE2	1:J:345:VAL:HG22	2.28	0.48
1:A:111:HIS:CD2	2:B:139:PRO:HG3	2.48	0.48
1:A:405:LEU:O	1:A:408:ASN:HB2	2.13	0.48
2:B:209:MET:SD	3:C:100:LYS:HG3	2.53	0.48
1:D:107:TRP:O	1:D:109:ARG:HD2	2.12	0.48
1:D:344:ASP:C	1:D:348:ILE:HG12	2.31	0.48
1:D:490:ALA:C	1:D:492:LYS:N	2.64	0.48
1:G:104:GLY:O	1:G:105:VAL:C	2.50	0.48
2:H:209:MET:SD	3:I:100:LYS:HG3	2.53	0.48
3:I:169:TRP:N	3:I:170:PRO:CD	2.76	0.48
3:I:161:PHE:CE2	3:I:246:LYS:HB2	2.48	0.48
1:J:48:GLN:HA	1:J:154:ASP:O	2.13	0.48
1:J:523:VAL:HB	1:J:524:PRO:HD3	1.94	0.48
1:J:464:PHE:CD1	2:K:45:GLU:HA	2.48	0.48
2:B:215:HIS:CD2	2:B:225:GLN:HB2	2.48	0.48
2:B:57:CYS:SG	2:B:61:ILE:HD12	2.53	0.48
3:C:126:TRP:O	3:C:127:TRP:C	2.51	0.48
11:C:303:LMT:C6	11:C:303:LMT:H101	2.43	0.48
1:D:306:ARG:HB2	1:D:307:ARG:HH12	1.78	0.48
3:F:161:PHE:CE2	3:F:246:LYS:HB2	2.48	0.48
1:G:112:LYS:HG3	1:G:133:HIS:HB2	1.95	0.48
2:H:157:CYS:SG	2:H:174:ALA:HB2	2.54	0.48
1:J:74:VAL:O	1:J:77:SER:OG	2.28	0.48
2:K:36:ILE:HG22	2:K:76:ALA:HB1	1.95	0.48
3:L:83:ALA:CA	10:L:303:HEM:HBB1	2.42	0.48
2:B:157:CYS:SG	2:B:174:ALA:HB2	2.54	0.48
1:D:278:ILE:HG21	1:D:286:ARG:HH11	1.78	0.48
1:D:616:ILE:HG23	1:D:637:LEU:HD22	1.94	0.48
1:D:410:VAL:HG13	4:D:701:FAD:N1	2.28	0.48
1:D:464:PHE:CD1	2:E:45:GLU:HA	2.48	0.48
2:E:209:MET:SD	3:F:100:LYS:HG3	2.53	0.48
3:F:87:PHE:HD2	3:F:144:LEU:HD13	1.76	0.48
1:G:108:THR:HG21	1:G:151:TYR:HE1	1.79	0.48
3:I:248:PHE:HB3	3:I:254:HIS:HD1	1.77	0.48
11:I:303:LMT:H101	11:I:303:LMT:C6	2.43	0.48
1:J:314:LYS:CB	1:J:314:LYS:HZ3	2.25	0.48
1:J:539:ASP:HB3	1:J:580:TYR:OH	2.14	0.48
1:J:247:GLN:HG2	1:J:567:SER:HB3	1.95	0.48
1:A:410:VAL:HG13	4:A:701:FAD:N1	2.28	0.48
3:C:161:PHE:CE2	3:C:246:LYS:HB2	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:ARG:HG2	1:D:115:ARG:HH11	1.79	0.48
1:G:51:MET:SD	1:G:97:ILE:HG13	2.53	0.48
1:G:464:PHE:CD1	2:H:45:GLU:HA	2.48	0.48
1:J:461:GLU:HB3	1:J:466:ILE:HD11	1.94	0.48
2:K:199:ILE:HD12	2:K:231:LEU:HD21	1.94	0.48
1:A:211:GLY:HA3	1:A:428:CYS:SG	2.53	0.48
1:A:303:VAL:O	1:A:305:SER:N	2.46	0.48
1:A:48:GLN:HA	1:A:154:ASP:O	2.13	0.48
1:A:48:GLN:NE2	1:A:345:VAL:HG22	2.28	0.48
1:A:57:ASN:OD1	1:A:135:LEU:HB3	2.13	0.48
2:B:46:THR:OG1	2:B:47:TYR:HD1	1.95	0.48
3:C:87:PHE:HD2	3:C:144:LEU:HD13	1.76	0.48
1:D:51:MET:SD	1:D:97:ILE:HG13	2.53	0.48
2:E:57:CYS:SG	2:E:61:ILE:HD12	2.53	0.48
1:G:303:VAL:O	1:G:305:SER:N	2.46	0.48
1:J:115:ARG:HG2	1:J:115:ARG:HH11	1.79	0.48
1:J:303:VAL:O	1:J:305:SER:N	2.46	0.48
2:K:57:CYS:SG	2:K:61:ILE:HD12	2.53	0.48
1:A:247:GLN:HG2	1:A:567:SER:HB3	1.95	0.48
1:D:52:GLN:CG	1:D:148:ARG:HG3	2.42	0.48
1:D:213:LEU:HD23	1:D:213:LEU:C	2.34	0.48
1:D:48:GLN:HA	1:D:154:ASP:O	2.13	0.48
1:D:48:GLN:NE2	1:D:345:VAL:HG22	2.28	0.48
1:D:518:GLU:O	1:D:522:ARG:HG3	2.14	0.48
3:F:248:PHE:HB3	3:F:254:HIS:HD1	1.77	0.48
3:F:95:PHE:CE1	11:F:301:LMT:H82	2.49	0.48
1:G:111:HIS:HD2	2:H:139:PRO:HG3	1.78	0.48
1:G:279:LEU:H	1:G:288:MET:HE1	1.76	0.48
1:J:344:ASP:C	1:J:348:ILE:HG12	2.31	0.48
1:J:585:VAL:HA	1:J:588:MET:HG3	1.95	0.48
2:B:191:THR:O	2:B:195:TYR:HD1	1.95	0.48
1:D:539:ASP:HB3	1:D:580:TYR:OH	2.14	0.48
1:D:585:VAL:HA	1:D:588:MET:HG3	1.95	0.48
2:E:144:GLU:C	2:E:146:PHE:N	2.68	0.48
2:E:157:CYS:SG	2:E:174:ALA:HB2	2.54	0.48
3:F:13:VAL:HG22	3:F:18:LYS:H	1.79	0.48
4:G:701:FAD:H9	4:G:701:FAD:H1'1	1.63	0.48
3:I:126:TRP:O	3:I:127:TRP:C	2.51	0.48
1:J:111:HIS:HD2	2:K:139:PRO:HG3	1.78	0.48
1:J:51:MET:SD	1:J:97:ILE:HG13	2.53	0.48
1:A:112:LYS:HG3	1:A:133:HIS:HB2	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:HB3	1:A:289:PRO:HD2	1.89	0.48
3:C:248:PHE:HB3	3:C:254:HIS:ND1	2.29	0.48
1:D:405:LEU:O	1:D:408:ASN:HB2	2.13	0.48
3:F:69:PHE:CD1	3:F:70:ILE:HG13	2.40	0.48
1:G:115:ARG:HG2	1:G:115:ARG:HH11	1.79	0.48
1:J:278:ILE:HB	1:J:288:MET:HE3	1.95	0.48
1:J:518:GLU:O	1:J:522:ARG:HG3	2.14	0.48
2:K:209:MET:SD	3:L:100:LYS:HG3	2.53	0.48
1:A:115:ARG:HH11	1:A:115:ARG:HG2	1.79	0.47
1:A:5:TYR:HD1	1:A:208:VAL:HG23	1.79	0.47
1:A:213:LEU:C	1:A:213:LEU:HD23	2.34	0.47
3:F:36:PHE:HD2	3:F:89:VAL:CG1	2.25	0.47
3:F:58:MET:HE3	3:F:156:PRO:HA	1.95	0.47
1:G:642:LEU:HB2	1:G:647:LYS:HE3	1.94	0.47
1:A:349:CYS:O	1:A:353:ALA:HB3	2.14	0.47
1:G:52:GLN:CG	1:G:148:ARG:HG3	2.42	0.47
1:G:48:GLN:NE2	1:G:345:VAL:HG22	2.28	0.47
2:H:57:CYS:SG	2:H:61:ILE:HD12	2.53	0.47
3:I:248:PHE:HB3	3:I:254:HIS:ND1	2.29	0.47
1:J:112:LYS:HG3	1:J:133:HIS:HB2	1.95	0.47
1:J:405:LEU:O	1:J:408:ASN:HB2	2.13	0.47
2:K:157:CYS:SG	2:K:174:ALA:HB2	2.54	0.47
2:K:34:MET:SD	2:K:39:VAL:HG22	2.55	0.47
1:G:278:ILE:HD12	1:G:286:ARG:NH1	2.29	0.47
1:J:233:GLU:HB3	1:J:526:MET:HE3	1.96	0.47
1:J:278:ILE:CD1	1:J:286:ARG:HH11	2.28	0.47
1:J:451:MET:O	1:J:455:VAL:HG23	2.15	0.47
2:K:144:GLU:C	2:K:146:PHE:N	2.67	0.47
1:A:255:GLN:HE21	1:A:403:ASN:ND2	2.12	0.47
1:A:518:GLU:O	1:A:522:ARG:HG3	2.14	0.47
1:A:464:PHE:CD1	2:B:45:GLU:HA	2.48	0.47
1:D:255:GLN:HE21	1:D:403:ASN:ND2	2.12	0.47
1:D:319:GLN:CA	1:D:324:GLN:HA	2.45	0.47
1:D:349:CYS:O	1:D:353:ALA:HB3	2.14	0.47
1:D:247:GLN:HG2	1:D:567:SER:HB3	1.95	0.47
2:E:166:MET:HE2	3:F:107:GLN:HB3	1.95	0.47
3:F:204:LYS:O	3:F:207:ALA:HB3	2.15	0.47
3:F:218:ALA:O	3:F:222:VAL:HG23	2.15	0.47
2:H:144:GLU:C	2:H:146:PHE:N	2.68	0.47
3:I:136:MET:CE	3:I:179:VAL:HA	2.45	0.47
3:I:69:PHE:CD1	3:I:70:ILE:HG13	2.40	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:168:MET:HB3	3:L:172:TYR:CE1	2.50	0.47
1:A:152:THR:O	1:A:153:ALA:HB3	2.15	0.47
1:A:319:GLN:CA	1:A:324:GLN:HA	2.45	0.47
1:A:357:PRO:C	1:A:359:GLU:H	2.18	0.47
1:A:251:MET:HE1	1:A:529:VAL:HG13	1.97	0.47
1:A:540:ARG:NH2	1:A:562:ASN:HD22	2.08	0.47
1:D:186:HIS:CD2	1:D:243:THR:HB	2.50	0.47
3:F:168:MET:HB3	3:F:172:TYR:CE1	2.50	0.47
3:F:136:MET:CE	3:F:179:VAL:HA	2.45	0.47
1:G:186:HIS:CD2	1:G:243:THR:HB	2.50	0.47
1:G:219:TYR:O	1:G:222:ILE:HG12	2.15	0.47
1:G:349:CYS:O	1:G:353:ALA:HB3	2.14	0.47
1:G:368:GLN:NE2	1:G:368:GLN:C	2.68	0.47
3:I:204:LYS:O	3:I:207:ALA:HB3	2.15	0.47
1:J:152:THR:O	1:J:153:ALA:HB3	2.15	0.47
1:J:278:ILE:HG21	1:J:286:ARG:HH11	1.77	0.47
1:J:356:ASP:HA	1:J:357:PRO:HD3	1.71	0.47
3:L:218:ALA:O	3:L:222:VAL:HG23	2.15	0.47
1:A:32:ILE:HD13	1:A:207:TYR:HE2	1.80	0.47
1:A:351:TYR:CD2	2:B:78:ARG:HD3	2.50	0.47
1:A:539:ASP:HB3	1:A:580:TYR:OH	2.14	0.47
3:C:14:THR:O	3:C:17:ARG:N	2.43	0.47
3:C:36:PHE:HD2	3:C:89:VAL:CG1	2.25	0.47
1:D:540:ARG:NH2	1:D:562:ASN:HD22	2.08	0.47
1:D:5:TYR:HD1	1:D:208:VAL:HG23	1.79	0.47
1:G:518:GLU:O	1:G:522:ARG:HG3	2.14	0.47
1:G:71:MET:O	1:G:75:LYS:HG3	2.15	0.47
2:H:34:MET:SD	2:H:39:VAL:HG22	2.55	0.47
1:J:108:THR:HG21	1:J:151:TYR:HE1	1.79	0.47
1:J:349:CYS:O	1:J:353:ALA:HB3	2.15	0.47
1:J:41:ARG:NH2	2:K:153:GLU:O	2.42	0.47
3:L:14:THR:O	3:L:17:ARG:N	2.42	0.47
3:L:136:MET:CE	3:L:179:VAL:HA	2.44	0.47
1:A:111:HIS:HD2	2:B:139:PRO:HG3	1.78	0.47
1:A:487:LEU:O	1:A:538:LEU:HD22	2.15	0.47
1:A:71:MET:O	1:A:75:LYS:HG3	2.15	0.47
1:D:278:ILE:CD1	1:D:286:ARG:HH11	2.28	0.47
1:D:37:ILE:O	1:D:38:PRO:C	2.53	0.47
2:E:34:MET:SD	2:E:39:VAL:HG22	2.55	0.47
1:G:152:THR:O	1:G:153:ALA:HB3	2.15	0.47
1:G:213:LEU:C	1:G:213:LEU:HD23	2.34	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:319:GLN:CA	1:G:324:GLN:HA	2.45	0.47
1:G:32:ILE:HD13	1:G:207:TYR:HE2	1.80	0.47
3:I:218:ALA:O	3:I:222:VAL:HG23	2.15	0.47
3:I:83:ALA:CA	10:I:302:HEM:HBB1	2.42	0.47
1:A:368:GLN:C	1:A:368:GLN:NE2	2.68	0.47
3:C:58:MET:HE3	3:C:156:PRO:HA	1.96	0.47
1:G:255:GLN:HE21	1:G:403:ASN:ND2	2.12	0.47
1:G:492:LYS:O	1:G:492:LYS:HD3	2.15	0.47
3:I:168:MET:HB3	3:I:172:TYR:CE1	2.50	0.47
1:J:58:SER:HA	1:J:110:ILE:CD1	2.45	0.47
1:J:213:LEU:HD23	1:J:213:LEU:C	2.34	0.47
1:J:319:GLN:CA	1:J:324:GLN:HA	2.45	0.47
1:J:5:TYR:HD1	1:J:208:VAL:HG23	1.79	0.47
1:A:451:MET:O	1:A:455:VAL:HG23	2.15	0.47
2:B:144:GLU:C	2:B:146:PHE:N	2.68	0.47
2:B:147:GLU:HA	2:B:150:ARG:HD3	1.97	0.47
1:G:355:ILE:C	1:G:355:ILE:HD12	2.35	0.47
1:G:539:ASP:HB3	1:G:580:TYR:OH	2.14	0.47
1:J:219:TYR:O	1:J:222:ILE:HG12	2.15	0.47
1:J:255:GLN:HE21	1:J:403:ASN:ND2	2.12	0.47
1:J:487:LEU:O	1:J:538:LEU:HD22	2.15	0.47
3:I:171:LEU:HD12	3:L:145:TYR:CE1	2.49	0.47
2:B:34:MET:SD	2:B:39:VAL:HG22	2.55	0.47
3:C:72:GLU:HB3	3:C:73:GLY:H	1.47	0.47
1:D:2:LYS:HB2	1:D:2:LYS:HZ3	1.76	0.47
1:D:351:TYR:CD2	2:E:78:ARG:HD3	2.50	0.47
2:E:232:ARG:HG2	3:F:194:TRP:CZ3	2.50	0.47
1:G:617:ASP:HA	1:G:620:GLN:HB2	1.97	0.47
3:I:103:ILE:H	3:I:107:GLN:HE21	1.62	0.47
1:J:10:VAL:O	1:J:10:VAL:HG12	2.15	0.47
1:J:288:MET:HB3	1:J:289:PRO:HD2	1.89	0.47
1:J:32:ILE:HD13	1:J:207:TYR:HE2	1.80	0.47
1:A:10:VAL:O	1:A:10:VAL:HG12	2.15	0.47
1:A:108:THR:HG21	1:A:151:TYR:HE1	1.79	0.47
1:A:186:HIS:CD2	1:A:243:THR:HB	2.50	0.47
3:C:85:PHE:C	3:C:87:PHE:H	2.19	0.47
1:D:10:VAL:HG12	1:D:10:VAL:O	2.15	0.47
1:D:108:THR:HG21	1:D:151:TYR:HE1	1.79	0.47
1:D:278:ILE:HD12	1:D:286:ARG:NH1	2.29	0.47
1:D:32:ILE:HD13	1:D:207:TYR:HE2	1.80	0.47
3:F:248:PHE:HB3	3:F:254:HIS:ND1	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:ILE:O	1:G:38:PRO:C	2.53	0.47
1:G:5:TYR:HD1	1:G:208:VAL:HG23	1.79	0.47
1:J:71:MET:O	1:J:75:LYS:HG3	2.15	0.47
2:K:114:MET:O	2:K:118:VAL:HG22	2.15	0.47
3:L:103:ILE:H	3:L:107:GLN:HE21	1.62	0.47
3:L:248:PHE:HB3	3:L:254:HIS:ND1	2.29	0.47
3:C:204:LYS:O	3:C:207:ALA:HB3	2.15	0.46
1:D:487:LEU:O	1:D:538:LEU:HD22	2.15	0.46
1:G:57:ASN:O	1:G:132:ARG:NH1	2.48	0.46
2:H:114:MET:O	2:H:118:VAL:HG22	2.15	0.46
2:H:147:GLU:HA	2:H:150:ARG:HD3	1.97	0.46
1:J:52:GLN:CG	1:J:148:ARG:HG3	2.42	0.46
1:J:278:ILE:HD12	1:J:286:ARG:NH1	2.29	0.46
1:J:368:GLN:NE2	1:J:368:GLN:C	2.68	0.46
1:A:281:ASP:CG	1:A:287:PHE:HB2	2.36	0.46
1:D:368:GLN:NE2	1:D:368:GLN:C	2.68	0.46
3:F:186:GLY:O	3:F:190:LEU:HB2	2.15	0.46
1:G:18:LEU:O	1:G:22:VAL:HG23	2.15	0.46
1:G:451:MET:O	1:G:455:VAL:HG23	2.15	0.46
2:H:222:LEU:HB3	2:H:223:PRO:HD2	1.97	0.46
2:H:230:TYR:CE1	2:H:234:LYS:HD2	2.50	0.46
2:H:232:ARG:HG2	3:I:194:TRP:CZ3	2.50	0.46
1:J:57:ASN:O	1:J:132:ARG:NH1	2.48	0.46
2:K:147:GLU:HA	2:K:150:ARG:HD3	1.97	0.46
3:L:13:VAL:HG22	3:L:18:LYS:H	1.79	0.46
3:L:186:GLY:O	3:L:190:LEU:HB2	2.15	0.46
3:L:204:LYS:O	3:L:207:ALA:HB3	2.15	0.46
1:A:355:ILE:HD12	1:A:355:ILE:C	2.35	0.46
3:C:13:VAL:HG22	3:C:18:LYS:H	1.79	0.46
3:C:168:MET:HB3	3:C:172:TYR:CE1	2.50	0.46
3:C:253:THR:HG22	3:C:254:HIS:N	2.21	0.46
3:C:83:ALA:CA	10:C:302:HEM:HBB1	2.42	0.46
1:D:58:SER:HA	1:D:110:ILE:CD1	2.45	0.46
1:D:110:ILE:HA	1:D:137:HIS:HD2	1.80	0.46
1:D:219:TYR:O	1:D:222:ILE:HG12	2.15	0.46
1:D:225:ASN:HB3	1:D:367:MET:CE	2.41	0.46
1:G:58:SER:HA	1:G:110:ILE:CD1	2.45	0.46
1:G:225:ASN:HB3	1:G:367:MET:CE	2.41	0.46
1:G:278:ILE:CD1	1:G:286:ARG:HH11	2.28	0.46
1:G:288:MET:HB3	1:G:289:PRO:HD2	1.89	0.46
1:G:351:TYR:CD2	2:H:78:ARG:HD3	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:281:ASP:CG	1:J:287:PHE:HB2	2.36	0.46
1:J:296:LYS:HG3	1:J:307:ARG:HE	1.81	0.46
1:J:351:TYR:CD2	2:K:78:ARG:HD3	2.50	0.46
1:J:37:ILE:O	1:J:38:PRO:C	2.53	0.46
2:K:222:LEU:HB3	2:K:223:PRO:HD2	1.97	0.46
2:B:114:MET:O	2:B:118:VAL:HG22	2.15	0.46
2:B:222:LEU:HB3	2:B:223:PRO:HD2	1.97	0.46
2:B:232:ARG:HG2	3:C:194:TRP:CZ3	2.50	0.46
2:E:145:VAL:O	2:E:145:VAL:CG1	2.64	0.46
2:E:230:TYR:CE1	2:E:234:LYS:HD2	2.51	0.46
1:G:233:GLU:HB3	1:G:526:MET:HE3	1.98	0.46
1:J:186:HIS:CD2	1:J:243:THR:HB	2.50	0.46
1:J:492:LYS:O	1:J:492:LYS:HD3	2.15	0.46
3:L:36:PHE:HD2	3:L:89:VAL:CG1	2.25	0.46
1:A:542:GLU:HG2	1:A:560:TRP:CD1	2.51	0.46
2:B:206:PHE:CE1	3:C:24:ALA:HB2	2.51	0.46
1:D:119:ILE:CG2	1:D:120:ASN:H	2.15	0.46
1:D:18:LEU:O	1:D:22:VAL:HG23	2.15	0.46
1:D:617:ASP:HA	1:D:620:GLN:HB2	1.97	0.46
2:E:206:PHE:CE1	3:F:24:ALA:HB2	2.51	0.46
2:E:222:LEU:HB3	2:E:223:PRO:HD2	1.97	0.46
3:F:83:ALA:CA	10:F:303:HEM:HBB1	2.42	0.46
1:G:487:LEU:O	1:G:538:LEU:HD22	2.15	0.46
2:H:145:VAL:O	2:H:145:VAL:CG1	2.64	0.46
2:H:1:MET:HE2	2:H:31:ALA:HA	1.95	0.46
3:I:98:MET:O	3:I:101:PHE:HB2	2.16	0.46
1:D:152:THR:O	1:D:153:ALA:HB3	2.15	0.46
1:D:57:ASN:O	1:D:132:ARG:NH1	2.48	0.46
1:G:173:VAL:HG12	1:G:174:SER:N	2.31	0.46
1:G:296:LYS:HG3	1:G:307:ARG:HE	1.81	0.46
3:I:186:GLY:O	3:I:190:LEU:HB2	2.15	0.46
1:J:18:LEU:O	1:J:22:VAL:HG23	2.15	0.46
1:J:41:ARG:HH11	1:J:41:ARG:CG	2.29	0.46
1:A:296:LYS:HG3	1:A:307:ARG:HE	1.81	0.46
1:A:226:THR:OG1	1:A:368:GLN:NE2	2.49	0.46
3:C:103:ILE:H	3:C:107:GLN:HE21	1.62	0.46
1:D:451:MET:O	1:D:455:VAL:HG23	2.15	0.46
2:E:114:MET:O	2:E:118:VAL:HG22	2.15	0.46
1:G:10:VAL:O	1:G:10:VAL:HG12	2.15	0.46
3:I:253:THR:HG22	3:I:254:HIS:N	2.21	0.46
1:J:478:VAL:O	1:J:478:VAL:HG12	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:84:LYS:HE3	1:J:638:MET:HG3	1.97	0.46
1:J:93:ALA:N	1:J:94:PRO:CD	2.79	0.46
1:A:219:TYR:O	1:A:222:ILE:HG12	2.15	0.46
1:A:281:ASP:CB	1:A:285:HIS:NE2	2.79	0.46
4:A:701:FAD:H1'1	4:A:701:FAD:H9	1.63	0.46
3:C:136:MET:CE	3:C:179:VAL:HA	2.45	0.46
1:D:295:LYS:HG3	1:D:297:GLU:O	2.16	0.46
1:D:478:VAL:O	1:D:478:VAL:HG12	2.16	0.46
3:F:146:ILE:C	3:F:148:MET:N	2.61	0.46
1:G:288:MET:O	1:G:290:ASP:N	2.48	0.46
1:G:295:LYS:HG3	1:G:297:GLU:O	2.16	0.46
1:J:617:ASP:HA	1:J:620:GLN:HB2	1.97	0.46
3:L:49:SER:HA	3:L:227:THR:HG21	1.98	0.46
1:A:295:LYS:HG3	1:A:297:GLU:O	2.16	0.46
2:B:82:LYS:HE3	2:B:83:ASP:OD2	2.16	0.46
3:C:218:ALA:O	3:C:222:VAL:HG23	2.15	0.46
3:C:61:VAL:HA	3:C:64:LYS:HG3	1.98	0.46
1:D:281:ASP:CB	1:D:285:HIS:NE2	2.79	0.46
1:D:288:MET:HB3	1:D:289:PRO:HD2	1.89	0.46
1:D:296:LYS:HG3	1:D:307:ARG:HE	1.81	0.46
1:D:84:LYS:HE3	1:D:638:MET:HG3	1.97	0.46
3:F:64:LYS:HB3	3:F:64:LYS:HE2	1.79	0.46
3:F:85:PHE:C	3:F:87:PHE:H	2.19	0.46
1:G:110:ILE:HA	1:G:137:HIS:HD2	1.80	0.46
1:G:281:ASP:CB	1:G:285:HIS:NE2	2.79	0.46
3:I:248:PHE:O	3:I:254:HIS:ND1	2.49	0.46
1:J:118:ILE:CD1	1:J:123:LYS:HE3	2.41	0.46
1:J:288:MET:O	1:J:290:ASP:N	2.48	0.46
2:K:230:TYR:CE1	2:K:234:LYS:HD2	2.50	0.46
2:K:166:MET:HE2	3:L:107:GLN:HB3	1.97	0.46
3:L:69:PHE:CD1	3:L:70:ILE:HG13	2.40	0.46
1:A:110:ILE:HA	1:A:137:HIS:HD2	1.80	0.46
1:A:57:ASN:O	1:A:132:ARG:NH1	2.48	0.46
1:A:173:VAL:HG12	1:A:174:SER:N	2.31	0.46
1:A:37:ILE:O	1:A:38:PRO:C	2.53	0.46
2:B:230:TYR:CE1	2:B:234:LYS:HD2	2.51	0.46
2:B:46:THR:OG1	2:B:47:TYR:N	2.49	0.46
1:D:281:ASP:CG	1:D:287:PHE:HB2	2.36	0.46
1:D:357:PRO:C	1:D:359:GLU:H	2.18	0.46
1:D:93:ALA:N	1:D:94:PRO:CD	2.79	0.46
3:F:103:ILE:H	3:F:107:GLN:HE21	1.62	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:ILE:HA	1:G:137:HIS:CD2	2.51	0.46
1:G:238:ALA:CB	1:G:525:MET:HB3	2.46	0.46
3:I:151:PRO:O	3:I:154:ILE:HG13	2.16	0.46
3:I:1:MET:HB3	3:L:112:LYS:NZ	2.31	0.46
1:J:355:ILE:C	1:J:355:ILE:HD12	2.35	0.46
1:J:226:THR:OG1	1:J:368:GLN:NE2	2.49	0.46
1:A:18:LEU:O	1:A:22:VAL:HG23	2.15	0.45
1:A:238:ALA:CB	1:A:525:MET:HB3	2.46	0.45
1:A:84:LYS:HE3	1:A:638:MET:HG3	1.97	0.45
1:D:71:MET:O	1:D:75:LYS:HG3	2.15	0.45
1:G:112:LYS:NZ	1:G:130:ASP:HB3	2.32	0.45
1:J:542:GLU:HG2	1:J:560:TRP:CD1	2.51	0.45
3:L:151:PRO:O	3:L:154:ILE:HG13	2.16	0.45
1:A:112:LYS:NZ	1:A:130:ASP:HB3	2.31	0.45
2:B:145:VAL:CG1	2:B:145:VAL:O	2.64	0.45
3:C:109:LEU:O	3:C:109:LEU:HD12	2.16	0.45
3:C:49:SER:HA	3:C:227:THR:HG21	1.98	0.45
1:D:238:ALA:CB	1:D:525:MET:HB3	2.46	0.45
1:D:355:ILE:C	1:D:355:ILE:HD12	2.35	0.45
1:D:613:GLN:O	1:D:616:ILE:HB	2.17	0.45
1:G:9:LEU:CD2	1:G:10:VAL:H	2.28	0.45
1:G:540:ARG:NH2	1:G:562:ASN:HD22	2.08	0.45
1:G:562:ASN:HD22	1:G:562:ASN:N	2.03	0.45
2:H:190:ARG:HB3	2:H:195:TYR:CE1	2.51	0.45
1:J:173:VAL:HG12	1:J:174:SER:N	2.31	0.45
1:J:295:LYS:HG3	1:J:297:GLU:O	2.16	0.45
1:J:311:HIS:HA	1:J:314:LYS:HD3	1.99	0.45
1:J:238:ALA:CB	1:J:525:MET:HB3	2.46	0.45
1:A:345:VAL:O	1:A:345:VAL:HG12	2.17	0.45
1:A:380:ARG:CB	1:A:423:TYR:CD1	3.00	0.45
2:B:122:ILE:HD13	2:B:188:ASP:HB2	1.99	0.45
1:D:112:LYS:HZ2	1:D:130:ASP:HB3	1.82	0.45
1:D:129:GLU:HG2	1:D:131:PHE:HE2	1.82	0.45
1:D:226:THR:OG1	1:D:368:GLN:NE2	2.49	0.45
1:D:288:MET:O	1:D:290:ASP:N	2.48	0.45
1:D:345:VAL:HG12	1:D:345:VAL:O	2.17	0.45
2:E:82:LYS:HE3	2:E:83:ASP:OD2	2.16	0.45
3:F:248:PHE:O	3:F:254:HIS:ND1	2.49	0.45
3:F:98:MET:O	3:F:101:PHE:HB2	2.16	0.45
1:J:129:GLU:HG2	1:J:131:PHE:HE2	1.82	0.45
3:L:13:VAL:CG2	3:L:18:LYS:N	2.79	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:248:PHE:O	3:L:254:HIS:ND1	2.49	0.45
3:L:63:LYS:O	3:L:66:GLN:N	2.45	0.45
1:A:478:VAL:O	1:A:478:VAL:HG12	2.16	0.45
1:A:93:ALA:N	1:A:94:PRO:CD	2.79	0.45
1:D:173:VAL:HG12	1:D:174:SER:N	2.31	0.45
1:D:380:ARG:CB	1:D:423:TYR:CD1	3.00	0.45
1:D:427:HIS:O	1:D:431:THR:HG22	2.17	0.45
3:F:13:VAL:CG2	3:F:18:LYS:N	2.79	0.45
1:G:478:VAL:O	1:G:478:VAL:HG12	2.16	0.45
2:H:206:PHE:CE1	3:I:24:ALA:HB2	2.51	0.45
2:H:46:THR:OG1	2:H:47:TYR:N	2.49	0.45
1:J:357:PRO:C	1:J:359:GLU:H	2.18	0.45
1:J:427:HIS:O	1:J:431:THR:HG22	2.17	0.45
1:A:311:HIS:HA	1:A:314:LYS:HD3	1.99	0.45
1:A:492:LYS:HD3	1:A:492:LYS:O	2.15	0.45
1:A:58:SER:HA	1:A:110:ILE:CD1	2.45	0.45
1:A:613:GLN:O	1:A:616:ILE:HB	2.16	0.45
3:C:160:SER:O	3:C:163:MET:HB3	2.17	0.45
1:D:279:LEU:H	1:D:288:MET:HE1	1.78	0.45
1:D:41:ARG:NH2	2:E:153:GLU:O	2.42	0.45
2:E:7:ILE:HG22	2:E:9:VAL:HG23	1.99	0.45
3:F:49:SER:HA	3:F:227:THR:HG21	1.98	0.45
1:G:84:LYS:HE3	1:G:638:MET:HG3	1.97	0.45
2:H:7:ILE:HG22	2:H:9:VAL:HG23	1.99	0.45
3:I:49:SER:HA	3:I:227:THR:HG21	1.98	0.45
3:I:161:PHE:CD1	3:I:245:TYR:HB2	2.52	0.45
1:J:110:ILE:HA	1:J:137:HIS:CD2	2.51	0.45
1:J:22:VAL:O	1:J:26:GLN:HG2	2.17	0.45
1:J:60:MET:HB2	1:J:147:TRP:HB2	1.99	0.45
2:K:145:VAL:CG1	2:K:145:VAL:O	2.64	0.45
3:L:161:PHE:CD1	3:L:245:TYR:HB2	2.52	0.45
3:L:85:PHE:C	3:L:87:PHE:H	2.19	0.45
3:L:98:MET:O	3:L:101:PHE:HB2	2.16	0.45
1:A:467:LYS:HG3	1:A:468:ASN:N	2.31	0.45
1:A:512:HIS:O	1:A:513:ALA:C	2.55	0.45
3:C:186:GLY:O	3:C:190:LEU:HB2	2.15	0.45
3:C:51:ILE:HG21	3:C:231:TYR:CE1	2.52	0.45
3:C:40:PHE:HE1	3:C:86:VAL:HG21	1.81	0.45
1:D:123:LYS:H	1:D:123:LYS:HG2	1.59	0.45
1:D:470:MET:SD	1:D:527:LEU:HD23	2.57	0.45
1:G:345:VAL:HG12	1:G:345:VAL:O	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:380:ARG:CB	1:G:423:TYR:CD1	3.00	0.45
2:H:82:LYS:HE3	2:H:83:ASP:OD2	2.16	0.45
3:I:95:PHE:CE1	11:I:303:LMT:H82	2.52	0.45
3:I:61:VAL:HA	3:I:64:LYS:HG3	1.98	0.45
1:J:112:LYS:NZ	1:J:130:ASP:HB3	2.32	0.45
1:J:281:ASP:CB	1:J:285:HIS:NE2	2.79	0.45
1:J:562:ASN:HA	1:J:583:LEU:CD1	2.47	0.45
1:J:562:ASN:HD22	1:J:562:ASN:N	2.03	0.45
1:J:613:GLN:O	1:J:616:ILE:HB	2.17	0.45
2:K:190:ARG:HB3	2:K:195:TYR:CE1	2.51	0.45
2:K:206:PHE:CE1	3:L:24:ALA:HB2	2.51	0.45
1:A:60:MET:HB2	1:A:147:TRP:HB2	1.99	0.45
1:A:278:ILE:HD12	1:A:286:ARG:NH1	2.29	0.45
1:A:562:ASN:H	1:A:562:ASN:ND2	2.12	0.45
1:A:617:ASP:HA	1:A:620:GLN:HB2	1.97	0.45
2:B:166:MET:HE2	3:C:107:GLN:HB3	1.98	0.45
2:B:190:ARG:HB3	2:B:195:TYR:CE1	2.51	0.45
2:B:226:SER:O	2:B:229:ALA:HB3	2.17	0.45
3:C:151:PRO:O	3:C:154:ILE:HG13	2.16	0.45
1:D:110:ILE:HA	1:D:137:HIS:CD2	2.51	0.45
1:D:492:LYS:HD3	1:D:492:LYS:O	2.15	0.45
2:E:190:ARG:HB3	2:E:195:TYR:CE1	2.51	0.45
2:E:213:ALA:HA	3:F:120:HIS:CE1	2.52	0.45
3:F:151:PRO:O	3:F:154:ILE:HG13	2.16	0.45
1:G:226:THR:OG1	1:G:368:GLN:NE2	2.49	0.45
1:G:281:ASP:CG	1:G:287:PHE:HB2	2.36	0.45
1:G:613:GLN:O	1:G:616:ILE:HB	2.17	0.45
1:G:93:ALA:N	1:G:94:PRO:CD	2.79	0.45
1:J:281:ASP:OD1	1:J:287:PHE:HB2	2.17	0.45
1:J:251:MET:HE1	1:J:529:VAL:HG13	1.98	0.45
2:K:122:ILE:HD13	2:K:188:ASP:HB2	1.99	0.45
2:K:232:ARG:HG2	3:L:194:TRP:CZ3	2.50	0.45
2:K:65:CYS:SG	2:K:65:CYS:O	2.75	0.45
2:K:82:LYS:HE3	2:K:83:ASP:OD2	2.16	0.45
1:A:110:ILE:HA	1:A:137:HIS:CD2	2.51	0.45
1:A:278:ILE:CD1	1:A:286:ARG:HH11	2.28	0.45
1:A:233:GLU:HB3	1:A:526:MET:HE3	1.98	0.45
1:A:562:ASN:HA	1:A:583:LEU:CD1	2.47	0.45
1:A:67:ASP:O	1:A:70:PHE:HB3	2.17	0.45
2:B:209:MET:O	2:B:211:LEU:HD23	2.17	0.45
3:C:95:PHE:CE1	11:C:303:LMT:H82	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:512:HIS:O	1:D:513:ALA:C	2.55	0.45
2:E:226:SER:O	2:E:229:ALA:HB3	2.17	0.45
1:G:288:MET:HA	1:G:296:LYS:HB3	1.99	0.45
1:G:348:ILE:O	1:G:352:PHE:HD1	2.00	0.45
1:G:427:HIS:O	1:G:431:THR:HG22	2.17	0.45
1:G:512:HIS:O	1:G:513:ALA:C	2.55	0.45
2:H:67:MET:CE	2:H:76:ALA:HB2	2.47	0.45
2:H:166:MET:HE2	3:I:107:GLN:HB3	1.99	0.45
1:J:345:VAL:HG12	1:J:345:VAL:O	2.17	0.45
1:J:467:LYS:HG3	1:J:468:ASN:N	2.31	0.45
2:K:213:ALA:HA	3:L:120:HIS:CE1	2.52	0.45
3:L:109:LEU:HD12	3:L:109:LEU:O	2.16	0.45
3:L:51:ILE:HG21	3:L:231:TYR:CE1	2.52	0.45
1:A:348:ILE:O	1:A:352:PHE:HD1	2.00	0.45
2:B:67:MET:CE	2:B:76:ALA:HB2	2.47	0.45
3:C:87:PHE:HA	3:C:144:LEU:HD13	1.99	0.45
3:C:161:PHE:CD1	3:C:245:TYR:HB2	2.52	0.45
3:C:248:PHE:O	3:C:254:HIS:ND1	2.49	0.45
3:C:98:MET:O	3:C:101:PHE:HB2	2.16	0.45
1:D:22:VAL:O	1:D:26:GLN:HG2	2.17	0.45
1:D:542:GLU:HG2	1:D:560:TRP:CD1	2.51	0.45
1:D:60:MET:HB2	1:D:147:TRP:HB2	1.99	0.45
2:E:122:ILE:HD13	2:E:188:ASP:HB2	1.99	0.45
2:E:209:MET:O	2:E:211:LEU:HD23	2.17	0.45
2:E:65:CYS:SG	2:E:65:CYS:O	2.75	0.45
3:F:61:VAL:HA	3:F:64:LYS:HG3	1.98	0.45
1:G:542:GLU:HG2	1:G:560:TRP:CD1	2.51	0.45
2:H:126:LYS:HE3	2:H:126:LYS:HB3	1.88	0.45
2:H:213:ALA:HA	3:I:120:HIS:CE1	2.52	0.45
3:I:142:VAL:CG2	3:I:143:HIS:N	2.66	0.45
3:I:160:SER:O	3:I:163:MET:HB3	2.17	0.45
3:I:36:PHE:HD2	3:I:89:VAL:CG1	2.25	0.45
1:J:9:LEU:CD2	1:J:10:VAL:H	2.28	0.45
1:J:512:HIS:O	1:J:513:ALA:C	2.55	0.45
2:K:158:ILE:CD1	2:K:172:GLY:HA3	2.47	0.45
1:A:111:HIS:CD2	1:A:133:HIS:HE1	2.35	0.45
1:A:356:ASP:HA	1:A:357:PRO:HD3	1.71	0.45
2:B:213:ALA:HA	3:C:120:HIS:CE1	2.52	0.45
2:B:65:CYS:SG	2:B:65:CYS:O	2.75	0.45
1:D:348:ILE:O	1:D:352:PHE:HD1	2.00	0.45
3:F:158:SER:H	3:F:254:HIS:CE1	2.35	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:PHE:CD1	3:F:245:TYR:HB2	2.52	0.45
1:G:118:ILE:HB	1:G:276:GLY:HA3	1.99	0.45
1:G:306:ARG:HB2	1:G:307:ARG:NH1	2.32	0.45
1:G:357:PRO:C	1:G:359:GLU:H	2.18	0.45
1:G:562:ASN:HA	1:G:583:LEU:CD1	2.47	0.45
1:G:84:LYS:HE2	1:G:639:PRO:O	2.17	0.45
3:I:25:LYS:O	3:I:29:TRP:HD1	2.00	0.45
3:I:51:ILE:HG21	3:I:231:TYR:CE1	2.52	0.45
1:J:110:ILE:HA	1:J:137:HIS:HD2	1.80	0.45
1:J:67:ASP:O	1:J:70:PHE:HB3	2.17	0.45
1:A:22:VAL:O	1:A:26:GLN:HG2	2.17	0.44
1:A:281:ASP:OD1	1:A:287:PHE:HB2	2.17	0.44
1:D:112:LYS:NZ	1:D:130:ASP:HB3	2.32	0.44
1:D:111:HIS:CD2	1:D:133:HIS:HE1	2.35	0.44
1:D:288:MET:HA	1:D:296:LYS:HB3	1.99	0.44
1:D:311:HIS:HA	1:D:314:LYS:HD3	1.99	0.44
1:D:542:GLU:OE1	1:D:544:ARG:NH1	2.50	0.44
1:D:98:ARG:NH2	2:E:133:LEU:CD1	2.81	0.44
2:E:147:GLU:HA	2:E:150:ARG:HD3	1.97	0.44
3:F:109:LEU:HD12	3:F:109:LEU:O	2.16	0.44
3:F:160:SER:O	3:F:163:MET:HB3	2.17	0.44
3:F:51:ILE:HG21	3:F:231:TYR:CE1	2.52	0.44
1:G:512:HIS:O	1:G:514:ASN:N	2.50	0.44
1:G:41:ARG:NH2	2:H:153:GLU:O	2.42	0.44
2:H:209:MET:O	2:H:211:LEU:HD23	2.16	0.44
3:I:72:GLU:HB3	3:I:73:GLY:H	1.47	0.44
1:J:118:ILE:HB	1:J:276:GLY:HA3	1.99	0.44
1:J:297:GLU:O	1:J:298:LEU:HB2	2.17	0.44
1:J:98:ARG:NH2	2:K:133:LEU:CD1	2.80	0.44
2:K:226:SER:O	2:K:229:ALA:HB3	2.17	0.44
2:K:67:MET:CE	2:K:76:ALA:HB2	2.47	0.44
3:L:25:LYS:O	3:L:29:TRP:HD1	2.00	0.44
3:L:61:VAL:HA	3:L:64:LYS:HG3	1.98	0.44
2:B:133:LEU:HD12	2:B:133:LEU:HA	1.84	0.44
2:B:7:ILE:HG22	2:B:9:VAL:HG23	1.99	0.44
3:C:158:SER:H	3:C:254:HIS:CE1	2.35	0.44
1:D:281:ASP:OD1	1:D:287:PHE:HB2	2.17	0.44
1:D:512:HIS:O	1:D:514:ASN:N	2.50	0.44
3:I:109:LEU:O	3:I:109:LEU:HD12	2.16	0.44
1:J:540:ARG:NH2	1:J:562:ASN:HD22	2.08	0.44
1:D:297:GLU:O	1:D:298:LEU:HB2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:ARG:HD3	2:E:181:ARG:C	2.38	0.44
2:E:46:THR:OG1	2:E:47:TYR:N	2.49	0.44
3:F:25:LYS:O	3:F:29:TRP:HD1	2.00	0.44
1:G:129:GLU:HG2	1:G:131:PHE:HE2	1.82	0.44
2:H:122:ILE:HD13	2:H:188:ASP:HB2	1.99	0.44
2:H:226:SER:O	2:H:229:ALA:HB3	2.17	0.44
3:I:158:SER:H	3:I:254:HIS:CE1	2.35	0.44
3:I:85:PHE:C	3:I:87:PHE:H	2.19	0.44
1:J:306:ARG:HB2	1:J:307:ARG:NH1	2.32	0.44
1:J:512:HIS:O	1:J:514:ASN:N	2.50	0.44
1:J:84:LYS:HE2	1:J:639:PRO:O	2.18	0.44
2:K:209:MET:O	2:K:211:LEU:HD23	2.17	0.44
2:K:7:ILE:HG22	2:K:9:VAL:HG23	1.99	0.44
1:A:288:MET:HA	1:A:296:LYS:HB3	1.99	0.44
1:A:490:ALA:C	1:A:492:LYS:H	2.21	0.44
1:A:470:MET:SD	1:A:527:LEU:HD23	2.57	0.44
1:D:118:ILE:HB	1:D:276:GLY:HA3	1.99	0.44
1:D:84:LYS:HE2	1:D:639:PRO:O	2.17	0.44
2:E:67:MET:CE	2:E:76:ALA:HB2	2.47	0.44
1:G:287:PHE:CA	1:G:290:ASP:HB3	2.48	0.44
1:G:67:ASP:O	1:G:70:PHE:HB3	2.17	0.44
2:H:158:ILE:CD1	2:H:172:GLY:HA3	2.47	0.44
3:I:232:VAL:O	3:I:236:LEU:HG	2.18	0.44
1:J:112:LYS:HZ2	1:J:130:ASP:HB3	1.83	0.44
1:J:111:HIS:CD2	1:J:133:HIS:HE1	2.35	0.44
1:J:147:TRP:N	1:J:147:TRP:CD1	2.86	0.44
3:L:160:SER:O	3:L:163:MET:HB3	2.17	0.44
1:A:118:ILE:HB	1:A:276:GLY:HA3	1.99	0.44
1:A:297:GLU:O	1:A:298:LEU:HB2	2.17	0.44
1:A:84:LYS:HE2	1:A:639:PRO:O	2.17	0.44
3:C:63:LYS:O	3:C:66:GLN:N	2.45	0.44
1:D:562:ASN:HA	1:D:583:LEU:CD1	2.47	0.44
2:E:158:ILE:CD1	2:E:172:GLY:HA3	2.47	0.44
1:G:111:HIS:CD2	1:G:133:HIS:HE1	2.35	0.44
1:G:281:ASP:OD1	1:G:287:PHE:HB2	2.17	0.44
1:G:311:HIS:HA	1:G:314:LYS:HD3	1.99	0.44
1:G:467:LYS:HG3	1:G:468:ASN:N	2.31	0.44
1:G:470:MET:SD	1:G:527:LEU:HD23	2.57	0.44
1:J:542:GLU:OE1	1:J:544:ARG:NH1	2.50	0.44
2:K:181:ARG:C	2:K:181:ARG:HD3	2.38	0.44
1:A:542:GLU:OE1	1:A:544:ARG:NH1	2.50	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:LYS:O	3:C:29:TRP:HD1	2.00	0.44
1:D:278:ILE:HD12	1:D:286:ARG:HD3	2.00	0.44
3:F:40:PHE:HE1	3:F:86:VAL:HG21	1.81	0.44
1:G:542:GLU:OE1	1:G:544:ARG:NH1	2.50	0.44
1:J:287:PHE:CA	1:J:290:ASP:HB3	2.48	0.44
3:L:158:SER:H	3:L:254:HIS:CE1	2.35	0.44
3:L:126:TRP:HE1	10:L:302:HEM:HBA1	1.83	0.44
1:A:287:PHE:CA	1:A:290:ASP:HB3	2.48	0.44
1:A:427:HIS:O	1:A:431:THR:HG22	2.17	0.44
3:C:232:VAL:O	3:C:236:LEU:HG	2.18	0.44
1:D:467:LYS:HG3	1:D:468:ASN:N	2.31	0.44
1:D:490:ALA:C	1:D:492:LYS:H	2.20	0.44
1:G:60:MET:HB2	1:G:147:TRP:HB2	1.99	0.44
1:G:98:ARG:NH2	2:H:133:LEU:CD1	2.81	0.44
1:J:380:ARG:CB	1:J:423:TYR:CD1	3.00	0.44
1:A:606:ASN:HB3	1:A:609:SER:OG	2.18	0.44
2:B:158:ILE:CD1	2:B:172:GLY:HA3	2.47	0.44
2:B:181:ARG:HD3	2:B:181:ARG:C	2.38	0.44
1:G:22:VAL:O	1:G:26:GLN:HG2	2.17	0.44
3:I:87:PHE:HA	3:I:144:LEU:HD13	1.99	0.44
3:I:40:PHE:HE1	3:I:86:VAL:HG21	1.81	0.44
1:J:348:ILE:O	1:J:352:PHE:HD1	2.00	0.44
1:J:470:MET:SD	1:J:527:LEU:HD23	2.57	0.44
1:J:606:ASN:HB3	1:J:609:SER:OG	2.18	0.44
2:K:46:THR:OG1	2:K:47:TYR:N	2.49	0.44
1:A:129:GLU:HG2	1:A:131:PHE:HE2	1.82	0.44
2:B:110:TRP:HZ3	2:B:111:PHE:CE2	2.36	0.44
2:E:40:LEU:HD22	2:E:53:PHE:CD2	2.53	0.44
3:F:126:TRP:HE1	10:F:302:HEM:HBA1	1.83	0.44
1:G:238:ALA:HB1	1:G:525:MET:HB3	2.00	0.44
2:H:65:CYS:O	2:H:65:CYS:SG	2.75	0.44
1:J:376:ARG:NH2	1:J:563:ARG:NH1	2.66	0.44
1:J:562:ASN:ND2	1:J:562:ASN:N	2.66	0.44
1:A:278:ILE:HB	1:A:288:MET:HE3	2.00	0.43
1:A:278:ILE:HD12	1:A:286:ARG:HD3	2.00	0.43
1:A:306:ARG:HB2	1:A:307:ARG:NH1	2.32	0.43
1:A:374:GLY:O	1:A:375:ILE:C	2.57	0.43
1:A:512:HIS:O	1:A:514:ASN:N	2.50	0.43
1:D:238:ALA:HB1	1:D:525:MET:HB3	2.00	0.43
3:F:112:LYS:O	3:F:113:THR:C	2.56	0.43
1:G:297:GLU:O	1:G:298:LEU:HB2	2.17	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:551:ASP:N	1:G:551:ASP:OD1	2.51	0.43
1:G:376:ARG:NH2	1:G:563:ARG:NH1	2.66	0.43
3:I:64:LYS:HE2	3:I:64:LYS:HB3	1.79	0.43
3:I:75:LYS:CA	3:I:75:LYS:HE2	2.48	0.43
2:K:110:TRP:HZ3	2:K:111:PHE:CE2	2.36	0.43
1:A:562:ASN:ND2	1:A:562:ASN:N	2.66	0.43
1:D:306:ARG:HB2	1:D:307:ARG:NH1	2.32	0.43
1:D:67:ASP:O	1:D:70:PHE:HB3	2.17	0.43
3:F:87:PHE:HA	3:F:144:LEU:HD13	1.99	0.43
1:G:147:TRP:CD1	1:G:147:TRP:N	2.86	0.43
1:G:484:GLY:HA2	1:G:549:ARG:HH12	1.83	0.43
1:G:490:ALA:C	1:G:492:LYS:H	2.20	0.43
1:G:606:ASN:HB3	1:G:609:SER:OG	2.18	0.43
3:I:13:VAL:CG2	3:I:18:LYS:N	2.79	0.43
3:L:232:VAL:O	3:L:236:LEU:HG	2.18	0.43
3:F:221:ILE:HA	3:F:221:ILE:HD13	1.90	0.43
1:J:490:ALA:C	1:J:492:LYS:H	2.20	0.43
2:K:179:VAL:HG11	2:K:199:ILE:HD11	2.01	0.43
3:L:40:PHE:HE1	3:L:86:VAL:HG21	1.81	0.43
1:A:250:ASN:OD1	1:A:563:ARG:HG3	2.18	0.43
2:B:179:VAL:HG11	2:B:199:ILE:HD11	2.01	0.43
2:B:40:LEU:HD22	2:B:53:PHE:CD2	2.53	0.43
1:D:147:TRP:N	1:D:147:TRP:CD1	2.86	0.43
1:D:164:VAL:O	1:D:167:GLU:HB2	2.19	0.43
1:D:250:ASN:OD1	1:D:563:ARG:HG3	2.19	0.43
3:F:118:MET:O	3:F:119:ARG:HB2	2.18	0.43
1:G:356:ASP:HA	1:G:357:PRO:HD3	1.71	0.43
2:H:40:LEU:HD22	2:H:53:PHE:CD2	2.53	0.43
3:I:221:ILE:HA	3:I:221:ILE:HD13	1.90	0.43
1:J:188:ASP:O	1:J:190:LYS:HG3	2.19	0.43
1:J:278:ILE:HD12	1:J:286:ARG:HD3	2.00	0.43
2:K:40:LEU:HD22	2:K:53:PHE:CD2	2.53	0.43
3:L:87:PHE:HA	3:L:144:LEU:HD13	1.99	0.43
1:A:9:LEU:CD2	1:A:10:VAL:H	2.28	0.43
1:A:41:ARG:HH11	1:A:41:ARG:CG	2.29	0.43
1:A:99:GLU:OE1	1:A:418:MET:HE3	2.18	0.43
1:D:356:ASP:HA	1:D:357:PRO:HD3	1.71	0.43
1:G:2:LYS:HB2	1:G:2:LYS:HZ3	1.82	0.43
1:G:562:ASN:H	1:G:562:ASN:ND2	2.12	0.43
3:I:126:TRP:HE1	10:I:301:HEM:HBA1	1.83	0.43
3:L:112:LYS:O	3:L:113:THR:C	2.56	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:189:ARG:NH1	3:C:189:ARG:HG3	2.26	0.43
1:D:288:MET:C	1:D:290:ASP:N	2.72	0.43
1:D:376:ARG:NH2	1:D:563:ARG:NH1	2.66	0.43
1:D:594:TYR:CE1	1:D:600:LYS:HG2	2.54	0.43
2:E:110:TRP:HZ3	2:E:111:PHE:CE2	2.36	0.43
1:G:188:ASP:O	1:G:190:LYS:HG3	2.19	0.43
1:G:278:ILE:HD12	1:G:286:ARG:HD3	2.00	0.43
1:G:415:VAL:O	1:G:418:MET:N	2.52	0.43
1:G:594:TYR:CE1	1:G:600:LYS:HG2	2.54	0.43
2:H:179:VAL:HG11	2:H:199:ILE:HD11	2.01	0.43
2:H:181:ARG:HD3	2:H:181:ARG:C	2.38	0.43
1:J:288:MET:HA	1:J:296:LYS:HB3	1.99	0.43
1:J:464:PHE:HE2	1:J:519:GLU:HG3	1.84	0.43
2:K:213:ALA:N	8:K:302:F3S:S4	2.91	0.43
1:A:164:VAL:O	1:A:167:GLU:HB2	2.19	0.43
1:A:238:ALA:HB1	1:A:525:MET:HB3	2.00	0.43
1:A:419:ILE:C	1:A:421:GLY:N	2.72	0.43
1:A:515:PRO:O	1:A:518:GLU:HB2	2.19	0.43
1:A:464:PHE:HE2	1:A:519:GLU:HG3	1.84	0.43
1:A:41:ARG:NH2	2:B:153:GLU:O	2.42	0.43
1:D:286:ARG:HD2	1:D:288:MET:HE2	1.99	0.43
1:D:562:ASN:N	1:D:562:ASN:ND2	2.66	0.43
1:G:164:VAL:O	1:G:167:GLU:HB2	2.19	0.43
1:G:419:ILE:C	1:G:421:GLY:N	2.72	0.43
1:J:515:PRO:O	1:J:518:GLU:HB2	2.19	0.43
1:J:562:ASN:H	1:J:562:ASN:ND2	2.12	0.43
2:K:176:LEU:HD13	2:K:228:ILE:HG23	2.01	0.43
3:L:118:MET:O	3:L:119:ARG:HB2	2.18	0.43
1:A:376:ARG:NH2	1:A:563:ARG:NH1	2.66	0.43
1:D:515:PRO:O	1:D:518:GLU:HB2	2.19	0.43
1:D:484:GLY:HA2	1:D:549:ARG:HH12	1.83	0.43
1:G:374:GLY:O	1:G:375:ILE:C	2.57	0.43
2:H:110:TRP:HZ3	2:H:111:PHE:CE2	2.36	0.43
3:I:112:LYS:O	3:I:113:THR:C	2.56	0.43
3:I:118:MET:O	3:I:119:ARG:HB2	2.18	0.43
1:J:287:PHE:O	1:J:290:ASP:HB3	2.19	0.43
1:J:531:LEU:O	1:J:535:LYS:HB3	2.19	0.43
1:A:288:MET:O	1:A:290:ASP:N	2.48	0.43
1:A:29:LEU:O	1:A:31:THR:HG23	2.19	0.43
1:A:594:TYR:CE1	1:A:600:LYS:HG2	2.54	0.43
1:A:98:ARG:NH2	2:B:133:LEU:CD1	2.81	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ARG:NH1	2:B:167:ARG:CG	2.82	0.43
3:C:69:PHE:CD1	3:C:70:ILE:HG13	2.40	0.43
1:D:374:GLY:O	1:D:375:ILE:C	2.57	0.43
1:D:531:LEU:O	1:D:535:LYS:HB3	2.19	0.43
1:D:551:ASP:OD1	1:D:551:ASP:N	2.51	0.43
1:D:591:ALA:HA	1:D:592:PRO:HD3	1.83	0.43
2:E:179:VAL:HG11	2:E:199:ILE:HD11	2.01	0.43
2:E:1:MET:HE2	2:E:31:ALA:HA	1.99	0.43
1:J:611:LYS:HE2	1:J:611:LYS:HB3	1.84	0.43
3:C:112:LYS:O	3:C:113:THR:C	2.56	0.43
1:D:464:PHE:HE2	1:D:519:GLU:HG3	1.84	0.43
1:G:251:MET:HE1	1:G:529:VAL:HG13	2.00	0.43
1:G:250:ASN:OD1	1:G:563:ARG:HG3	2.18	0.43
1:G:611:LYS:HB3	1:G:611:LYS:HE2	1.84	0.43
3:I:104:ASN:OD1	3:I:107:GLN:HB2	2.19	0.43
3:I:171:LEU:HB2	3:L:145:TYR:OH	2.18	0.43
3:C:253:THR:CG2	3:C:254:HIS:H	2.20	0.42
2:E:191:THR:O	2:E:195:TYR:CD1	2.72	0.42
3:F:253:THR:CG2	3:F:254:HIS:H	2.20	0.42
3:I:63:LYS:O	3:I:66:GLN:N	2.45	0.42
1:A:484:GLY:HA2	1:A:549:ARG:HH12	1.83	0.42
2:E:176:LEU:HD13	2:E:228:ILE:HG23	2.01	0.42
1:G:531:LEU:O	1:G:535:LYS:HB3	2.19	0.42
1:G:562:ASN:ND2	1:G:562:ASN:N	2.66	0.42
3:I:13:VAL:HG22	3:I:18:LYS:H	1.79	0.42
1:J:328:LEU:O	1:J:361:TRP:HA	2.20	0.42
1:A:147:TRP:CD1	1:A:147:TRP:N	2.86	0.42
1:D:6:CYS:O	1:D:209:ALA:CB	2.68	0.42
2:E:20:LYS:HA	2:E:21:PRO:HD3	1.93	0.42
3:F:104:ASN:OD1	3:F:107:GLN:HB2	2.19	0.42
3:F:75:LYS:HE2	3:F:75:LYS:CA	2.48	0.42
2:H:176:LEU:HD13	2:H:228:ILE:HG23	2.01	0.42
1:J:338:ILE:HD13	1:J:358:ALA:HA	2.02	0.42
1:J:250:ASN:OD1	1:J:563:ARG:HG3	2.18	0.42
2:K:191:THR:O	2:K:195:TYR:CD1	2.72	0.42
3:L:104:ASN:OD1	3:L:107:GLN:HB2	2.19	0.42
1:A:551:ASP:OD1	1:A:551:ASP:N	2.51	0.42
3:C:118:MET:O	3:C:119:ARG:HB2	2.18	0.42
3:F:189:ARG:NH1	3:F:189:ARG:HG3	2.26	0.42
3:F:232:VAL:O	3:F:236:LEU:HG	2.18	0.42
1:G:270:GLU:C	1:G:272:CYS:N	2.73	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:338:ILE:HD13	1:G:358:ALA:HA	2.01	0.42
1:J:164:VAL:O	1:J:167:GLU:HB2	2.19	0.42
1:J:238:ALA:HB1	1:J:525:MET:HB3	2.00	0.42
1:J:225:ASN:HB3	1:J:367:MET:HG2	2.01	0.42
1:J:478:VAL:CG1	1:J:482:ARG:HE	2.33	0.42
1:A:188:ASP:O	1:A:190:LYS:HG3	2.19	0.42
2:B:176:LEU:HD13	2:B:228:ILE:HG23	2.01	0.42
1:D:287:PHE:CA	1:D:290:ASP:HB3	2.48	0.42
1:D:2:LYS:HB2	1:D:2:LYS:HZ2	1.80	0.42
1:D:606:ASN:HB3	1:D:609:SER:OG	2.18	0.42
2:E:199:ILE:O	2:E:205:VAL:HG12	2.20	0.42
2:E:213:ALA:N	8:E:302:F3S:S4	2.91	0.42
3:F:72:GLU:HB3	3:F:73:GLY:H	1.47	0.42
1:G:515:PRO:O	1:G:518:GLU:HB2	2.19	0.42
2:H:199:ILE:O	2:H:205:VAL:HG12	2.20	0.42
3:I:29:TRP:HA	3:I:32:ALA:CB	2.45	0.42
1:J:126:ILE:CG2	1:J:127:THR:N	2.83	0.42
1:J:484:GLY:HA2	1:J:549:ARG:HH12	1.83	0.42
1:J:594:TYR:CE1	1:J:600:LYS:HG2	2.54	0.42
2:K:129:ASP:OD1	2:K:131:SER:HB3	2.20	0.42
3:L:75:LYS:CA	3:L:75:LYS:HE2	2.48	0.42
3:C:75:LYS:CA	3:C:75:LYS:HE2	2.48	0.42
3:I:209:LEU:HD23	3:I:209:LEU:HA	1.92	0.42
2:K:199:ILE:O	2:K:205:VAL:HG12	2.20	0.42
1:A:126:ILE:CG2	1:A:127:THR:N	2.83	0.42
3:C:104:ASN:OD1	3:C:107:GLN:HB2	2.19	0.42
3:C:13:VAL:CG2	3:C:18:LYS:N	2.79	0.42
3:C:21:ARG:N	3:C:21:ARG:HD2	2.35	0.42
1:D:126:ILE:CG2	1:D:127:THR:N	2.83	0.42
1:D:287:PHE:O	1:D:290:ASP:HB3	2.19	0.42
1:D:420:VAL:HG12	1:D:420:VAL:O	2.19	0.42
2:E:188:ASP:OD1	2:E:190:ARG:HB2	2.20	0.42
1:J:6:CYS:O	1:J:209:ALA:CB	2.68	0.42
1:J:228:ASN:HD22	1:J:228:ASN:N	2.17	0.42
1:A:316:LYS:CE	1:A:316:LYS:HA	2.49	0.42
1:A:531:LEU:O	1:A:535:LYS:HB3	2.19	0.42
3:C:103:ILE:O	3:C:104:ASN:CB	2.67	0.42
3:F:21:ARG:HD2	3:F:21:ARG:N	2.35	0.42
3:F:69:PHE:C	3:F:70:ILE:HG13	2.40	0.42
1:G:287:PHE:O	1:G:290:ASP:HB3	2.19	0.42
1:G:225:ASN:HB3	1:G:367:MET:HG2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:490:ALA:O	1:G:492:LYS:N	2.53	0.42
2:H:197:GLU:HA	3:I:19:LYS:HD3	2.02	0.42
3:I:21:ARG:HD2	3:I:21:ARG:N	2.35	0.42
1:J:316:LYS:HA	1:J:316:LYS:CE	2.49	0.42
1:J:420:VAL:HG12	1:J:420:VAL:O	2.19	0.42
2:K:67:MET:HA	2:K:94:LEU:HD23	2.02	0.42
1:A:225:ASN:HB3	1:A:367:MET:HG2	2.01	0.42
1:A:490:ALA:O	1:A:492:LYS:N	2.53	0.42
1:A:83:GLN:HE21	1:A:588:MET:CB	2.26	0.42
2:B:164:LYS:HD3	2:B:164:LYS:O	2.20	0.42
1:D:29:LEU:O	1:D:31:THR:HG23	2.19	0.42
1:D:562:ASN:H	1:D:562:ASN:ND2	2.12	0.42
1:D:60:MET:C	1:D:62:ASP:N	2.73	0.42
2:E:197:GLU:HA	3:F:19:LYS:HD3	2.02	0.42
1:G:141:PHE:HZ	5:G:702:MLA:C2	2.31	0.42
1:G:41:ARG:HG2	1:G:41:ARG:NH1	2.33	0.42
1:G:591:ALA:HA	1:G:592:PRO:HD3	1.83	0.42
2:H:123:HIS:HD2	2:H:190:ARG:CZ	2.32	0.42
1:J:374:GLY:O	1:J:375:ILE:C	2.57	0.42
1:A:270:GLU:C	1:A:272:CYS:N	2.73	0.42
1:A:287:PHE:O	1:A:290:ASP:HB3	2.19	0.42
1:A:478:VAL:CG1	1:A:482:ARG:HE	2.33	0.42
1:A:6:CYS:O	1:A:209:ALA:CB	2.68	0.42
3:F:44:HIS:CE1	10:F:303:HEM:ND	2.88	0.42
1:G:328:LEU:O	1:G:361:TRP:HA	2.19	0.42
3:I:103:ILE:O	3:I:104:ASN:CB	2.67	0.42
3:I:216:MET:O	3:I:220:LEU:HG	2.20	0.42
3:I:69:PHE:C	3:I:70:ILE:HG13	2.40	0.42
1:J:225:ASN:CB	1:J:367:MET:HE2	2.43	0.42
3:L:253:THR:HG22	3:L:254:HIS:N	2.21	0.42
1:A:380:ARG:HA	1:A:423:TYR:CD1	2.55	0.41
1:D:188:ASP:O	1:D:190:LYS:HG3	2.19	0.41
1:D:490:ALA:O	1:D:492:LYS:N	2.53	0.41
2:E:150:ARG:O	2:E:151:CYS:C	2.59	0.41
3:F:216:MET:O	3:F:220:LEU:HG	2.20	0.41
3:F:63:LYS:O	3:F:66:GLN:N	2.45	0.41
1:G:41:ARG:CG	1:G:41:ARG:HH11	2.29	0.41
1:G:420:VAL:HG12	1:G:420:VAL:O	2.20	0.41
1:G:464:PHE:HE2	1:G:519:GLU:HG3	1.84	0.41
2:H:188:ASP:OD1	2:H:190:ARG:HB2	2.20	0.41
1:J:164:VAL:O	1:J:167:GLU:N	2.53	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:380:ARG:HA	1:J:423:TYR:CD1	2.55	0.41
1:J:551:ASP:N	1:J:551:ASP:OD1	2.51	0.41
4:J:701:FAD:H1'1	4:J:701:FAD:H9	1.63	0.41
2:K:188:ASP:OD1	2:K:190:ARG:HB2	2.20	0.41
1:A:306:ARG:HG2	1:A:481:PHE:CZ	2.55	0.41
1:D:228:ASN:HD22	1:D:228:ASN:N	2.17	0.41
2:E:129:ASP:OD1	2:E:131:SER:HB3	2.20	0.41
3:F:136:MET:HE2	3:F:179:VAL:N	2.35	0.41
3:F:29:TRP:HA	3:F:32:ALA:CB	2.45	0.41
1:G:251:MET:O	1:G:533:VAL:HG13	2.21	0.41
1:G:29:LEU:O	1:G:31:THR:HG23	2.19	0.41
1:G:633:ILE:O	1:G:636:ALA:HB3	2.20	0.41
1:G:6:CYS:O	1:G:209:ALA:CB	2.68	0.41
2:H:191:THR:O	2:H:195:TYR:CD1	2.72	0.41
2:H:213:ALA:N	8:H:302:F3S:S4	2.91	0.41
1:J:29:LEU:O	1:J:31:THR:HG23	2.19	0.41
3:L:21:ARG:HD2	3:L:21:ARG:N	2.35	0.41
1:A:338:ILE:HD13	1:A:358:ALA:HA	2.01	0.41
2:B:129:ASP:OD1	2:B:131:SER:HB3	2.20	0.41
2:B:150:ARG:O	2:B:151:CYS:C	2.59	0.41
2:B:209:MET:O	2:B:210:THR:C	2.59	0.41
3:C:216:MET:O	3:C:220:LEU:HG	2.20	0.41
1:D:222:ILE:HG13	1:D:223:TYR:CD1	2.56	0.41
1:D:338:ILE:HD13	1:D:358:ALA:HA	2.01	0.41
1:D:419:ILE:C	1:D:421:GLY:N	2.72	0.41
1:D:531:LEU:HD13	1:D:574:THR:O	2.21	0.41
1:D:423:TYR:CZ	1:D:643:PRO:HG3	2.55	0.41
1:G:164:VAL:O	1:G:167:GLU:N	2.53	0.41
1:G:281:ASP:HB3	1:G:282:VAL:H	1.74	0.41
1:G:303:VAL:CG1	1:G:304:VAL:N	2.80	0.41
3:I:44:HIS:CE1	10:I:302:HEM:ND	2.88	0.41
1:J:306:ARG:HG2	1:J:481:PHE:CZ	2.55	0.41
1:J:347:GLU:O	1:J:351:TYR:HD1	2.03	0.41
1:J:490:ALA:O	1:J:492:LYS:N	2.53	0.41
3:L:69:PHE:C	3:L:70:ILE:HG13	2.40	0.41
3:L:72:GLU:HB3	3:L:73:GLY:H	1.47	0.41
1:A:420:VAL:O	1:A:420:VAL:HG12	2.20	0.41
2:B:191:THR:O	2:B:195:TYR:CD1	2.72	0.41
3:C:44:HIS:CE1	10:C:302:HEM:ND	2.88	0.41
1:D:164:VAL:O	1:D:167:GLU:N	2.53	0.41
3:F:175:LEU:HG	10:F:303:HEM:HMD2	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:ILE:CG2	1:G:127:THR:N	2.83	0.41
1:G:216:THR:CB	1:G:236:GLY:HA3	2.51	0.41
1:G:478:VAL:CG1	1:G:482:ARG:HE	2.33	0.41
2:H:167:ARG:NH1	2:H:167:ARG:CG	2.82	0.41
3:L:175:LEU:HG	10:L:303:HEM:HMD2	2.01	0.41
1:A:164:VAL:O	1:A:167:GLU:N	2.53	0.41
1:A:375:ILE:O	1:A:395:ALA:HB1	2.21	0.41
1:A:423:TYR:CZ	1:A:643:PRO:HG3	2.55	0.41
1:A:433:VAL:CG1	1:A:434:ASP:N	2.84	0.41
1:A:506:ILE:HG22	1:A:516:GLU:HG2	2.03	0.41
1:A:5:TYR:CG	1:A:6:CYS:N	2.89	0.41
2:B:188:ASP:OD1	2:B:190:ARG:HB2	2.20	0.41
3:C:126:TRP:HE1	10:C:301:HEM:HBA1	1.83	0.41
1:D:225:ASN:HB3	1:D:367:MET:HG2	2.01	0.41
1:D:415:VAL:O	1:D:418:MET:N	2.52	0.41
4:D:701:FAD:H1'1	4:D:701:FAD:H9	1.63	0.41
2:E:67:MET:HA	2:E:94:LEU:HD23	2.02	0.41
3:F:253:THR:HG22	3:F:254:HIS:N	2.20	0.41
1:G:506:ILE:HG22	1:G:516:GLU:HG2	2.03	0.41
1:J:270:GLU:C	1:J:272:CYS:N	2.73	0.41
1:J:506:ILE:HG22	1:J:516:GLU:HG2	2.03	0.41
3:L:22:MET:HB2	3:L:23:PRO:HD3	2.02	0.41
1:A:222:ILE:HG13	1:A:223:TYR:CD1	2.56	0.41
1:A:228:ASN:N	1:A:228:ASN:HD22	2.17	0.41
1:A:408:ASN:HA	1:A:408:ASN:HD22	1.65	0.41
1:A:419:ILE:O	1:A:421:GLY:N	2.54	0.41
1:A:251:MET:O	1:A:533:VAL:HG13	2.21	0.41
1:D:380:ARG:HA	1:D:423:TYR:CD1	2.55	0.41
1:D:41:ARG:NH1	1:D:41:ARG:CG	2.83	0.41
1:D:486:HIS:N	1:D:486:HIS:CD2	2.88	0.41
3:F:22:MET:HB2	3:F:23:PRO:HD3	2.03	0.41
1:G:222:ILE:HG13	1:G:223:TYR:CD1	2.56	0.41
1:G:419:ILE:O	1:G:421:GLY:N	2.54	0.41
1:G:306:ARG:HG2	1:G:481:PHE:CZ	2.55	0.41
1:G:423:TYR:CZ	1:G:643:PRO:HG3	2.55	0.41
2:H:24:GLN:HG2	2:H:26:TYR:CZ	2.56	0.41
2:K:150:ARG:O	2:K:151:CYS:C	2.59	0.41
2:K:209:MET:O	2:K:210:THR:C	2.59	0.41
3:L:136:MET:HE2	3:L:179:VAL:N	2.35	0.41
3:L:44:HIS:CE1	10:L:303:HEM:ND	2.88	0.41
2:B:199:ILE:O	2:B:205:VAL:HG12	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:LEU:HG	10:C:302:HEM:HMD2	2.02	0.41
1:D:3:VAL:HG22	1:D:206:ALA:HB3	2.02	0.41
2:E:123:HIS:HD2	2:E:190:ARG:CZ	2.32	0.41
2:E:24:GLN:HG2	2:E:26:TYR:CZ	2.56	0.41
3:F:22:MET:CB	3:F:23:PRO:HD3	2.51	0.41
2:H:129:ASP:OD1	2:H:131:SER:HB3	2.20	0.41
1:G:111:HIS:HD2	2:H:139:PRO:CG	2.34	0.41
1:J:222:ILE:HG13	1:J:223:TYR:CD1	2.56	0.41
1:J:375:ILE:O	1:J:395:ALA:HB1	2.21	0.41
1:J:39:VAL:O	1:J:41:ARG:N	2.54	0.41
1:G:210:LYS:NZ	1:J:441:GLU:OE2	2.52	0.41
1:J:423:TYR:CZ	1:J:643:PRO:HG3	2.55	0.41
1:J:64:ASP:OD1	1:J:148:ARG:HB3	2.21	0.41
3:L:22:MET:CB	3:L:23:PRO:HD3	2.51	0.41
1:A:328:LEU:O	1:A:361:TRP:HA	2.20	0.41
1:A:3:VAL:HG22	1:A:206:ALA:HB3	2.02	0.41
1:A:415:VAL:O	1:A:418:MET:N	2.52	0.41
1:A:60:MET:C	1:A:62:ASP:H	2.24	0.41
1:D:216:THR:CB	1:D:236:GLY:HA3	2.51	0.41
1:D:375:ILE:O	1:D:395:ALA:HB1	2.21	0.41
1:D:433:VAL:CG1	1:D:434:ASP:N	2.84	0.41
3:I:253:THR:CG2	3:I:254:HIS:H	2.20	0.41
1:J:3:VAL:HG22	1:J:206:ALA:HB3	2.03	0.41
1:J:39:VAL:C	1:J:41:ARG:H	2.24	0.41
1:J:463:VAL:O	1:J:467:LYS:HB3	2.21	0.41
1:A:107:TRP:HA	1:A:152:THR:CG2	2.38	0.41
1:A:216:THR:CB	1:A:236:GLY:HA3	2.51	0.41
1:A:41:ARG:NH1	1:A:41:ARG:CG	2.83	0.41
1:D:141:PHE:CE1	1:D:270:GLU:HB3	2.56	0.41
1:D:478:VAL:CG1	1:D:482:ARG:HE	2.33	0.41
1:G:288:MET:C	1:G:290:ASP:N	2.71	0.41
1:G:3:VAL:HG22	1:G:206:ALA:HB3	2.03	0.41
1:G:39:VAL:C	1:G:41:ARG:H	2.24	0.41
1:G:433:VAL:CG1	1:G:434:ASP:N	2.84	0.41
1:G:644:ALA:HA	1:G:647:LYS:HG3	2.03	0.41
2:H:206:PHE:HE1	3:I:24:ALA:HB2	1.86	0.41
1:J:141:PHE:CE1	1:J:270:GLU:HB3	2.56	0.41
1:J:415:VAL:O	1:J:418:MET:N	2.52	0.41
1:J:589:GLU:C	1:J:590:ILE:HG13	2.41	0.41
2:K:141:VAL:C	2:K:143:GLN:N	2.75	0.41
2:K:197:GLU:HA	3:L:19:LYS:HD3	2.02	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:HIS:HD2	2:B:139:PRO:CG	2.34	0.41
1:A:531:LEU:HD13	1:A:574:THR:O	2.21	0.41
1:A:60:MET:C	1:A:62:ASP:N	2.73	0.41
3:C:64:LYS:HE2	3:C:64:LYS:HB3	1.79	0.41
3:C:69:PHE:C	3:C:70:ILE:HG13	2.40	0.41
1:D:347:GLU:O	1:D:351:TYR:HD1	2.03	0.41
1:D:463:VAL:O	1:D:467:LYS:HB3	2.21	0.41
1:D:611:LYS:HB3	1:D:611:LYS:HE2	1.84	0.41
1:D:64:ASP:OD1	1:D:148:ARG:HB3	2.21	0.41
2:E:141:VAL:C	2:E:143:GLN:H	2.25	0.41
3:F:93:HIS:CD2	10:F:302:HEM:NB	2.89	0.41
1:G:265:GLY:HA3	1:G:367:MET:HE1	2.03	0.41
1:G:380:ARG:HA	1:G:423:TYR:CD1	2.56	0.41
1:G:41:ARG:CG	1:G:41:ARG:NH1	2.83	0.41
1:G:463:VAL:O	1:G:467:LYS:HB3	2.21	0.41
1:J:216:THR:CB	1:J:236:GLY:HA3	2.51	0.41
1:J:542:GLU:HG2	1:J:560:TRP:CG	2.56	0.41
1:A:349:CYS:CB	1:A:357:PRO:HG3	2.51	0.41
1:A:589:GLU:C	1:A:590:ILE:HG13	2.41	0.41
1:A:64:ASP:OD1	1:A:148:ARG:HB3	2.21	0.41
2:B:148:LEU:HD22	2:B:177:ASN:OD1	2.21	0.41
2:B:192:ASP:OD2	2:B:234:LYS:HE2	2.21	0.41
2:B:24:GLN:HG2	2:B:26:TYR:CZ	2.56	0.41
2:B:213:ALA:N	8:B:302:F3S:S4	2.91	0.41
3:C:1:MET:HB3	3:F:112:LYS:NZ	2.35	0.41
1:D:328:LEU:O	1:D:361:TRP:HA	2.20	0.41
1:D:306:ARG:HG2	1:D:481:PHE:CZ	2.55	0.41
1:D:542:GLU:HG2	1:D:560:TRP:CG	2.56	0.41
1:D:87:ARG:HD2	1:D:640:TYR:CD2	2.56	0.41
2:E:164:LYS:HD3	2:E:164:LYS:O	2.20	0.41
2:E:192:ASP:OD2	2:E:234:LYS:HE2	2.21	0.41
3:F:19:LYS:O	3:F:20:SER:C	2.60	0.41
1:G:64:ASP:OD1	1:G:148:ARG:HB3	2.21	0.41
1:G:392:GLY:O	1:G:393:GLU:C	2.60	0.41
1:G:589:GLU:C	1:G:590:ILE:HG13	2.41	0.41
1:J:120:ASN:CG	1:J:121:ALA:H	2.25	0.41
1:J:251:MET:O	1:J:533:VAL:HG13	2.21	0.41
1:J:419:ILE:C	1:J:421:GLY:N	2.72	0.41
1:J:644:ALA:HA	1:J:647:LYS:HG3	2.03	0.41
1:A:262:PHE:H	1:A:364:VAL:HA	1.86	0.40
1:A:347:GLU:O	1:A:351:TYR:HD1	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:ILE:O	1:A:636:ALA:HB3	2.20	0.40
2:B:93:PRO:HB3	2:B:103:LEU:HA	2.03	0.40
3:C:19:LYS:O	3:C:20:SER:C	2.60	0.40
3:C:3:ASN:HD21	2:E:8:ARG:HH12	1.69	0.40
3:C:71:PHE:HB3	3:C:75:LYS:CG	2.51	0.40
1:D:118:ILE:CD1	1:D:123:LYS:HE3	2.41	0.40
1:D:282:VAL:HG13	1:D:318:VAL:HB	2.03	0.40
2:E:141:VAL:C	2:E:143:GLN:N	2.74	0.40
3:F:142:VAL:CG2	3:F:143:HIS:N	2.66	0.40
1:G:228:ASN:N	1:G:228:ASN:HD22	2.17	0.40
1:G:141:PHE:CE1	1:G:270:GLU:HB3	2.56	0.40
1:G:278:ILE:HG22	1:G:297:GLU:HG3	2.03	0.40
1:G:542:GLU:HG2	1:G:560:TRP:CG	2.56	0.40
1:G:60:MET:C	1:G:62:ASP:N	2.73	0.40
2:H:93:PRO:HB3	2:H:103:LEU:HA	2.03	0.40
3:I:26:LEU:HB3	3:I:99:ARG:HH12	1.86	0.40
1:J:333:LEU:O	1:J:337:HIS:HB2	2.21	0.40
1:J:392:GLY:O	1:J:393:GLU:C	2.59	0.40
1:J:99:GLU:OE1	1:J:418:MET:HE3	2.21	0.40
2:K:164:LYS:HD3	2:K:164:LYS:O	2.20	0.40
1:A:141:PHE:CE1	1:A:270:GLU:HB3	2.56	0.40
1:A:268:LEU:HA	1:A:345:VAL:HG13	2.04	0.40
1:A:463:VAL:O	1:A:467:LYS:HB3	2.21	0.40
2:B:141:VAL:C	2:B:143:GLN:N	2.74	0.40
3:C:22:MET:HB2	3:C:23:PRO:HD3	2.02	0.40
1:D:120:ASN:CG	1:D:121:ALA:H	2.24	0.40
2:E:93:PRO:HB3	2:E:103:LEU:HA	2.03	0.40
2:E:129:ASP:HB3	2:E:132:LYS:HB2	2.04	0.40
1:G:333:LEU:O	1:G:337:HIS:HB2	2.21	0.40
1:G:603:TYR:O	1:G:603:TYR:CD1	2.74	0.40
3:I:145:TYR:CE1	3:L:171:LEU:HD12	2.56	0.40
3:I:19:LYS:O	3:I:20:SER:C	2.60	0.40
1:J:111:HIS:HD2	2:K:139:PRO:CG	2.34	0.40
1:J:299:ALA:HB1	1:J:303:VAL:CG1	2.48	0.40
1:J:385:LEU:O	1:J:386:LYS:C	2.59	0.40
1:J:5:TYR:CG	1:J:6:CYS:N	2.89	0.40
2:K:148:LEU:HD22	2:K:177:ASN:OD1	2.21	0.40
2:K:24:GLN:HG2	2:K:26:TYR:CZ	2.56	0.40
3:L:155:GLY:O	3:L:159:SER:HB2	2.22	0.40
1:A:540:ARG:NH2	1:A:562:ASN:O	2.54	0.40
2:B:176:LEU:CD1	2:B:228:ILE:HG23	2.52	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:HIS:HD2	2:B:190:ARG:CZ	2.32	0.40
3:C:155:GLY:O	3:C:159:SER:HB2	2.21	0.40
1:D:349:CYS:CB	1:D:357:PRO:HG3	2.51	0.40
1:D:39:VAL:O	1:D:41:ARG:N	2.54	0.40
1:D:589:GLU:C	1:D:590:ILE:HG13	2.41	0.40
1:D:633:ILE:O	1:D:636:ALA:HB3	2.20	0.40
1:D:5:TYR:CG	1:D:6:CYS:N	2.89	0.40
2:E:176:LEU:CD1	2:E:228:ILE:HG23	2.52	0.40
3:F:26:LEU:HB3	3:F:99:ARG:HH12	1.86	0.40
1:G:375:ILE:O	1:G:395:ALA:HB1	2.21	0.40
1:G:434:ASP:OD1	1:J:434:ASP:OD1	2.39	0.40
1:G:531:LEU:HD13	1:G:574:THR:O	2.21	0.40
1:G:87:ARG:HA	1:G:87:ARG:HD3	1.95	0.40
2:H:164:LYS:HD3	2:H:164:LYS:O	2.20	0.40
2:H:67:MET:HA	2:H:94:LEU:HD23	2.02	0.40
3:I:125:LEU:HD23	3:I:125:LEU:HA	1.91	0.40
1:J:107:TRP:HA	1:J:152:THR:CG2	2.38	0.40
1:J:262:PHE:H	1:J:364:VAL:HA	1.86	0.40
1:J:268:LEU:HA	1:J:345:VAL:HG13	2.04	0.40
1:J:140:ASP:O	1:J:274:GLY:HA3	2.22	0.40
1:J:282:VAL:HG13	1:J:318:VAL:HB	2.03	0.40
1:J:531:LEU:HD13	1:J:574:THR:O	2.21	0.40
3:L:19:LYS:O	3:L:20:SER:C	2.60	0.40
3:L:77:ILE:O	3:L:77:ILE:HG12	2.22	0.40
3:L:99:ARG:HH21	3:L:100:LYS:NZ	2.20	0.40
1:A:385:LEU:O	1:A:386:LYS:C	2.59	0.40
1:A:542:GLU:HG2	1:A:560:TRP:CG	2.56	0.40
2:B:206:PHE:HE1	3:C:24:ALA:HB2	1.86	0.40
1:D:506:ILE:HG22	1:D:516:GLU:HG2	2.03	0.40
1:G:129:GLU:HG2	1:G:131:PHE:CE2	2.57	0.40
1:G:262:PHE:H	1:G:364:VAL:HA	1.86	0.40
2:H:129:ASP:HB3	2:H:132:LYS:HB2	2.04	0.40
2:H:141:VAL:C	2:H:143:GLN:H	2.25	0.40
2:H:148:LEU:HD22	2:H:177:ASN:OD1	2.21	0.40
2:H:64:SER:O	2:H:66:GLY:N	2.54	0.40
3:I:99:ARG:HH21	3:I:100:LYS:NZ	2.20	0.40
1:J:419:ILE:O	1:J:421:GLY:N	2.54	0.40
2:K:99:LEU:HD12	2:K:100:ILE:H	1.87	0.40
2:K:167:ARG:CG	2:K:167:ARG:NH1	2.82	0.40
2:K:192:ASP:OD2	2:K:234:LYS:HE2	2.21	0.40
3:L:216:MET:O	3:L:220:LEU:HG	2.20	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ILE:CD1	1:A:123:LYS:HE3	2.41	0.40
1:A:344:ASP:O	1:A:346:GLN:N	2.53	0.40
3:C:221:ILE:HA	3:C:221:ILE:HD13	1.90	0.40
3:C:29:TRP:HA	3:C:32:ALA:CB	2.45	0.40
3:C:44:HIS:O	3:C:48:VAL:HB	2.22	0.40
3:C:77:ILE:HG12	3:C:77:ILE:O	2.22	0.40
3:C:85:PHE:C	3:C:87:PHE:N	2.75	0.40
1:D:9:LEU:CD2	1:D:10:VAL:H	2.28	0.40
1:D:129:GLU:HG2	1:D:131:PHE:CE2	2.57	0.40
1:D:251:MET:O	1:D:533:VAL:HG13	2.21	0.40
1:D:26:GLN:HE21	1:D:27:LYS:HE3	1.87	0.40
1:D:39:VAL:C	1:D:41:ARG:H	2.24	0.40
1:D:419:ILE:O	1:D:421:GLY:N	2.54	0.40
2:E:64:SER:O	2:E:66:GLY:N	2.54	0.40
3:F:155:GLY:O	3:F:159:SER:HB2	2.22	0.40
1:G:14:GLY:O	1:G:18:LEU:HG	2.22	0.40
1:G:385:LEU:O	1:G:386:LYS:C	2.59	0.40
2:H:141:VAL:C	2:H:143:GLN:N	2.75	0.40
3:I:85:PHE:C	3:I:87:PHE:N	2.75	0.40
3:I:93:HIS:CD2	10:I:301:HEM:NB	2.89	0.40
1:J:257:HIS:CE1	1:J:267:LEU:HD11	2.57	0.40
2:K:64:SER:O	2:K:66:GLY:N	2.54	0.40
3:L:103:ILE:O	3:L:104:ASN:CB	2.67	0.40

All (27) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:580:TYR:C	1:G:122:GLN:NE2[1_455]	0.81	1.39
1:A:122:GLN:NE2	1:J:581:GLU:N[1_554]	0.84	1.36
1:D:581:GLU:N	1:G:122:GLN:NE2[1_455]	1.03	1.17
1:A:122:GLN:NE2	1:J:580:TYR:C[1_554]	1.10	1.10
1:A:122:GLN:OE1	1:J:581:GLU:CA[1_554]	1.30	0.90
1:D:580:TYR:C	1:G:122:GLN:CD[1_455]	1.35	0.85
1:D:580:TYR:O	1:G:122:GLN:CD[1_455]	1.38	0.82
1:D:581:GLU:CA	1:G:122:GLN:OE1[1_455]	1.44	0.76
1:D:116:MET:CE	1:J:332:ILE:CD1[2_546]	1.45	0.75
1:A:122:GLN:CD	1:J:581:GLU:N[1_554]	1.62	0.58
1:A:122:GLN:CD	1:J:580:TYR:C[1_554]	1.62	0.58
1:D:581:GLU:N	1:G:122:GLN:CD[1_455]	1.63	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:580:TYR:CA	1:G:122:GLN:NE2[1_455]	1.68	0.52
1:A:122:GLN:CD	1:J:580:TYR:O[1_554]	1.70	0.50
1:D:116:MET:CE	1:J:332:ILE:CG1[2_546]	1.71	0.49
1:A:122:GLN:CD	1:J:581:GLU:CA[1_554]	1.80	0.40
1:D:122:GLN:NE2	1:J:359:GLU:CB[2_546]	1.83	0.37
1:D:580:TYR:O	1:G:122:GLN:OE1[1_455]	1.87	0.33
1:D:580:TYR:O	1:G:122:GLN:NE2[1_455]	1.90	0.30
1:D:581:GLU:N	1:G:122:GLN:OE1[1_455]	1.96	0.24
1:D:581:GLU:CA	1:G:122:GLN:CD[1_455]	2.03	0.17
1:A:122:GLN:NE2	1:J:581:GLU:CA[1_554]	2.04	0.16
1:A:122:GLN:NE2	1:J:580:TYR:CA[1_554]	2.05	0.15
1:A:122:GLN:OE1	1:J:581:GLU:N[1_554]	2.07	0.13
1:D:580:TYR:O	1:G:122:GLN:CG[1_455]	2.08	0.12
1:A:122:GLN:NE2	1:J:580:TYR:O[1_554]	2.09	0.11
1:D:580:TYR:C	1:G:122:GLN:OE1[1_455]	2.13	0.07

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	653/656 (100%)	499 (76%)	113 (17%)	41 (6%)	1	8
1	D	653/656 (100%)	499 (76%)	112 (17%)	42 (6%)	1	8
1	G	653/656 (100%)	499 (76%)	113 (17%)	41 (6%)	1	8
1	J	653/656 (100%)	499 (76%)	112 (17%)	42 (6%)	1	8
2	B	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
2	E	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
2	H	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
2	K	237/239 (99%)	190 (80%)	37 (16%)	10 (4%)	3	16
3	C	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14
3	F	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14
3	L	252/256 (98%)	200 (79%)	40 (16%)	12 (5%)	2	14
All	All	4568/4604 (99%)	3556 (78%)	758 (17%)	254 (6%)	2	11

All (254) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	THR
1	A	288	MET
1	A	294	GLU
1	A	319	GLN
1	A	333	LEU
1	A	345	VAL
2	B	65	CYS
2	B	85	GLU
2	B	109	ASN
2	B	132	LYS
3	C	54	GLY
3	C	103	ILE
3	C	104	ASN
3	C	147	MET
1	D	269	THR
1	D	288	MET
1	D	294	GLU
1	D	319	GLN
1	D	333	LEU
1	D	345	VAL
2	E	65	CYS
2	E	85	GLU
2	E	109	ASN
2	E	132	LYS
3	F	54	GLY
3	F	103	ILE
3	F	104	ASN
3	F	147	MET
1	G	269	THR
1	G	288	MET
1	G	294	GLU
1	G	319	GLN
1	G	333	LEU
1	G	345	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	65	CYS
2	H	85	GLU
2	H	109	ASN
2	H	132	LYS
3	I	54	GLY
3	I	103	ILE
3	I	104	ASN
3	I	147	MET
1	J	269	THR
1	J	288	MET
1	J	294	GLU
1	J	319	GLN
1	J	333	LEU
1	J	345	VAL
2	K	65	CYS
2	K	85	GLU
2	K	109	ASN
2	K	132	LYS
3	L	54	GLY
3	L	103	ILE
3	L	104	ASN
3	L	147	MET
1	A	14	GLY
1	A	49	GLY
1	A	119	ILE
1	A	129	GLU
1	A	218	GLY
1	A	304	VAL
1	A	334	GLY
1	A	375	ILE
1	A	393	GLU
1	A	513	ALA
1	A	573	GLN
2	B	47	TYR
2	B	108	GLY
2	B	147	GLU
3	C	253	THR
1	D	14	GLY
1	D	49	GLY
1	D	119	ILE
1	D	129	GLU
1	D	218	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	304	VAL
1	D	334	GLY
1	D	375	ILE
1	D	393	GLU
1	D	513	ALA
1	D	573	GLN
2	E	47	TYR
2	E	108	GLY
2	E	147	GLU
3	F	253	THR
1	G	14	GLY
1	G	49	GLY
1	G	119	ILE
1	G	129	GLU
1	G	218	GLY
1	G	304	VAL
1	G	334	GLY
1	G	375	ILE
1	G	393	GLU
1	G	513	ALA
1	G	573	GLN
2	H	47	TYR
2	H	108	GLY
2	H	147	GLU
3	I	253	THR
1	J	14	GLY
1	J	49	GLY
1	J	119	ILE
1	J	129	GLU
1	J	218	GLY
1	J	304	VAL
1	J	334	GLY
1	J	375	ILE
1	J	393	GLU
1	J	513	ALA
1	J	573	GLN
2	K	47	TYR
2	K	108	GLY
2	K	147	GLU
3	L	253	THR
1	A	10	VAL
1	A	40	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	42	SER
1	A	54	SER
1	A	125	THR
1	A	146	LYS
1	A	540	ARG
1	A	553	PRO
1	A	555	ARG
1	A	620	GLN
1	A	648	ALA
2	B	64	SER
2	B	102	ASP
3	C	198	ASP
1	D	10	VAL
1	D	40	LYS
1	D	42	SER
1	D	54	SER
1	D	125	THR
1	D	146	LYS
1	D	540	ARG
1	D	553	PRO
1	D	555	ARG
1	D	620	GLN
1	D	648	ALA
2	E	64	SER
2	E	102	ASP
3	F	198	ASP
1	G	10	VAL
1	G	40	LYS
1	G	42	SER
1	G	54	SER
1	G	125	THR
1	G	146	LYS
1	G	540	ARG
1	G	553	PRO
1	G	555	ARG
1	G	620	GLN
1	G	648	ALA
2	H	64	SER
2	H	102	ASP
3	I	198	ASP
1	J	10	VAL
1	J	40	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	42	SER
1	J	54	SER
1	J	125	THR
1	J	146	LYS
1	J	540	ARG
1	J	553	PRO
1	J	555	ARG
1	J	620	GLN
1	J	648	ALA
2	K	64	SER
2	K	102	ASP
3	L	198	ASP
1	A	89	PHE
1	A	261	LEU
1	A	286	ARG
1	A	564	THR
3	C	214	THR
1	D	89	PHE
1	D	261	LEU
1	D	286	ARG
1	D	564	THR
3	F	214	THR
1	G	89	PHE
1	G	261	LEU
1	G	286	ARG
1	G	564	THR
3	I	214	THR
1	J	89	PHE
1	J	261	LEU
1	J	286	ARG
1	J	564	THR
3	L	214	THR
1	A	198	ASP
1	A	281	ASP
1	A	295	LYS
1	A	365	LEU
3	C	70	ILE
3	C	112	LYS
1	D	198	ASP
1	D	281	ASP
1	D	295	LYS
1	D	365	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	F	70	ILE
1	G	198	ASP
1	G	281	ASP
1	G	295	LYS
1	G	365	LEU
3	I	70	ILE
3	I	112	LYS
1	J	198	ASP
1	J	281	ASP
1	J	295	LYS
1	J	365	LEU
3	L	70	ILE
3	L	112	LYS
1	A	153	ALA
3	C	121	GLY
3	C	127	TRP
1	D	153	ALA
3	F	112	LYS
3	F	121	GLY
3	F	127	TRP
1	G	153	ALA
3	I	121	GLY
3	I	127	TRP
1	J	153	ALA
3	L	121	GLY
3	L	127	TRP
1	A	419	ILE
1	D	419	ILE
1	G	419	ILE
1	J	419	ILE
1	A	303	VAL
1	A	406	GLY
1	D	303	VAL
1	D	406	GLY
1	G	303	VAL
1	G	406	GLY
1	J	303	VAL
1	J	406	GLY
2	B	21	PRO
3	C	142	VAL
2	E	21	PRO
3	F	142	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	21	PRO
3	I	142	VAL
2	K	21	PRO
3	L	142	VAL
1	A	592	PRO
1	D	592	PRO
1	G	592	PRO
1	J	592	PRO
1	D	105	VAL
1	J	105	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	532/533 (100%)	497 (93%)	35 (7%)	16	47
1	D	532/533 (100%)	497 (93%)	35 (7%)	16	47
1	G	532/533 (100%)	497 (93%)	35 (7%)	16	47
1	J	532/533 (100%)	497 (93%)	35 (7%)	16	47
2	B	211/211 (100%)	199 (94%)	12 (6%)	20	52
2	E	211/211 (100%)	199 (94%)	12 (6%)	20	52
2	H	211/211 (100%)	199 (94%)	12 (6%)	20	52
2	K	211/211 (100%)	199 (94%)	12 (6%)	20	52
3	C	221/223 (99%)	198 (90%)	23 (10%)	7	27
3	F	221/223 (99%)	198 (90%)	23 (10%)	7	27
3	I	221/223 (99%)	198 (90%)	23 (10%)	7	27
3	L	221/223 (99%)	198 (90%)	23 (10%)	7	27
All	All	3856/3868 (100%)	3576 (93%)	280 (7%)	14	43

All (280) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	9	LEU
1	A	40	LYS
1	A	72	ASP
1	A	84	LYS
1	A	97	ILE
1	A	109	ARG
1	A	116	MET
1	A	141	PHE
1	A	145	LYS
1	A	268	LEU
1	A	278	ILE
1	A	285	HIS
1	A	286	ARG
1	A	287	PHE
1	A	294	GLU
1	A	302	ASP
1	A	307	ARG
1	A	314	LYS
1	A	322	TYR
1	A	337	HIS
1	A	361	TRP
1	A	368	GLN
1	A	371	SER
1	A	385	LEU
1	A	390	SER
1	A	398	ASP
1	A	403	ASN
1	A	408	ASN
1	A	426	GLU
1	A	467	LYS
1	A	509	LYS
1	A	511	LEU
1	A	562	ASN
1	A	628	LYS
2	B	1	MET
2	B	40	LEU
2	B	41	ASN
2	B	50	ASP
2	B	79	THR
2	B	101	LYS
2	B	114	MET
2	B	140	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	147	GLU
2	B	167	ARG
2	B	181	ARG
2	B	189	GLU
3	C	1	MET
3	C	14	THR
3	C	40	PHE
3	C	47	PHE
3	C	56	ASN
3	C	58	MET
3	C	65	PHE
3	C	69	PHE
3	C	75	LYS
3	C	78	VAL
3	C	100	LYS
3	C	101	PHE
3	C	106	ARG
3	C	123	THR
3	C	137	PHE
3	C	154	ILE
3	C	164	VAL
3	C	197	PHE
3	C	203	ASP
3	C	212	LEU
3	C	223	LEU
3	C	234	LYS
3	C	239	THR
1	D	2	LYS
1	D	9	LEU
1	D	40	LYS
1	D	72	ASP
1	D	84	LYS
1	D	97	ILE
1	D	109	ARG
1	D	116	MET
1	D	141	PHE
1	D	145	LYS
1	D	268	LEU
1	D	278	ILE
1	D	285	HIS
1	D	286	ARG
1	D	287	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	294	GLU
1	D	302	ASP
1	D	307	ARG
1	D	314	LYS
1	D	322	TYR
1	D	337	HIS
1	D	361	TRP
1	D	368	GLN
1	D	371	SER
1	D	385	LEU
1	D	390	SER
1	D	398	ASP
1	D	403	ASN
1	D	408	ASN
1	D	426	GLU
1	D	467	LYS
1	D	509	LYS
1	D	511	LEU
1	D	562	ASN
1	D	628	LYS
2	E	1	MET
2	E	40	LEU
2	E	41	ASN
2	E	50	ASP
2	E	79	THR
2	E	101	LYS
2	E	114	MET
2	E	140	GLU
2	E	147	GLU
2	E	167	ARG
2	E	181	ARG
2	E	189	GLU
3	F	1	MET
3	F	14	THR
3	F	40	PHE
3	F	47	PHE
3	F	56	ASN
3	F	58	MET
3	F	65	PHE
3	F	69	PHE
3	F	75	LYS
3	F	78	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	F	100	LYS
3	F	101	PHE
3	F	106	ARG
3	F	123	THR
3	F	137	PHE
3	F	154	ILE
3	F	164	VAL
3	F	197	PHE
3	F	203	ASP
3	F	212	LEU
3	F	223	LEU
3	F	234	LYS
3	F	239	THR
1	G	2	LYS
1	G	9	LEU
1	G	40	LYS
1	G	72	ASP
1	G	84	LYS
1	G	97	ILE
1	G	109	ARG
1	G	116	MET
1	G	141	PHE
1	G	145	LYS
1	G	268	LEU
1	G	278	ILE
1	G	285	HIS
1	G	286	ARG
1	G	287	PHE
1	G	294	GLU
1	G	302	ASP
1	G	307	ARG
1	G	314	LYS
1	G	322	TYR
1	G	337	HIS
1	G	361	TRP
1	G	368	GLN
1	G	371	SER
1	G	385	LEU
1	G	390	SER
1	G	398	ASP
1	G	403	ASN
1	G	408	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	G	426	GLU
1	G	467	LYS
1	G	509	LYS
1	G	511	LEU
1	G	562	ASN
1	G	628	LYS
2	H	1	MET
2	H	40	LEU
2	H	41	ASN
2	H	50	ASP
2	H	79	THR
2	H	101	LYS
2	H	114	MET
2	H	140	GLU
2	H	147	GLU
2	H	167	ARG
2	H	181	ARG
2	H	189	GLU
3	I	1	MET
3	I	14	THR
3	I	40	PHE
3	I	47	PHE
3	I	56	ASN
3	I	58	MET
3	I	65	PHE
3	I	69	PHE
3	I	75	LYS
3	I	78	VAL
3	I	100	LYS
3	I	101	PHE
3	I	106	ARG
3	I	123	THR
3	I	137	PHE
3	I	154	ILE
3	I	164	VAL
3	I	197	PHE
3	I	203	ASP
3	I	212	LEU
3	I	223	LEU
3	I	234	LYS
3	I	239	THR
1	J	2	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	9	LEU
1	J	40	LYS
1	J	72	ASP
1	J	84	LYS
1	J	97	ILE
1	J	109	ARG
1	J	116	MET
1	J	141	PHE
1	J	145	LYS
1	J	268	LEU
1	J	278	ILE
1	J	285	HIS
1	J	286	ARG
1	J	287	PHE
1	J	294	GLU
1	J	302	ASP
1	J	307	ARG
1	J	314	LYS
1	J	322	TYR
1	J	337	HIS
1	J	361	TRP
1	J	368	GLN
1	J	371	SER
1	J	385	LEU
1	J	390	SER
1	J	398	ASP
1	J	403	ASN
1	J	408	ASN
1	J	426	GLU
1	J	467	LYS
1	J	509	LYS
1	J	511	LEU
1	J	562	ASN
1	J	628	LYS
2	K	1	MET
2	K	40	LEU
2	K	41	ASN
2	K	50	ASP
2	K	79	THR
2	K	101	LYS
2	K	114	MET
2	K	140	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	K	147	GLU
2	K	167	ARG
2	K	181	ARG
2	K	189	GLU
3	L	1	MET
3	L	14	THR
3	L	40	PHE
3	L	47	PHE
3	L	56	ASN
3	L	58	MET
3	L	65	PHE
3	L	69	PHE
3	L	75	LYS
3	L	78	VAL
3	L	100	LYS
3	L	101	PHE
3	L	106	ARG
3	L	123	THR
3	L	137	PHE
3	L	154	ILE
3	L	164	VAL
3	L	197	PHE
3	L	203	ASP
3	L	212	LEU
3	L	223	LEU
3	L	234	LYS
3	L	239	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	48	GLN
1	A	83	GLN
1	A	91	ASN
1	A	111	HIS
1	A	158	HIS
1	A	228	ASN
1	A	257	HIS
1	A	325	HIS
1	A	368	GLN
1	A	403	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	408	ASN
1	A	468	ASN
1	A	486	HIS
1	A	547	HIS
1	A	548	ASN
1	A	562	ASN
1	A	631	HIS
2	B	116	GLN
2	B	225	GLN
3	C	3	ASN
3	C	30	GLN
3	C	107	GLN
3	C	152	GLN
1	D	26	GLN
1	D	48	GLN
1	D	83	GLN
1	D	91	ASN
1	D	111	HIS
1	D	158	HIS
1	D	228	ASN
1	D	257	HIS
1	D	325	HIS
1	D	368	GLN
1	D	403	ASN
1	D	408	ASN
1	D	468	ASN
1	D	486	HIS
1	D	547	HIS
1	D	548	ASN
1	D	562	ASN
1	D	631	HIS
2	E	116	GLN
2	E	225	GLN
3	F	3	ASN
3	F	30	GLN
3	F	107	GLN
3	F	152	GLN
1	G	26	GLN
1	G	48	GLN
1	G	83	GLN
1	G	91	ASN
1	G	111	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	158	HIS
1	G	228	ASN
1	G	257	HIS
1	G	325	HIS
1	G	368	GLN
1	G	403	ASN
1	G	408	ASN
1	G	468	ASN
1	G	486	HIS
1	G	547	HIS
1	G	548	ASN
1	G	562	ASN
1	G	631	HIS
2	H	116	GLN
2	H	225	GLN
3	I	3	ASN
3	I	30	GLN
3	I	107	GLN
3	I	152	GLN
1	J	26	GLN
1	J	48	GLN
1	J	83	GLN
1	J	91	ASN
1	J	111	HIS
1	J	158	HIS
1	J	228	ASN
1	J	257	HIS
1	J	325	HIS
1	J	368	GLN
1	J	403	ASN
1	J	408	ASN
1	J	468	ASN
1	J	486	HIS
1	J	547	HIS
1	J	548	ASN
1	J	562	ASN
1	J	631	HIS
2	K	116	GLN
2	K	225	GLN
3	L	3	ASN
3	L	30	GLN
3	L	107	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	L	152	GLN

### 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 ⓘ

Of 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	F3S	B	302	2	0,9,9	0.00	-	-		
8	F3S	E	302	2	0,9,9	0.00	-	-		
10	HEM	L	302	3	27,50,50	2.08	8 (29%)	17,82,82	1.66	2 (11%)
10	HEM	I	302	3	27,50,50	1.80	7 (25%)	17,82,82	1.48	2 (11%)
5	MLA	D	702	-	0,6,6	0.00	-	0,7,7	0.00	-
7	FES	B	301	2	0,4,4	0.00	-	-		
9	SF4	H	303	2	0,12,12	0.00	-	-		
9	SF4	B	303	2	0,12,12	0.00	-	-		
4	FAD	G	701	1	51,58,58	2.38	15 (29%)	60,89,89	2.14	10 (16%)
10	HEM	I	301	3	27,50,50	2.08	8 (29%)	17,82,82	1.66	2 (11%)
5	MLA	A	702	-	0,6,6	0.00	-	0,7,7	0.00	-
8	F3S	H	302	2	0,9,9	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FAD	J	701	1	51,58,58	2.39	15 (29%)	60,89,89	2.14	10 (16%)
7	FES	E	301	2	0,4,4	0.00	-	-	-	-
11	LMT	I	303	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
9	SF4	K	303	2	0,12,12	0.00	-	-	-	-
8	F3S	K	302	2	0,9,9	0.00	-	-	-	-
10	HEM	F	302	3	27,50,50	2.09	8 (29%)	17,82,82	1.65	2 (11%)
7	FES	H	301	2	0,4,4	0.00	-	-	-	-
7	FES	K	301	2	0,4,4	0.00	-	-	-	-
11	LMT	C	303	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
10	HEM	F	303	3	27,50,50	1.81	7 (25%)	17,82,82	1.47	2 (11%)
11	LMT	L	301	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
9	SF4	E	303	2	0,12,12	0.00	-	-	-	-
4	FAD	D	701	1	51,58,58	2.38	15 (29%)	60,89,89	2.14	10 (16%)
4	FAD	A	701	1	51,58,58	2.38	15 (29%)	60,89,89	2.14	10 (16%)
10	HEM	C	301	3	27,50,50	2.08	8 (29%)	17,82,82	1.66	2 (11%)
11	LMT	F	301	-	36,36,36	1.15	2 (5%)	47,47,47	1.23	4 (8%)
10	HEM	C	302	3	27,50,50	1.81	7 (25%)	17,82,82	1.47	2 (11%)
5	MLA	G	702	-	0,6,6	0.00	-	0,7,7	0.00	-
10	HEM	L	303	3	27,50,50	1.80	7 (25%)	17,82,82	1.47	2 (11%)
5	MLA	J	702	-	0,6,6	0.00	-	0,7,7	0.00	-

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
8	F3S	B	302	2	-	-	0/3/3/3
10	HEM	L	302	3	-	1/6/54/54	-
10	HEM	I	302	3	-	0/6/54/54	-
5	MLA	D	702	-	-	0/0/4/4	-
7	FES	B	301	2	-	-	0/1/1/1
4	FAD	J	701	1	-	9/30/50/50	0/6/6/6
11	LMT	F	301	-	-	10/21/61/61	0/2/2/2
5	MLA	J	702	-	-	0/0/4/4	-
10	HEM	I	301	3	-	1/6/54/54	-
5	MLA	A	702	-	-	0/0/4/4	-
8	F3S	H	302	2	-	-	0/3/3/3
10	HEM	C	301	3	-	1/6/54/54	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	FES	E	301	2	-	-	0/1/1/1
9	SF4	H	303	2	-	-	0/6/5/5
11	LMT	I	303	-	-	10/21/61/61	0/2/2/2
9	SF4	K	303	2	-	-	0/6/5/5
9	SF4	E	303	2	-	-	0/6/5/5
8	F3S	K	302	2	-	-	0/3/3/3
10	HEM	F	302	3	-	1/6/54/54	-
7	FES	H	301	2	-	-	0/1/1/1
7	FES	K	301	2	-	-	0/1/1/1
11	LMT	C	303	-	-	10/21/61/61	0/2/2/2
10	HEM	F	303	3	-	0/6/54/54	-
11	LMT	L	301	-	-	10/21/61/61	0/2/2/2
4	FAD	G	701	1	-	9/30/50/50	0/6/6/6
4	FAD	D	701	1	-	9/30/50/50	0/6/6/6
4	FAD	A	701	1	-	9/30/50/50	0/6/6/6
8	F3S	E	302	2	-	-	0/3/3/3
9	SF4	B	303	2	-	-	0/6/5/5
10	HEM	C	302	3	-	0/6/54/54	-
5	MLA	G	702	-	-	0/0/4/4	-
10	HEM	L	303	3	-	0/6/54/54	-

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	701	FAD	C4X-C10	9.34	1.48	1.38
4	A	701	FAD	C4X-C10	9.31	1.48	1.38
4	G	701	FAD	C4X-C10	9.29	1.48	1.38
4	D	701	FAD	C4X-C10	9.23	1.48	1.38
10	F	302	HEM	C3B-CAB	-5.37	1.37	1.47
10	L	302	HEM	C3B-CAB	-5.35	1.37	1.47
10	C	301	HEM	C3B-CAB	-5.34	1.37	1.47
10	I	301	HEM	C3B-CAB	-5.34	1.37	1.47
4	G	701	FAD	C9A-N10	5.10	1.45	1.38
4	D	701	FAD	O4B-C1B	5.09	1.48	1.41
4	J	701	FAD	C9A-N10	5.08	1.45	1.38
4	G	701	FAD	O4B-C1B	5.05	1.48	1.41
4	A	701	FAD	C9A-N10	5.05	1.45	1.38
4	A	701	FAD	O4B-C1B	5.05	1.48	1.41
4	D	701	FAD	C9A-N10	5.03	1.45	1.38
4	J	701	FAD	O4B-C1B	5.01	1.48	1.41
10	L	303	HEM	C3C-CAC	-4.76	1.38	1.47

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	303	HEM	C3C-CAC	-4.74	1.38	1.47
10	C	302	HEM	C3C-CAC	-4.73	1.38	1.47
10	I	302	HEM	C3C-CAC	-4.71	1.38	1.47
10	F	302	HEM	C3B-C2B	-4.51	1.34	1.40
10	I	301	HEM	C3B-C2B	-4.50	1.34	1.40
10	C	301	HEM	C3B-C2B	-4.47	1.34	1.40
10	L	302	HEM	C3B-C2B	-4.44	1.34	1.40
4	A	701	FAD	PA-O2A	-4.14	1.35	1.55
4	J	701	FAD	PA-O2A	-4.13	1.35	1.55
4	G	701	FAD	PA-O2A	-4.13	1.35	1.55
4	D	701	FAD	PA-O2A	-4.13	1.35	1.55
4	J	701	FAD	O5'-C5'	4.11	1.60	1.44
4	G	701	FAD	O5'-C5'	4.10	1.60	1.44
4	A	701	FAD	O5'-C5'	4.10	1.60	1.44
4	D	701	FAD	O5'-C5'	4.09	1.60	1.44
10	I	301	HEM	C3C-CAC	-3.87	1.39	1.47
10	C	301	HEM	C3C-CAC	-3.87	1.39	1.47
10	F	302	HEM	C3C-CAC	-3.87	1.39	1.47
10	L	302	HEM	C3C-CAC	-3.84	1.39	1.47
10	C	302	HEM	C3B-C2B	-3.57	1.35	1.40
10	F	303	HEM	C3B-C2B	-3.55	1.35	1.40
10	I	302	HEM	C3B-C2B	-3.54	1.35	1.40
10	L	303	HEM	C3B-C2B	-3.52	1.35	1.40
4	G	701	FAD	P-O2P	-3.47	1.39	1.55
4	J	701	FAD	P-O2P	-3.47	1.39	1.55
4	A	701	FAD	P-O2P	-3.47	1.39	1.55
4	D	701	FAD	P-O2P	-3.47	1.39	1.55
4	D	701	FAD	C2B-C1B	-3.46	1.48	1.53
10	L	302	HEM	CAA-C2A	3.42	1.57	1.52
4	J	701	FAD	C2B-C1B	-3.41	1.48	1.53
10	I	301	HEM	CAA-C2A	3.41	1.57	1.52
4	A	701	FAD	C2B-C1B	-3.40	1.48	1.53
10	F	302	HEM	CAA-C2A	3.39	1.57	1.52
4	G	701	FAD	C2B-C1B	-3.39	1.48	1.53
10	C	301	HEM	CAA-C2A	3.38	1.57	1.52
10	F	302	HEM	C3C-C2C	-3.35	1.35	1.40
11	C	303	LMT	O5B-C1B	3.33	1.50	1.41
11	I	303	LMT	O5B-C1B	3.32	1.50	1.41
10	C	301	HEM	C3C-C2C	-3.32	1.35	1.40
11	L	301	LMT	O5B-C1B	3.32	1.50	1.41
11	F	301	LMT	O5B-C1B	3.32	1.50	1.41
10	L	302	HEM	C3C-C2C	-3.31	1.35	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	301	HEM	C3C-C2C	-3.28	1.35	1.40
10	I	302	HEM	C3B-CAB	-3.24	1.41	1.47
10	C	302	HEM	C3B-CAB	-3.23	1.41	1.47
10	L	303	HEM	C3B-CAB	-3.23	1.41	1.47
10	F	303	HEM	C3B-CAB	-3.22	1.41	1.47
10	F	303	HEM	C3C-C2C	-3.21	1.35	1.40
10	C	302	HEM	C3C-C2C	-3.19	1.35	1.40
10	I	302	HEM	C3C-C2C	-3.16	1.36	1.40
10	L	303	HEM	C3C-C2C	-3.16	1.36	1.40
4	D	701	FAD	C4-C4X	3.06	1.46	1.41
4	A	701	FAD	C4-C4X	3.04	1.46	1.41
4	G	701	FAD	C4-C4X	3.02	1.46	1.41
4	J	701	FAD	C4-C4X	3.02	1.46	1.41
4	D	701	FAD	C5'-C4'	2.96	1.56	1.51
11	C	303	LMT	C3'-C4'	2.95	1.60	1.52
4	G	701	FAD	C5'-C4'	2.95	1.56	1.51
11	L	301	LMT	C3'-C4'	2.95	1.60	1.52
11	F	301	LMT	C3'-C4'	2.95	1.60	1.52
11	I	303	LMT	C3'-C4'	2.94	1.60	1.52
4	A	701	FAD	C5'-C4'	2.93	1.55	1.51
10	L	303	HEM	CBB-CAB	2.91	1.48	1.29
10	C	302	HEM	CBB-CAB	2.91	1.48	1.29
10	I	302	HEM	CBB-CAB	2.91	1.48	1.29
10	F	303	HEM	CBB-CAB	2.90	1.48	1.29
4	J	701	FAD	C5'-C4'	2.90	1.55	1.51
4	D	701	FAD	C10-N1	2.90	1.37	1.33
4	A	701	FAD	C10-N1	2.86	1.36	1.33
4	J	701	FAD	C10-N1	2.85	1.36	1.33
4	G	701	FAD	C10-N1	2.84	1.36	1.33
10	F	302	HEM	CBC-CAC	2.72	1.47	1.29
10	C	301	HEM	CBC-CAC	2.71	1.47	1.29
10	I	301	HEM	CBC-CAC	2.70	1.47	1.29
10	L	302	HEM	CBC-CAC	2.70	1.47	1.29
10	F	302	HEM	CBB-CAB	2.56	1.46	1.29
10	L	302	HEM	CBB-CAB	2.55	1.46	1.29
10	I	301	HEM	CBB-CAB	2.55	1.46	1.29
10	C	301	HEM	CBB-CAB	2.55	1.46	1.29
4	J	701	FAD	C2A-N3A	2.36	1.35	1.32
4	D	701	FAD	C2A-N3A	2.35	1.35	1.32
4	A	701	FAD	C2A-N3A	2.34	1.35	1.32
4	G	701	FAD	C2A-N3A	2.30	1.35	1.32
10	C	302	HEM	CMB-C2B	2.27	1.57	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	701	FAD	C8-C7	2.27	1.46	1.40
4	G	701	FAD	C8-C7	2.27	1.46	1.40
4	D	701	FAD	C8-C7	2.26	1.46	1.40
10	L	303	HEM	CMB-C2B	2.25	1.56	1.51
10	F	303	HEM	CMB-C2B	2.25	1.56	1.51
10	I	302	HEM	CMB-C2B	2.24	1.56	1.51
4	A	701	FAD	C8-C7	2.24	1.46	1.40
10	F	303	HEM	CBC-CAC	2.22	1.44	1.29
10	I	302	HEM	CBC-CAC	2.22	1.43	1.29
10	C	302	HEM	CBC-CAC	2.21	1.43	1.29
10	L	303	HEM	CBC-CAC	2.21	1.43	1.29
4	J	701	FAD	C4-N3	2.19	1.36	1.33
4	G	701	FAD	C4A-N3A	2.17	1.38	1.35
4	G	701	FAD	C4-N3	2.14	1.36	1.33
4	A	701	FAD	C4-N3	2.12	1.36	1.33
4	A	701	FAD	C4A-N3A	2.10	1.38	1.35
4	D	701	FAD	C4A-N3A	2.09	1.38	1.35
4	D	701	FAD	C4-N3	2.09	1.36	1.33
4	J	701	FAD	C4A-N3A	2.07	1.38	1.35
4	J	701	FAD	C4X-N5	2.07	1.36	1.33
4	G	701	FAD	C4X-N5	2.07	1.36	1.33
4	A	701	FAD	C4X-N5	2.06	1.36	1.33
4	D	701	FAD	C4X-N5	2.02	1.36	1.33
10	C	301	HEM	CAD-C3D	2.02	1.55	1.52
10	L	302	HEM	CAD-C3D	2.01	1.55	1.52
10	F	302	HEM	CAD-C3D	2.01	1.55	1.52
10	I	301	HEM	CAD-C3D	2.00	1.55	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	701	FAD	C1'-N10-C10	9.14	126.60	118.41
4	G	701	FAD	C1'-N10-C10	9.13	126.59	118.41
4	J	701	FAD	C1'-N10-C10	9.12	126.58	118.41
4	A	701	FAD	C1'-N10-C10	9.10	126.56	118.41
4	G	701	FAD	C4-N3-C2	6.92	120.98	115.14
4	A	701	FAD	C4-N3-C2	6.91	120.98	115.14
4	J	701	FAD	C4-N3-C2	6.88	120.95	115.14
4	D	701	FAD	C4-N3-C2	6.83	120.91	115.14
4	G	701	FAD	C1'-N10-C9A	-6.80	112.94	118.29
4	D	701	FAD	C1'-N10-C9A	-6.79	112.95	118.29
4	A	701	FAD	C1'-N10-C9A	-6.77	112.96	118.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	701	FAD	C1'-N10-C9A	-6.76	112.97	118.29
10	I	301	HEM	CBA-CAA-C2A	5.95	123.46	112.49
10	L	302	HEM	CBA-CAA-C2A	5.95	123.45	112.49
10	C	301	HEM	CBA-CAA-C2A	5.94	123.44	112.49
10	F	302	HEM	CBA-CAA-C2A	5.93	123.42	112.49
11	L	301	LMT	C1-O1'-C1'	4.89	121.95	113.84
11	I	303	LMT	C1-O1'-C1'	4.88	121.93	113.84
11	F	301	LMT	C1-O1'-C1'	4.88	121.93	113.84
11	C	303	LMT	C1-O1'-C1'	4.88	121.93	113.84
10	I	302	HEM	CBA-CAA-C2A	4.53	120.84	112.49
10	C	302	HEM	CBA-CAA-C2A	4.53	120.84	112.49
10	L	303	HEM	CBA-CAA-C2A	4.52	120.82	112.49
10	F	303	HEM	CBA-CAA-C2A	4.51	120.80	112.49
4	J	701	FAD	C4X-C4-N3	-4.05	117.89	123.43
4	G	701	FAD	C4X-C4-N3	-4.05	117.90	123.43
4	A	701	FAD	C4X-C4-N3	-4.03	117.92	123.43
4	D	701	FAD	C4X-C4-N3	-3.98	117.98	123.43
4	J	701	FAD	C5'-C4'-C3'	-3.23	105.97	112.20
4	A	701	FAD	C5'-C4'-C3'	-3.23	105.97	112.20
4	G	701	FAD	C5'-C4'-C3'	-3.22	105.98	112.20
4	D	701	FAD	C5'-C4'-C3'	-3.21	106.00	112.20
11	I	303	LMT	C3'-C4'-C5'	-3.10	103.82	110.93
11	L	301	LMT	C3'-C4'-C5'	-3.10	103.83	110.93
11	F	301	LMT	C3'-C4'-C5'	-3.09	103.84	110.93
11	C	303	LMT	C3'-C4'-C5'	-3.08	103.86	110.93
4	G	701	FAD	C5A-C6A-N6A	2.58	124.28	120.35
4	J	701	FAD	C5A-C6A-N6A	2.58	124.28	120.35
4	A	701	FAD	C5A-C6A-N6A	2.58	124.27	120.35
4	D	701	FAD	C5A-C6A-N6A	2.58	124.27	120.35
4	G	701	FAD	O4B-C1B-C2B	-2.40	103.42	106.93
4	A	701	FAD	O4B-C1B-C2B	-2.40	103.42	106.93
4	D	701	FAD	O4B-C1B-C2B	-2.39	103.43	106.93
4	J	701	FAD	O4B-C1B-C2B	-2.39	103.44	106.93
11	F	301	LMT	O1'-C1'-C2'	-2.29	104.72	108.30
11	L	301	LMT	O1'-C1'-C2'	-2.29	104.73	108.30
11	I	303	LMT	O1'-C1'-C2'	-2.29	104.73	108.30
11	C	303	LMT	O1'-C1'-C2'	-2.29	104.73	108.30
4	D	701	FAD	C4-C4X-C10	-2.21	118.49	119.95
4	D	701	FAD	C2A-N1A-C6A	2.19	122.50	118.75
4	A	701	FAD	C2A-N1A-C6A	2.19	122.49	118.75
4	J	701	FAD	C2A-N1A-C6A	2.18	122.47	118.75
4	G	701	FAD	C2A-N1A-C6A	2.17	122.46	118.75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	FAD	C4-C4X-C10	-2.17	118.52	119.95
10	I	302	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
10	L	303	HEM	CMA-C3A-C4A	-2.16	125.15	128.46
10	C	302	HEM	CMA-C3A-C4A	-2.16	125.15	128.46
4	J	701	FAD	C5A-C6A-N1A	-2.15	115.48	120.35
4	A	701	FAD	C5A-C6A-N1A	-2.14	115.49	120.35
4	G	701	FAD	C5A-C6A-N1A	-2.14	115.50	120.35
4	G	701	FAD	C4-C4X-C10	-2.14	118.53	119.95
4	D	701	FAD	C5A-C6A-N1A	-2.14	115.50	120.35
10	F	303	HEM	CMA-C3A-C4A	-2.14	125.18	128.46
10	L	302	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
4	J	701	FAD	C4-C4X-C10	-2.10	118.56	119.95
10	C	301	HEM	CMA-C3A-C4A	-2.08	125.27	128.46
10	I	301	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
10	F	302	HEM	CMA-C3A-C4A	-2.06	125.30	128.46
11	F	301	LMT	O1B-C4'-C3'	2.03	112.67	107.28
11	L	301	LMT	O1B-C4'-C3'	2.02	112.66	107.28
11	I	303	LMT	O1B-C4'-C3'	2.02	112.66	107.28
11	C	303	LMT	O1B-C4'-C3'	2.01	112.64	107.28

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	701	FAD	C2'-C1'-N10-C9A
4	G	701	FAD	C2'-C1'-N10-C10
4	G	701	FAD	C5'-O5'-P-O1P
4	G	701	FAD	C5'-O5'-P-O3P
4	A	701	FAD	C2'-C1'-N10-C9A
4	A	701	FAD	C2'-C1'-N10-C10
4	A	701	FAD	C5'-O5'-P-O1P
4	A	701	FAD	C5'-O5'-P-O3P
4	J	701	FAD	C2'-C1'-N10-C9A
4	J	701	FAD	C2'-C1'-N10-C10
4	J	701	FAD	C5'-O5'-P-O1P
4	J	701	FAD	C5'-O5'-P-O3P
4	D	701	FAD	C2'-C1'-N10-C9A
4	D	701	FAD	C2'-C1'-N10-C10
4	D	701	FAD	C5'-O5'-P-O1P
4	D	701	FAD	C5'-O5'-P-O3P
11	C	303	LMT	O5'-C5'-C6'-O6'
11	I	303	LMT	O5'-C5'-C6'-O6'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
11	L	301	LMT	O5'-C5'-C6'-O6'
11	F	301	LMT	O5'-C5'-C6'-O6'
11	C	303	LMT	C4'-C5'-C6'-O6'
11	I	303	LMT	C4'-C5'-C6'-O6'
11	L	301	LMT	C4'-C5'-C6'-O6'
11	F	301	LMT	C4'-C5'-C6'-O6'
11	L	301	LMT	O1'-C1-C2-C3
11	C	303	LMT	O1'-C1-C2-C3
11	I	303	LMT	O1'-C1-C2-C3
11	F	301	LMT	O1'-C1-C2-C3
11	C	303	LMT	C2-C3-C4-C5
11	I	303	LMT	C2-C3-C4-C5
11	L	301	LMT	C2-C3-C4-C5
11	F	301	LMT	C2-C3-C4-C5
4	G	701	FAD	C4'-C5'-O5'-P
4	A	701	FAD	C4'-C5'-O5'-P
4	J	701	FAD	C4'-C5'-O5'-P
4	D	701	FAD	C4'-C5'-O5'-P
4	G	701	FAD	P-O3P-PA-O2A
4	A	701	FAD	P-O3P-PA-O2A
4	J	701	FAD	P-O3P-PA-O2A
4	D	701	FAD	P-O3P-PA-O2A
11	C	303	LMT	C5'-C4'-O1B-C1B
11	I	303	LMT	C5'-C4'-O1B-C1B
11	L	301	LMT	C5'-C4'-O1B-C1B
11	F	301	LMT	C5'-C4'-O1B-C1B
10	L	302	HEM	C4D-C3D-CAD-CBD
10	I	301	HEM	C4D-C3D-CAD-CBD
10	F	302	HEM	C4D-C3D-CAD-CBD
10	C	301	HEM	C4D-C3D-CAD-CBD
4	G	701	FAD	P-O3P-PA-O1A
4	A	701	FAD	P-O3P-PA-O1A
4	J	701	FAD	P-O3P-PA-O1A
4	D	701	FAD	P-O3P-PA-O1A
11	I	303	LMT	C2B-C1B-O1B-C4'
11	C	303	LMT	C2B-C1B-O1B-C4'
11	L	301	LMT	C2B-C1B-O1B-C4'
11	F	301	LMT	C2B-C1B-O1B-C4'
11	L	301	LMT	O5B-C1B-O1B-C4'
11	C	303	LMT	O5B-C1B-O1B-C4'
11	I	303	LMT	O5B-C1B-O1B-C4'
11	F	301	LMT	O5B-C1B-O1B-C4'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
11	I	303	LMT	C7-C8-C9-C10
11	L	301	LMT	C7-C8-C9-C10
11	C	303	LMT	C7-C8-C9-C10
11	F	301	LMT	C7-C8-C9-C10
11	C	303	LMT	C9-C10-C11-C12
11	F	301	LMT	C9-C10-C11-C12
11	I	303	LMT	C9-C10-C11-C12
11	L	301	LMT	C9-C10-C11-C12
11	F	301	LMT	C3'-C4'-O1B-C1B
11	C	303	LMT	C3'-C4'-O1B-C1B
11	L	301	LMT	C3'-C4'-O1B-C1B
11	I	303	LMT	C3'-C4'-O1B-C1B
4	G	701	FAD	PA-O3P-P-O2P
4	A	701	FAD	PA-O3P-P-O2P
4	J	701	FAD	PA-O3P-P-O2P
4	D	701	FAD	PA-O3P-P-O2P
4	G	701	FAD	O4B-C4B-C5B-O5B
4	A	701	FAD	O4B-C4B-C5B-O5B
4	J	701	FAD	O4B-C4B-C5B-O5B
4	D	701	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

24 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	302	F3S	2	0
8	E	302	F3S	2	0
10	L	302	HEM	4	0
10	I	302	HEM	6	0
5	D	702	MLA	5	0
4	G	701	FAD	4	0
10	I	301	HEM	5	0
5	A	702	MLA	5	0
8	H	302	F3S	2	0
4	J	701	FAD	4	0
11	I	303	LMT	3	0
8	K	302	F3S	2	0
10	F	302	HEM	5	0
11	C	303	LMT	3	0
10	F	303	HEM	7	0
11	L	301	LMT	3	0
4	D	701	FAD	4	0

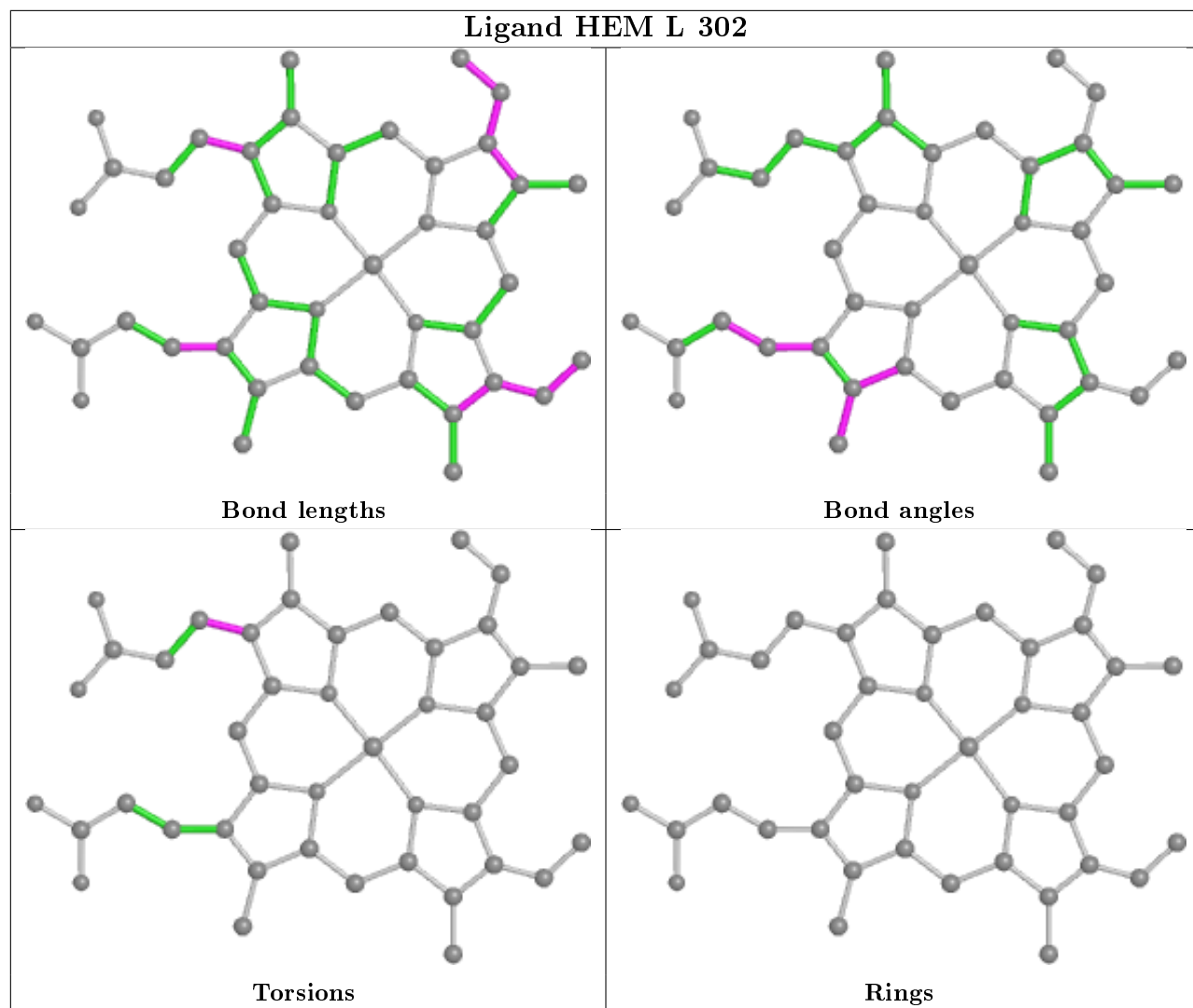
*Continued on next page...*

*Continued from previous page...*

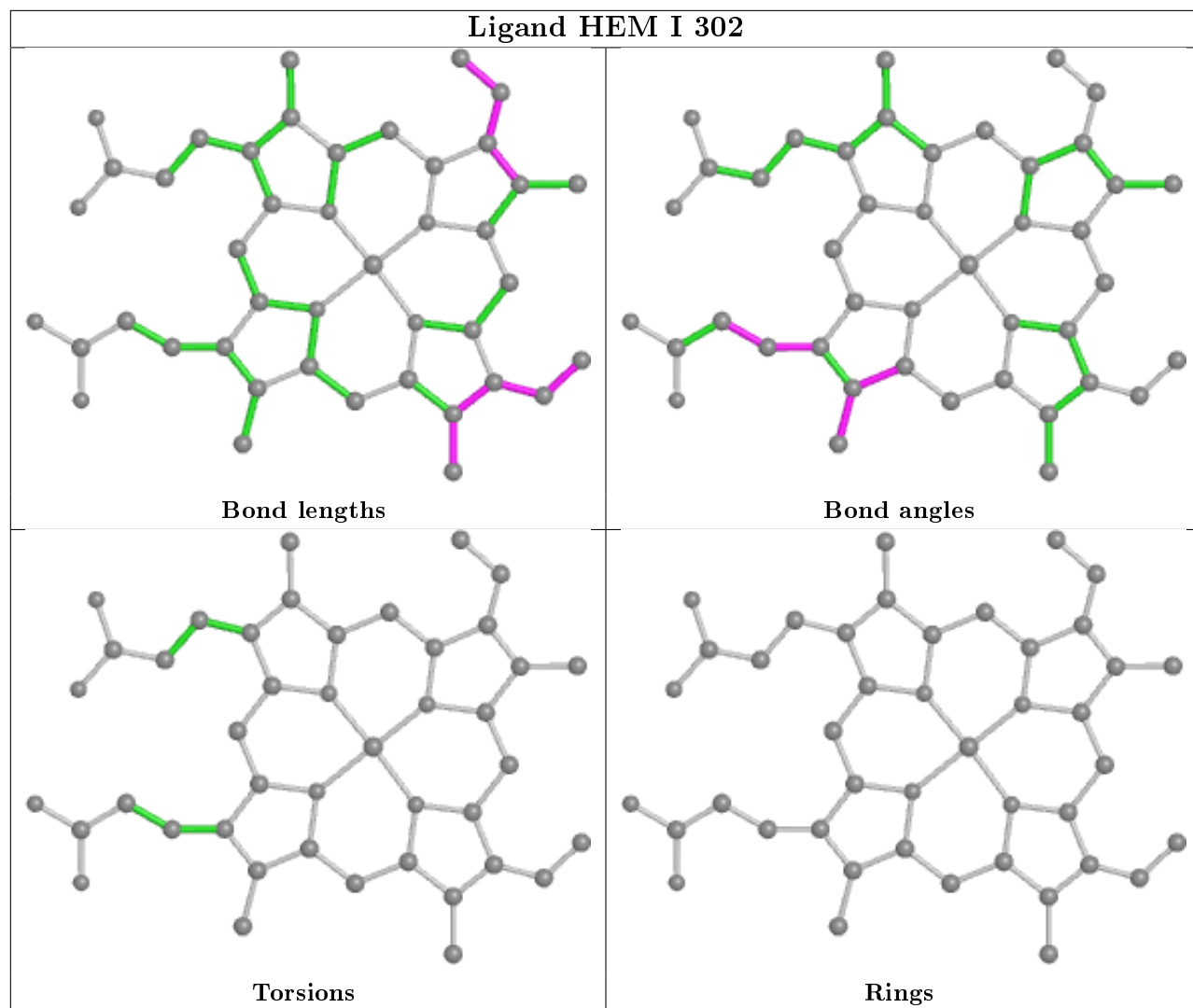
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	FAD	4	0
10	C	301	HEM	4	0
11	F	301	LMT	3	0
10	C	302	HEM	7	0
5	G	702	MLA	6	0
10	L	303	HEM	7	0
5	J	702	MLA	5	0

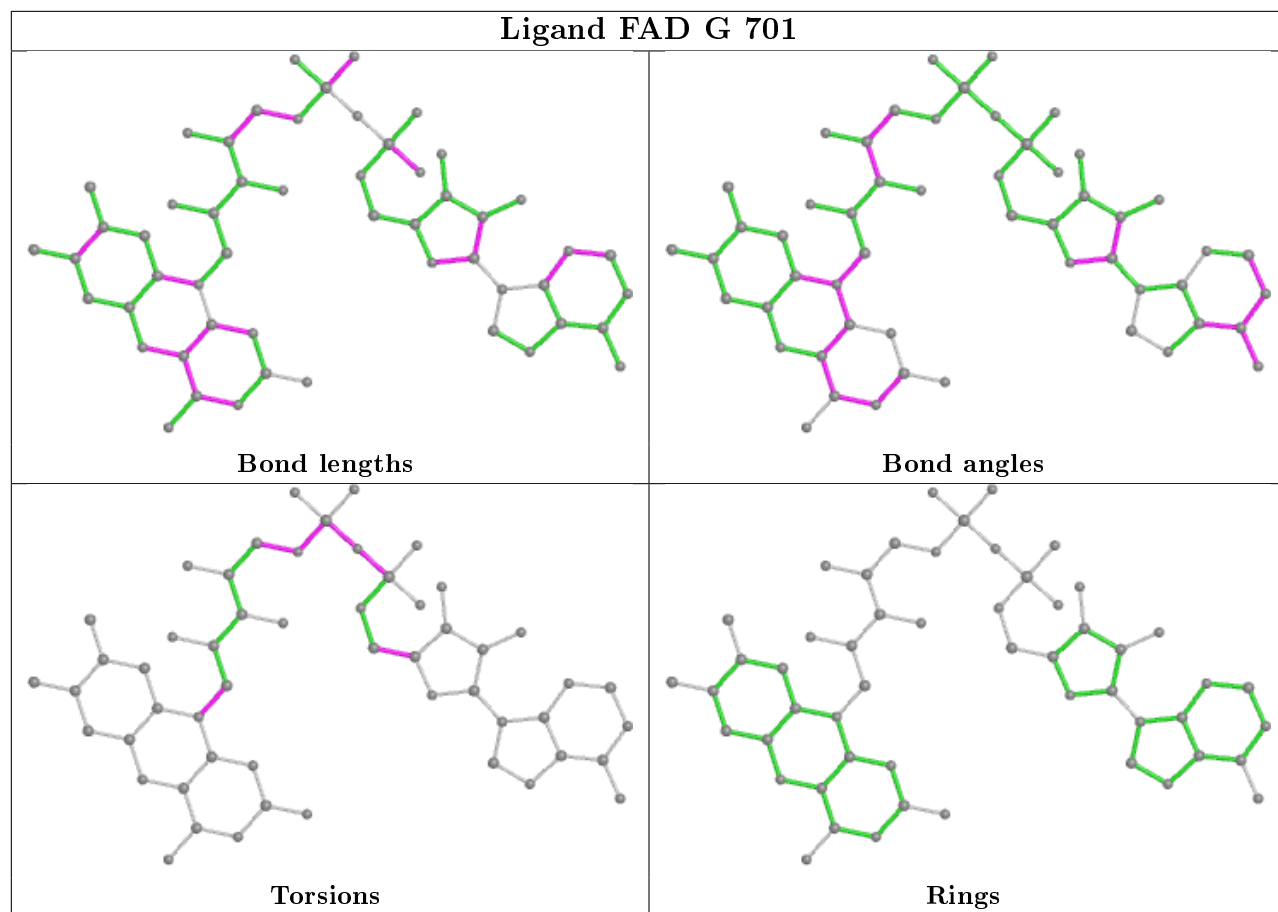
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



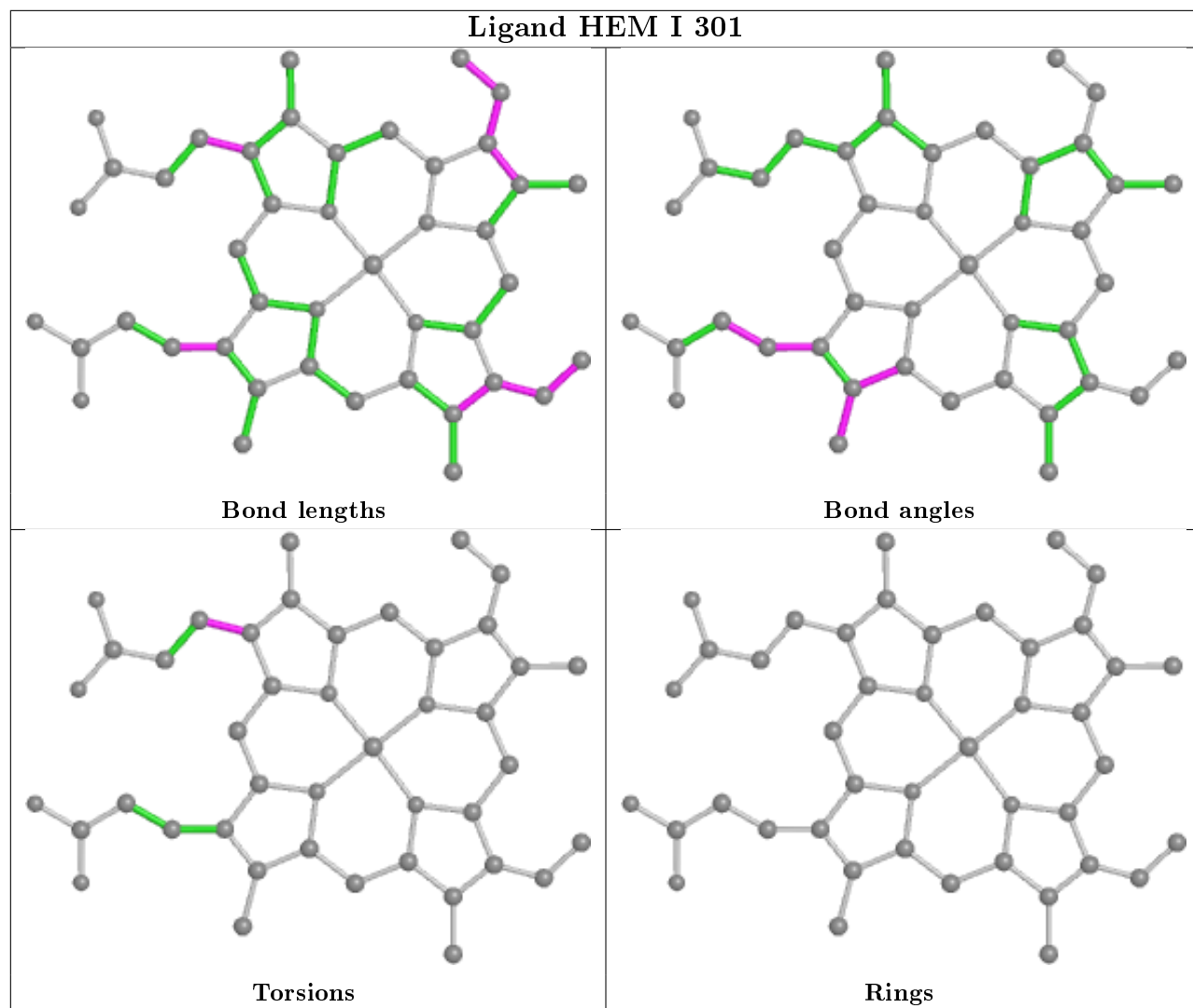


## Ligand HEM I 302

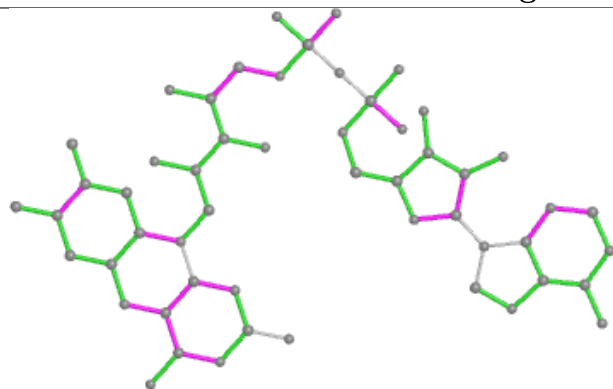




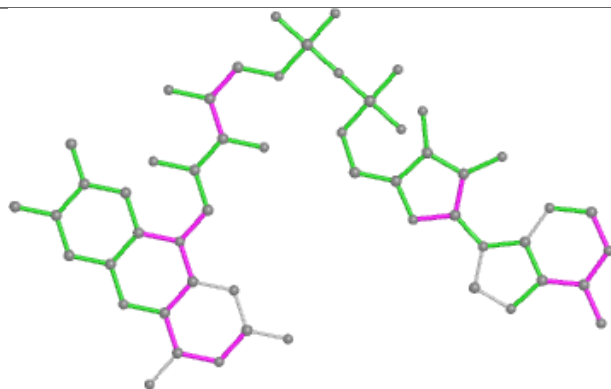
## Ligand HEM I 301



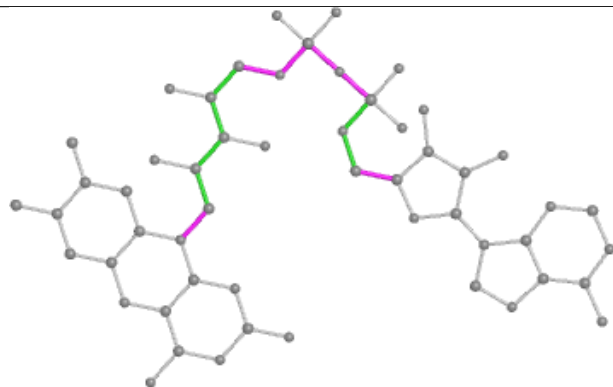
## Ligand FAD J 701



Bond lengths



Bond angles

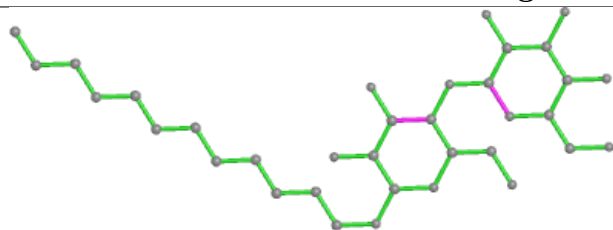


Torsions

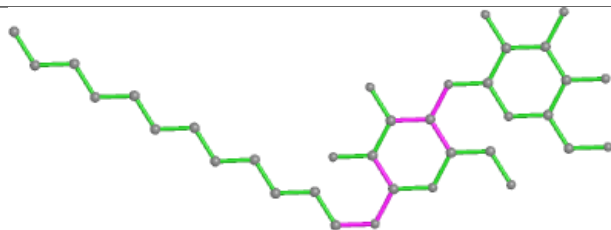


Rings

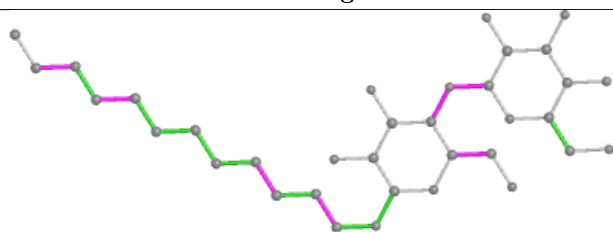
## Ligand LMT I 303



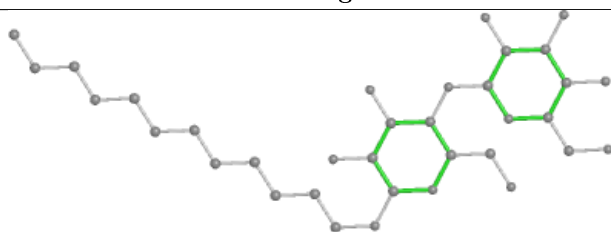
Bond lengths



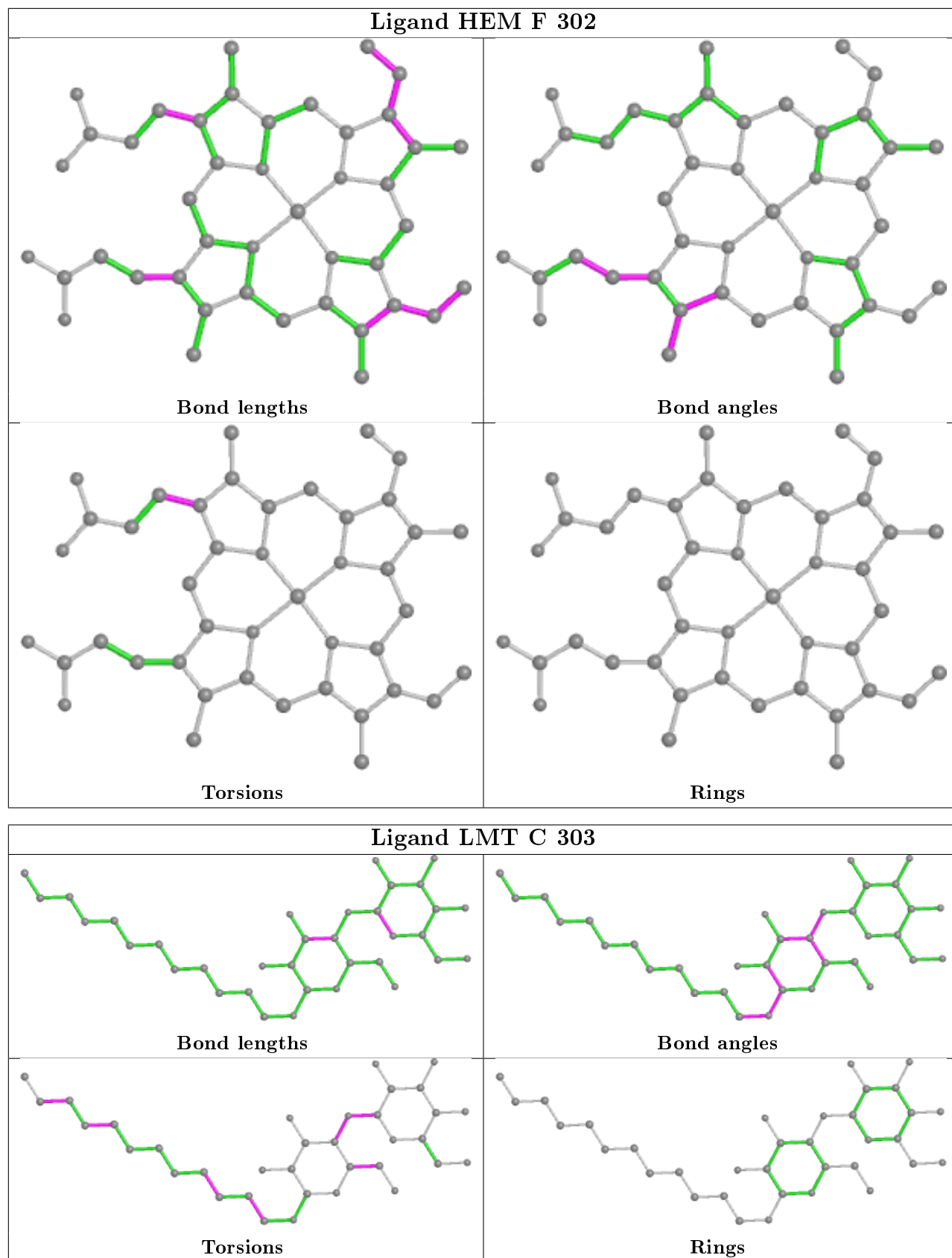
Bond angles

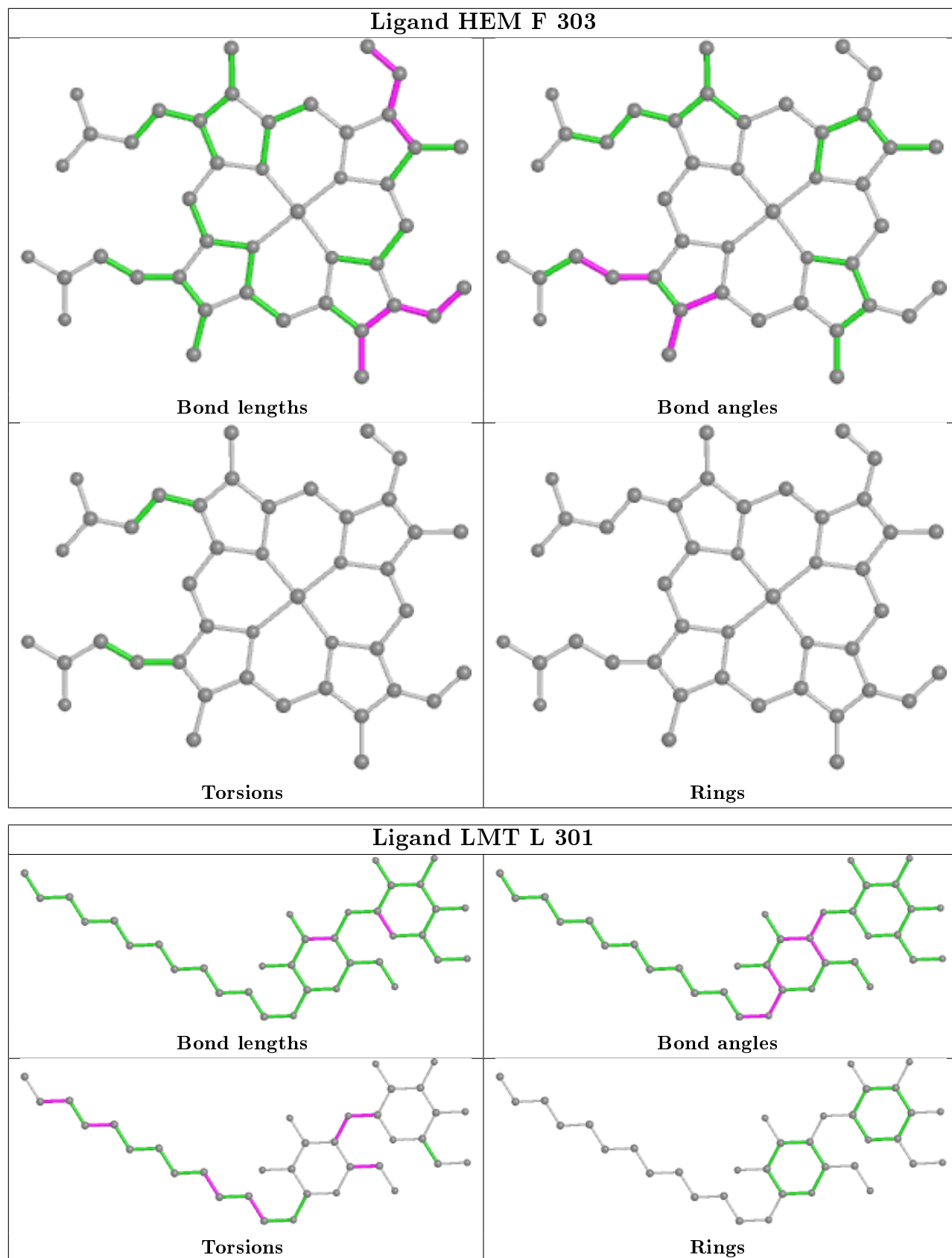


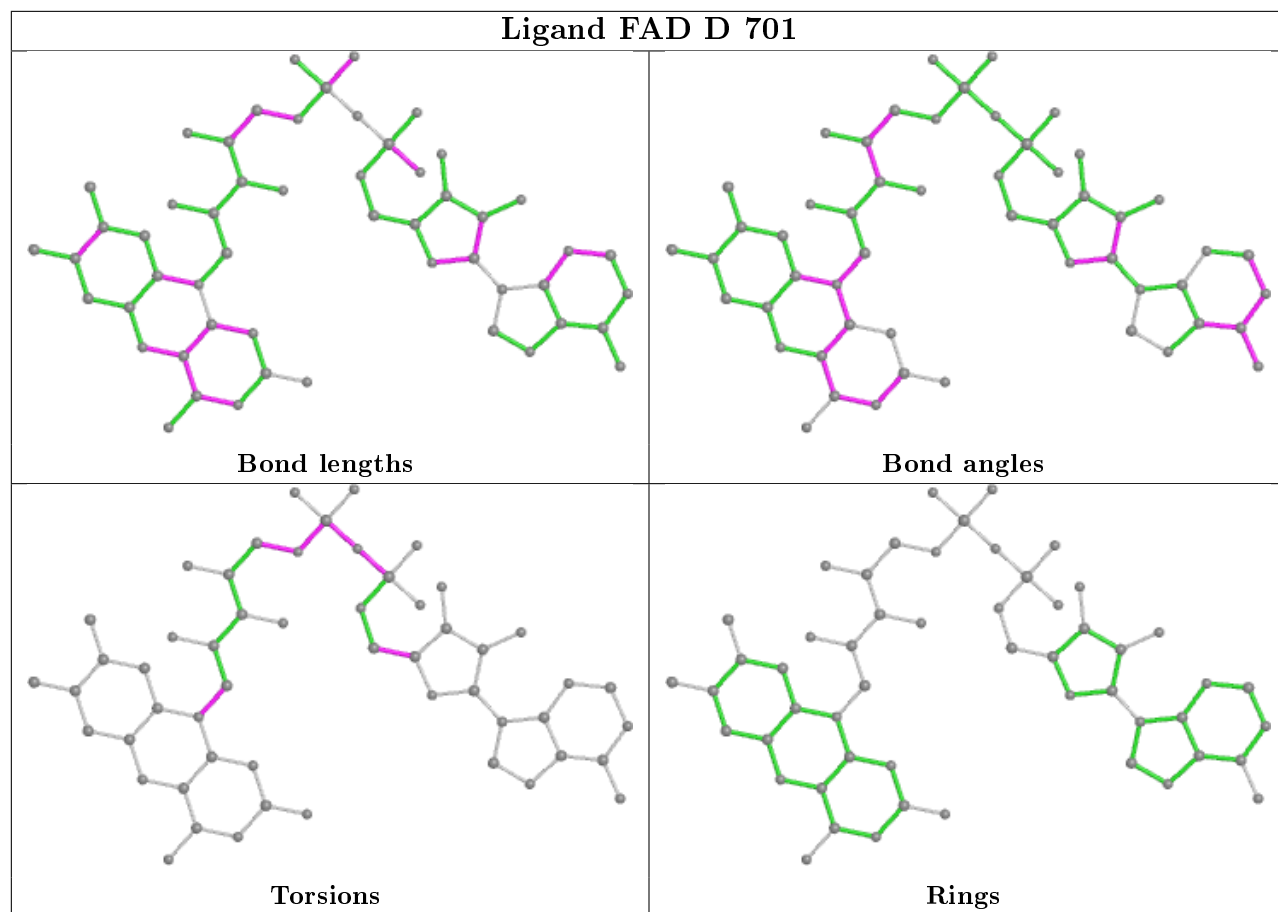
Torsions



Rings

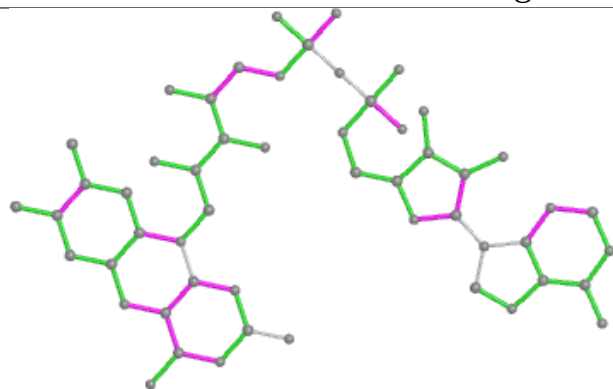




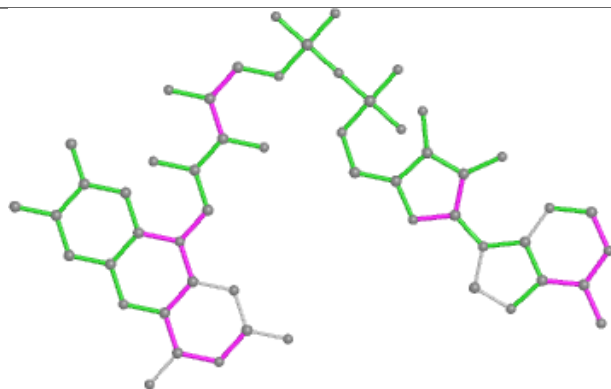




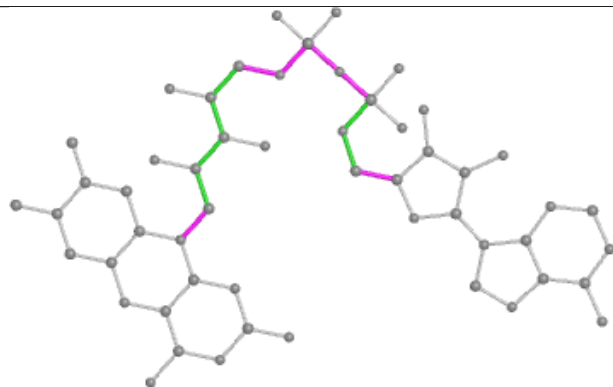
## Ligand FAD A 701



Bond lengths



Bond angles

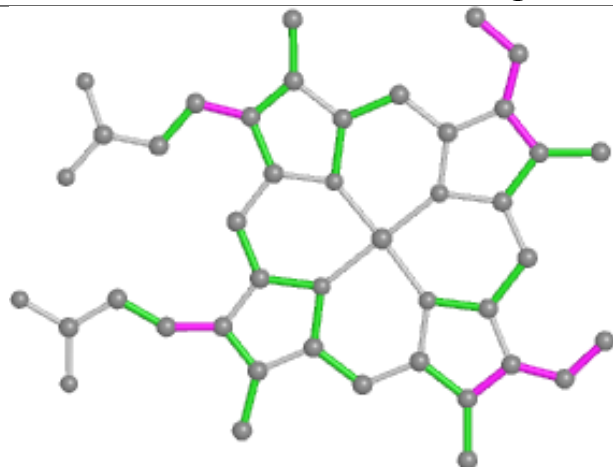


Torsions

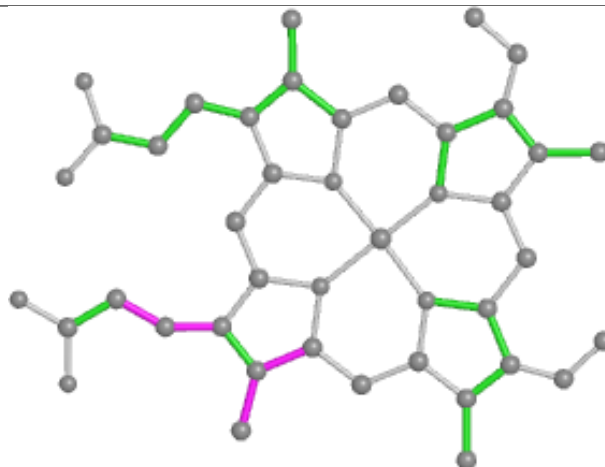


Rings

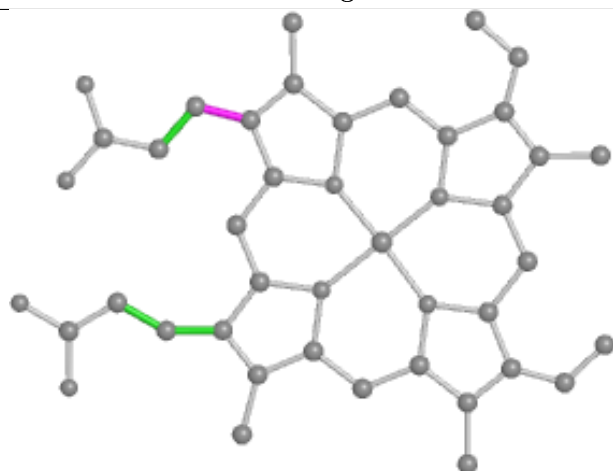
## Ligand HEM C 301



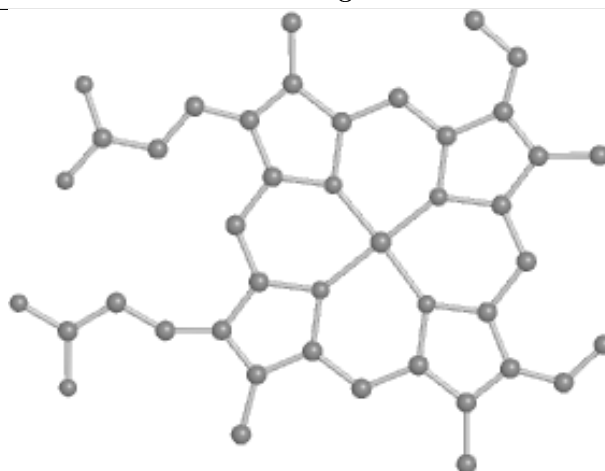
Bond lengths



Bond angles

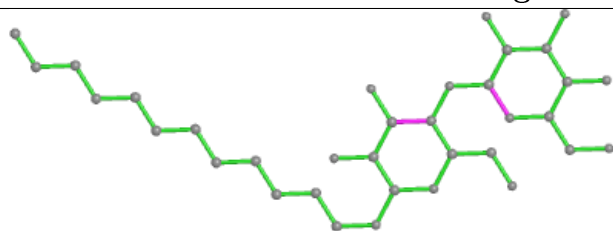


Torsions

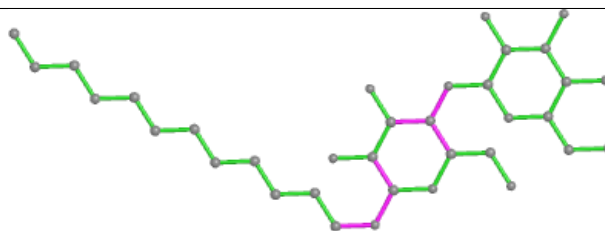


Rings

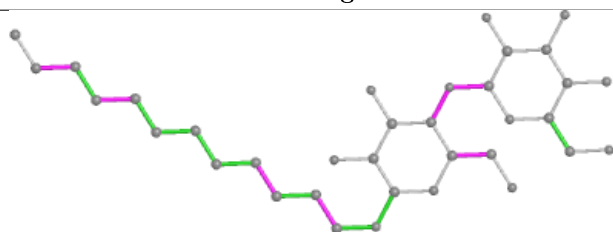
## Ligand LMT F 301



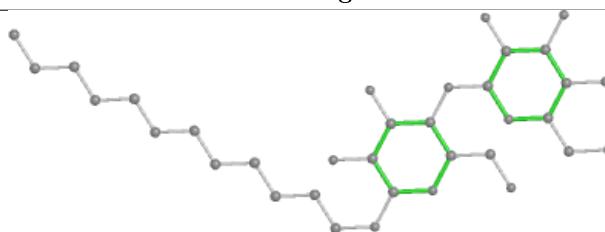
Bond lengths



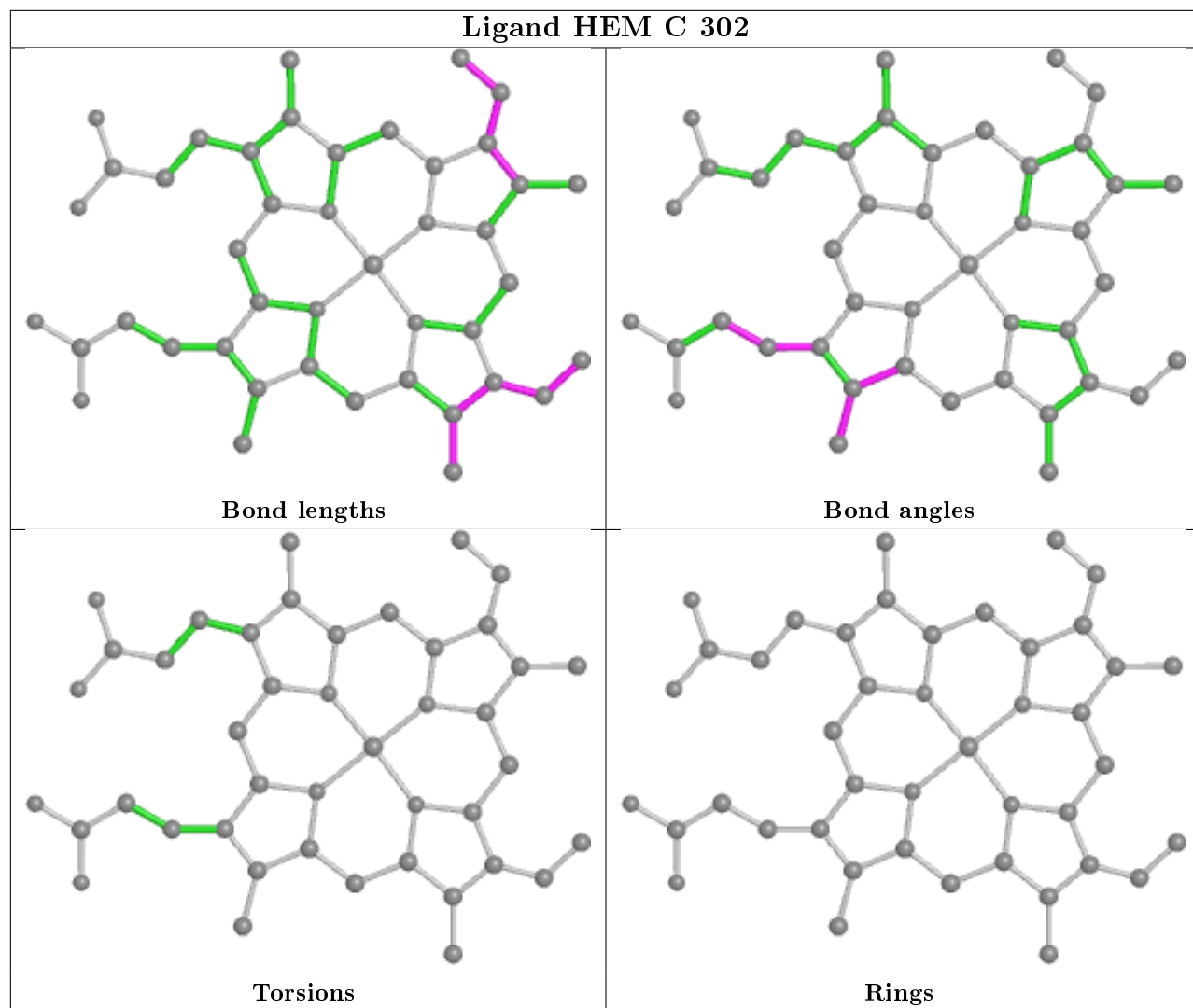
Bond angles

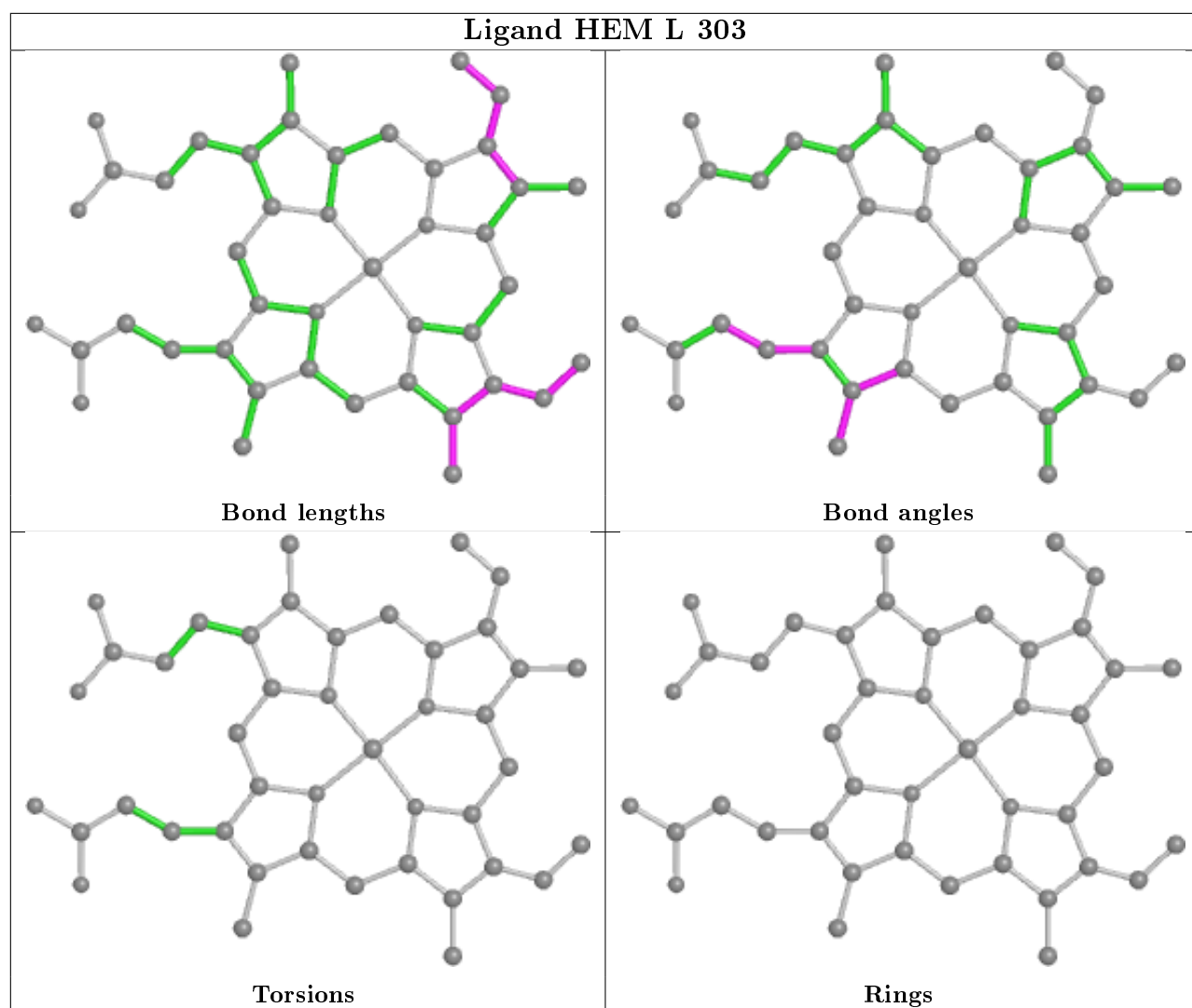


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.