



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 12:17 AM EST

PDB ID : 3UKP  
Title : Crystal structure of R327A UDP-galactopyranose mutase from *Aspergillus fumigatus* in complex with UDPgalp  
Authors : Van Straaten, K.E.; Sanders, D.A.R.  
Deposited on : 2011-11-09  
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

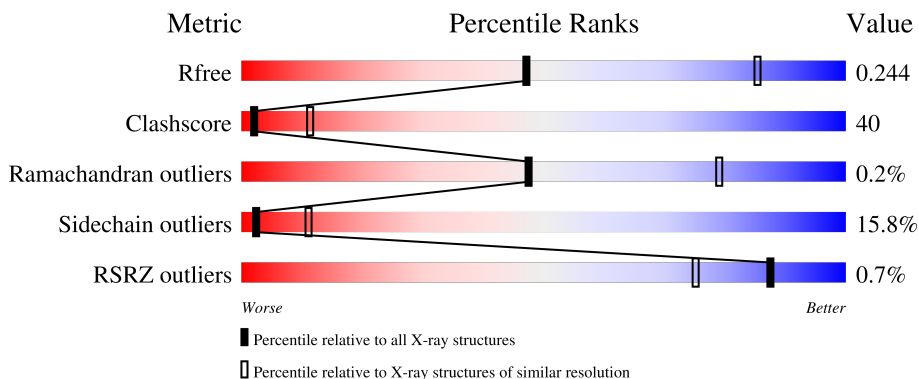
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	509	 50% 43% 7%
1	B	509	 48% 44% 8%
1	C	509	 49% 45% 6%
1	D	509	 50% 43% 7%
1	E	509	 37% 55% 9%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	509	<p>%</p>
1	G	509	
1	H	509	

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
2	FAD	A	601	X	-	-	-
2	FAD	D	601	-	-	X	-
2	FAD	F	601	X	-	-	-

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 32560 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 UDP-galactopyranose mutase.

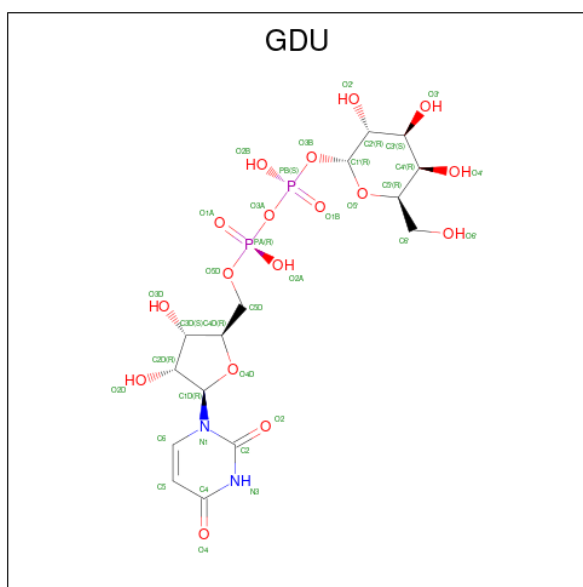
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	509	3990	2531	683	755	21	0	0	0
1	B	509	3990	2531	683	755	21	0	0	0
1	C	509	3990	2531	683	755	21	0	0	0
1	D	509	3990	2531	683	755	21	0	0	0
1	E	509	3990	2531	683	755	21	0	0	0
1	F	509	3990	2531	683	755	21	0	0	0
1	G	509	3990	2531	683	755	21	0	0	0
1	H	509	3990	2531	683	755	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

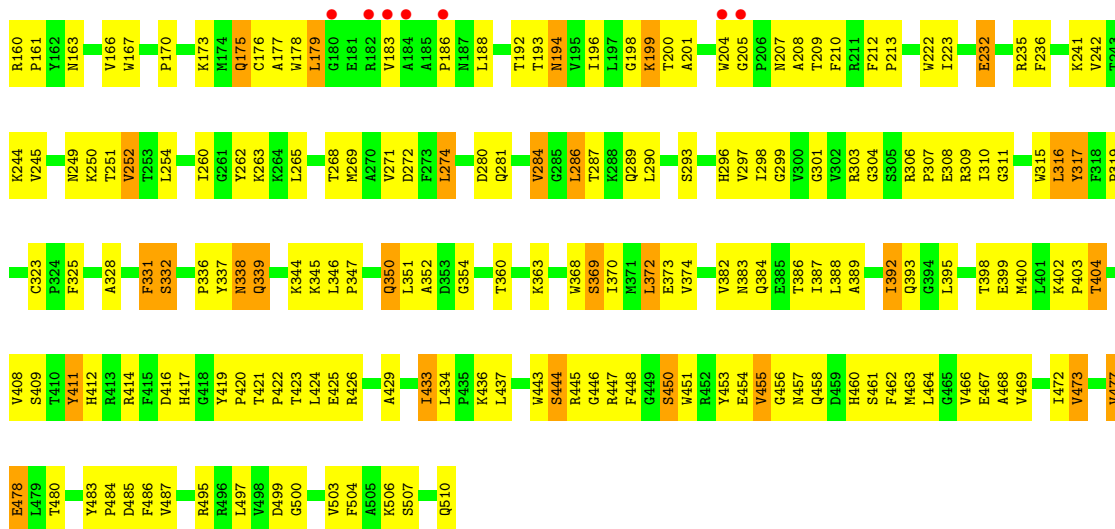
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	ARG	engineered mutation	UNP Q4W1X2
B	327	ALA	ARG	engineered mutation	UNP Q4W1X2
C	327	ALA	ARG	engineered mutation	UNP Q4W1X2
D	327	ALA	ARG	engineered mutation	UNP Q4W1X2
E	327	ALA	ARG	engineered mutation	UNP Q4W1X2
F	327	ALA	ARG	engineered mutation	UNP Q4W1X2
G	327	ALA	ARG	engineered mutation	UNP Q4W1X2
H	327	ALA	ARG	engineered mutation	UNP Q4W1X2

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

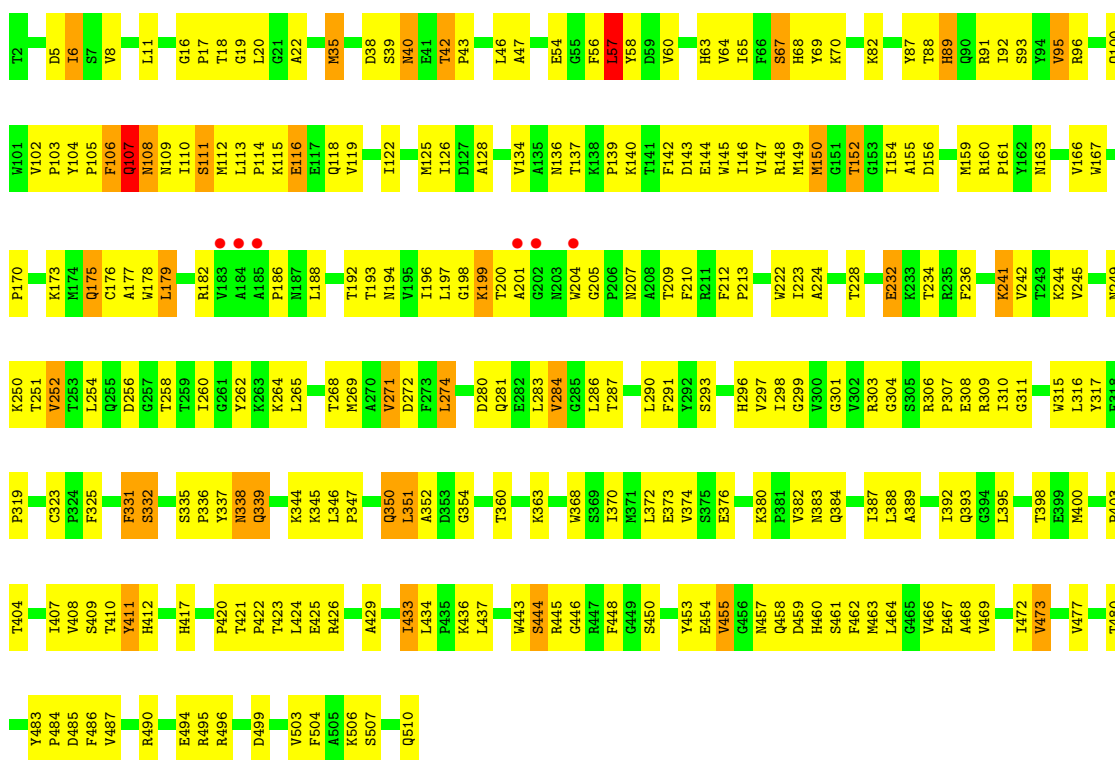




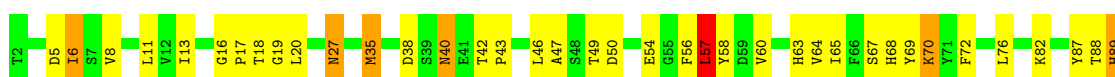




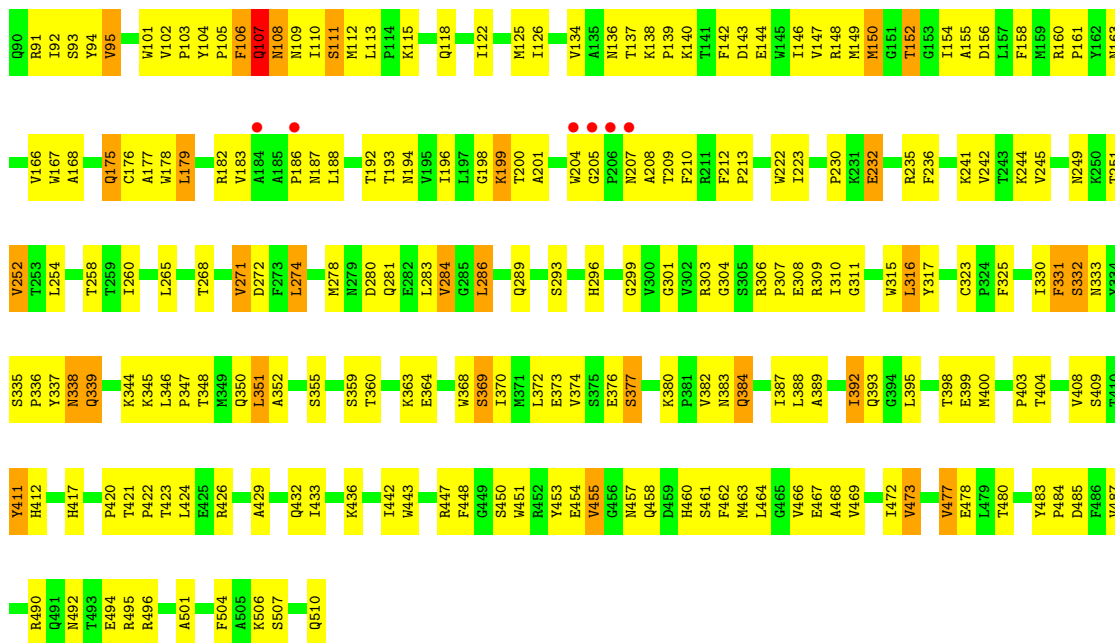
● Molecule 1: UDP-galactopyranose mutase



● Molecule 1: UDP-galactopyranose mutase

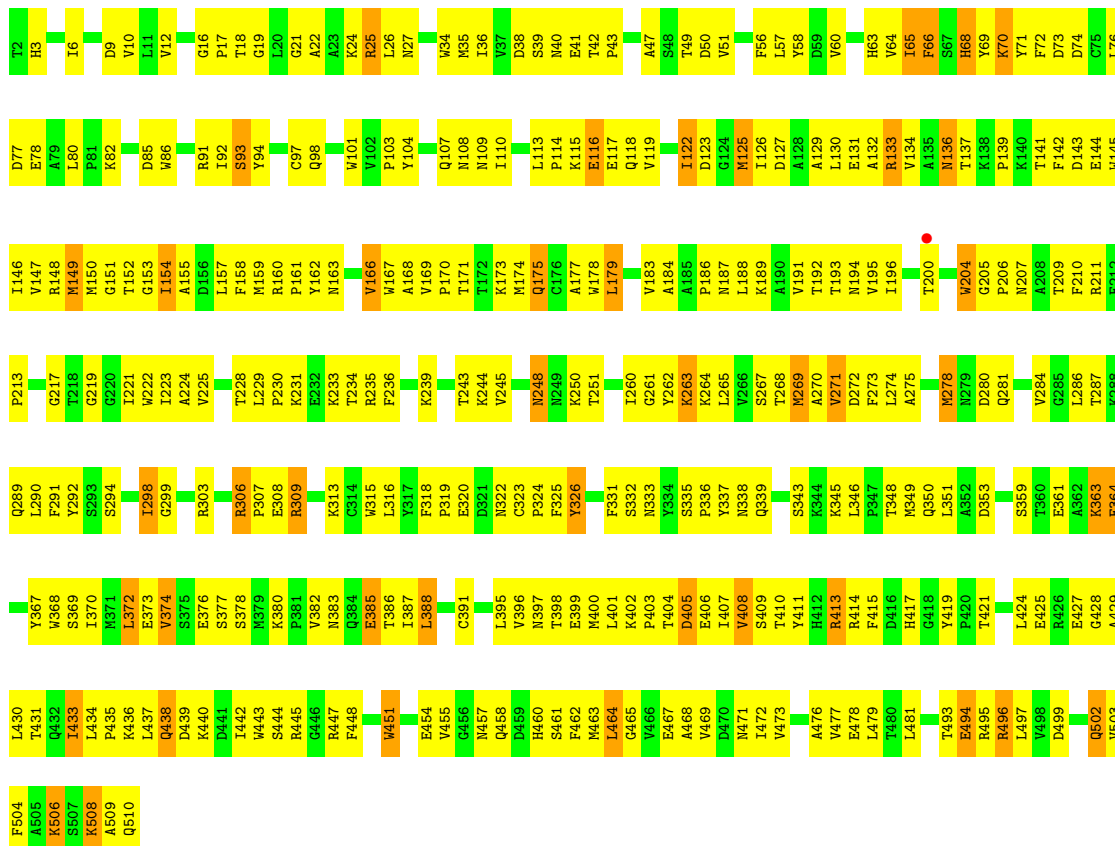




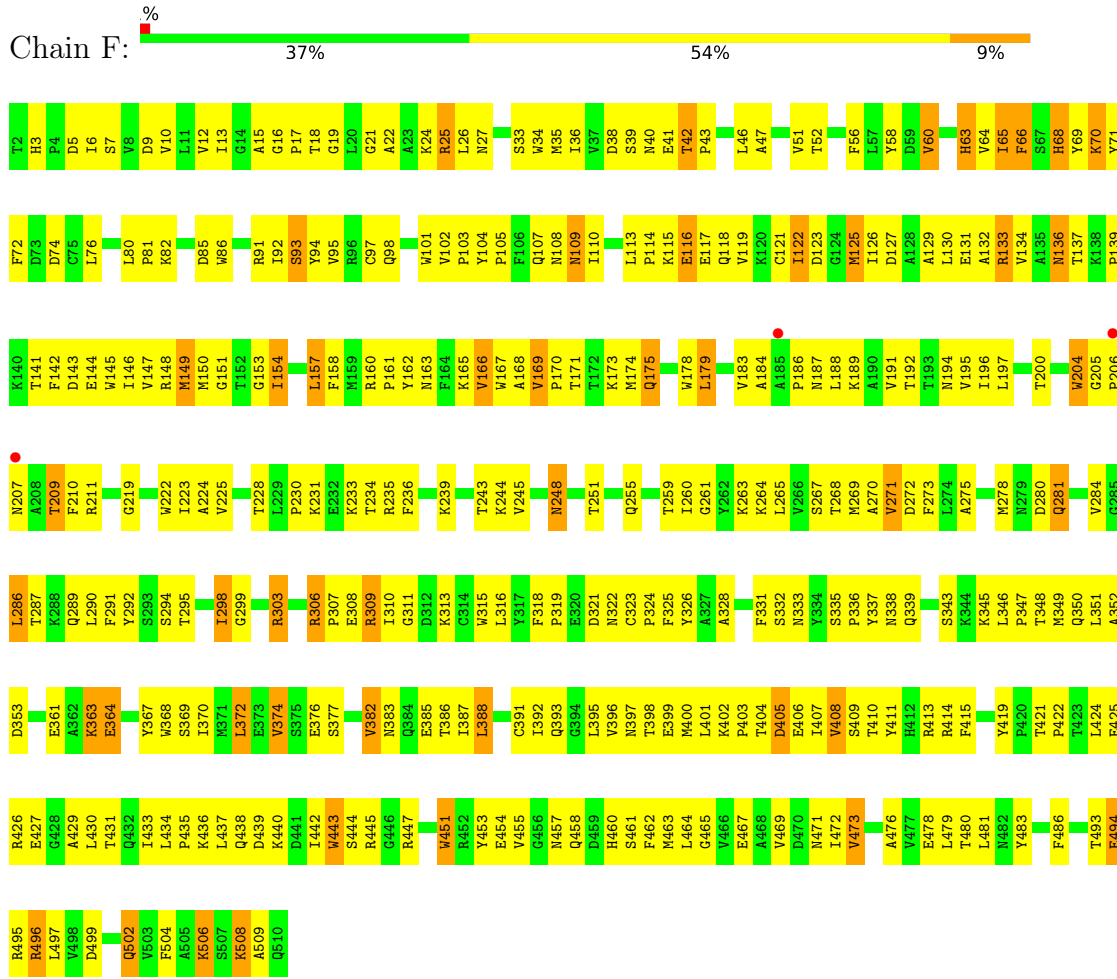


- Molecule 1: UDP-galactopyranose mutase

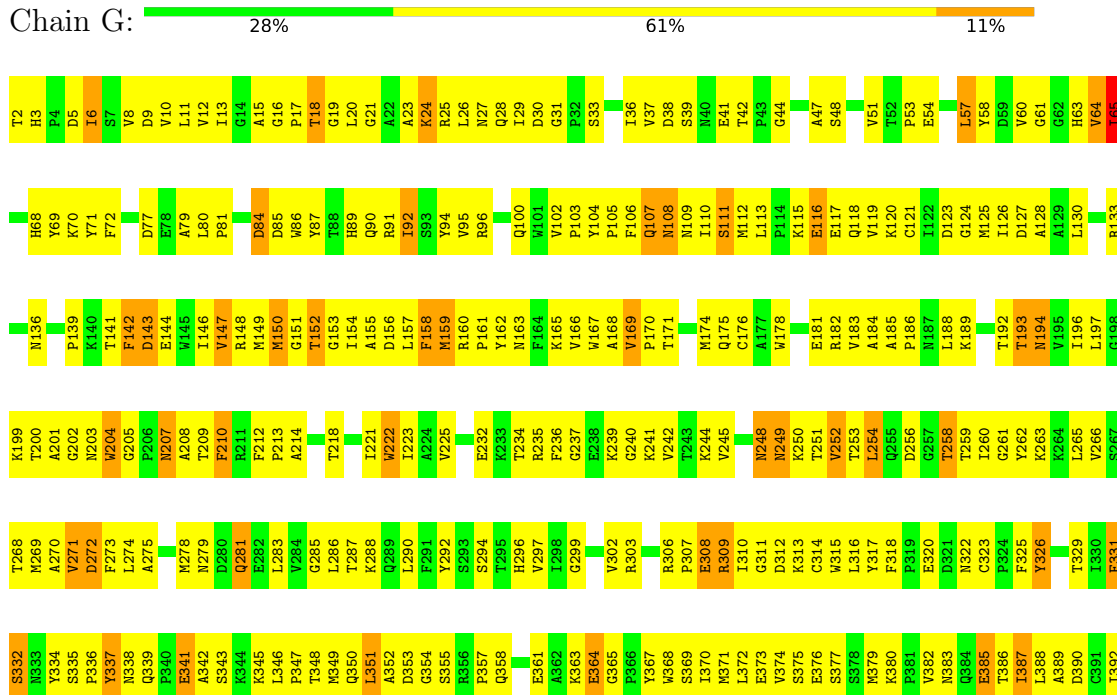
Chain E:

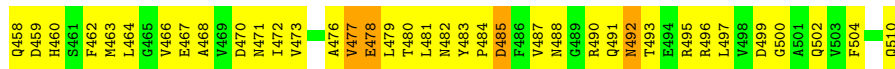


- Molecule 1: UDP-galactopyranose mutase

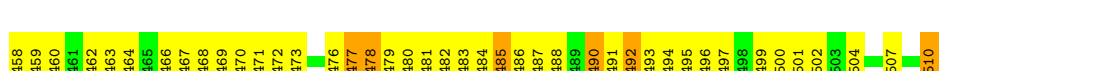
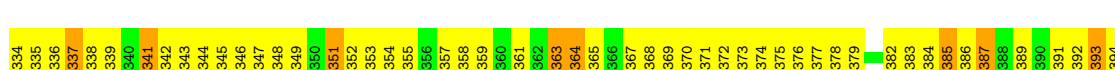
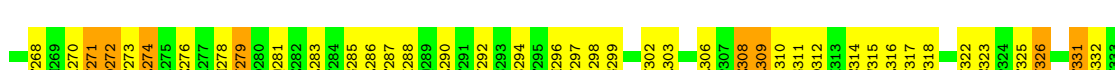
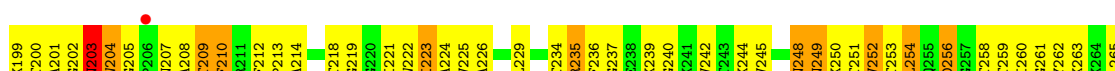
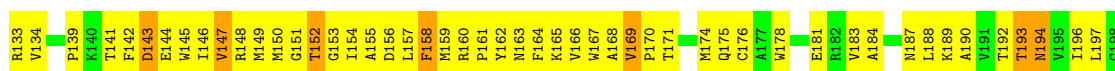
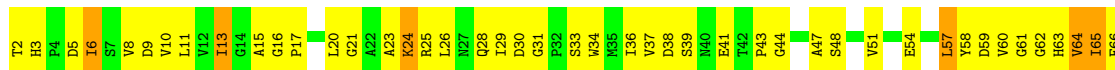
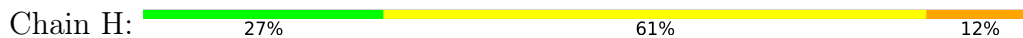


• Molecule 1: UDP-galactopyranose mutase





● Molecule 1: UDP-galactopyranose mutase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.60Å 175.71Å 135.35Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	34.77 – 3.10 34.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (34.77-3.10) 96.2 (34.77-3.10)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	0.24	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, $R_{free}$	0.202 , 0.260 0.201 , 0.244	Depositor DCC
$R_{free}$ test set	5333 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.6	Xtrriage
Anisotropy	0.517	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.000 for l,k,-h 0.327 for h,-k,-l 0.000 for l,-k,h	Xtrriage
Reported twinning fraction	0.479 for h,-k,-l	Depositor
Outliers	2 of 105627 reflections (0.002%)	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	32560	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6278e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDU, 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	0.30	0/4089	0.55	1/5558 (0.0%)
1	B	0.30	0/4089	0.55	1/5558 (0.0%)
1	C	0.30	0/4089	0.55	1/5558 (0.0%)
1	D	0.30	0/4089	0.55	1/5558 (0.0%)
1	E	0.32	0/4089	0.57	0/5558
1	F	0.32	0/4089	0.58	0/5558
1	G	0.32	0/4089	0.61	2/5558 (0.0%)
1	H	0.31	0/4089	0.59	1/5558 (0.0%)
All	All	0.31	0/32712	0.57	7/44464 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	LEU	CA-CB-CG	6.50	130.25	115.30
1	G	205	GLY	O-C-N	-6.40	108.95	121.10
1	B	57	LEU	CA-CB-CG	6.33	129.85	115.30
1	H	205	GLY	N-CA-C	-5.37	99.66	113.10
1	A	57	LEU	CA-CB-CG	5.24	127.35	115.30
1	G	205	GLY	CA-C-N	5.20	131.67	117.10
1	D	57	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	65	ILE	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3990	0	3906	244	0
1	B	3990	0	3906	267	0
1	C	3990	0	3906	265	0
1	D	3990	0	3906	233	0
1	E	3990	0	3906	386	0
1	F	3990	0	3906	359	0
1	G	3990	0	3906	446	0
1	H	3990	0	3906	430	0
2	A	53	0	29	10	0
2	B	53	0	30	14	0
2	C	53	0	30	12	0
2	D	53	0	30	22	0
2	E	53	0	30	20	0
2	F	53	0	29	14	0
2	G	53	0	29	13	0
2	H	53	0	30	10	0
3	A	36	0	22	9	0
3	B	36	0	22	15	0
3	C	36	0	22	9	0
3	D	36	0	22	4	0
3	E	36	0	22	14	0
3	F	36	0	22	8	0
All	All	32560	0	31617	2587	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (2587) 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:E:70:LYS:HG3	1:E:496:ARG:HH22	0.96	1.10
1:F:70:LYS:HG3	1:F:496:ARG:HH22	1.12	1.10
1:F:461:SER:HA	1:F:464:LEU:HD12	1.37	1.06
1:D:303:ARG:NH2	1:D:346:LEU:O	1.90	1.05
1:E:461:SER:HA	1:E:464:LEU:HD12	1.38	1.05
1:B:332:SER:HA	1:B:339:GLN:HE21	1.20	1.04
1:E:133:ARG:HH11	1:E:133:ARG:HG3	1.24	1.02
1:F:16:GLY:HA3	2:F:601:FAD:O1P	1.59	1.02
1:B:62:GLY:O	3:B:602:GDU:O4'	1.76	1.01
1:B:183:VAL:HG22	3:B:602:GDU:H1D	1.36	1.01
1:A:303:ARG:NH2	1:A:346:LEU:O	1.95	1.00
1:H:149:MET:SD	1:H:184:ALA:HA	2.01	1.00
1:G:17:PRO:HD2	2:G:601:FAD:O1P	1.60	0.99
1:D:332:SER:HA	1:D:339:GLN:HE21	1.24	0.99
1:A:104:TYR:HE1	3:A:602:GDU:H5	1.26	0.98
1:A:183:VAL:HG13	3:A:602:GDU:O2	1.65	0.96
1:A:104:TYR:CE1	3:A:602:GDU:H5	2.00	0.96
1:G:115:LYS:HA	1:G:118:GLN:HG3	1.47	0.95
1:C:332:SER:HA	1:C:339:GLN:HE21	1.30	0.95
1:G:18:THR:HG22	1:G:268:THR:HG21	1.49	0.94
1:F:154:ILE:HD13	1:F:154:ILE:H	1.31	0.94
1:G:197:LEU:C	1:G:199:LYS:H	1.70	0.94
1:G:292:TYR:HB2	1:G:419:TYR:O	1.67	0.94
1:E:70:LYS:HG3	1:E:496:ARG:NH2	1.81	0.94
1:A:244:LYS:HB2	1:F:255:GLN:HE21	1.30	0.94
1:H:292:TYR:HB2	1:H:419:TYR:O	1.69	0.93
1:A:332:SER:HA	1:A:339:GLN:HE21	1.34	0.93
1:F:445:ARG:HB3	1:F:464:LEU:HB3	1.51	0.92
1:G:47:ALA:HB3	1:G:222:TRP:HE1	1.34	0.92
1:H:150:MET:HG3	1:H:154:ILE:HB	1.51	0.92
1:F:133:ARG:HH11	1:F:133:ARG:HG3	1.31	0.92
1:F:467:GLU:HG3	1:F:495:ARG:HH12	1.36	0.91
1:B:183:VAL:HG13	3:B:602:GDU:C2	2.01	0.91
1:F:9:ASP:HA	1:F:263:LYS:HD3	1.52	0.90
1:E:445:ARG:HB3	1:E:464:LEU:HB3	1.52	0.90
1:G:105:PRO:HB2	1:G:107:GLN:HG2	1.52	0.89
1:H:29:ILE:HG22	1:H:31:GLY:H	1.36	0.89
1:G:309:ARG:H	1:G:309:ARG:HD3	1.38	0.89
1:H:115:LYS:HA	1:H:118:GLN:HG3	1.53	0.89
1:B:38:ASP:OD1	2:B:601:FAD:H1B	1.73	0.88
1:E:162:TYR:O	1:E:166:VAL:HG12	1.73	0.88
1:H:376:GLU:HG3	1:H:382:VAL:HG13	1.54	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:LEU:O	1:F:192:THR:HG23	1.74	0.88
1:G:17:PRO:CD	2:G:601:FAD:O1P	2.20	0.88
1:G:121:CYS:HB3	1:G:154:ILE:HG13	1.56	0.88
1:C:332:SER:HA	1:C:339:GLN:NE2	1.89	0.88
1:G:445:ARG:HA	1:G:450:SER:HB2	1.53	0.88
1:H:455:VAL:O	1:H:460:HIS:HB3	1.74	0.88
1:H:47:ALA:HB3	1:H:222:TRP:HE1	1.36	0.87
1:E:149:MET:SD	1:E:186:PRO:HD2	2.14	0.87
1:C:110:ILE:HA	1:C:113:LEU:HD12	1.57	0.87
1:H:271:VAL:HG12	1:H:448:PHE:O	1.75	0.87
1:H:59:ASP:HB3	1:H:63:HIS:HD2	1.40	0.87
1:H:309:ARG:HD3	1:H:309:ARG:H	1.41	0.86
1:D:122:ILE:O	1:D:126:ILE:HG13	1.76	0.86
1:B:110:ILE:HA	1:B:113:LEU:HD12	1.57	0.86
1:G:121:CYS:HA	1:G:153:GLY:HA3	1.58	0.86
1:C:178:TRP:HB2	1:C:454:GLU:HG3	1.57	0.86
1:D:105:PRO:O	1:D:109:ASN:ND2	2.09	0.86
1:D:178:TRP:HB2	1:D:454:GLU:HG3	1.57	0.86
1:G:69:TYR:CD2	1:G:463:MET:HG3	2.11	0.86
1:G:376:GLU:HG3	1:G:382:VAL:HG13	1.57	0.86
1:B:193:THR:HG23	1:H:119:VAL:HG11	1.58	0.85
1:G:150:MET:HG3	1:G:154:ILE:HB	1.58	0.85
1:C:494:GLU:HG2	1:G:477:VAL:HA	1.56	0.85
1:A:122:ILE:O	1:A:126:ILE:HG13	1.77	0.85
1:B:178:TRP:HB2	1:B:454:GLU:HG3	1.57	0.85
1:E:9:ASP:HA	1:E:263:LYS:HD3	1.57	0.85
1:E:63:HIS:CE1	2:E:601:FAD:C9A	2.59	0.85
1:A:111:SER:HB3	1:A:198:GLY:HA2	1.58	0.85
1:A:243:THR:HB	1:F:243:THR:HG21	1.56	0.85
3:A:602:GDU:H5'1	3:A:602:GDU:H6	1.59	0.84
1:F:56:PHE:CE1	1:F:339:GLN:HB3	2.12	0.84
2:A:601:FAD:H9	2:A:601:FAD:O2'	1.77	0.84
1:G:91:ARG:HH21	1:G:203:ASN:HA	1.40	0.84
1:G:149:MET:SD	1:G:184:ALA:HA	2.17	0.84
1:H:121:CYS:HA	1:H:153:GLY:HA3	1.60	0.84
1:D:332:SER:HA	1:D:339:GLN:NE2	1.92	0.84
1:H:332:SER:HA	1:H:339:GLN:NE2	1.92	0.84
1:E:154:ILE:HD13	1:E:154:ILE:H	1.44	0.83
1:G:17:PRO:HD2	2:G:601:FAD:O1A	1.78	0.83
1:G:281:GLN:OE1	1:G:281:GLN:HA	1.75	0.83
1:F:175:GLN:OE1	1:F:178:TRP:HD1	1.59	0.83

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:VAL:HG23	1:E:196:ILE:HG21	1.61	0.83
1:H:109:ASN:ND2	1:H:201:ALA:O	2.12	0.83
1:E:455:VAL:HA	1:E:460:HIS:HD1	1.44	0.82
1:F:187:ASN:OD1	1:F:189:LYS:HB2	1.79	0.82
1:H:57:LEU:HD11	1:H:338:ASN:HA	1.61	0.82
1:H:121:CYS:HB3	1:H:154:ILE:HG13	1.61	0.82
1:A:178:TRP:HB2	1:A:454:GLU:HG3	1.60	0.82
1:A:280:ASP:O	1:A:284:VAL:HG23	1.78	0.82
1:E:458:GLN:HG3	2:E:601:FAD:H2'	1.62	0.82
1:E:332:SER:HA	1:E:339:GLN:NE2	1.95	0.82
1:E:338:ASN:HB2	1:E:339:GLN:NE2	1.94	0.81
1:G:411:TYR:HD1	1:G:412:HIS:N	1.78	0.81
1:H:69:TYR:CD2	1:H:463:MET:HG3	2.16	0.81
1:A:332:SER:HA	1:A:339:GLN:NE2	1.94	0.81
1:B:332:SER:HA	1:B:339:GLN:NE2	1.94	0.81
1:D:91:ARG:HG3	1:D:315:TRP:CH2	2.16	0.81
1:H:468:ALA:O	1:H:471:ASN:HB3	1.80	0.81
1:A:244:LYS:HB2	1:F:255:GLN:NE2	1.96	0.81
1:E:281:GLN:OE1	1:E:281:GLN:HA	1.79	0.81
1:F:430:LEU:HD22	1:F:434:LEU:HG	1.61	0.81
1:D:16:GLY:HA3	2:D:601:FAD:H52A	1.62	0.80
1:G:332:SER:HA	1:G:339:GLN:NE2	1.96	0.80
1:B:111:SER:HB3	1:B:198:GLY:HA2	1.64	0.80
1:D:91:ARG:HD3	1:D:207:ASN:HB2	1.64	0.80
1:A:350:GLN:HE22	1:A:354:GLY:HA2	1.46	0.80
1:F:70:LYS:HG3	1:F:496:ARG:NH2	1.93	0.80
1:F:467:GLU:HG3	1:F:495:ARG:NH1	1.96	0.80
1:G:197:LEU:C	1:G:199:LYS:N	2.35	0.80
1:D:280:ASP:O	1:D:284:VAL:HG23	1.81	0.80
1:F:27:ASN:HB2	1:F:34:TRP:CZ2	2.16	0.80
1:H:411:TYR:HD1	1:H:412:HIS:N	1.80	0.80
1:E:457:ASN:HB3	2:E:601:FAD:C2	2.12	0.79
1:D:458:GLN:HG3	2:D:601:FAD:H2'	1.63	0.79
1:H:105:PRO:HB2	1:H:107:GLN:HG2	1.64	0.79
1:H:144:GLU:O	1:H:148:ARG:HG3	1.83	0.79
1:F:63:HIS:H	1:F:63:HIS:CD2	1.98	0.79
1:G:57:LEU:HD11	1:G:338:ASN:HA	1.65	0.79
1:H:271:VAL:N	1:H:448:PHE:O	2.14	0.79
1:H:389:ALA:HA	1:H:392:ILE:HD12	1.63	0.79
1:G:154:ILE:H	1:G:154:ILE:HD12	1.45	0.79
1:H:417:HIS:HB3	1:H:448:PHE:CE2	2.17	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:VAL:HG22	1:G:57:LEU:HB3	1.64	0.78
1:C:91:ARG:HG3	1:C:315:TRP:CH2	2.19	0.78
1:A:110:ILE:HA	1:A:113:LEU:HD12	1.64	0.78
1:A:188:LEU:O	1:A:192:THR:HG23	1.83	0.78
1:G:218:THR:HA	1:G:221:ILE:HD12	1.64	0.78
1:A:91:ARG:HH12	1:A:205:GLY:HA3	1.49	0.78
1:D:111:SER:HB3	1:D:198:GLY:HA2	1.65	0.78
1:G:29:ILE:HG22	1:G:31:GLY:H	1.49	0.78
1:G:346:LEU:HD23	1:G:347:PRO:HD2	1.65	0.78
1:F:230:PRO:HG2	1:F:233:LYS:HD2	1.66	0.78
1:H:418:GLY:C	1:H:419:TYR:HD1	1.86	0.78
1:B:398:THR:HG22	1:B:400:MET:HG2	1.64	0.78
1:E:188:LEU:O	1:E:192:THR:HG23	1.84	0.78
1:G:314:CYS:HB3	1:G:315:TRP:HE3	1.49	0.78
1:H:359:SER:HB3	1:H:363:LYS:HE2	1.66	0.78
1:E:22:ALA:HA	1:E:469:VAL:CG2	2.14	0.77
1:H:194:ASN:ND2	1:H:199:LYS:HB3	1.99	0.77
1:D:110:ILE:HA	1:D:113:LEU:HD12	1.67	0.77
1:F:178:TRP:HB2	1:F:454:GLU:HG3	1.65	0.77
1:A:91:ARG:HD3	1:A:207:ASN:HB2	1.67	0.77
1:B:122:ILE:O	1:B:126:ILE:HG13	1.84	0.77
1:G:18:THR:HG22	1:G:268:THR:CG2	2.14	0.77
1:H:314:CYS:HB3	1:H:315:TRP:HE3	1.49	0.77
1:C:188:LEU:O	1:C:192:THR:HG23	1.84	0.77
1:H:17:PRO:HG3	1:H:222:TRP:CZ2	2.20	0.77
1:F:151:GLY:O	1:F:154:ILE:HG12	1.85	0.77
1:G:79:ALA:HB2	1:G:225:VAL:HG23	1.65	0.77
1:B:188:LEU:O	1:B:192:THR:HG23	1.85	0.77
1:A:420:PRO:HG2	1:A:453:TYR:HB2	1.66	0.77
1:C:398:THR:O	1:C:398:THR:HG22	1.84	0.77
1:G:18:THR:CG2	1:G:268:THR:HG21	2.14	0.77
1:H:51:VAL:HG22	1:H:57:LEU:HB3	1.66	0.77
1:C:122:ILE:O	1:C:126:ILE:HG13	1.84	0.76
1:F:101:TRP:CZ3	1:F:316:LEU:HD13	2.19	0.76
1:G:96:ARG:HG2	1:G:398:THR:HG22	1.67	0.76
1:H:249:ASN:HB2	1:H:251:THR:HG23	1.66	0.76
1:F:108:ASN:HB3	1:F:194:ASN:ND2	2.00	0.76
1:H:47:ALA:HB3	1:H:222:TRP:NE1	2.00	0.76
1:A:91:ARG:HG3	1:A:315:TRP:CH2	2.20	0.76
1:E:398:THR:OG1	1:E:400:MET:HG2	1.85	0.76
1:F:332:SER:HA	1:F:339:GLN:NE2	1.99	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:SER:HB3	1:C:198:GLY:HA2	1.67	0.76
1:E:353:ASP:HB3	1:E:403:PRO:CB	2.15	0.76
1:E:267:SER:O	1:E:444:SER:HA	1.86	0.76
1:F:149:MET:SD	1:F:186:PRO:HD2	2.25	0.76
1:G:468:ALA:O	1:G:471:ASN:HB3	1.84	0.76
1:E:19:GLY:N	1:E:268:THR:HG21	2.01	0.76
1:E:280:ASP:O	1:E:284:VAL:HG23	1.86	0.76
1:G:348:THR:O	1:G:357:PRO:HG3	1.85	0.76
1:E:178:TRP:HB2	1:E:454:GLU:HG3	1.65	0.76
1:F:22:ALA:HA	1:F:469:VAL:CG2	2.15	0.76
1:F:338:ASN:HB2	1:F:339:GLN:NE2	2.01	0.75
1:H:130:LEU:O	1:H:133:ARG:HB3	1.86	0.75
1:G:18:THR:CG2	1:G:268:THR:CG2	2.63	0.75
1:E:127:ASP:O	1:E:131:GLU:HG2	1.86	0.75
1:H:155:ALA:O	1:H:160:ARG:HG3	1.86	0.75
1:A:414:ARG:HD3	1:F:281:GLN:HB3	1.68	0.75
1:E:56:PHE:CE1	1:E:339:GLN:HB3	2.21	0.75
1:G:47:ALA:HB3	1:G:222:TRP:NE1	2.02	0.75
1:G:351:LEU:O	1:G:354:GLY:N	2.19	0.75
1:B:91:ARG:HD3	1:B:207:ASN:HB2	1.67	0.75
1:F:91:ARG:HD3	1:F:207:ASN:HB2	1.67	0.75
1:A:60:VAL:O	1:A:63:HIS:NE2	2.20	0.75
1:C:280:ASP:O	1:C:284:VAL:HG23	1.86	0.75
1:B:47:ALA:HB1	1:B:222:TRP:HE1	1.51	0.75
1:H:446:GLY:H	1:H:450:SER:HB3	1.52	0.75
1:D:188:LEU:O	1:D:192:THR:HG23	1.87	0.74
1:F:80:LEU:HD12	1:F:86:TRP:CZ2	2.22	0.74
1:D:420:PRO:HG2	1:D:453:TYR:HB2	1.69	0.74
1:F:127:ASP:O	1:F:131:GLU:HG2	1.88	0.74
1:G:271:VAL:HG12	1:G:448:PHE:O	1.87	0.74
1:G:338:ASN:HB2	1:G:339:GLN:NE2	2.03	0.74
1:H:393:GLN:O	1:H:396:VAL:N	2.19	0.74
1:B:280:ASP:O	1:B:284:VAL:HG23	1.86	0.74
1:G:109:ASN:ND2	1:G:201:ALA:O	2.21	0.74
1:D:462:PHE:O	1:D:466:VAL:HG23	1.88	0.74
1:E:60:VAL:O	1:E:63:HIS:NE2	2.21	0.74
1:G:393:GLN:O	1:G:396:VAL:N	2.19	0.74
1:D:104:TYR:CD1	1:D:105:PRO:HA	2.22	0.73
1:G:249:ASN:HB2	1:G:251:THR:HG23	1.69	0.73
1:G:17:PRO:HG3	1:G:222:TRP:CZ2	2.22	0.73
1:G:271:VAL:N	1:G:448:PHE:O	2.20	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:443:TRP:HA	1:H:445:ARG:HH21	1.54	0.73
1:E:71:TYR:O	1:E:74:ASP:HB2	1.87	0.73
1:E:383:ASN:HB3	1:E:386:THR:OG1	1.88	0.73
1:H:303:ARG:NH1	1:H:406:GLU:OE2	2.21	0.73
1:H:338:ASN:HB2	1:H:339:GLN:NE2	2.03	0.73
1:B:159:MET:HE3	3:B:602:GDU:HN3	1.53	0.73
1:B:91:ARG:HG3	1:B:315:TRP:CH2	2.24	0.73
1:B:108:ASN:OD1	1:B:108:ASN:N	2.20	0.73
1:H:79:ALA:HB2	1:H:225:VAL:HG23	1.70	0.73
1:C:421:THR:HG22	1:C:423:THR:HG23	1.69	0.72
1:G:418:GLY:C	1:G:419:TYR:HD1	1.91	0.72
1:F:93:SER:OG	1:F:315:TRP:NE1	2.22	0.72
1:G:37:VAL:HG12	1:G:235:ARG:HB2	1.71	0.72
1:G:104:TYR:O	1:G:203:ASN:N	2.22	0.72
1:F:303:ARG:HH21	1:F:363:LYS:HB2	1.52	0.72
1:E:471:ASN:ND2	1:E:476:ALA:O	2.20	0.72
1:G:18:THR:HG21	1:G:268:THR:HG22	1.72	0.72
1:B:130:LEU:HD23	1:H:130:LEU:HD23	1.72	0.72
1:G:181:GLU:N	1:G:485:ASP:OD1	2.21	0.72
1:B:420:PRO:HG2	1:B:453:TYR:HB2	1.70	0.72
1:C:104:TYR:CD1	1:C:105:PRO:HA	2.25	0.72
1:E:91:ARG:HD3	1:E:207:ASN:HB2	1.71	0.72
1:G:48:SER:O	1:G:60:VAL:HG23	1.89	0.72
1:A:104:TYR:CD1	1:A:105:PRO:HA	2.23	0.72
1:C:350:GLN:HE22	1:C:354:GLY:HA2	1.55	0.72
1:E:80:LEU:HD12	1:E:86:TRP:CZ2	2.23	0.72
1:F:398:THR:OG1	1:F:400:MET:HG2	1.90	0.72
1:H:402:LYS:NZ	1:H:405:ASP:OD1	2.21	0.72
1:C:303:ARG:NH2	1:C:363:LYS:O	2.22	0.72
1:E:303:ARG:NH2	1:E:363:LYS:HG3	2.04	0.72
1:E:457:ASN:HA	2:E:601:FAD:H1'2	1.71	0.72
1:E:465:GLY:O	1:E:469:VAL:HG23	1.90	0.72
1:E:133:ARG:HG3	1:E:133:ARG:NH1	2.03	0.72
1:F:19:GLY:N	1:F:268:THR:HG21	2.04	0.71
1:G:142:PHE:HB3	1:G:171:THR:O	1.89	0.71
1:G:417:HIS:HB3	1:G:448:PHE:CE2	2.24	0.71
1:H:59:ASP:HB3	1:H:63:HIS:CD2	2.23	0.71
1:A:104:TYR:HE1	3:A:602:GDU:C5	2.03	0.71
1:D:91:ARG:HH12	1:D:205:GLY:HA3	1.54	0.71
1:E:230:PRO:HG2	1:E:233:LYS:HD2	1.71	0.71
1:E:9:ASP:O	1:E:263:LYS:HB2	1.91	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:494:GLU:H	1:F:494:GLU:CD	1.91	0.71
1:G:130:LEU:O	1:G:133:ARG:HB3	1.90	0.71
1:C:420:PRO:HG2	1:C:453:TYR:HB2	1.70	0.71
1:F:353:ASP:HB3	1:F:403:PRO:CB	2.20	0.71
1:F:465:GLY:O	1:F:469:VAL:HG23	1.90	0.71
1:G:314:CYS:HB3	1:G:315:TRP:CE3	2.26	0.71
1:A:462:PHE:O	1:A:466:VAL:HG23	1.89	0.71
1:H:181:GLU:OE1	1:H:181:GLU:HA	1.91	0.71
1:H:212:PHE:CG	1:H:213:PRO:HD2	2.25	0.71
1:A:421:THR:HG22	1:A:423:THR:HG23	1.72	0.71
1:C:91:ARG:HD3	1:C:207:ASN:HB2	1.73	0.71
1:G:143:ASP:HA	1:G:146:ILE:HD12	1.71	0.71
1:H:188:LEU:O	1:H:192:THR:HG23	1.90	0.71
1:A:473:VAL:O	1:E:499:ASP:HB3	1.91	0.71
1:E:122:ILE:O	1:E:126:ILE:HG13	1.91	0.71
1:G:188:LEU:O	1:G:192:THR:HG23	1.91	0.71
1:G:447:ARG:O	1:G:451:TRP:HA	1.91	0.71
1:B:183:VAL:HG22	3:B:602:GDU:C1D	2.18	0.70
1:F:27:ASN:HB2	1:F:34:TRP:HZ2	1.55	0.70
1:G:28:GLN:HE21	1:G:497:LEU:C	1.93	0.70
1:H:218:THR:HA	1:H:221:ILE:HD12	1.73	0.70
1:E:265:LEU:HD23	1:E:442:ILE:HG12	1.72	0.70
1:G:303:ARG:NH1	1:G:406:GLU:OE2	2.23	0.70
1:A:455:VAL:O	1:A:460:HIS:HB3	1.90	0.70
1:G:171:THR:HA	1:G:174:MET:HE2	1.72	0.70
1:G:392:ILE:O	1:G:395:LEU:HB2	1.92	0.70
1:H:54:GLU:HB3	1:H:346:LEU:HD11	1.71	0.70
1:H:482:ASN:HB2	1:H:483:TYR:CE2	2.27	0.70
1:C:115:LYS:HD3	1:E:196:ILE:O	1.90	0.70
1:E:70:LYS:HB3	1:E:496:ARG:HH12	1.56	0.70
1:H:467:GLU:OE1	1:H:480:THR:N	2.21	0.70
1:H:37:VAL:HG12	1:H:235:ARG:HB2	1.73	0.70
1:D:463:MET:O	1:D:467:GLU:HG3	1.92	0.70
1:B:419:TYR:HE1	2:B:601:FAD:HM73	1.54	0.70
1:C:47:ALA:HB1	1:C:222:TRP:HE1	1.56	0.70
1:E:142:PHE:O	1:E:145:TRP:HB3	1.91	0.70
1:F:267:SER:O	1:F:444:SER:HA	1.90	0.70
1:F:303:ARG:HH21	1:F:363:LYS:CB	2.05	0.70
1:G:25:ARG:HH11	1:G:470:ASP:CG	1.94	0.70
1:G:468:ALA:O	1:G:472:ILE:HD12	1.92	0.70
1:H:96:ARG:HG2	1:H:398:THR:HG22	1.74	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:PRO:HG2	1:C:109:ASN:ND2	2.06	0.70
1:H:274:LEU:O	1:H:278:MET:HG2	1.92	0.70
1:H:440:LYS:HB2	1:H:442:ILE:HD12	1.74	0.70
1:A:91:ARG:NH2	1:A:204:TRP:O	2.24	0.70
1:G:142:PHE:O	1:G:146:ILE:HG13	1.92	0.70
1:G:445:ARG:HA	1:G:450:SER:CB	2.21	0.70
1:E:175:GLN:HE22	1:E:177:ALA:HB3	1.56	0.69
1:H:84:ASP:OD2	1:H:84:ASP:N	2.22	0.69
1:E:455:VAL:HG23	1:E:455:VAL:O	1.91	0.69
1:B:350:GLN:HE22	1:B:354:GLY:HA2	1.57	0.69
1:H:107:GLN:H	1:H:107:GLN:CD	1.94	0.69
1:H:308:GLU:HG3	1:H:309:ARG:HD3	1.74	0.69
1:B:104:TYR:CD1	1:B:105:PRO:HA	2.28	0.69
1:E:118:GLN:OE1	1:E:195:VAL:HG13	1.92	0.69
1:B:176:CYS:O	1:B:179:LEU:HD12	1.93	0.69
1:F:280:ASP:O	1:F:284:VAL:HG23	1.93	0.69
1:H:484:PRO:HA	1:H:487:VAL:HG22	1.74	0.69
1:G:84:ASP:OD2	1:G:84:ASP:N	2.24	0.69
1:H:103:PRO:HB2	1:H:202:GLY:HA2	1.75	0.69
1:B:91:ARG:HH12	1:B:205:GLY:HA3	1.56	0.69
1:B:398:THR:CG2	1:B:398:THR:O	2.40	0.69
1:E:22:ALA:HA	1:E:469:VAL:HG22	1.75	0.69
1:E:313:LYS:O	1:E:333:ASN:ND2	2.26	0.69
1:G:144:GLU:O	1:G:148:ARG:HG3	1.93	0.69
1:G:159:MET:O	1:G:163:ASN:HB2	1.91	0.69
1:G:207:ASN:C	1:G:207:ASN:OD1	2.31	0.69
1:H:314:CYS:HB3	1:H:315:TRP:CE3	2.26	0.69
1:D:421:THR:HG22	1:D:423:THR:HG23	1.74	0.69
1:E:419:TYR:HE1	2:E:601:FAD:HM73	1.58	0.69
1:C:455:VAL:O	1:C:460:HIS:HB3	1.93	0.69
1:F:63:HIS:H	1:F:63:HIS:HD2	1.40	0.69
1:F:105:PRO:O	1:F:109:ASN:ND2	2.26	0.69
1:F:163:ASN:OD1	3:F:602:GDU:O3D	2.09	0.69
1:G:389:ALA:HA	1:G:392:ILE:HD12	1.75	0.69
1:E:350:GLN:O	1:E:407:ILE:HB	1.93	0.68
1:F:133:ARG:HG3	1:F:133:ARG:NH1	2.04	0.68
1:G:322:ASN:HD22	1:G:397:ASN:HB3	1.58	0.68
1:G:341:GLU:HG3	1:G:343:SER:H	1.59	0.68
1:G:492:ASN:HD22	1:G:492:ASN:H	1.42	0.68
1:H:203:ASN:HD22	1:H:204:TRP:H	1.39	0.68
1:E:18:THR:OG1	1:E:461:SER:HB3	1.92	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:GLU:HB3	1:G:346:LEU:HD11	1.76	0.68
1:H:142:PHE:O	1:H:146:ILE:HG13	1.93	0.68
1:C:19:GLY:N	1:C:268:THR:HG21	2.09	0.68
1:C:429:ALA:O	1:C:433:ILE:HD12	1.93	0.68
1:E:101:TRP:CZ3	1:E:316:LEU:HD13	2.29	0.68
1:H:445:ARG:HA	1:H:450:SER:HB2	1.73	0.68
1:C:462:PHE:O	1:C:466:VAL:HG23	1.93	0.68
1:E:104:TYR:HE1	3:E:602:GDU:C5	2.06	0.68
1:G:331:PHE:CD2	1:G:338:ASN:HB3	2.29	0.68
1:C:136:ASN:OD1	1:C:137:THR:HG23	1.92	0.68
1:E:143:ASP:HA	1:E:146:ILE:HD12	1.76	0.68
1:H:159:MET:O	1:H:163:ASN:HB2	1.93	0.68
1:C:453:TYR:OH	3:C:602:GDU:O3A	2.10	0.68
1:G:245:VAL:O	1:G:278:MET:HA	1.93	0.68
1:B:40:ASN:O	1:B:236:PHE:HB3	1.94	0.68
1:E:27:ASN:HB2	1:E:34:TRP:CZ2	2.29	0.68
1:A:18:THR:OG1	1:A:461:SER:HB3	1.94	0.68
1:D:455:VAL:O	1:D:460:HIS:HB3	1.93	0.68
1:E:93:SER:OG	1:E:315:TRP:NE1	2.27	0.68
1:H:60:VAL:O	1:H:63:HIS:NE2	2.27	0.68
1:H:68:HIS:O	1:H:492:ASN:ND2	2.27	0.68
1:B:462:PHE:O	1:B:466:VAL:HG23	1.94	0.67
1:D:54:GLU:HB3	1:D:346:LEU:HD11	1.76	0.67
1:F:71:TYR:O	1:F:74:ASP:HB2	1.93	0.67
1:F:431:THR:O	1:F:435:PRO:HG2	1.94	0.67
1:H:281:GLN:OE1	1:H:281:GLN:HA	1.93	0.67
1:E:12:VAL:HB	1:E:36:ILE:HG13	1.75	0.67
1:E:16:GLY:HA3	2:E:601:FAD:O1P	1.94	0.67
1:F:5:ASP:H	1:F:259:THR:HG1	1.40	0.67
1:B:271:VAL:HA	1:B:274:LEU:HB2	1.77	0.67
1:B:421:THR:HG22	1:B:423:THR:HG23	1.76	0.67
1:C:103:PRO:HB2	1:C:109:ASN:ND2	2.10	0.67
1:E:437:LEU:HB3	1:E:442:ILE:HB	1.75	0.67
1:B:142:PHE:O	1:B:146:ILE:HG13	1.94	0.67
1:G:445:ARG:NH1	1:G:481:LEU:HD22	2.10	0.67
1:H:447:ARG:O	1:H:451:TRP:HA	1.95	0.67
1:A:136:ASN:OD1	1:A:137:THR:HG23	1.95	0.67
1:B:107:GLN:NE2	3:B:602:GDU:O4	2.27	0.67
1:D:63:HIS:CD2	2:D:601:FAD:C5X	2.78	0.67
1:D:91:ARG:NH1	1:D:205:GLY:HA3	2.09	0.67
1:D:115:LYS:HB3	1:F:197:LEU:HD23	1.77	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ILE:HG23	1:F:126:ILE:HD11	1.76	0.67
1:F:336:PRO:HG2	1:F:337:TYR:CD1	2.30	0.67
1:G:204:TRP:HB3	1:G:208:ALA:HB2	1.76	0.67
1:G:353:ASP:HB3	1:G:403:PRO:HB3	1.77	0.67
1:B:159:MET:CE	3:B:602:GDU:HN3	2.08	0.67
1:B:398:THR:HG22	1:B:398:THR:O	1.93	0.67
1:H:297:VAL:HB	1:H:415:PHE:HE2	1.59	0.67
1:A:358:GLN:OE1	1:A:358:GLN:N	2.28	0.67
1:B:43:PRO:HG2	1:B:223:ILE:HD13	1.77	0.67
1:E:179:LEU:N	1:E:179:LEU:HD23	2.09	0.67
1:E:494:GLU:H	1:E:494:GLU:CD	1.98	0.67
1:B:91:ARG:NH2	1:B:204:TRP:O	2.28	0.67
1:C:108:ASN:OD1	1:C:108:ASN:N	2.21	0.67
1:A:58:TYR:HA	1:A:331:PHE:HE2	1.59	0.67
1:G:155:ALA:O	1:G:160:ARG:HG3	1.95	0.67
1:H:392:ILE:O	1:H:395:LEU:HB2	1.95	0.67
1:E:187:ASN:OD1	1:E:189:LYS:HB2	1.95	0.67
1:F:184:ALA:HA	1:F:204:TRP:CZ2	2.29	0.67
1:E:17:PRO:O	1:E:462:PHE:HA	1.95	0.66
1:F:104:TYR:CE1	3:F:602:GDU:O4	2.48	0.66
1:C:303:ARG:HH21	1:C:363:LYS:C	1.98	0.66
1:F:12:VAL:HB	1:F:36:ILE:HG13	1.76	0.66
1:F:91:ARG:HG3	1:F:315:TRP:CH2	2.29	0.66
1:F:142:PHE:O	1:F:145:TRP:HB3	1.95	0.66
1:B:119:VAL:HG22	1:H:193:THR:HG22	1.76	0.66
1:H:57:LEU:CD1	1:H:338:ASN:HA	2.25	0.66
1:A:45:GLY:HA3	2:A:601:FAD:O1A	1.96	0.66
1:A:54:GLU:HB3	1:A:346:LEU:HD11	1.77	0.66
1:E:429:ALA:O	1:E:433:ILE:HG13	1.95	0.66
1:D:63:HIS:HD2	2:D:601:FAD:C5X	2.08	0.66
1:F:281:GLN:HA	1:F:281:GLN:OE1	1.96	0.66
1:H:204:TRP:HA	1:H:204:TRP:CE3	2.29	0.66
1:C:176:CYS:O	1:C:179:LEU:HD12	1.96	0.66
1:D:46:LEU:HG	2:D:601:FAD:O1A	1.95	0.66
1:E:353:ASP:HB3	1:E:403:PRO:HB2	1.77	0.66
1:E:457:ASN:HB3	2:E:601:FAD:O2	1.94	0.66
1:G:306:ARG:HH11	1:G:312:ASP:HA	1.61	0.66
1:E:269:MET:HE2	1:E:273:PHE:HB3	1.76	0.66
1:G:149:MET:O	1:G:186:PRO:HB3	1.95	0.66
1:G:432:GLN:O	1:G:436:LYS:HG2	1.96	0.66
1:D:271:VAL:HG12	1:D:448:PHE:O	1.95	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:430:LEU:HD22	1:E:434:LEU:HG	1.77	0.66
1:G:308:GLU:HG3	1:G:309:ARG:HD3	1.78	0.66
1:H:47:ALA:HB2	2:H:601:FAD:H4'	1.78	0.66
1:G:254:LEU:HG	1:G:258:THR:HG22	1.78	0.66
1:G:446:GLY:H	1:G:450:SER:HB3	1.60	0.66
1:H:9:ASP:HA	1:H:263:LYS:HD3	1.78	0.66
1:H:306:ARG:HD2	1:H:311:GLY:O	1.94	0.66
1:C:58:TYR:HA	1:C:331:PHE:HE2	1.59	0.66
1:D:458:GLN:HA	2:D:601:FAD:O3'	1.97	0.66
1:G:58:TYR:CE2	1:G:299:GLY:HA3	2.31	0.66
1:G:345:LYS:HD3	1:G:364:GLU:HG2	1.77	0.66
1:B:455:VAL:O	1:B:460:HIS:HB3	1.95	0.65
1:E:326:TYR:CD2	1:E:374:VAL:HA	2.31	0.65
1:E:349:MET:N	1:E:407:ILE:O	2.27	0.65
1:F:383:ASN:HB3	1:F:386:THR:OG1	1.96	0.65
1:B:19:GLY:N	1:B:268:THR:HG21	2.11	0.65
1:B:108:ASN:ND2	1:B:201:ALA:HB3	2.11	0.65
1:E:137:THR:O	1:E:148:ARG:NH1	2.28	0.65
1:E:336:PRO:HG2	1:E:337:TYR:CD1	2.31	0.65
1:A:91:ARG:NH1	1:A:205:GLY:HA3	2.11	0.65
1:H:139:PRO:HB2	1:H:176:CYS:SG	2.36	0.65
1:H:325:PHE:CD2	1:H:372:LEU:HD22	2.31	0.65
1:G:162:TYR:CZ	1:G:166:VAL:HG11	2.31	0.65
1:F:413:ARG:HD3	1:F:415:PHE:CE2	2.31	0.65
1:H:346:LEU:HD23	1:H:347:PRO:HD2	1.78	0.65
1:H:71:TYR:CD2	1:H:495:ARG:HG2	2.32	0.65
1:A:336:PRO:HG2	1:A:337:TYR:CE1	2.31	0.65
1:B:69:TYR:CG	1:B:463:MET:HG3	2.32	0.65
1:E:51:VAL:HA	1:E:56:PHE:O	1.97	0.65
1:F:331:PHE:CE2	1:F:338:ASN:ND2	2.65	0.65
1:F:429:ALA:O	1:F:433:ILE:HG13	1.97	0.65
1:H:245:VAL:O	1:H:278:MET:HA	1.97	0.65
1:F:440:LYS:HB2	1:F:442:ILE:HD12	1.79	0.64
1:H:29:ILE:HG22	1:H:31:GLY:N	2.12	0.64
1:C:40:ASN:O	1:C:236:PHE:HB3	1.97	0.64
1:F:419:TYR:HE1	2:F:601:FAD:HM73	1.62	0.64
1:D:47:ALA:HB1	1:D:222:TRP:HE1	1.63	0.64
1:D:136:ASN:OD1	1:D:137:THR:HG23	1.98	0.64
1:E:368:TRP:CZ3	1:E:370:ILE:HD11	2.32	0.64
1:F:51:VAL:HA	1:F:56:PHE:O	1.96	0.64
1:H:348:THR:O	1:H:357:PRO:HG3	1.96	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:GLU:O	1:C:148:ARG:HG3	1.98	0.64
1:D:108:ASN:OD1	1:D:108:ASN:N	2.20	0.64
1:F:326:TYR:CD2	1:F:374:VAL:HA	2.32	0.64
1:D:398:THR:HB	1:D:400:MET:CG	2.28	0.64
1:H:21:GLY:HA2	1:H:462:PHE:CE1	2.32	0.64
1:C:43:PRO:HG2	1:C:223:ILE:HD13	1.80	0.64
1:C:119:VAL:HA	1:E:196:ILE:HD13	1.78	0.64
1:D:69:TYR:CG	1:D:463:MET:HG3	2.33	0.64
1:F:179:LEU:N	1:F:179:LEU:HD23	2.12	0.64
1:G:44:GLY:HA3	1:G:222:TRP:CD1	2.33	0.64
1:C:91:ARG:HH12	1:C:205:GLY:HA3	1.61	0.64
1:E:175:GLN:NE2	1:E:177:ALA:H	1.94	0.64
1:E:184:ALA:HA	1:E:204:TRP:CZ2	2.32	0.64
1:F:18:THR:OG1	1:F:461:SER:HB3	1.97	0.64
1:H:251:THR:HA	1:H:260:ILE:O	1.98	0.64
1:H:484:PRO:O	1:H:488:ASN:HB2	1.96	0.64
1:A:197:LEU:HD23	1:G:115:LYS:HD3	1.80	0.64
1:C:69:TYR:CG	1:C:463:MET:HG3	2.33	0.64
1:F:17:PRO:HD2	2:F:601:FAD:O5'	1.98	0.64
1:G:91:ARG:HH21	1:G:203:ASN:CA	2.11	0.64
1:C:271:VAL:HG12	1:C:448:PHE:O	1.98	0.64
1:E:115:LYS:O	1:E:119:VAL:HG23	1.97	0.64
1:G:71:TYR:CD2	1:G:495:ARG:HG2	2.33	0.64
1:A:325:PHE:HA	1:A:374:VAL:HG22	1.80	0.63
1:B:11:LEU:O	1:B:265:LEU:HD12	1.99	0.63
1:F:184:ALA:HB2	1:F:204:TRP:CD2	2.32	0.63
1:G:484:PRO:O	1:G:488:ASN:HB2	1.97	0.63
1:F:56:PHE:HE1	1:F:339:GLN:HB3	1.62	0.63
1:F:457:ASN:HB3	2:F:601:FAD:C2	2.28	0.63
1:G:58:TYR:HD2	1:G:411:TYR:HD2	1.46	0.63
1:H:171:THR:HA	1:H:174:MET:HE2	1.79	0.63
1:H:268:THR:HA	1:H:445:ARG:O	1.98	0.63
1:B:104:TYR:HE1	3:B:602:GDU:H5	1.62	0.63
1:B:504:PHE:HZ	1:F:264:LYS:HG2	1.63	0.63
1:D:301:GLY:HA3	1:D:409:SER:HB3	1.80	0.63
1:E:413:ARG:HD3	1:E:415:PHE:CE2	2.32	0.63
1:G:44:GLY:CA	1:G:222:TRP:CD1	2.81	0.63
1:H:336:PRO:HG2	1:H:337:TYR:CE1	2.33	0.63
1:E:326:TYR:H	1:E:374:VAL:HG13	1.64	0.63
1:H:142:PHE:HB3	1:H:171:THR:O	1.98	0.63
1:B:58:TYR:HA	1:B:331:PHE:HE2	1.63	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:PRO:HB2	1:G:109:ASN:ND2	2.14	0.63
1:A:69:TYR:CG	1:A:463:MET:HG3	2.34	0.63
1:B:486:PHE:HE1	1:F:483:TYR:CD1	2.16	0.63
1:D:19:GLY:N	1:D:268:THR:HG21	2.13	0.63
1:E:16:GLY:HA3	2:E:601:FAD:O5B	1.98	0.63
1:F:97:CYS:SG	1:F:98:GLN:HG3	2.38	0.63
1:G:326:TYR:CE2	1:G:375:SER:HB3	2.32	0.63
1:H:326:TYR:HE2	1:H:375:SER:N	1.96	0.63
1:A:176:CYS:O	1:A:179:LEU:HD12	1.98	0.63
1:C:103:PRO:O	1:C:109:ASN:ND2	2.26	0.63
1:F:63:HIS:CD2	1:F:63:HIS:N	2.66	0.63
1:F:142:PHE:O	1:F:146:ILE:HG13	1.99	0.63
1:C:17:PRO:HD2	2:C:601:FAD:O5'	1.98	0.63
1:E:348:THR:OG1	1:E:406:GLU:HB3	1.99	0.63
1:H:322:ASN:HD22	1:H:397:ASN:HB3	1.64	0.63
1:F:143:ASP:HA	1:F:146:ILE:HD12	1.80	0.62
1:G:11:LEU:HD21	1:G:252:VAL:HG11	1.80	0.62
1:E:133:ARG:HH11	1:E:133:ARG:CG	2.06	0.62
1:F:348:THR:OG1	1:F:406:GLU:HB3	1.99	0.62
1:G:18:THR:CG2	1:G:268:THR:HG22	2.29	0.62
1:G:91:ARG:NH2	1:G:203:ASN:HA	2.14	0.62
1:H:336:PRO:HG2	1:H:337:TYR:CD1	2.33	0.62
1:F:353:ASP:HB3	1:F:403:PRO:HB2	1.81	0.62
1:G:68:HIS:O	1:G:492:ASN:ND2	2.32	0.62
1:G:393:GLN:OE1	1:G:393:GLN:HA	1.99	0.62
1:H:194:ASN:HD22	1:H:199:LYS:HB3	1.63	0.62
1:A:19:GLY:N	1:A:268:THR:HG21	2.14	0.62
1:A:301:GLY:HA3	1:A:409:SER:HB3	1.81	0.62
1:A:398:THR:HB	1:A:400:MET:CG	2.29	0.62
1:B:332:SER:CA	1:B:339:GLN:HE21	2.05	0.62
1:F:125:MET:HG2	1:F:188:LEU:HD13	1.80	0.62
1:F:326:TYR:H	1:F:374:VAL:HG13	1.65	0.62
1:G:254:LEU:HG	1:G:258:THR:CG2	2.30	0.62
1:A:309:ARG:HG3	1:A:310:ILE:HG13	1.80	0.62
1:B:103:PRO:O	1:B:109:ASN:ND2	2.31	0.62
1:B:308:GLU:CD	1:B:308:GLU:H	2.03	0.62
1:B:398:THR:CG2	1:B:400:MET:HG2	2.30	0.62
1:C:398:THR:O	1:C:398:THR:CG2	2.47	0.62
1:E:271:VAL:HG13	1:E:287:THR:HG22	1.81	0.62
1:F:22:ALA:HA	1:F:469:VAL:HG22	1.80	0.62
1:G:395:LEU:HD23	1:G:400:MET:HG3	1.82	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:LEU:HD12	1:G:452:ARG:HE	1.65	0.62
1:H:103:PRO:HB2	1:H:109:ASN:ND2	2.14	0.62
1:A:142:PHE:O	1:A:146:ILE:HG13	1.98	0.62
1:D:422:PRO:HA	1:D:426:ARG:HD3	1.82	0.62
1:E:25:ARG:HG2	1:E:469:VAL:HB	1.81	0.62
1:H:69:TYR:OH	1:H:487:VAL:HB	1.99	0.62
1:G:336:PRO:HG2	1:G:337:TYR:CD1	2.35	0.62
1:C:38:ASP:OD2	1:C:40:ASN:HB2	2.00	0.62
1:F:17:PRO:O	1:F:462:PHE:HA	1.99	0.62
1:G:482:ASN:HB2	1:G:483:TYR:CE2	2.35	0.62
1:E:440:LYS:HB2	1:E:442:ILE:HD12	1.82	0.62
1:H:143:ASP:HA	1:H:146:ILE:HD12	1.82	0.62
1:A:125:MET:HE3	1:A:186:PRO:HB2	1.81	0.61
1:C:91:ARG:NH1	1:C:205:GLY:HA3	2.15	0.61
1:C:490:ARG:NH2	1:G:483:TYR:OH	2.27	0.61
1:F:402:LYS:O	1:F:405:ASP:HB2	2.00	0.61
1:G:326:TYR:HE2	1:G:375:SER:N	1.98	0.61
1:H:154:ILE:H	1:H:154:ILE:HD12	1.63	0.61
1:A:108:ASN:OD1	1:A:108:ASN:N	2.20	0.61
1:B:271:VAL:HG12	1:B:448:PHE:O	2.00	0.61
1:E:178:TRP:CB	1:E:454:GLU:HG3	2.30	0.61
1:F:115:LYS:O	1:F:119:VAL:HG23	1.99	0.61
1:F:367:TYR:CE1	1:F:408:VAL:HG21	2.35	0.61
1:G:323:CYS:HB2	1:G:325:PHE:CZ	2.35	0.61
1:A:107:GLN:O	1:A:110:ILE:HG13	2.00	0.61
1:B:296:HIS:CE1	1:B:382:VAL:HG21	2.34	0.61
1:C:296:HIS:CE1	1:C:382:VAL:HG21	2.36	0.61
1:E:461:SER:HA	1:E:464:LEU:CD1	2.24	0.61
1:H:432:GLN:O	1:H:436:LYS:HG2	2.00	0.61
1:B:125:MET:HE3	1:B:186:PRO:HB2	1.82	0.61
1:C:336:PRO:HG2	1:C:337:TYR:CE1	2.34	0.61
1:E:178:TRP:CE3	1:E:179:LEU:HD22	2.36	0.61
1:G:222:TRP:HA	1:G:222:TRP:HE3	1.65	0.61
1:G:268:THR:HA	1:G:445:ARG:O	1.99	0.61
1:G:367:TYR:HD1	1:G:408:VAL:HG21	1.65	0.61
1:H:58:TYR:CE2	1:H:299:GLY:HA3	2.36	0.61
1:H:212:PHE:CD2	1:H:213:PRO:HD2	2.35	0.61
1:H:443:TRP:HB3	1:H:445:ARG:HE	1.65	0.61
1:E:169:VAL:HG23	1:E:170:PRO:O	2.01	0.61
1:F:271:VAL:HG13	1:F:287:THR:HG22	1.83	0.61
1:G:47:ALA:CB	1:G:222:TRP:HE1	2.11	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:VAL:O	1:G:60:VAL:HG12	2.01	0.61
1:A:40:ASN:O	1:A:236:PHE:HB3	2.01	0.61
1:C:271:VAL:HA	1:C:274:LEU:HB2	1.82	0.61
1:F:147:VAL:HG22	1:F:160:ARG:HH21	1.65	0.61
1:H:58:TYR:HD2	1:H:411:TYR:HD2	1.49	0.61
1:A:108:ASN:ND2	1:A:201:ALA:HB3	2.15	0.61
1:B:60:VAL:O	1:B:63:HIS:NE2	2.34	0.61
1:C:468:ALA:O	1:C:472:ILE:HG13	2.01	0.61
1:F:118:GLN:OE1	1:F:195:VAL:HG13	2.00	0.61
1:G:57:LEU:CD1	1:G:338:ASN:HA	2.30	0.61
1:H:70:LYS:HE2	1:H:496:ARG:NH1	2.16	0.61
1:H:430:LEU:HD12	1:H:452:ARG:HE	1.64	0.61
1:C:175:GLN:NE2	1:C:178:TRP:HD1	1.98	0.61
1:E:91:ARG:HG3	1:E:315:TRP:CH2	2.35	0.61
1:F:437:LEU:HB3	1:F:442:ILE:HB	1.81	0.61
1:G:222:TRP:HA	1:G:222:TRP:CE3	2.34	0.61
1:G:443:TRP:HB3	1:G:445:ARG:HE	1.66	0.61
1:G:492:ASN:ND2	1:G:492:ASN:N	2.49	0.61
1:H:446:GLY:N	1:H:450:SER:H	1.99	0.61
1:B:144:GLU:O	1:B:148:ARG:HG3	2.00	0.61
1:D:58:TYR:HA	1:D:331:PHE:HE2	1.66	0.61
1:E:91:ARG:CD	1:E:207:ASN:HB2	2.31	0.61
1:F:178:TRP:CB	1:F:454:GLU:HG3	2.30	0.61
1:G:297:VAL:HB	1:G:415:PHE:HE2	1.64	0.61
1:H:359:SER:HB3	1:H:363:LYS:CE	2.31	0.61
1:B:338:ASN:N	1:B:338:ASN:OD1	2.34	0.61
1:C:178:TRP:HB2	1:C:454:GLU:CG	2.30	0.61
1:D:232:GLU:H	1:D:232:GLU:CD	2.04	0.61
1:G:69:TYR:OH	1:G:487:VAL:HB	2.01	0.61
1:H:25:ARG:HD3	1:H:470:ASP:OD1	2.01	0.61
1:H:445:ARG:NH1	1:H:481:LEU:HD22	2.16	0.61
1:A:398:THR:HB	1:A:400:MET:HG3	1.82	0.60
1:C:60:VAL:O	1:C:63:HIS:NE2	2.34	0.60
1:E:125:MET:HG2	1:E:188:LEU:HD13	1.82	0.60
1:E:207:ASN:ND2	3:E:602:GDU:O4'	2.33	0.60
1:F:69:TYR:CZ	1:F:463:MET:HG3	2.36	0.60
1:G:115:LYS:O	1:G:118:GLN:HB2	2.01	0.60
1:G:457:ASN:HB3	1:G:459:ASP:OD1	2.00	0.60
1:H:150:MET:CG	1:H:154:ILE:HB	2.30	0.60
1:C:91:ARG:NH2	1:C:204:TRP:O	2.32	0.60
1:D:245:VAL:HG22	1:D:252:VAL:HG23	1.81	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:GLY:C	1:G:151:GLY:HA3	2.20	0.60
1:G:478:GLU:HB2	1:G:481:LEU:HB3	1.83	0.60
1:D:108:ASN:ND2	1:D:201:ALA:HB3	2.16	0.60
1:G:338:ASN:HB2	1:G:339:GLN:HE22	1.66	0.60
1:E:6:ILE:HG22	1:E:260:ILE:HG23	1.82	0.60
1:B:170:PRO:HG2	1:B:173:LYS:HG3	1.83	0.60
1:C:251:THR:HA	1:C:260:ILE:O	2.01	0.60
1:D:163:ASN:HA	1:D:166:VAL:HG12	1.83	0.60
1:E:145:TRP:CH2	1:E:183:VAL:HG21	2.36	0.60
1:F:145:TRP:CH2	1:F:183:VAL:HG21	2.36	0.60
1:B:411:TYR:C	1:B:411:TYR:CD2	2.75	0.60
1:D:18:THR:OG1	1:D:461:SER:HB3	2.01	0.60
1:D:107:GLN:O	1:D:110:ILE:HG13	2.01	0.60
1:D:176:CYS:O	1:D:179:LEU:HD12	2.01	0.60
1:E:122:ILE:HG23	1:E:126:ILE:HD11	1.83	0.60
1:E:183:VAL:HG11	3:E:602:GDU:O2	2.02	0.60
1:E:346:LEU:HD12	1:E:367:TYR:CZ	2.37	0.60
1:F:9:ASP:O	1:F:263:LYS:HB2	2.02	0.60
1:F:64:VAL:HB	3:F:602:GDU:O6'	2.02	0.60
1:F:265:LEU:HD23	1:F:442:ILE:HG12	1.82	0.60
1:G:336:PRO:HG2	1:G:337:TYR:CE1	2.36	0.60
1:H:203:ASN:O	1:H:204:TRP:HB2	2.01	0.60
1:F:322:ASN:ND2	1:F:398:THR:HG22	2.16	0.60
2:F:601:FAD:O4	3:F:602:GDU:H2'	2.02	0.60
1:G:168:ALA:HB1	1:G:377:SER:OG	2.02	0.60
1:C:504:PHE:HA	1:C:507:SER:HB3	1.84	0.60
1:H:47:ALA:CB	1:H:222:TRP:HE1	2.09	0.60
1:C:411:TYR:C	1:C:411:TYR:CD2	2.74	0.60
1:D:57:LEU:HD22	1:D:338:ASN:HA	1.84	0.60
1:D:411:TYR:C	1:D:411:TYR:CD2	2.75	0.60
1:G:325:PHE:CD2	1:G:372:LEU:HD22	2.37	0.60
1:H:162:TYR:CZ	1:H:166:VAL:HG11	2.36	0.60
1:H:457:ASN:HB3	1:H:459:ASP:OD1	2.02	0.60
1:B:91:ARG:NH1	1:B:205:GLY:HA3	2.17	0.60
1:C:125:MET:HE3	1:C:186:PRO:HB2	1.84	0.60
1:F:122:ILE:HG22	1:F:123:ASP:N	2.17	0.60
1:F:471:ASN:ND2	1:F:476:ALA:O	2.25	0.60
1:G:53:PRO:HB2	1:G:54:GLU:OE2	2.02	0.60
1:G:274:LEU:O	1:G:278:MET:HG2	2.02	0.60
1:H:250:LYS:HB3	1:H:262:TYR:O	2.02	0.60
1:H:309:ARG:HG2	1:H:310:ILE:HD12	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ALA:O	1:A:433:ILE:HD12	2.03	0.59
1:F:167:TRP:CD2	1:F:174:MET:HE1	2.36	0.59
1:G:91:ARG:N	1:G:208:ALA:O	2.30	0.59
1:A:271:VAL:HA	1:A:274:LEU:HB2	1.83	0.59
1:E:322:ASN:ND2	1:E:398:THR:HG22	2.18	0.59
1:F:91:ARG:CD	1:F:207:ASN:HB2	2.32	0.59
1:G:248:ASN:N	1:G:248:ASN:OD1	2.34	0.59
1:H:204:TRP:HA	1:H:204:TRP:HE3	1.66	0.59
1:H:395:LEU:HD23	1:H:400:MET:HG3	1.85	0.59
1:A:336:PRO:HG2	1:A:337:TYR:CD1	2.37	0.59
1:B:245:VAL:HG22	1:B:252:VAL:HG23	1.84	0.59
1:B:301:GLY:HA3	1:B:409:SER:HB3	1.85	0.59
1:C:242:VAL:HG23	2:C:601:FAD:N1A	2.16	0.59
1:E:402:LYS:O	1:E:405:ASP:HB2	2.02	0.59
1:G:170:PRO:HD2	1:G:379:MET:SD	2.42	0.59
1:D:43:PRO:HG2	1:D:223:ILE:HD13	1.84	0.59
1:D:143:ASP:HA	1:D:146:ILE:HD12	1.84	0.59
1:D:336:PRO:HG2	1:D:337:TYR:CE1	2.36	0.59
1:H:285:GLY:O	1:H:288:LYS:HB2	2.02	0.59
1:H:303:ARG:NH2	1:H:346:LEU:O	2.35	0.59
1:C:455:VAL:CG1	1:C:464:LEU:HD11	2.32	0.59
1:E:94:TYR:HB2	1:E:316:LEU:HD22	1.82	0.59
1:B:107:GLN:O	1:B:110:ILE:HG13	2.01	0.59
1:F:38:ASP:HB3	1:F:236:PHE:HD1	1.67	0.59
1:F:160:ARG:N	1:F:161:PRO:HD2	2.18	0.59
1:G:443:TRP:HA	1:G:445:ARG:HH21	1.68	0.59
1:H:70:LYS:HE2	1:H:496:ARG:HH12	1.67	0.59
1:B:419:TYR:CE1	2:B:601:FAD:HM73	2.36	0.59
1:C:346:LEU:HD23	1:C:347:PRO:HD2	1.85	0.59
1:F:350:GLN:O	1:F:407:ILE:HB	2.02	0.59
1:F:437:LEU:O	1:F:442:ILE:N	2.35	0.59
1:G:353:ASP:HB3	1:G:403:PRO:CB	2.32	0.59
1:A:32:PRO:HB3	1:E:504:PHE:CD2	2.37	0.59
1:B:54:GLU:HB3	1:B:346:LEU:HD11	1.84	0.59
1:B:422:PRO:HA	1:B:426:ARG:HD3	1.84	0.59
1:F:69:TYR:CE1	1:F:463:MET:HG3	2.37	0.59
1:F:154:ILE:H	1:F:154:ILE:CD1	1.99	0.59
1:H:383:ASN:HD22	1:H:386:THR:HG23	1.67	0.59
1:H:445:ARG:HA	1:H:450:SER:CB	2.32	0.59
1:B:57:LEU:H	1:B:57:LEU:HD13	1.67	0.59
1:B:463:MET:O	1:B:467:GLU:HG3	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:ALA:O	1:F:228:THR:HG23	2.03	0.59
1:G:25:ARG:HA	1:G:28:GLN:HB2	1.84	0.59
1:G:250:LYS:HB3	1:G:262:TYR:O	2.02	0.59
1:G:471:ASN:HA	1:G:476:ALA:H	1.68	0.59
1:A:109:ASN:OD1	1:A:200:THR:HG22	2.03	0.59
1:A:411:TYR:C	1:A:411:TYR:CD2	2.76	0.59
1:B:429:ALA:O	1:B:433:ILE:HD12	2.03	0.59
1:C:308:GLU:H	1:C:308:GLU:CD	2.06	0.59
1:F:69:TYR:HB2	1:F:72:PHE:HB3	1.85	0.59
1:G:23:ALA:HA	1:G:26:LEU:HD12	1.84	0.59
1:G:492:ASN:HD22	1:G:492:ASN:N	2.00	0.59
1:H:142:PHE:HA	1:H:176:CYS:HB3	1.85	0.59
1:A:126:ILE:HD12	1:G:189:LYS:HG2	1.84	0.58
1:B:383:ASN:O	1:B:387:ILE:HB	2.03	0.58
1:C:170:PRO:HG2	1:C:173:LYS:HG3	1.84	0.58
1:F:178:TRP:CE3	1:F:179:LEU:HD22	2.38	0.58
1:F:346:LEU:HD12	1:F:367:TYR:CZ	2.38	0.58
1:G:58:TYR:HE1	1:G:369:SER:OG	1.85	0.58
1:H:348:THR:HG21	1:H:406:GLU:HG2	1.83	0.58
1:A:95:VAL:HG23	1:A:102:VAL:O	2.02	0.58
1:B:309:ARG:HG3	1:B:310:ILE:HG13	1.86	0.58
1:E:97:CYS:SG	1:E:98:GLN:HG3	2.43	0.58
1:F:70:LYS:HB3	1:F:496:ARG:HH12	1.67	0.58
1:F:502:GLN:O	1:F:506:LYS:HD3	2.03	0.58
1:G:462:PHE:O	1:G:466:VAL:HG23	2.03	0.58
1:G:464:LEU:HG	1:G:480:THR:HB	1.85	0.58
1:H:341:GLU:HG3	1:H:343:SER:H	1.68	0.58
1:A:57:LEU:HD22	1:A:338:ASN:HA	1.85	0.58
1:G:107:GLN:CD	1:G:107:GLN:H	2.06	0.58
1:G:411:TYR:C	1:G:411:TYR:CD1	2.75	0.58
1:A:178:TRP:HB2	1:A:454:GLU:CG	2.32	0.58
1:A:197:LEU:CD2	1:G:115:LYS:HD3	2.33	0.58
1:B:352:ALA:HB3	1:B:403:PRO:HA	1.86	0.58
1:D:16:GLY:H	2:D:601:FAD:H4B	1.68	0.58
1:D:338:ASN:N	1:D:338:ASN:OD1	2.36	0.58
1:D:457:ASN:O	1:D:460:HIS:HB2	2.03	0.58
1:E:184:ALA:HB2	1:E:204:TRP:CD2	2.38	0.58
1:E:303:ARG:HH21	1:E:363:LYS:CB	2.17	0.58
1:G:197:LEU:O	1:G:199:LYS:N	2.37	0.58
1:H:341:GLU:HG3	1:H:342:ALA:N	2.18	0.58
1:B:504:PHE:HA	1:B:507:SER:HB3	1.85	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:SER:HB2	1:C:104:TYR:HB3	1.83	0.58
1:C:182:ARG:HD2	3:C:602:GDU:O1A	2.04	0.58
1:C:453:TYR:OH	3:C:602:GDU:O2B	2.22	0.58
3:C:602:GDU:H5'2	3:C:602:GDU:O1B	2.04	0.58
1:E:207:ASN:HB3	1:E:315:TRP:CH2	2.39	0.58
1:G:367:TYR:HE1	1:G:408:VAL:HG11	1.68	0.58
1:H:11:LEU:O	1:H:265:LEU:HD12	2.04	0.58
1:H:44:GLY:HA3	1:H:222:TRP:CD1	2.38	0.58
1:A:303:ARG:NH1	1:A:348:THR:OG1	2.37	0.58
1:C:16:GLY:H	2:C:601:FAD:H52A	1.68	0.58
1:C:103:PRO:CB	1:C:109:ASN:ND2	2.66	0.58
1:C:232:GLU:CD	1:C:232:GLU:H	2.07	0.58
1:E:163:ASN:HA	1:E:166:VAL:HG13	1.85	0.58
1:F:94:TYR:HB2	1:F:316:LEU:HD22	1.84	0.58
1:H:103:PRO:CB	1:H:202:GLY:HA2	2.33	0.58
1:A:416:ASP:HB2	1:F:281:GLN:NE2	2.19	0.58
1:C:113:LEU:O	1:C:118:GLN:NE2	2.29	0.58
1:C:245:VAL:HG22	1:C:252:VAL:HG23	1.85	0.58
1:C:301:GLY:HA3	1:C:409:SER:HB3	1.85	0.58
1:E:160:ARG:N	1:E:161:PRO:HD2	2.18	0.58
1:E:248:ASN:OD1	1:E:248:ASN:N	2.37	0.58
1:H:44:GLY:CA	1:H:222:TRP:CD1	2.86	0.58
1:H:85:ASP:HA	1:H:214:ALA:HB2	1.86	0.58
1:H:124:GLY:C	1:H:151:GLY:HA3	2.22	0.58
1:H:331:PHE:CD2	1:H:338:ASN:HB3	2.39	0.58
1:H:418:GLY:C	1:H:419:TYR:CD1	2.75	0.58
1:H:433:ILE:O	1:H:436:LYS:HB2	2.03	0.58
1:B:20:LEU:HD23	1:B:20:LEU:N	2.19	0.58
1:C:54:GLU:HB3	1:C:346:LEU:HD11	1.86	0.58
1:C:136:ASN:OD1	1:C:136:ASN:N	2.35	0.58
1:D:91:ARG:HD3	1:D:207:ASN:CB	2.34	0.58
1:E:26:LEU:HD13	1:E:34:TRP:HB2	1.86	0.58
1:C:11:LEU:O	1:C:265:LEU:HD12	2.04	0.58
1:C:411:TYR:C	1:C:411:TYR:HD2	2.07	0.58
1:C:455:VAL:HG21	1:C:480:THR:O	2.04	0.58
1:C:499:ASP:O	1:C:503:VAL:HG23	2.04	0.58
1:D:60:VAL:O	1:D:63:HIS:NE2	2.37	0.58
1:D:325:PHE:HA	1:D:374:VAL:HG22	1.85	0.58
1:E:103:PRO:HB2	1:E:109:ASN:OD1	2.04	0.58
1:A:47:ALA:HB1	1:A:222:TRP:HE1	1.69	0.57
1:A:143:ASP:O	1:A:147:VAL:HG23	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PRO:HG2	1:A:173:LYS:HG3	1.86	0.57
1:A:350:GLN:NE2	1:A:354:GLY:HA2	2.16	0.57
1:B:303:ARG:HH21	1:B:363:LYS:C	2.06	0.57
1:D:455:VAL:CG1	1:D:464:LEU:HD11	2.33	0.57
1:D:466:VAL:HG12	1:D:495:ARG:NH1	2.19	0.57
1:E:64:VAL:HG22	1:E:210:PHE:CE1	2.39	0.57
1:E:351:LEU:HA	1:E:405:ASP:O	2.04	0.57
2:E:601:FAD:O4	3:E:602:GDU:H2'	2.04	0.57
1:G:446:GLY:N	1:G:450:SER:H	2.01	0.57
1:B:163:ASN:HA	1:B:166:VAL:HG12	1.86	0.57
1:B:411:TYR:C	1:B:411:TYR:HD2	2.07	0.57
1:C:463:MET:O	1:C:467:GLU:HG3	2.04	0.57
1:D:309:ARG:HG3	1:D:310:ILE:HG13	1.85	0.57
1:H:89:HIS:HB2	1:H:210:PHE:CE2	2.39	0.57
1:H:149:MET:SD	1:H:184:ALA:CA	2.86	0.57
1:H:249:ASN:OD1	1:H:249:ASN:N	2.37	0.57
1:G:285:GLY:O	1:G:288:LYS:HB2	2.05	0.57
1:G:383:ASN:HD22	1:G:386:THR:HG23	1.69	0.57
1:H:189:LYS:O	1:H:193:THR:OG1	2.21	0.57
1:A:271:VAL:HG12	1:A:448:PHE:O	2.04	0.57
1:C:309:ARG:HG3	1:C:310:ILE:HG13	1.87	0.57
1:G:467:GLU:OE1	1:G:480:THR:N	2.24	0.57
1:H:248:ASN:OD1	1:H:248:ASN:N	2.37	0.57
1:B:47:ALA:HB1	1:B:222:TRP:NE1	2.19	0.57
1:C:107:GLN:O	1:C:110:ILE:HG13	2.04	0.57
1:D:142:PHE:O	1:D:146:ILE:HG13	2.05	0.57
1:D:483:TYR:OH	1:H:490:ARG:NH2	2.22	0.57
1:E:10:VAL:HG22	1:E:264:LYS:HG3	1.86	0.57
1:E:69:TYR:CZ	1:E:463:MET:HG3	2.39	0.57
1:E:263:LYS:HD2	1:E:263:LYS:N	2.19	0.57
1:E:303:ARG:NH2	1:E:363:LYS:CG	2.67	0.57
1:F:445:ARG:CZ	1:F:481:LEU:HD22	2.34	0.57
1:H:25:ARG:HH11	1:H:470:ASP:CG	2.07	0.57
1:H:158:PHE:HE1	1:H:162:TYR:CG	2.22	0.57
1:H:222:TRP:HA	1:H:222:TRP:CE3	2.39	0.57
1:H:344:LYS:O	1:H:367:TYR:OH	2.22	0.57
1:H:492:ASN:HD22	1:H:492:ASN:H	1.52	0.57
1:A:20:LEU:N	1:A:20:LEU:HD23	2.19	0.57
1:A:338:ASN:N	1:A:338:ASN:OD1	2.37	0.57
1:B:109:ASN:OD1	1:B:200:THR:HG22	2.04	0.57
1:B:175:GLN:NE2	1:B:178:TRP:HD1	2.03	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:HD13	1:C:338:ASN:O	2.03	0.57
1:C:196:ILE:HG21	1:E:119:VAL:HG23	1.84	0.57
1:D:199:LYS:HD2	1:D:200:THR:O	2.04	0.57
1:E:167:TRP:CE3	1:E:421:THR:HG22	2.39	0.57
1:F:154:ILE:HD13	1:F:154:ILE:N	2.12	0.57
1:F:368:TRP:CZ3	1:F:370:ILE:HD11	2.40	0.57
1:H:28:GLN:HG2	1:H:497:LEU:O	2.05	0.57
1:D:458:GLN:CG	2:D:601:FAD:H2'	2.34	0.57
1:E:71:TYR:CD2	1:E:496:ARG:HA	2.39	0.57
1:F:150:MET:HG3	1:F:154:ILE:HB	1.85	0.57
1:F:167:TRP:CE3	1:F:421:THR:HG22	2.39	0.57
1:H:17:PRO:HD2	2:H:601:FAD:O5'	2.03	0.57
1:H:25:ARG:NH1	1:H:470:ASP:OD1	2.25	0.57
1:H:91:ARG:N	1:H:208:ALA:O	2.30	0.57
1:A:183:VAL:HG13	3:A:602:GDU:C2	2.32	0.57
1:A:306:ARG:CZ	1:A:311:GLY:HA2	2.34	0.57
1:C:47:ALA:HB1	1:C:222:TRP:NE1	2.19	0.57
1:C:58:TYR:HA	1:C:331:PHE:CE2	2.40	0.57
1:D:429:ALA:O	1:D:433:ILE:HD12	2.04	0.57
1:E:143:ASP:O	1:E:147:VAL:HG23	2.04	0.57
1:F:19:GLY:O	1:F:22:ALA:HB3	2.05	0.57
1:F:26:LEU:HD13	1:F:34:TRP:HB2	1.87	0.57
1:G:11:LEU:O	1:G:265:LEU:HD12	2.05	0.57
1:G:103:PRO:CB	1:G:202:GLY:HA3	2.34	0.57
1:G:292:TYR:CE1	1:G:417:HIS:ND1	2.70	0.57
1:G:438:GLN:HA	1:G:442:ILE:O	2.05	0.57
1:E:502:GLN:O	1:E:506:LYS:HD3	2.03	0.57
1:F:6:ILE:HG22	1:F:260:ILE:HG23	1.87	0.57
1:F:72:PHE:CZ	1:F:76:LEU:HD11	2.40	0.57
1:A:175:GLN:NE2	1:A:178:TRP:HD1	2.03	0.57
1:B:136:ASN:OD1	1:B:136:ASN:N	2.32	0.57
1:B:136:ASN:OD1	1:B:137:THR:HG23	2.05	0.57
1:E:323:CYS:HB2	1:E:324:PRO:HD2	1.86	0.57
1:D:344:LYS:HD2	1:D:345:LYS:N	2.20	0.56
1:E:104:TYR:HE1	3:E:602:GDU:C4	2.18	0.56
1:E:325:PHE:HA	1:E:374:VAL:CG1	2.35	0.56
1:F:9:ASP:N	1:F:33:SER:OG	2.28	0.56
1:F:467:GLU:CG	1:F:495:ARG:HH12	2.12	0.56
1:H:58:TYR:HE1	1:H:369:SER:OG	1.88	0.56
1:H:455:VAL:O	1:H:460:HIS:CB	2.49	0.56
1:B:455:VAL:CG1	1:B:464:LEU:HD11	2.35	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:GLY:O	2:B:601:FAD:O3'	2.22	0.56
1:E:326:TYR:OH	1:E:373:GLU:OE2	2.23	0.56
1:F:335:SER:HB3	1:F:338:ASN:OD1	2.05	0.56
1:G:162:TYR:O	1:G:165:LYS:N	2.38	0.56
1:G:458:GLN:HG2	2:G:601:FAD:H2'	1.86	0.56
1:H:162:TYR:O	1:H:165:LYS:N	2.37	0.56
1:H:480:THR:HA	1:H:487:VAL:HG21	1.87	0.56
1:A:134:VAL:O	1:A:134:VAL:CG1	2.53	0.56
1:A:163:ASN:HA	1:A:166:VAL:HG12	1.87	0.56
1:A:212:PHE:CG	1:A:213:PRO:HD2	2.40	0.56
1:A:388:LEU:O	1:A:392:ILE:HG13	2.04	0.56
1:A:411:TYR:C	1:A:411:TYR:HD2	2.08	0.56
1:B:163:ASN:HA	1:B:166:VAL:CG1	2.35	0.56
1:C:352:ALA:HB3	1:C:403:PRO:HA	1.87	0.56
1:D:125:MET:HE3	1:D:186:PRO:HB2	1.87	0.56
1:F:427:GLU:O	1:F:431:THR:HG23	2.05	0.56
1:H:13:ILE:HD12	1:H:265:LEU:HD11	1.88	0.56
1:H:58:TYR:HD2	1:H:411:TYR:CD2	2.22	0.56
1:H:141:THR:OG1	1:H:144:GLU:HB2	2.05	0.56
1:H:353:ASP:HB3	1:H:403:PRO:HB3	1.87	0.56
1:H:411:TYR:CD1	1:H:411:TYR:C	2.77	0.56
1:H:462:PHE:O	1:H:466:VAL:HG23	2.05	0.56
1:A:91:ARG:HD3	1:A:207:ASN:CB	2.34	0.56
1:B:395:LEU:HD22	1:B:400:MET:HE2	1.86	0.56
1:E:21:GLY:HA2	1:E:462:PHE:CE1	2.41	0.56
1:E:151:GLY:O	1:E:154:ILE:HG12	2.05	0.56
1:G:38:ASP:OD1	2:G:601:FAD:O3B	2.23	0.56
1:G:402:LYS:HD3	1:G:405:ASP:OD2	2.04	0.56
1:H:306:ARG:HH11	1:H:312:ASP:HA	1.68	0.56
1:B:183:VAL:CG2	3:B:602:GDU:H1D	2.24	0.56
1:B:466:VAL:HG12	1:B:495:ARG:NH1	2.20	0.56
1:C:422:PRO:HA	1:C:426:ARG:HD3	1.86	0.56
1:D:457:ASN:HA	2:D:601:FAD:H1'2	1.88	0.56
1:F:6:ILE:O	1:F:260:ILE:HA	2.05	0.56
1:F:169:VAL:HG23	1:F:170:PRO:O	2.05	0.56
1:A:64:VAL:HG13	1:A:210:PHE:CD1	2.41	0.56
1:A:433:ILE:O	1:A:436:LYS:HB2	2.05	0.56
1:B:139:PRO:HB2	1:B:176:CYS:SG	2.46	0.56
1:C:38:ASP:HA	2:C:601:FAD:H2A	1.87	0.56
1:C:103:PRO:C	1:C:109:ASN:HD22	2.07	0.56
1:D:144:GLU:O	1:D:148:ARG:HG3	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:GLU:H	1:D:308:GLU:CD	2.09	0.56
1:D:411:TYR:C	1:D:411:TYR:HD2	2.09	0.56
1:E:27:ASN:HB2	1:E:34:TRP:HZ2	1.70	0.56
1:E:72:PHE:CZ	1:E:76:LEU:HD11	2.41	0.56
1:E:147:VAL:HG22	1:E:160:ARG:HH21	1.71	0.56
1:F:17:PRO:O	1:F:462:PHE:HD1	1.88	0.56
1:F:64:VAL:HG22	1:F:210:PHE:CE1	2.41	0.56
1:F:303:ARG:NH2	1:F:363:LYS:HB2	2.19	0.56
1:G:204:TRP:CE3	1:G:204:TRP:HA	2.39	0.56
1:G:250:LYS:O	1:G:261:GLY:HA2	2.06	0.56
1:H:453:TYR:C	1:H:453:TYR:CD2	2.79	0.56
1:B:336:PRO:HG2	1:B:337:TYR:CE1	2.41	0.56
1:D:93:SER:HB2	1:D:104:TYR:HB3	1.88	0.56
1:F:101:TRP:HZ3	1:F:316:LEU:HD13	1.71	0.56
1:F:353:ASP:HB3	1:F:403:PRO:HB3	1.87	0.56
1:A:143:ASP:HA	1:A:146:ILE:HD12	1.88	0.56
1:B:18:THR:OG1	1:B:461:SER:HB3	2.05	0.56
1:B:143:ASP:HA	1:B:146:ILE:HD12	1.87	0.56
1:C:160:ARG:N	1:C:161:PRO:HD2	2.21	0.56
1:C:163:ASN:HA	1:C:166:VAL:CG1	2.35	0.56
1:C:346:LEU:HD23	1:C:347:PRO:CD	2.36	0.56
1:E:367:TYR:CE1	1:E:408:VAL:HG21	2.40	0.56
1:E:424:LEU:HB2	1:E:425:GLU:OE1	2.06	0.56
1:E:460:HIS:O	1:E:463:MET:HB2	2.05	0.56
1:F:109:ASN:HD22	1:F:109:ASN:H	1.54	0.56
1:F:270:ALA:HB3	1:F:273:PHE:CD2	2.41	0.56
1:A:308:GLU:H	1:A:308:GLU:CD	2.09	0.56
1:A:398:THR:HG22	1:A:398:THR:O	2.05	0.56
1:B:93:SER:HB2	1:B:104:TYR:HB3	1.86	0.56
1:B:504:PHE:HZ	1:F:264:LYS:CG	2.20	0.56
1:D:20:LEU:N	1:D:20:LEU:HD23	2.20	0.56
1:F:47:ALA:HB1	1:F:222:TRP:NE1	2.21	0.56
1:F:163:ASN:HA	1:F:166:VAL:HG13	1.88	0.56
1:A:105:PRO:O	1:A:109:ASN:ND2	2.38	0.55
1:A:352:ALA:HB3	1:A:403:PRO:HA	1.87	0.55
1:D:64:VAL:HG13	1:D:210:PHE:CD1	2.40	0.55
1:E:69:TYR:CE1	1:E:463:MET:HG3	2.41	0.55
1:F:63:HIS:CE1	2:F:601:FAD:C9A	2.89	0.55
1:G:272:ASP:OD1	1:G:272:ASP:N	2.38	0.55
1:G:349:MET:SD	1:G:409:SER:HA	2.46	0.55
1:H:96:ARG:HA	1:H:100:GLN:O	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ASP:OD1	2:A:601:FAD:H1B	2.06	0.55
1:B:8:VAL:HG11	1:B:35:MET:HG2	1.88	0.55
1:B:480:THR:HA	1:B:487:VAL:HG11	1.88	0.55
1:C:163:ASN:HA	1:C:166:VAL:HG12	1.87	0.55
1:D:344:LYS:HD2	1:D:345:LYS:H	1.72	0.55
1:E:17:PRO:O	1:E:462:PHE:HD1	1.88	0.55
1:G:96:ARG:HA	1:G:100:GLN:O	2.07	0.55
1:H:222:TRP:HA	1:H:222:TRP:HE3	1.71	0.55
1:H:383:ASN:ND2	1:H:386:THR:HG23	2.21	0.55
1:A:383:ASN:O	1:A:387:ILE:HB	2.06	0.55
1:D:398:THR:HB	1:D:400:MET:HG2	1.87	0.55
1:D:398:THR:HB	1:D:400:MET:HG3	1.89	0.55
1:E:114:PRO:O	1:E:118:GLN:HG3	2.06	0.55
1:E:230:PRO:CG	1:E:233:LYS:HD2	2.36	0.55
1:G:158:PHE:C	1:G:158:PHE:CD1	2.80	0.55
1:H:64:VAL:HG22	1:H:210:PHE:CD1	2.41	0.55
1:B:468:ALA:O	1:B:472:ILE:HG13	2.06	0.55
1:D:27:ASN:OD1	1:D:230:PRO:HD2	2.07	0.55
1:D:64:VAL:O	2:D:601:FAD:N3	2.37	0.55
1:D:91:ARG:NH2	1:D:204:TRP:O	2.32	0.55
1:D:242:VAL:HB	2:D:601:FAD:H62A	1.69	0.55
1:E:26:LEU:HG	1:E:469:VAL:HG13	1.89	0.55
1:E:27:ASN:OD1	1:E:27:ASN:C	2.44	0.55
1:E:116:GLU:HG2	1:E:117:GLU:N	2.20	0.55
1:F:116:GLU:HG2	1:F:117:GLU:N	2.19	0.55
1:G:212:PHE:CG	1:G:213:PRO:HD2	2.41	0.55
1:G:458:GLN:HA	2:G:601:FAD:O3'	2.07	0.55
1:H:25:ARG:HA	1:H:28:GLN:HB2	1.89	0.55
1:B:16:GLY:HA3	2:B:601:FAD:O1A	2.06	0.55
1:C:494:GLU:OE2	1:G:477:VAL:HB	2.07	0.55
1:D:187:ASN:C	1:D:187:ASN:OD1	2.44	0.55
1:A:87:TYR:HB3	1:A:89:HIS:CE1	2.42	0.55
1:C:338:ASN:OD1	1:C:338:ASN:N	2.40	0.55
1:D:69:TYR:CD1	1:D:463:MET:HG3	2.41	0.55
1:H:115:LYS:O	1:H:118:GLN:HB2	2.07	0.55
1:A:11:LEU:O	1:A:265:LEU:HD12	2.07	0.55
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.42	0.55
1:B:251:THR:HA	1:B:260:ILE:O	2.06	0.55
1:B:455:VAL:HG21	1:B:480:THR:O	2.06	0.55
1:C:134:VAL:O	1:C:134:VAL:CG1	2.54	0.55
1:F:332:SER:HA	1:F:339:GLN:HE21	1.71	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:LEU:CD2	1:G:347:PRO:HD2	2.35	0.55
1:G:358:GLN:OE1	1:G:358:GLN:HA	2.06	0.55
1:G:453:TYR:C	1:G:453:TYR:CD2	2.79	0.55
1:H:478:GLU:HB2	1:H:481:LEU:HB3	1.88	0.55
1:A:38:ASP:OD2	1:A:40:ASN:HB2	2.06	0.55
1:B:306:ARG:CZ	1:B:311:GLY:HA2	2.37	0.55
1:C:20:LEU:N	1:C:20:LEU:HD23	2.21	0.55
1:D:251:THR:HA	1:D:260:ILE:O	2.06	0.55
1:E:68:HIS:CE1	1:E:460:HIS:NE2	2.75	0.55
1:E:136:ASN:OD1	1:E:137:THR:HG23	2.07	0.55
1:H:458:GLN:HG3	2:H:601:FAD:O2	2.07	0.55
1:A:107:GLN:NE2	3:A:602:GDU:O4	2.40	0.55
1:G:158:PHE:C	1:G:158:PHE:HD1	2.10	0.55
1:G:484:PRO:HA	1:G:487:VAL:HG22	1.89	0.55
1:H:79:ALA:HB2	1:H:225:VAL:CG2	2.36	0.55
1:H:207:ASN:C	1:H:207:ASN:OD1	2.45	0.55
1:A:251:THR:HA	1:A:260:ILE:O	2.07	0.55
1:A:422:PRO:HA	1:A:426:ARG:HD3	1.88	0.55
1:E:179:LEU:HD23	1:E:179:LEU:H	1.70	0.55
1:E:383:ASN:ND2	1:E:386:THR:HG23	2.22	0.55
1:F:147:VAL:CG2	1:F:160:ARG:HH21	2.20	0.55
1:F:219:GLY:O	1:F:223:ILE:HG12	2.07	0.55
1:G:103:PRO:HB3	1:G:202:GLY:HA3	1.89	0.55
1:G:232:GLU:OE1	1:G:232:GLU:N	2.25	0.55
1:H:464:LEU:HG	1:H:480:THR:HB	1.88	0.55
1:B:160:ARG:N	1:B:161:PRO:HD2	2.23	0.54
1:C:143:ASP:HA	1:C:146:ILE:HD12	1.89	0.54
1:E:110:ILE:HG23	1:E:195:VAL:HG22	1.89	0.54
1:F:150:MET:O	1:F:154:ILE:HG13	2.07	0.54
1:H:11:LEU:HD21	1:H:252:VAL:HG11	1.87	0.54
1:H:170:PRO:HD2	1:H:379:MET:SD	2.47	0.54
1:H:299:GLY:HA2	1:H:371:MET:HA	1.89	0.54
1:A:46:LEU:N	2:A:601:FAD:O1A	2.35	0.54
1:B:62:GLY:O	3:B:602:GDU:H6'1	2.07	0.54
1:C:457:ASN:O	1:C:460:HIS:HB2	2.08	0.54
1:E:26:LEU:HD22	1:E:34:TRP:HB3	1.90	0.54
1:E:376:GLU:HB2	1:E:382:VAL:CG1	2.37	0.54
1:F:298:ILE:CD1	1:F:388:LEU:HD13	2.38	0.54
1:F:457:ASN:HB3	2:F:601:FAD:O2	2.06	0.54
1:A:144:GLU:O	1:A:148:ARG:HG3	2.07	0.54
1:C:125:MET:CE	1:C:186:PRO:HB2	2.38	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:TYR:OH	3:C:602:GDU:PB	2.64	0.54
1:C:455:VAL:O	1:C:455:VAL:HG13	2.05	0.54
1:C:494:GLU:HG2	1:G:477:VAL:CA	2.32	0.54
1:E:19:GLY:CA	1:E:268:THR:HG21	2.37	0.54
1:B:155:ALA:O	1:B:160:ARG:HG3	2.07	0.54
1:C:95:VAL:HG23	1:C:102:VAL:O	2.07	0.54
1:D:17:PRO:HD2	2:D:601:FAD:O5'	2.06	0.54
1:H:8:VAL:O	1:H:262:TYR:HA	2.07	0.54
1:A:468:ALA:O	1:A:472:ILE:HG13	2.06	0.54
1:C:57:LEU:HD22	1:C:338:ASN:HA	1.89	0.54
1:C:336:PRO:HG2	1:C:337:TYR:CD1	2.42	0.54
1:G:89:HIS:HB2	1:G:210:PHE:CE2	2.42	0.54
1:G:143:ASP:O	1:G:147:VAL:HG23	2.08	0.54
1:B:178:TRP:HB2	1:B:454:GLU:CG	2.33	0.54
1:C:57:LEU:HD13	1:C:57:LEU:H	1.73	0.54
1:C:182:ARG:HD2	3:C:602:GDU:O2A	2.08	0.54
1:F:204:TRP:CE3	1:F:205:GLY:HA2	2.43	0.54
1:F:303:ARG:NH2	1:F:363:LYS:CB	2.71	0.54
1:G:303:ARG:NH1	1:G:348:THR:OG1	2.26	0.54
1:G:411:TYR:CD1	1:G:412:HIS:N	2.69	0.54
1:G:418:GLY:C	1:G:419:TYR:CD1	2.79	0.54
1:H:337:TYR:CD1	1:H:337:TYR:N	2.75	0.54
1:A:455:VAL:O	1:A:455:VAL:HG13	2.08	0.54
1:B:457:ASN:O	1:B:460:HIS:HB2	2.08	0.54
1:F:25:ARG:HG2	1:F:469:VAL:HB	1.90	0.54
1:G:29:ILE:HG22	1:G:31:GLY:N	2.22	0.54
1:G:341:GLU:HG3	1:G:342:ALA:N	2.21	0.54
1:G:411:TYR:HD1	1:G:411:TYR:C	2.10	0.54
1:G:434:LEU:HB2	1:G:435:PRO:HD3	1.90	0.54
1:A:446:GLY:H	1:A:450:SER:HB2	1.72	0.54
1:C:60:VAL:O	1:C:63:HIS:CD2	2.61	0.54
1:C:64:VAL:HG13	1:C:210:PHE:CD1	2.42	0.54
1:C:142:PHE:O	1:C:146:ILE:HG13	2.07	0.54
1:D:168:ALA:CB	1:D:377:SER:HB3	2.38	0.54
1:F:248:ASN:OD1	1:F:248:ASN:N	2.40	0.54
1:F:309:ARG:H	1:F:309:ARG:HD3	1.73	0.54
2:F:601:FAD:C2'	2:F:601:FAD:H9	2.38	0.54
1:H:23:ALA:HA	1:H:26:LEU:HD12	1.89	0.54
1:A:504:PHE:HA	1:A:507:SER:HB3	1.88	0.54
1:C:175:GLN:HE21	1:C:178:TRP:HD1	1.56	0.54
1:D:143:ASP:O	1:D:147:VAL:HG23	2.08	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ASN:O	1:D:387:ILE:HB	2.07	0.54
1:F:207:ASN:HB3	1:F:315:TRP:CH2	2.42	0.54
1:G:58:TYR:HD2	1:G:411:TYR:CD2	2.25	0.54
1:H:426:ARG:O	1:H:430:LEU:HG	2.08	0.54
1:A:433:ILE:HG22	1:A:434:LEU:N	2.23	0.54
1:B:344:LYS:HD2	1:B:345:LYS:N	2.23	0.54
1:C:18:THR:OG1	1:C:461:SER:HB3	2.07	0.54
1:D:136:ASN:OD1	1:D:136:ASN:N	2.34	0.54
1:G:480:THR:HA	1:G:487:VAL:HG21	1.90	0.54
1:H:54:GLU:HB3	1:H:346:LEU:CD1	2.38	0.54
1:H:402:LYS:HD3	1:H:405:ASP:OD2	2.07	0.54
1:A:46:LEU:HD13	2:A:601:FAD:HM81	1.89	0.53
1:E:291:PHE:CG	1:E:292:TYR:N	2.76	0.53
1:E:454:GLU:OE2	1:E:454:GLU:N	2.20	0.53
1:H:500:GLY:O	1:H:504:PHE:CD2	2.61	0.53
1:B:159:MET:CE	3:B:602:GDU:N3	2.71	0.53
1:B:325:PHE:HA	1:B:374:VAL:HG22	1.89	0.53
1:D:134:VAL:O	1:D:134:VAL:CG1	2.56	0.53
1:D:178:TRP:CB	1:D:454:GLU:HG3	2.35	0.53
1:F:122:ILE:O	1:F:126:ILE:HG13	2.08	0.53
1:G:158:PHE:CG	1:G:159:MET:SD	3.01	0.53
1:H:95:VAL:HG22	1:H:317:TYR:HD2	1.72	0.53
1:H:158:PHE:CD1	1:H:158:PHE:C	2.82	0.53
1:H:471:ASN:HA	1:H:476:ALA:H	1.73	0.53
1:A:269:MET:HG2	1:A:274:LEU:HD22	1.91	0.53
1:A:455:VAL:CG1	1:A:464:LEU:HD11	2.38	0.53
1:D:6:ILE:O	1:D:260:ILE:HA	2.09	0.53
1:D:242:VAL:HA	1:D:254:LEU:CD2	2.38	0.53
1:D:398:THR:HG22	1:D:398:THR:O	2.08	0.53
1:G:367:TYR:CE1	1:G:408:VAL:HG11	2.43	0.53
1:G:500:GLY:O	1:G:504:PHE:CD2	2.62	0.53
1:H:283:LEU:O	1:H:287:THR:HG23	2.08	0.53
1:H:348:THR:HB	1:H:357:PRO:HB3	1.90	0.53
1:A:155:ALA:O	1:A:160:ARG:HG3	2.08	0.53
1:B:395:LEU:HA	1:B:400:MET:HG3	1.91	0.53
1:C:417:HIS:HB3	1:C:448:PHE:CZ	2.44	0.53
1:F:162:TYR:O	1:F:166:VAL:HG12	2.08	0.53
1:G:306:ARG:HD2	1:G:311:GLY:O	2.09	0.53
1:H:28:GLN:NE2	1:H:502:GLN:OE1	2.41	0.53
1:H:417:HIS:HB3	1:H:448:PHE:CZ	2.42	0.53
1:B:91:ARG:HD3	1:B:207:ASN:CB	2.36	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:GLN:NE2	1:C:354:GLY:HA2	2.21	0.53
1:D:175:GLN:HG3	1:D:422:PRO:O	2.09	0.53
1:D:468:ALA:O	1:D:472:ILE:HG13	2.09	0.53
1:H:58:TYR:CE1	1:H:369:SER:OG	2.61	0.53
1:H:342:ALA:O	1:H:365:GLY:O	2.27	0.53
1:H:479:LEU:HA	1:H:483:TYR:HD2	1.74	0.53
1:A:93:SER:HB2	1:A:104:TYR:HB3	1.90	0.53
1:A:108:ASN:HD22	1:A:201:ALA:HB3	1.73	0.53
1:A:419:TYR:HE1	2:A:601:FAD:HM73	1.74	0.53
1:B:16:GLY:HA3	2:B:601:FAD:PA	2.48	0.53
1:C:63:HIS:CD2	2:C:601:FAD:C5X	2.92	0.53
1:C:455:VAL:O	1:C:455:VAL:CG1	2.55	0.53
1:D:113:LEU:O	1:D:118:GLN:NE2	2.31	0.53
1:E:137:THR:C	1:E:148:ARG:HH12	2.11	0.53
1:E:219:GLY:O	1:E:223:ILE:HG12	2.09	0.53
1:E:353:ASP:HB3	1:E:403:PRO:HB3	1.89	0.53
1:F:165:LYS:HZ3	1:F:318:PHE:HB3	1.74	0.53
1:G:17:PRO:N	2:G:601:FAD:O1P	2.42	0.53
1:G:63:HIS:HB2	1:G:218:THR:HG21	1.91	0.53
1:G:116:GLU:OE2	1:G:117:GLU:HG2	2.08	0.53
1:G:250:LYS:HD2	1:G:262:TYR:CE1	2.44	0.53
1:A:43:PRO:HG2	1:A:223:ILE:HD13	1.89	0.53
1:A:163:ASN:HA	1:A:166:VAL:CG1	2.38	0.53
1:C:39:SER:HB3	1:C:241:LYS:HG2	1.90	0.53
1:C:344:LYS:HD2	1:C:345:LYS:N	2.24	0.53
1:D:107:GLN:CD	1:D:107:GLN:H	2.10	0.53
1:F:192:THR:O	1:F:196:ILE:HG13	2.08	0.53
1:G:351:LEU:HD12	1:G:404:THR:HA	1.90	0.53
1:A:58:TYR:HA	1:A:331:PHE:CE2	2.42	0.53
1:D:196:ILE:HD12	1:F:119:VAL:HG22	1.91	0.53
1:D:242:VAL:HA	1:D:254:LEU:HD22	1.90	0.53
1:E:387:ILE:HG23	1:E:388:LEU:H	1.71	0.53
1:H:28:GLN:HG3	1:H:497:LEU:HD12	1.91	0.53
1:C:182:ARG:HD2	3:C:602:GDU:PA	2.49	0.53
1:E:326:TYR:N	1:E:374:VAL:HG13	2.23	0.53
1:F:142:PHE:CB	1:F:174:MET:HB2	2.39	0.53
1:G:149:MET:SD	1:G:184:ALA:CA	2.94	0.53
1:A:242:VAL:HA	1:A:254:LEU:CD2	2.39	0.53
1:C:242:VAL:H	2:C:601:FAD:H62A	1.55	0.53
1:C:383:ASN:O	1:C:387:ILE:HB	2.08	0.53
1:E:66:PHE:CB	1:E:206:PRO:O	2.57	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:CYS:HB2	1:F:324:PRO:HD2	1.90	0.53
1:G:337:TYR:CD1	1:G:337:TYR:N	2.76	0.53
1:H:323:CYS:HB2	1:H:325:PHE:CZ	2.44	0.53
1:B:143:ASP:O	1:B:147:VAL:HG23	2.08	0.52
1:D:38:ASP:HA	2:D:601:FAD:H2A	1.91	0.52
1:F:70:LYS:HB3	1:F:496:ARG:NH1	2.25	0.52
1:G:322:ASN:ND2	1:G:397:ASN:HB3	2.23	0.52
1:G:389:ALA:O	1:G:392:ILE:HB	2.09	0.52
1:H:28:GLN:NE2	1:H:497:LEU:O	2.37	0.52
1:H:160:ARG:HB2	1:H:161:PRO:HD3	1.91	0.52
1:H:338:ASN:HB2	1:H:339:GLN:HE22	1.73	0.52
1:H:349:MET:SD	1:H:409:SER:HA	2.49	0.52
1:H:411:TYR:HD1	1:H:411:TYR:C	2.11	0.52
1:A:455:VAL:O	1:A:455:VAL:CG1	2.56	0.52
1:B:38:ASP:OD2	1:B:40:ASN:HB2	2.08	0.52
1:B:87:TYR:HB3	1:B:89:HIS:CE1	2.44	0.52
1:E:38:ASP:OD2	1:E:40:ASN:N	2.42	0.52
1:E:159:MET:CE	3:E:602:GDU:C2	2.88	0.52
1:F:129:ALA:O	1:F:132:ALA:HB3	2.08	0.52
1:G:64:VAL:HG22	1:G:210:PHE:CD1	2.44	0.52
1:G:249:ASN:N	1:G:249:ASN:OD1	2.42	0.52
1:H:492:ASN:ND2	1:H:492:ASN:N	2.56	0.52
1:D:11:LEU:O	1:D:265:LEU:HD12	2.09	0.52
1:E:12:VAL:O	1:E:36:ILE:HA	2.09	0.52
1:G:18:THR:HG21	1:G:268:THR:CG2	2.32	0.52
1:G:25:ARG:HD3	1:G:470:ASP:OD1	2.09	0.52
1:G:189:LYS:O	1:G:193:THR:OG1	2.23	0.52
1:G:194:ASN:ND2	1:G:199:LYS:O	2.42	0.52
1:A:152:THR:HG22	1:A:156:ASP:OD2	2.09	0.52
1:E:19:GLY:H	1:E:268:THR:HG21	1.72	0.52
1:E:167:TRP:CD2	1:E:174:MET:HE1	2.44	0.52
1:G:160:ARG:HB2	1:G:161:PRO:HD3	1.92	0.52
1:H:70:LYS:HB2	1:H:493:THR:HA	1.90	0.52
1:A:466:VAL:HG12	1:A:495:ARG:NH1	2.25	0.52
1:C:110:ILE:CA	1:C:113:LEU:HD12	2.35	0.52
1:C:242:VAL:HA	1:C:254:LEU:HD22	1.91	0.52
1:D:68:HIS:O	1:D:492:ASN:ND2	2.40	0.52
1:D:163:ASN:HA	1:D:166:VAL:CG1	2.39	0.52
1:E:204:TRP:CE3	1:E:205:GLY:HA2	2.44	0.52
1:F:349:MET:N	1:F:407:ILE:O	2.36	0.52
1:H:163:ASN:O	1:H:167:TRP:HB2	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:283:LEU:HD22	1:H:433:ILE:HG23	1.91	0.52
1:A:245:VAL:HG22	1:A:252:VAL:HG23	1.90	0.52
1:B:103:PRO:HB2	1:B:109:ASN:ND2	2.25	0.52
1:D:16:GLY:CA	2:D:601:FAD:H52A	2.38	0.52
1:E:22:ALA:O	1:E:26:LEU:HB2	2.08	0.52
1:F:313:LYS:O	1:F:333:ASN:ND2	2.42	0.52
1:F:325:PHE:HA	1:F:374:VAL:CG1	2.40	0.52
1:G:253:THR:HA	1:G:259:THR:HG22	1.92	0.52
1:H:389:ALA:O	1:H:392:ILE:HB	2.10	0.52
1:H:455:VAL:HG13	1:H:484:PRO:HB3	1.91	0.52
1:A:199:LYS:HD2	1:A:200:THR:O	2.09	0.52
1:A:416:ASP:HB2	1:F:281:GLN:HE21	1.75	0.52
1:C:114:PRO:O	1:C:118:GLN:HG3	2.09	0.52
1:E:69:TYR:HB2	1:E:72:PHE:HB3	1.91	0.52
1:E:427:GLU:O	1:E:431:THR:HG23	2.09	0.52
1:G:89:HIS:NE2	1:G:334:TYR:HA	2.25	0.52
1:A:28:GLN:NE2	1:A:502:GLN:OE1	2.42	0.52
1:A:395:LEU:HD22	1:A:400:MET:HE2	1.92	0.52
1:B:125:MET:CE	1:B:186:PRO:HB2	2.40	0.52
1:B:134:VAL:CG1	1:B:134:VAL:O	2.57	0.52
1:C:175:GLN:HG3	1:C:422:PRO:O	2.10	0.52
1:C:307:PRO:HD2	1:C:310:ILE:HD12	1.91	0.52
1:E:142:PHE:O	1:E:146:ILE:HG13	2.10	0.52
1:E:167:TRP:HE3	1:E:421:THR:HG22	1.74	0.52
1:E:335:SER:HB3	1:E:338:ASN:OD1	2.09	0.52
1:F:82:LYS:HB2	1:F:85:ASP:OD2	2.09	0.52
1:F:303:ARG:HH21	1:F:363:LYS:C	2.13	0.52
1:G:8:VAL:O	1:G:262:TYR:HA	2.10	0.52
1:G:79:ALA:HB2	1:G:225:VAL:CG2	2.38	0.52
1:A:183:VAL:HG22	3:A:602:GDU:H1D	1.92	0.52
1:B:504:PHE:CZ	1:F:264:LYS:HG2	2.43	0.52
1:E:24:LYS:HE3	1:E:229:LEU:HD21	1.92	0.52
1:E:298:ILE:CD1	1:E:388:LEU:HD13	2.40	0.52
1:F:19:GLY:CA	1:F:268:THR:HG21	2.40	0.52
1:F:306:ARG:NH1	1:F:333:ASN:OD1	2.42	0.52
1:A:344:LYS:HD2	1:A:345:LYS:N	2.25	0.52
1:B:346:LEU:HD23	1:B:347:PRO:HD2	1.91	0.52
1:D:336:PRO:HG2	1:D:337:TYR:CD1	2.45	0.52
1:D:455:VAL:HG21	1:D:480:THR:O	2.10	0.52
1:F:10:VAL:HG22	1:F:264:LYS:HG3	1.92	0.52
1:F:158:PHE:O	1:F:161:PRO:HG2	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:453:TYR:CD2	1:F:453:TYR:O	2.62	0.52
1:G:210:PHE:HZ	1:G:334:TYR:CE1	2.28	0.52
1:H:254:LEU:HB2	1:H:258:THR:HB	1.91	0.52
1:H:270:ALA:HB1	1:H:272:ASP:OD1	2.09	0.52
1:B:199:LYS:HD2	1:B:200:THR:O	2.10	0.51
1:D:40:ASN:O	1:D:236:PHE:HB3	2.09	0.51
1:D:271:VAL:HA	1:D:274:LEU:HB2	1.92	0.51
1:E:18:THR:HA	1:E:461:SER:O	2.09	0.51
1:E:504:PHE:N	1:E:504:PHE:CD1	2.78	0.51
1:F:110:ILE:HG23	1:F:195:VAL:HG22	1.93	0.51
1:G:244:LYS:HB3	1:G:253:THR:HB	1.91	0.51
1:G:453:TYR:CD2	1:G:453:TYR:O	2.63	0.51
1:C:155:ALA:O	1:C:160:ARG:HG3	2.10	0.51
1:G:283:LEU:O	1:G:287:THR:HG23	2.10	0.51
1:G:375:SER:OG	1:G:380:LYS:HE3	2.11	0.51
1:G:455:VAL:HA	1:G:460:HIS:ND1	2.24	0.51
1:D:325:PHE:CZ	1:D:395:LEU:HD23	2.45	0.51
1:E:150:MET:O	1:E:154:ILE:HG13	2.10	0.51
1:F:21:GLY:HA2	1:F:462:PHE:CE1	2.45	0.51
1:F:38:ASP:OD1	2:F:601:FAD:H1B	2.11	0.51
1:G:38:ASP:OD2	1:G:39:SER:N	2.43	0.51
1:G:376:GLU:CG	1:G:382:VAL:HG13	2.37	0.51
1:H:272:ASP:OD1	1:H:272:ASP:N	2.40	0.51
1:B:232:GLU:H	1:B:232:GLU:CD	2.13	0.51
1:B:242:VAL:HA	1:B:254:LEU:HD22	1.93	0.51
1:B:346:LEU:HD23	1:B:347:PRO:CD	2.40	0.51
1:D:183:VAL:HG22	3:D:602:GDU:H1D	1.93	0.51
1:E:269:MET:CE	1:E:273:PHE:HB3	2.39	0.51
1:B:395:LEU:HD22	1:B:400:MET:CE	2.40	0.51
1:E:133:ARG:NH1	1:E:133:ARG:CG	2.71	0.51
1:H:143:ASP:O	1:H:147:VAL:HG23	2.10	0.51
1:A:32:PRO:HG3	1:E:504:PHE:HD2	1.75	0.51
1:C:398:THR:HB	1:C:400:MET:HG3	1.93	0.51
1:E:291:PHE:CE1	1:E:292:TYR:O	2.64	0.51
1:H:250:LYS:O	1:H:261:GLY:HA2	2.10	0.51
1:C:242:VAL:HA	1:C:254:LEU:CD2	2.41	0.51
1:E:320:GLU:HB2	1:E:322:ASN:OD1	2.11	0.51
1:F:272:ASP:N	1:F:272:ASP:OD1	2.43	0.51
1:F:458:GLN:HG3	2:F:601:FAD:H1'2	1.91	0.51
1:A:192:THR:OG1	1:A:193:THR:N	2.43	0.51
1:C:306:ARG:CZ	1:C:311:GLY:HA2	2.40	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:GLY:HA3	2:D:601:FAD:O1P	2.11	0.51
1:D:212:PHE:CG	1:D:213:PRO:HD2	2.46	0.51
1:D:272:ASP:OD1	1:D:272:ASP:N	2.44	0.51
1:E:281:GLN:OE1	1:E:284:VAL:HB	2.11	0.51
1:F:167:TRP:HE3	1:F:421:THR:HG22	1.75	0.51
1:F:391:CYS:O	1:F:395:LEU:HG	2.11	0.51
1:G:9:ASP:OD1	1:G:33:SER:N	2.43	0.51
1:A:69:TYR:CD2	1:A:463:MET:HG3	2.46	0.51
1:A:189:LYS:HE2	1:G:123:ASP:HA	1.92	0.51
1:D:494:GLU:HG2	1:H:477:VAL:HA	1.93	0.51
1:F:204:TRP:CE3	1:F:205:GLY:N	2.79	0.51
1:G:18:THR:HB	2:G:601:FAD:O2P	2.11	0.51
1:G:95:VAL:HG22	1:G:317:TYR:HD2	1.75	0.51
1:H:244:LYS:HB3	1:H:253:THR:HB	1.92	0.51
1:D:63:HIS:HB3	1:D:458:GLN:NE2	2.26	0.51
1:D:192:THR:OG1	1:D:193:THR:N	2.44	0.51
1:F:15:ALA:H	2:F:601:FAD:H4B	1.75	0.51
1:F:149:MET:O	1:F:149:MET:HG2	2.11	0.51
1:G:383:ASN:ND2	1:G:386:THR:HG23	2.25	0.51
1:G:447:ARG:HG2	1:G:448:PHE:CE2	2.45	0.51
2:G:601:FAD:O1P	2:G:601:FAD:O1A	2.29	0.51
1:B:303:ARG:NH2	1:B:363:LYS:O	2.43	0.50
1:B:455:VAL:O	1:B:455:VAL:CG1	2.59	0.50
1:C:325:PHE:CZ	1:C:395:LEU:HD23	2.45	0.50
1:D:91:ARG:O	1:D:92:ILE:HD13	2.11	0.50
1:F:230:PRO:CG	1:F:233:LYS:HD2	2.37	0.50
1:G:15:ALA:HB2	1:G:38:ASP:HB2	1.91	0.50
1:H:175:GLN:O	1:H:178:TRP:NE1	2.44	0.50
1:H:253:THR:HA	1:H:259:THR:HG22	1.93	0.50
1:H:438:GLN:HA	1:H:442:ILE:O	2.10	0.50
1:B:304:GLY:O	1:B:368:TRP:HD1	1.95	0.50
1:C:212:PHE:CG	1:C:213:PRO:HD2	2.46	0.50
1:D:155:ALA:O	1:D:160:ARG:HG3	2.12	0.50
1:D:432:GLN:O	1:D:436:LYS:HB2	2.11	0.50
1:E:309:ARG:HD3	1:E:309:ARG:H	1.76	0.50
1:E:467:GLU:HG2	1:E:495:ARG:NH1	2.26	0.50
1:G:16:GLY:O	1:G:20:LEU:HG	2.10	0.50
1:G:39:SER:HB3	1:G:241:LYS:CB	2.41	0.50
1:G:158:PHE:HE1	1:G:162:TYR:CG	2.28	0.50
1:G:204:TRP:HA	1:G:204:TRP:HE3	1.75	0.50
1:A:307:PRO:HD2	1:A:310:ILE:HD12	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:VAL:HG13	1:B:210:PHE:CD1	2.46	0.50
1:B:95:VAL:HG23	1:B:102:VAL:O	2.10	0.50
1:B:192:THR:O	1:B:196:ILE:HG13	2.12	0.50
1:B:244:LYS:HG2	1:B:245:VAL:N	2.26	0.50
1:C:6:ILE:O	1:C:260:ILE:HA	2.10	0.50
1:C:182:ARG:NH1	3:C:602:GDU:O2'	2.43	0.50
1:D:87:TYR:HB3	1:D:89:HIS:CE1	2.46	0.50
1:D:108:ASN:HD22	1:D:201:ALA:HB3	1.75	0.50
1:D:150:MET:HG2	1:D:154:ILE:HG21	1.93	0.50
1:D:306:ARG:CZ	1:D:311:GLY:HA2	2.41	0.50
1:E:204:TRP:CE3	1:E:205:GLY:N	2.79	0.50
1:E:324:PRO:O	1:E:374:VAL:HG11	2.10	0.50
1:F:18:THR:HA	1:F:461:SER:O	2.10	0.50
1:F:82:LYS:HB2	1:F:85:ASP:CG	2.30	0.50
1:F:454:GLU:OE2	1:F:454:GLU:N	2.26	0.50
1:B:455:VAL:O	1:B:455:VAL:HG13	2.11	0.50
1:C:139:PRO:HB2	1:C:176:CYS:SG	2.51	0.50
1:D:447:ARG:O	1:D:451:TRP:HA	2.11	0.50
1:E:244:LYS:HG2	1:E:245:VAL:N	2.26	0.50
1:F:38:ASP:OD2	1:F:40:ASN:N	2.41	0.50
1:F:397:ASN:C	1:F:399:GLU:H	2.14	0.50
1:F:411:TYR:OH	1:F:413:ARG:HB3	2.11	0.50
1:F:443:TRP:N	1:F:443:TRP:CE3	2.79	0.50
1:H:38:ASP:OD1	2:H:601:FAD:O3B	2.23	0.50
1:H:309:ARG:HG2	1:H:310:ILE:CD1	2.42	0.50
1:B:183:VAL:HG13	3:B:602:GDU:O2	2.09	0.50
1:B:346:LEU:HD13	1:B:408:VAL:HG13	1.93	0.50
1:D:504:PHE:HA	1:D:507:SER:HB3	1.92	0.50
1:G:299:GLY:HA2	1:G:370:ILE:O	2.11	0.50
1:H:425:GLU:CD	1:H:425:GLU:N	2.64	0.50
1:H:464:LEU:HD21	1:H:481:LEU:CA	2.41	0.50
1:C:103:PRO:CG	1:C:109:ASN:ND2	2.72	0.50
1:C:199:LYS:HD2	1:C:200:THR:O	2.12	0.50
1:E:270:ALA:HB3	1:E:273:PHE:CD2	2.47	0.50
1:F:76:LEU:HD12	1:F:211:ARG:NH2	2.27	0.50
1:F:136:ASN:OD1	1:F:137:THR:HG23	2.10	0.50
2:F:601:FAD:H9	2:F:601:FAD:O2'	2.11	0.50
1:G:150:MET:O	1:G:154:ILE:HD13	2.11	0.50
1:G:181:GLU:OE1	1:G:181:GLU:HA	2.12	0.50
1:H:335:SER:HB3	1:H:338:ASN:OD1	2.11	0.50
1:H:453:TYR:CD2	1:H:453:TYR:O	2.64	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:TRP:CB	1:B:454:GLU:HG3	2.35	0.50
1:B:212:PHE:CG	1:B:213:PRO:HD2	2.47	0.50
1:C:152:THR:HG22	1:C:156:ASP:OD2	2.11	0.50
1:E:122:ILE:HG22	1:E:123:ASP:N	2.27	0.50
1:E:224:ALA:O	1:E:228:THR:HG23	2.12	0.50
1:E:359:SER:HB3	1:E:363:LYS:HE2	1.93	0.50
1:F:166:VAL:HA	1:F:326:TYR:CD2	2.47	0.50
1:G:332:SER:HA	1:G:339:GLN:HE22	1.76	0.50
1:G:455:VAL:HG21	1:G:480:THR:O	2.12	0.50
1:G:479:LEU:HA	1:G:483:TYR:HD2	1.76	0.50
1:H:181:GLU:N	1:H:485:ASP:OD1	2.44	0.50
1:B:16:GLY:HA3	2:B:601:FAD:O5B	2.11	0.50
1:C:69:TYR:CD2	1:C:463:MET:HG3	2.47	0.50
1:C:143:ASP:O	1:C:147:VAL:HG23	2.11	0.50
1:C:192:THR:O	1:C:196:ILE:HG13	2.11	0.50
1:D:160:ARG:N	1:D:161:PRO:HD2	2.26	0.50
1:D:455:VAL:O	1:D:455:VAL:CG1	2.59	0.50
1:D:483:TYR:N	1:D:484:PRO:HD3	2.27	0.50
1:E:413:ARG:HG2	1:E:414:ARG:N	2.26	0.50
1:E:467:GLU:HG2	1:E:495:ARG:NH2	2.26	0.50
1:F:71:TYR:HB2	1:F:495:ARG:O	2.11	0.50
1:F:122:ILE:CG2	1:F:123:ASP:N	2.75	0.50
1:G:128:ALA:HB2	1:G:151:GLY:HA2	1.93	0.50
1:H:61:GLY:HA3	2:H:601:FAD:C6	2.41	0.50
1:H:178:TRP:HD1	1:H:178:TRP:H	1.60	0.50
1:H:351:LEU:HD12	1:H:404:THR:HA	1.93	0.50
1:B:175:GLN:HG3	1:B:422:PRO:O	2.12	0.50
1:B:296:HIS:NE2	1:B:382:VAL:HG21	2.27	0.50
1:C:108:ASN:ND2	1:C:201:ALA:HB3	2.27	0.50
1:D:244:LYS:HG2	1:D:245:VAL:N	2.27	0.50
1:F:110:ILE:CG2	1:F:195:VAL:HG22	2.42	0.50
1:G:109:ASN:HD21	1:G:201:ALA:C	2.14	0.50
1:H:167:TRP:O	1:H:169:VAL:HG12	2.12	0.50
1:H:345:LYS:HE3	1:H:364:GLU:OE1	2.12	0.50
1:C:103:PRO:HB2	1:C:109:ASN:HD21	1.73	0.49
1:F:114:PRO:O	1:F:118:GLN:HG3	2.11	0.49
1:F:326:TYR:N	1:F:374:VAL:HG13	2.26	0.49
1:G:251:THR:HA	1:G:260:ILE:O	2.12	0.49
1:G:262:TYR:CE1	1:G:265:LEU:HB2	2.47	0.49
1:G:351:LEU:HD13	1:G:404:THR:O	2.11	0.49
1:H:455:VAL:HA	1:H:460:HIS:ND1	2.27	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:MET:HG2	1:B:274:LEU:HD22	1.94	0.49
1:B:499:ASP:O	1:B:503:VAL:HG23	2.11	0.49
1:C:57:LEU:N	1:C:57:LEU:CD1	2.75	0.49
1:D:152:THR:HG22	1:D:156:ASP:OD2	2.11	0.49
1:D:455:VAL:O	1:D:455:VAL:HG13	2.11	0.49
1:F:16:GLY:HA3	2:F:601:FAD:O5B	2.11	0.49
1:F:396:VAL:HA	1:F:401:LEU:HB2	1.94	0.49
1:G:270:ALA:HB1	1:G:272:ASP:OD1	2.12	0.49
1:H:61:GLY:HA2	1:H:373:GLU:OE1	2.12	0.49
1:H:292:TYR:CE1	1:H:417:HIS:ND1	2.79	0.49
1:H:411:TYR:CD1	1:H:412:HIS:N	2.70	0.49
1:B:72:PHE:CE2	1:B:76:LEU:HD11	2.48	0.49
1:D:58:TYR:HA	1:D:331:PHE:CE2	2.46	0.49
1:F:91:ARG:CZ	1:F:93:SER:HB2	2.42	0.49
1:G:64:VAL:HG22	1:G:210:PHE:CE1	2.47	0.49
1:G:71:TYR:CE2	1:G:497:LEU:HA	2.47	0.49
1:G:292:TYR:CZ	1:G:417:HIS:CE1	3.00	0.49
1:G:401:LEU:HA	1:G:405:ASP:OD2	2.13	0.49
1:G:402:LYS:HD3	1:G:402:LYS:H	1.78	0.49
1:A:241:LYS:HE3	2:A:601:FAD:N6A	2.28	0.49
1:E:303:ARG:NH1	1:E:348:THR:OG1	2.45	0.49
1:F:269:MET:CE	1:F:273:PHE:HB3	2.42	0.49
1:G:28:GLN:NE2	1:G:502:GLN:OE1	2.45	0.49
1:G:63:HIS:H	1:G:63:HIS:CD2	2.30	0.49
1:G:104:TYR:CD2	1:G:105:PRO:HA	2.46	0.49
1:G:125:MET:HG2	1:G:188:LEU:HG	1.94	0.49
1:H:11:LEU:HB3	1:H:265:LEU:HD12	1.93	0.49
1:A:244:LYS:HG2	1:A:245:VAL:N	2.27	0.49
1:A:325:PHE:CZ	1:A:395:LEU:HD23	2.48	0.49
1:B:196:ILE:HG21	1:H:119:VAL:HG22	1.95	0.49
1:E:397:ASN:C	1:E:399:GLU:H	2.16	0.49
1:E:411:TYR:OH	1:E:413:ARG:HB3	2.13	0.49
1:F:15:ALA:N	2:F:601:FAD:H4B	2.27	0.49
1:F:460:HIS:O	1:F:463:MET:HB2	2.11	0.49
1:G:71:TYR:HB2	1:G:495:ARG:O	2.11	0.49
1:G:393:GLN:NE2	1:G:397:ASN:OD1	2.45	0.49
1:D:95:VAL:HG23	1:D:102:VAL:O	2.13	0.49
1:D:178:TRP:HB2	1:D:454:GLU:CG	2.38	0.49
1:D:352:ALA:HB3	1:D:403:PRO:HA	1.93	0.49
1:F:424:LEU:HB2	1:F:425:GLU:OE1	2.12	0.49
1:F:508:LYS:HG3	1:F:509:ALA:N	2.27	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:GLU:OE2	1:G:54:GLU:N	2.45	0.49
1:A:346:LEU:HD23	1:A:347:PRO:HD2	1.93	0.49
1:B:307:PRO:HB2	1:B:309:ARG:HG2	1.95	0.49
1:D:388:LEU:O	1:D:392:ILE:HG13	2.13	0.49
1:E:173:LYS:HA	1:E:424:LEU:HD11	1.95	0.49
1:F:56:PHE:CE2	1:F:409:SER:HB3	2.46	0.49
1:H:28:GLN:HE21	1:H:497:LEU:C	2.15	0.49
1:H:48:SER:O	1:H:60:VAL:HG23	2.13	0.49
1:H:460:HIS:CE1	1:H:488:ASN:OD1	2.66	0.49
1:B:414:ARG:HH12	1:B:416:ASP:HA	1.78	0.49
1:B:504:PHE:CZ	1:F:264:LYS:CG	2.96	0.49
1:C:103:PRO:HG2	1:C:109:ASN:CG	2.33	0.49
1:C:142:PHE:HE2	1:C:163:ASN:ND2	2.10	0.49
1:C:178:TRP:CB	1:C:454:GLU:CG	2.90	0.49
1:D:330:ILE:HB	1:D:333:ASN:OD1	2.13	0.49
1:F:26:LEU:HG	1:F:469:VAL:HG13	1.94	0.49
1:G:58:TYR:CE1	1:G:369:SER:OG	2.63	0.49
1:H:11:LEU:HB3	1:H:265:LEU:CD1	2.43	0.49
1:H:104:TYR:CD2	1:H:105:PRO:HA	2.46	0.49
1:A:178:TRP:CH2	1:A:179:LEU:HD23	2.48	0.49
1:A:346:LEU:HD23	1:A:347:PRO:CD	2.43	0.49
1:B:57:LEU:HD13	1:B:338:ASN:O	2.13	0.49
1:D:69:TYR:CD2	1:D:463:MET:HG3	2.48	0.49
1:D:351:LEU:HB2	1:D:355:SER:OG	2.13	0.49
1:E:9:ASP:CA	1:E:263:LYS:HD3	2.37	0.49
1:E:18:THR:O	1:E:465:GLY:HA3	2.13	0.49
1:F:179:LEU:HD23	1:F:179:LEU:H	1.78	0.49
1:G:11:LEU:HD21	1:G:252:VAL:CG1	2.43	0.49
1:G:126:ILE:HA	1:G:188:LEU:HD11	1.95	0.49
1:G:418:GLY:O	1:G:419:TYR:HD1	1.96	0.49
1:G:467:GLU:CD	1:G:480:THR:H	2.12	0.49
1:H:322:ASN:ND2	1:H:397:ASN:HB3	2.26	0.49
1:H:332:SER:OG	1:H:368:TRP:HB2	2.13	0.49
1:A:346:LEU:HD13	1:A:408:VAL:HG13	1.94	0.49
1:C:455:VAL:O	1:C:460:HIS:CB	2.61	0.49
1:D:175:GLN:NE2	1:D:178:TRP:HD1	2.10	0.49
1:D:480:THR:HA	1:D:487:VAL:HG11	1.95	0.49
1:E:17:PRO:O	1:E:462:PHE:CD1	2.66	0.49
1:F:19:GLY:H	1:F:268:THR:HG21	1.73	0.49
1:F:187:ASN:O	1:F:191:VAL:HG23	2.13	0.49
1:G:2:THR:OG1	1:G:3:HIS:N	2.46	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:PHE:HA	1:G:176:CYS:HB3	1.94	0.49
1:G:290:LEU:HD21	1:G:430:LEU:HD23	1.94	0.49
1:H:38:ASP:OD2	1:H:39:SER:N	2.46	0.49
1:H:203:ASN:ND2	1:H:204:TRP:H	2.08	0.49
1:H:290:LEU:HD21	1:H:430:LEU:HD23	1.95	0.49
1:H:484:PRO:HA	1:H:487:VAL:CG2	2.43	0.49
1:A:178:TRP:CB	1:A:454:GLU:HG3	2.38	0.48
1:A:272:ASP:OD1	1:A:272:ASP:N	2.45	0.48
1:A:463:MET:O	1:A:467:GLU:HG3	2.13	0.48
1:B:17:PRO:HG2	2:B:601:FAD:O4'	2.13	0.48
1:C:346:LEU:HD13	1:C:408:VAL:HG13	1.95	0.48
1:F:108:ASN:C	1:F:194:ASN:HD22	2.17	0.48
1:F:163:ASN:ND2	3:F:602:GDU:O2D	2.42	0.48
1:G:28:GLN:HG3	1:G:497:LEU:HD12	1.95	0.48
1:G:71:TYR:CD2	1:G:496:ARG:C	2.86	0.48
1:G:332:SER:OG	1:G:368:TRP:HB2	2.13	0.48
1:H:100:GLN:HA	1:H:100:GLN:OE1	2.13	0.48
1:A:395:LEU:HA	1:A:400:MET:HG3	1.94	0.48
1:B:272:ASP:OD1	1:B:272:ASP:N	2.47	0.48
1:C:178:TRP:CB	1:C:454:GLU:HG3	2.36	0.48
1:D:125:MET:CE	1:D:186:PRO:HB2	2.43	0.48
1:F:303:ARG:HH21	1:F:363:LYS:CA	2.26	0.48
1:F:350:GLN:NE2	1:F:407:ILE:HD12	2.28	0.48
1:G:464:LEU:HD21	1:G:481:LEU:CA	2.44	0.48
1:H:28:GLN:CG	1:H:497:LEU:O	2.62	0.48
1:B:250:LYS:HD3	1:B:262:TYR:O	2.13	0.48
1:C:116:GLU:O	1:C:119:VAL:HB	2.13	0.48
1:C:458:GLN:HG3	2:C:601:FAD:N1	2.28	0.48
1:D:477:VAL:HA	1:H:494:GLU:HG2	1.93	0.48
1:E:434:LEU:N	1:E:435:PRO:HD2	2.28	0.48
1:E:443:TRP:N	1:E:443:TRP:CE3	2.81	0.48
1:F:69:TYR:CD1	1:F:463:MET:HG3	2.48	0.48
1:G:197:LEU:HB2	1:G:199:LYS:HB3	1.95	0.48
1:H:86:TRP:HA	1:H:86:TRP:CE3	2.49	0.48
1:H:492:ASN:HD22	1:H:492:ASN:N	2.10	0.48
2:B:601:FAD:H6	3:B:602:GDU:O3'	2.12	0.48
1:C:5:ASP:OD2	1:C:258:THR:HA	2.12	0.48
1:C:87:TYR:HB3	1:C:89:HIS:CE1	2.48	0.48
1:C:232:GLU:OE2	1:C:232:GLU:N	2.45	0.48
1:D:395:LEU:HD22	1:D:400:MET:HE2	1.95	0.48
1:G:242:VAL:HG13	1:G:252:VAL:HG22	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PHE:CE1	1:A:339:GLN:HB3	2.49	0.48
1:A:475:GLY:O	1:E:494:GLU:HB2	2.14	0.48
1:B:196:ILE:HD12	1:H:119:VAL:HG22	1.96	0.48
1:B:336:PRO:HG2	1:B:337:TYR:CD1	2.49	0.48
1:E:322:ASN:HD21	1:E:398:THR:HG22	1.77	0.48
1:E:331:PHE:CE2	1:E:338:ASN:ND2	2.82	0.48
1:G:28:GLN:HG2	1:G:497:LEU:O	2.13	0.48
1:G:234:THR:HB	1:G:236:PHE:CE2	2.48	0.48
1:C:8:VAL:HG11	1:C:35:MET:HG2	1.96	0.48
1:D:47:ALA:HB1	1:D:222:TRP:NE1	2.27	0.48
1:E:63:HIS:CE1	2:E:601:FAD:C5X	2.97	0.48
1:G:141:THR:OG1	1:G:144:GLU:HB2	2.13	0.48
1:H:242:VAL:HG13	1:H:252:VAL:HG22	1.96	0.48
1:H:250:LYS:HD2	1:H:262:TYR:CE1	2.48	0.48
1:H:425:GLU:CD	1:H:425:GLU:H	2.17	0.48
1:A:39:SER:HB3	1:A:241:LYS:HG2	1.95	0.48
1:B:437:LEU:CD1	1:B:444:SER:HB2	2.44	0.48
1:C:224:ALA:O	1:C:228:THR:HG23	2.14	0.48
1:D:56:PHE:CE1	1:D:339:GLN:HB3	2.49	0.48
1:E:70:LYS:HD2	1:E:70:LYS:HA	1.55	0.48
1:E:189:LYS:O	1:E:192:THR:OG1	2.20	0.48
1:E:269:MET:HE1	2:E:601:FAD:H61A	1.79	0.48
1:F:324:PRO:O	1:F:374:VAL:HG11	2.13	0.48
1:F:387:ILE:HG23	1:F:388:LEU:N	2.28	0.48
1:G:270:ALA:HA	1:G:448:PHE:C	2.34	0.48
1:B:47:ALA:CB	1:B:222:TRP:NE1	2.76	0.48
1:E:376:GLU:HG2	1:E:377:SER:N	2.28	0.48
1:G:17:PRO:HG2	2:G:601:FAD:H4'	1.96	0.48
1:G:58:TYR:CZ	1:G:299:GLY:HA3	2.48	0.48
1:H:158:PHE:C	1:H:158:PHE:HD1	2.15	0.48
1:H:467:GLU:CD	1:H:480:THR:H	2.10	0.48
1:A:32:PRO:HB3	1:E:504:PHE:HD2	1.78	0.48
1:A:39:SER:CB	1:A:241:LYS:HG2	2.43	0.48
1:A:87:TYR:HB3	1:A:89:HIS:HE1	1.79	0.48
1:C:388:LEU:O	1:C:392:ILE:HG13	2.13	0.48
1:C:466:VAL:HG12	1:C:495:ARG:NH1	2.29	0.48
1:F:69:TYR:CE2	1:F:463:MET:HG3	2.48	0.48
1:F:167:TRP:O	1:F:169:VAL:HG13	2.13	0.48
1:F:235:ARG:HG2	1:F:239:LYS:HD2	1.95	0.48
1:G:394:GLY:HA2	1:G:397:ASN:HB2	1.95	0.48
1:B:388:LEU:O	1:B:392:ILE:HG13	2.14	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:LYS:HG2	1:E:364:GLU:HG3	1.95	0.48
1:F:113:LEU:HB3	1:F:114:PRO:HD2	1.96	0.48
1:F:143:ASP:O	1:F:147:VAL:HG23	2.14	0.48
1:G:65:ILE:HD12	1:G:65:ILE:HA	1.64	0.48
1:G:352:ALA:HB2	1:G:405:ASP:HB2	1.96	0.48
1:H:71:TYR:CE2	1:H:497:LEU:HA	2.49	0.48
1:H:507:SER:O	1:H:510:GLN:HB2	2.14	0.48
1:A:395:LEU:HD22	1:A:400:MET:CE	2.44	0.47
1:C:250:LYS:HD3	1:C:262:TYR:O	2.14	0.47
1:D:72:PHE:CE2	1:D:76:LEU:HD11	2.48	0.47
1:E:272:ASP:N	1:E:272:ASP:OD1	2.47	0.47
1:E:387:ILE:HG23	1:E:388:LEU:N	2.28	0.47
1:E:431:THR:O	1:E:435:PRO:HG3	2.14	0.47
1:F:91:ARG:O	1:F:92:ILE:HD13	2.14	0.47
1:F:158:PHE:CD1	1:F:319:PRO:HG3	2.49	0.47
1:F:447:ARG:O	1:F:451:TRP:HA	2.14	0.47
1:G:21:GLY:HA2	1:G:462:PHE:CE1	2.48	0.47
1:G:146:ILE:O	1:G:149:MET:HB2	2.14	0.47
1:G:149:MET:HG2	1:G:184:ALA:HB1	1.96	0.47
1:G:401:LEU:HB3	1:G:405:ASP:HB2	1.96	0.47
1:H:139:PRO:CB	1:H:145:TRP:HB2	2.44	0.47
1:H:383:ASN:O	1:H:387:ILE:HB	2.14	0.47
1:B:249:ASN:O	1:B:251:THR:HG23	2.14	0.47
1:C:57:LEU:CD2	1:C:338:ASN:HA	2.43	0.47
1:C:420:PRO:O	1:C:422:PRO:HD3	2.14	0.47
1:E:134:VAL:CG1	1:E:134:VAL:O	2.61	0.47
1:E:391:CYS:O	1:E:395:LEU:HG	2.14	0.47
1:F:173:LYS:HA	1:F:424:LEU:HD11	1.95	0.47
1:F:402:LYS:HE3	1:F:404:THR:OG1	2.13	0.47
1:G:212:PHE:CD2	1:G:213:PRO:HD2	2.49	0.47
1:G:433:ILE:O	1:G:436:LYS:HB2	2.14	0.47
1:H:43:PRO:HG2	1:H:223:ILE:HD13	1.95	0.47
1:A:115:LYS:O	1:A:118:GLN:HB2	2.15	0.47
1:A:126:ILE:CD1	1:G:189:LYS:HG2	2.45	0.47
1:F:126:ILE:O	1:F:130:LEU:HG	2.14	0.47
1:G:296:HIS:HB2	1:G:374:VAL:HB	1.95	0.47
1:G:350:GLN:OE1	1:G:354:GLY:HA2	2.15	0.47
1:H:149:MET:SD	1:H:184:ALA:O	2.72	0.47
1:A:199:LYS:HD2	1:A:200:THR:N	2.30	0.47
1:A:351:LEU:HB2	1:A:355:SER:OG	2.14	0.47
2:A:601:FAD:H9	2:A:601:FAD:C2'	2.43	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.48	0.47
1:E:154:ILE:HD13	1:E:154:ILE:N	2.22	0.47
1:E:175:GLN:OE1	1:E:178:TRP:HD1	1.97	0.47
1:F:56:PHE:CD2	1:F:409:SER:HB3	2.49	0.47
1:F:455:VAL:HA	1:F:460:HIS:HD1	1.79	0.47
1:A:331:PHE:HB3	1:A:369:SER:HB3	1.96	0.47
1:B:175:GLN:HE22	1:B:177:ALA:HB3	1.80	0.47
1:B:179:LEU:HD23	1:B:183:VAL:HG21	1.96	0.47
1:C:106:PHE:C	1:C:106:PHE:CD2	2.88	0.47
1:C:150:MET:HE3	1:C:159:MET:HG3	1.97	0.47
1:E:19:GLY:O	1:E:22:ALA:HB3	2.15	0.47
1:E:63:HIS:CE1	2:E:601:FAD:N10	2.82	0.47
1:G:24:LYS:HD3	1:G:24:LYS:HA	1.67	0.47
1:G:302:VAL:HA	1:G:406:GLU:O	2.14	0.47
1:G:342:ALA:O	1:G:365:GLY:O	2.32	0.47
1:G:447:ARG:NH1	2:G:601:FAD:H1'1	2.28	0.47
1:H:292:TYR:HB3	1:H:451:TRP:CZ2	2.49	0.47
1:A:455:VAL:HG21	1:A:480:THR:O	2.15	0.47
1:B:108:ASN:HB2	1:B:194:ASN:OD1	2.14	0.47
1:B:175:GLN:NE2	1:B:177:ALA:HB3	2.30	0.47
1:B:207:ASN:O	1:B:208:ALA:C	2.53	0.47
1:B:306:ARG:HA	1:B:307:PRO:HD3	1.79	0.47
1:C:175:GLN:NE2	1:C:177:ALA:HB3	2.30	0.47
1:D:420:PRO:O	1:D:422:PRO:HD3	2.14	0.47
1:E:56:PHE:HE1	1:E:339:GLN:HB3	1.75	0.47
1:E:179:LEU:N	1:E:179:LEU:CD2	2.77	0.47
1:F:51:VAL:HG12	1:F:52:THR:O	2.14	0.47
1:F:286:LEU:O	1:F:289:GLN:HB2	2.14	0.47
1:G:165:LYS:HD3	1:G:318:PHE:O	2.14	0.47
1:G:351:LEU:HB2	1:G:355:SER:H	1.78	0.47
1:H:62:GLY:O	2:H:601:FAD:O4	2.31	0.47
1:A:178:TRP:CB	1:A:454:GLU:CG	2.92	0.47
1:B:57:LEU:CD2	1:B:338:ASN:HA	2.45	0.47
1:B:87:TYR:HB3	1:B:89:HIS:HE1	1.80	0.47
1:B:192:THR:OG1	1:B:193:THR:N	2.47	0.47
1:C:483:TYR:N	1:C:484:PRO:HD3	2.30	0.47
1:E:47:ALA:HB1	1:E:222:TRP:NE1	2.30	0.47
1:E:63:HIS:CD2	1:E:63:HIS:N	2.81	0.47
1:F:109:ASN:ND2	1:F:109:ASN:N	2.63	0.47
1:F:244:LYS:HG2	1:F:245:VAL:N	2.30	0.47
1:F:265:LEU:O	1:F:442:ILE:HA	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:460:HIS:NE2	1:G:488:ASN:OD1	2.47	0.47
1:H:72:PHE:CE1	1:H:459:ASP:HA	2.50	0.47
1:H:187:ASN:OD1	1:H:190:ALA:CB	2.63	0.47
1:H:332:SER:HA	1:H:339:GLN:HE22	1.75	0.47
1:H:337:TYR:N	1:H:337:TYR:HD1	2.12	0.47
1:H:418:GLY:O	1:H:419:TYR:HD1	1.96	0.47
1:A:344:LYS:HD2	1:A:345:LYS:H	1.79	0.47
1:B:130:LEU:HD23	1:H:130:LEU:CD2	2.44	0.47
1:C:269:MET:HG2	1:C:274:LEU:HD22	1.96	0.47
1:C:395:LEU:HD22	1:C:400:MET:CE	2.45	0.47
1:D:103:PRO:HB2	1:D:109:ASN:OD1	2.15	0.47
1:D:168:ALA:HB1	1:D:377:SER:HB3	1.97	0.47
1:D:417:HIS:HB3	1:D:448:PHE:CZ	2.49	0.47
1:E:82:LYS:HB2	1:E:85:ASP:OD2	2.15	0.47
1:G:426:ARG:O	1:G:430:LEU:HG	2.15	0.47
1:H:221:ILE:O	1:H:224:ALA:HB3	2.15	0.47
1:B:107:GLN:CD	1:B:107:GLN:H	2.17	0.47
1:C:437:LEU:HD12	1:C:444:SER:HB2	1.96	0.47
1:D:17:PRO:HG2	2:D:601:FAD:H4'	1.96	0.47
1:E:6:ILE:O	1:E:260:ILE:HA	2.14	0.47
1:E:63:HIS:ND1	2:E:601:FAD:C10	2.78	0.47
1:E:274:LEU:O	1:E:278:MET:HG2	2.13	0.47
1:F:139:PRO:HA	1:F:144:GLU:OE2	2.14	0.47
1:G:420:PRO:HB2	1:G:451:TRP:CD1	2.50	0.47
1:H:64:VAL:HG22	1:H:210:PHE:CE1	2.49	0.47
1:H:175:GLN:HG3	1:H:178:TRP:CD1	2.50	0.47
1:A:494:GLU:HG2	1:E:477:VAL:HB	1.96	0.47
1:B:17:PRO:O	1:B:462:PHE:HA	2.15	0.47
1:B:242:VAL:HA	1:B:254:LEU:CD2	2.45	0.47
1:B:346:LEU:HD13	1:B:408:VAL:CG1	2.45	0.47
1:D:57:LEU:HD13	1:D:338:ASN:C	2.35	0.47
1:E:158:PHE:O	1:E:161:PRO:HG2	2.15	0.47
1:E:508:LYS:HG3	1:E:509:ALA:N	2.29	0.47
1:F:22:ALA:O	1:F:26:LEU:HB2	2.14	0.47
1:H:65:ILE:HG22	1:H:65:ILE:O	2.14	0.47
1:H:96:ARG:HB2	1:H:101:TRP:CZ3	2.50	0.47
1:H:467:GLU:OE1	1:H:479:LEU:N	2.48	0.47
1:A:136:ASN:OD1	1:A:136:ASN:N	2.33	0.46
1:B:473:VAL:O	1:F:499:ASP:HB3	2.16	0.46
1:C:119:VAL:HA	1:E:196:ILE:CD1	2.44	0.46
1:D:278:MET:HE2	1:D:442:ILE:HD12	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:LEU:HD22	1:D:400:MET:CE	2.45	0.46
1:E:207:ASN:HB3	1:E:315:TRP:HH2	1.78	0.46
1:F:351:LEU:HA	1:F:405:ASP:O	2.14	0.46
1:G:210:PHE:HD2	1:G:210:PHE:N	2.13	0.46
1:A:106:PHE:C	1:A:106:PHE:CD2	2.87	0.46
1:A:113:LEU:O	1:A:118:GLN:NE2	2.34	0.46
1:A:119:VAL:HG22	1:G:193:THR:HG22	1.96	0.46
1:A:358:GLN:N	1:A:358:GLN:CD	2.64	0.46
1:B:178:TRP:CB	1:B:454:GLU:CG	2.92	0.46
1:B:287:THR:O	1:B:290:LEU:HD12	2.16	0.46
1:C:39:SER:CB	1:C:241:LYS:HG2	2.45	0.46
1:C:335:SER:HB3	1:C:338:ASN:OD1	2.14	0.46
1:E:139:PRO:HA	1:E:144:GLU:OE2	2.16	0.46
1:F:95:VAL:HG23	1:F:102:VAL:O	2.16	0.46
1:G:106:PHE:CZ	1:G:113:LEU:HD11	2.50	0.46
1:G:425:GLU:N	1:G:425:GLU:CD	2.69	0.46
1:H:326:TYR:CE2	1:H:375:SER:HB3	2.50	0.46
1:A:207:ASN:O	1:A:208:ALA:C	2.53	0.46
1:C:234:THR:HB	1:C:236:PHE:CZ	2.51	0.46
1:D:304:GLY:O	1:D:368:TRP:CD1	2.68	0.46
1:E:17:PRO:C	1:E:462:PHE:HA	2.35	0.46
1:E:275:ALA:HB1	1:E:284:VAL:HG22	1.97	0.46
1:F:467:GLU:HG2	1:F:495:ARG:HH22	1.79	0.46
1:G:323:CYS:HB2	1:G:325:PHE:CE1	2.49	0.46
1:H:58:TYR:CZ	1:H:299:GLY:HA3	2.50	0.46
1:A:46:LEU:O	1:A:63:HIS:HE1	1.98	0.46
1:B:350:GLN:NE2	1:B:351:LEU:O	2.49	0.46
1:C:196:ILE:HG21	1:E:119:VAL:CG2	2.44	0.46
1:D:94:TYR:CD1	1:D:101:TRP:HB3	2.51	0.46
1:E:10:VAL:O	1:E:34:TRP:HA	2.15	0.46
1:E:70:LYS:HB3	1:E:496:ARG:NH1	2.27	0.46
1:E:402:LYS:HE3	1:E:404:THR:OG1	2.15	0.46
1:E:457:ASN:HB3	2:E:601:FAD:N1	2.31	0.46
1:A:106:PHE:C	1:A:106:PHE:HD2	2.19	0.46
1:A:417:HIS:HB3	1:A:448:PHE:CZ	2.50	0.46
1:D:175:GLN:HE22	1:D:177:ALA:HB3	1.80	0.46
1:F:376:GLU:HB2	1:F:382:VAL:CG1	2.45	0.46
1:G:351:LEU:CD1	1:G:404:THR:HA	2.46	0.46
1:H:376:GLU:CG	1:H:382:VAL:HG13	2.35	0.46
1:A:94:TYR:CD1	1:A:101:TRP:HB3	2.50	0.46
3:C:602:GDU:O2A	3:C:602:GDU:H4D	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:PHE:CE2	1:E:409:SER:HB3	2.50	0.46
1:E:167:TRP:O	1:E:169:VAL:HG13	2.16	0.46
1:E:454:GLU:H	1:E:454:GLU:CD	2.12	0.46
1:G:70:LYS:HB2	1:G:493:THR:HA	1.98	0.46
1:G:171:THR:HG22	1:G:174:MET:HE3	1.97	0.46
1:G:210:PHE:N	1:G:210:PHE:CD2	2.83	0.46
1:G:499:ASP:HB2	1:G:502:GLN:OE1	2.16	0.46
1:G:499:ASP:O	1:G:502:GLN:N	2.48	0.46
1:H:70:LYS:HA	1:H:70:LYS:HD2	1.62	0.46
1:H:210:PHE:HD2	1:H:210:PHE:N	2.13	0.46
1:H:367:TYR:HD1	1:H:408:VAL:HG21	1.80	0.46
1:A:232:GLU:H	1:A:232:GLU:CD	2.19	0.46
1:D:207:ASN:O	1:D:208:ALA:C	2.54	0.46
1:D:304:GLY:O	1:D:368:TRP:HD1	1.97	0.46
1:D:473:VAL:HG12	1:H:501:ALA:HA	1.98	0.46
1:E:56:PHE:CD2	1:E:409:SER:HB3	2.51	0.46
1:E:167:TRP:CG	1:E:174:MET:HE3	2.51	0.46
1:G:292:TYR:HB3	1:G:451:TRP:CZ2	2.50	0.46
1:H:2:THR:OG1	1:H:3:HIS:N	2.47	0.46
1:H:469:VAL:HA	1:H:472:ILE:HD12	1.98	0.46
1:A:193:THR:O	1:A:196:ILE:HB	2.15	0.46
1:C:395:LEU:HD22	1:C:400:MET:HE2	1.97	0.46
1:D:303:ARG:NH2	1:D:363:LYS:O	2.43	0.46
1:D:303:ARG:NH1	1:D:348:THR:OG1	2.49	0.46
1:E:38:ASP:HB3	1:E:236:PHE:HD1	1.79	0.46
1:E:250:LYS:O	1:E:261:GLY:HA2	2.16	0.46
1:E:467:GLU:CG	1:E:495:ARG:HH12	2.29	0.46
1:F:332:SER:HB3	1:F:369:SER:H	1.80	0.46
1:G:143:ASP:HA	1:G:146:ILE:CD1	2.43	0.46
1:H:197:LEU:C	1:H:199:LYS:N	2.67	0.46
1:A:125:MET:CE	1:A:186:PRO:HB2	2.44	0.46
1:B:45:GLY:HA3	2:B:601:FAD:O1A	2.16	0.46
1:B:57:LEU:CD1	1:B:57:LEU:N	2.79	0.46
1:B:60:VAL:O	1:B:61:GLY:O	2.34	0.46
1:B:152:THR:HG22	1:B:156:ASP:OD2	2.16	0.46
1:C:344:LYS:HD2	1:C:345:LYS:H	1.79	0.46
1:C:398:THR:HB	1:C:400:MET:CG	2.46	0.46
1:E:63:HIS:CE1	2:E:601:FAD:C9	2.99	0.46
1:E:69:TYR:CE2	1:E:463:MET:HG3	2.51	0.46
1:G:25:ARG:NH1	1:G:470:ASP:OD2	2.49	0.46
1:G:28:GLN:NE2	1:G:497:LEU:O	2.43	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:ILE:HG22	1:G:197:LEU:N	2.31	0.46
1:G:467:GLU:OE1	1:G:480:THR:OG1	2.27	0.46
1:H:63:HIS:HB2	1:H:218:THR:HG21	1.97	0.46
1:H:109:ASN:C	1:H:111:SER:N	2.69	0.46
1:H:419:TYR:CD1	1:H:419:TYR:N	2.84	0.46
1:A:398:THR:HB	1:A:400:MET:HG2	1.98	0.46
1:B:136:ASN:ND2	1:F:133:ARG:HE	2.14	0.46
1:B:325:PHE:CZ	1:B:395:LEU:HD23	2.50	0.46
1:B:455:VAL:O	1:B:460:HIS:CB	2.62	0.46
1:D:38:ASP:OD1	2:D:601:FAD:H1B	2.15	0.46
1:E:349:MET:O	1:E:350:GLN:HB3	2.16	0.46
1:F:9:ASP:H	1:F:33:SER:HG	1.55	0.46
1:F:12:VAL:O	1:F:36:ILE:HA	2.15	0.46
1:G:44:GLY:HA2	1:G:222:TRP:CD1	2.51	0.46
1:G:460:HIS:CE1	1:G:488:ASN:OD1	2.68	0.46
1:H:178:TRP:CD1	1:H:178:TRP:N	2.84	0.46
1:H:192:THR:OG1	1:H:193:THR:N	2.49	0.46
1:A:204:TRP:CE3	1:A:205:GLY:N	2.85	0.45
1:B:443:TRP:N	1:B:443:TRP:CE3	2.84	0.45
1:B:500:GLY:HA3	1:F:472:ILE:O	2.16	0.45
1:C:244:LYS:HG2	1:C:245:VAL:N	2.30	0.45
1:E:71:TYR:HB2	1:E:495:ARG:O	2.16	0.45
1:E:143:ASP:OD2	1:E:171:THR:OG1	2.30	0.45
1:E:430:LEU:HD23	1:E:430:LEU:HA	1.73	0.45
1:F:18:THR:O	1:F:465:GLY:HA3	2.16	0.45
1:G:103:PRO:HB2	1:G:202:GLY:HA3	1.97	0.45
1:H:299:GLY:HA2	1:H:370:ILE:O	2.16	0.45
1:A:301:GLY:HA3	1:A:409:SER:CB	2.46	0.45
1:A:483:TYR:N	1:A:484:PRO:HD3	2.30	0.45
1:C:100:GLN:OE1	1:C:100:GLN:HA	2.17	0.45
1:E:306:ARG:NH1	1:E:333:ASN:OD1	2.49	0.45
1:F:64:VAL:CG1	1:F:65:ILE:N	2.79	0.45
1:G:92:ILE:HB	1:G:314:CYS:H	1.81	0.45
1:G:273:PHE:N	1:G:273:PHE:CD1	2.81	0.45
1:H:126:ILE:HA	1:H:188:LEU:HD11	1.98	0.45
1:A:150:MET:HG2	1:A:154:ILE:HG21	1.97	0.45
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.52	0.45
1:C:469:VAL:O	1:C:472:ILE:N	2.48	0.45
1:E:66:PHE:HB3	1:E:206:PRO:O	2.15	0.45
1:E:187:ASN:CG	1:E:189:LYS:HB2	2.36	0.45
1:F:91:ARG:HG2	1:F:92:ILE:N	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:PHE:HB2	1:F:174:MET:HB2	1.96	0.45
1:G:12:VAL:HA	1:G:266:VAL:O	2.17	0.45
1:G:54:GLU:HB3	1:G:346:LEU:CD1	2.45	0.45
1:G:271:VAL:HB	1:G:449:GLY:O	2.16	0.45
1:H:196:ILE:HG22	1:H:197:LEU:N	2.31	0.45
1:H:401:LEU:HB3	1:H:405:ASP:HB2	1.99	0.45
1:A:160:ARG:N	1:A:161:PRO:HD2	2.31	0.45
1:A:457:ASN:O	1:A:460:HIS:HB2	2.16	0.45
1:B:443:TRP:CD1	1:B:445:ARG:NH2	2.84	0.45
1:C:480:THR:HA	1:C:487:VAL:HG11	1.97	0.45
1:E:51:VAL:HG22	1:E:57:LEU:HG	1.97	0.45
1:F:22:ALA:HA	1:F:469:VAL:HG21	1.97	0.45
1:G:69:TYR:HD1	1:G:492:ASN:HB2	1.81	0.45
1:G:156:ASP:HB2	1:G:157:LEU:HD12	1.98	0.45
1:G:207:ASN:OD1	1:G:208:ALA:N	2.49	0.45
1:G:306:ARG:HA	1:G:307:PRO:HD3	1.55	0.45
1:H:44:GLY:HA2	1:H:222:TRP:CD1	2.52	0.45
1:H:106:PHE:CZ	1:H:113:LEU:HD11	2.51	0.45
1:H:292:TYR:CZ	1:H:417:HIS:CE1	3.04	0.45
1:H:417:HIS:HB3	1:H:448:PHE:CD2	2.50	0.45
1:A:6:ILE:HD13	1:A:6:ILE:N	2.32	0.45
1:A:110:ILE:CA	1:A:113:LEU:HD12	2.42	0.45
1:A:296:HIS:CE1	1:A:382:VAL:HG21	2.50	0.45
1:F:17:PRO:O	1:F:462:PHE:CD1	2.69	0.45
1:F:336:PRO:HG2	1:F:337:TYR:CE1	2.52	0.45
1:A:199:LYS:HE2	1:A:199:LYS:HB3	1.67	0.45
1:A:325:PHE:CA	1:A:374:VAL:HG22	2.46	0.45
1:B:106:PHE:C	1:B:106:PHE:CD2	2.90	0.45
1:B:344:LYS:HD2	1:B:345:LYS:H	1.81	0.45
1:C:196:ILE:HD12	1:E:119:VAL:HG22	1.98	0.45
1:C:301:GLY:HA3	1:C:409:SER:CB	2.45	0.45
1:C:304:GLY:O	1:C:368:TRP:HD1	1.99	0.45
1:C:307:PRO:HB2	1:C:309:ARG:HG2	1.99	0.45
1:D:242:VAL:HG23	2:D:601:FAD:N1A	2.31	0.45
1:E:264:LYS:HD3	1:E:472:ILE:HG23	1.98	0.45
1:E:265:LEU:O	1:E:442:ILE:HA	2.17	0.45
1:E:499:ASP:O	1:E:503:VAL:HG23	2.16	0.45
1:F:286:LEU:HD21	1:F:436:LYS:HE3	1.98	0.45
1:G:70:LYS:HD2	1:G:70:LYS:HA	1.77	0.45
1:G:483:TYR:N	1:G:484:PRO:HD3	2.31	0.45
2:G:601:FAD:O1A	2:G:601:FAD:O5'	2.30	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:181:GLU:HG3	1:H:181:GLU:O	2.16	0.45
1:H:219:GLY:O	1:H:223:ILE:HG12	2.16	0.45
1:H:464:LEU:HD21	1:H:481:LEU:N	2.32	0.45
1:H:486:PHE:CE2	1:H:490:ARG:HD2	2.52	0.45
1:C:19:GLY:H	1:C:268:THR:HG21	1.81	0.45
1:C:272:ASP:N	1:C:272:ASP:OD1	2.48	0.45
1:C:455:VAL:HG11	1:C:464:LEU:HD11	1.99	0.45
1:D:395:LEU:HA	1:D:400:MET:HG3	1.97	0.45
1:E:70:LYS:NZ	1:E:73:ASP:HB2	2.32	0.45
1:F:504:PHE:CD1	1:F:504:PHE:N	2.82	0.45
1:A:312:ASP:OD1	1:A:312:ASP:N	2.44	0.45
1:B:119:VAL:HG13	1:H:193:THR:CG2	2.47	0.45
1:B:350:GLN:NE2	1:B:354:GLY:HA2	2.28	0.45
1:C:96:ARG:O	1:C:319:PRO:HD2	2.16	0.45
1:C:192:THR:OG1	1:C:193:THR:N	2.49	0.45
1:D:335:SER:OG	1:D:336:PRO:HD2	2.17	0.45
1:E:70:LYS:HE3	1:E:70:LYS:O	2.17	0.45
1:E:107:GLN:O	1:E:110:ILE:HG22	2.16	0.45
1:F:207:ASN:HB3	1:F:315:TRP:CZ2	2.52	0.45
1:F:269:MET:HE3	1:F:273:PHE:HB3	1.99	0.45
1:G:72:PHE:CE1	1:G:459:ASP:HA	2.51	0.45
1:H:69:TYR:HD1	1:H:492:ASN:HB2	1.80	0.45
1:H:130:LEU:O	1:H:133:ARG:CB	2.63	0.45
1:H:181:GLU:OE1	1:H:181:GLU:CA	2.62	0.45
1:H:210:PHE:HZ	1:H:334:TYR:CE1	2.34	0.45
1:A:150:MET:HE3	1:A:159:MET:HG3	1.98	0.45
1:C:346:LEU:HD13	1:C:408:VAL:CG1	2.47	0.45
1:C:395:LEU:HA	1:C:400:MET:HG3	1.99	0.45
1:D:35:MET:HE1	1:D:235:ARG:HG3	1.98	0.45
1:D:194:ASN:HD22	1:D:194:ASN:HA	1.55	0.45
1:E:91:ARG:O	1:E:92:ILE:HD13	2.16	0.45
1:E:109:ASN:N	1:E:109:ASN:ND2	2.62	0.45
1:E:318:PHE:CZ	1:E:325:PHE:HE1	2.35	0.45
1:G:86:TRP:CE3	1:G:86:TRP:HA	2.52	0.45
1:G:130:LEU:O	1:G:133:ARG:N	2.50	0.45
1:G:150:MET:CG	1:G:154:ILE:HB	2.36	0.45
1:H:351:LEU:O	1:H:354:GLY:N	2.43	0.45
1:H:353:ASP:HB3	1:H:403:PRO:CB	2.46	0.45
1:H:421:THR:HA	1:H:422:PRO:HD3	1.74	0.45
1:B:28:GLN:NE2	1:B:497:LEU:O	2.50	0.45
1:B:116:GLU:O	1:B:119:VAL:HB	2.17	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:MET:HG2	1:B:188:LEU:HD13	1.99	0.45
1:C:425:GLU:H	1:C:425:GLU:CD	2.20	0.45
1:D:70:LYS:HD2	1:D:70:LYS:HA	1.51	0.45
1:D:115:LYS:HB3	1:F:197:LEU:CD2	2.46	0.45
1:D:175:GLN:NE2	1:D:177:ALA:HB3	2.32	0.45
1:E:166:VAL:HA	1:E:326:TYR:CD2	2.52	0.45
1:E:235:ARG:HG2	1:E:239:LYS:HD2	1.98	0.45
1:E:325:PHE:HA	1:E:374:VAL:CG2	2.47	0.45
1:F:209:THR:O	1:F:210:PHE:HB3	2.17	0.45
1:F:436:LYS:O	1:F:439:ASP:HB2	2.16	0.45
1:G:30:ASP:OD1	1:G:30:ASP:O	2.35	0.45
1:H:61:GLY:HA3	2:H:601:FAD:H6	1.98	0.45
1:H:187:ASN:OD1	1:H:190:ALA:HB2	2.17	0.45
1:H:273:PHE:N	1:H:273:PHE:CD1	2.82	0.45
1:A:339:GLN:CD	1:A:339:GLN:N	2.71	0.44
1:B:304:GLY:O	1:B:368:TRP:CD1	2.70	0.44
1:C:376:GLU:HA	1:C:380:LYS:O	2.17	0.44
1:C:434:LEU:HD23	1:C:434:LEU:HA	1.84	0.44
1:D:307:PRO:HD2	1:D:310:ILE:HD12	1.98	0.44
1:D:323:CYS:HB2	1:D:325:PHE:CE2	2.52	0.44
1:E:332:SER:CB	1:E:369:SER:H	2.29	0.44
1:H:104:TYR:CG	1:H:105:PRO:HA	2.52	0.44
1:H:134:VAL:O	1:H:134:VAL:CG1	2.64	0.44
1:H:443:TRP:N	1:H:443:TRP:HE3	2.15	0.44
1:A:106:PHE:HD2	1:A:106:PHE:O	2.01	0.44
1:B:138:LYS:HE3	1:B:138:LYS:HB2	1.86	0.44
1:C:19:GLY:O	1:C:22:ALA:HB3	2.17	0.44
1:C:91:ARG:O	1:C:92:ILE:HD13	2.17	0.44
1:D:115:LYS:HD3	1:F:197:LEU:HA	1.98	0.44
1:E:63:HIS:CD2	1:E:63:HIS:H	2.33	0.44
1:E:163:ASN:HA	1:E:166:VAL:CG1	2.46	0.44
1:E:187:ASN:O	1:E:191:VAL:HG23	2.18	0.44
1:E:385:GLU:H	1:E:385:GLU:HG2	1.47	0.44
1:G:139:PRO:HA	1:G:144:GLU:OE2	2.17	0.44
1:G:312:ASP:OD1	1:G:312:ASP:N	2.37	0.44
1:G:417:HIS:HB3	1:G:448:PHE:CD2	2.52	0.44
1:G:417:HIS:HB3	1:G:448:PHE:CZ	2.51	0.44
1:A:57:LEU:HD13	1:A:338:ASN:C	2.38	0.44
1:B:6:ILE:O	1:B:260:ILE:HA	2.17	0.44
1:C:299:GLY:HA2	1:C:370:ILE:O	2.17	0.44
1:C:325:PHE:HA	1:C:374:VAL:HG22	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:LYS:HA	1:D:139:PRO:HD3	1.83	0.44
1:D:398:THR:O	1:D:399:GLU:HB2	2.17	0.44
1:E:10:VAL:HG13	1:E:264:LYS:HB2	2.00	0.44
1:E:104:TYR:CE1	3:E:602:GDU:H5	2.52	0.44
1:E:445:ARG:CZ	1:E:481:LEU:HD22	2.46	0.44
1:F:134:VAL:O	1:F:134:VAL:CG1	2.65	0.44
1:F:167:TRP:CG	1:F:174:MET:HE1	2.53	0.44
1:F:307:PRO:HD3	1:F:368:TRP:CE2	2.52	0.44
1:G:254:LEU:HB2	1:G:258:THR:HB	1.98	0.44
1:G:283:LEU:HD22	1:G:433:ILE:HG23	1.99	0.44
1:G:299:GLY:HA2	1:G:371:MET:HA	1.98	0.44
1:G:348:THR:HG21	1:G:406:GLU:HG2	2.00	0.44
1:H:107:GLN:CD	1:H:107:GLN:N	2.66	0.44
1:H:210:PHE:N	1:H:210:PHE:CD2	2.84	0.44
1:A:91:ARG:O	1:A:92:ILE:HD13	2.18	0.44
1:A:178:TRP:CZ3	1:A:179:LEU:HD23	2.52	0.44
1:B:58:TYR:HA	1:B:331:PHE:CE2	2.47	0.44
1:C:106:PHE:C	1:C:106:PHE:HD2	2.20	0.44
1:C:350:GLN:HE21	1:C:350:GLN:HB2	1.57	0.44
1:D:108:ASN:HB2	1:D:194:ASN:OD1	2.18	0.44
1:E:159:MET:HE3	3:E:602:GDU:C2	2.47	0.44
1:E:467:GLU:HG2	1:E:495:ARG:CZ	2.48	0.44
1:F:151:GLY:C	1:F:154:ILE:HG12	2.36	0.44
1:G:148:ARG:O	1:G:186:PRO:HD3	2.18	0.44
1:G:341:GLU:CG	1:G:343:SER:H	2.27	0.44
1:H:9:ASP:OD1	1:H:33:SER:N	2.49	0.44
1:H:276:GLU:O	1:H:279:ASN:N	2.48	0.44
1:A:5:ASP:N	1:A:259:THR:OG1	2.41	0.44
1:C:42:THR:HG22	1:C:223:ILE:HD11	1.98	0.44
1:C:57:LEU:HD13	1:C:338:ASN:C	2.38	0.44
1:C:194:ASN:HD22	1:C:194:ASN:HA	1.59	0.44
1:E:58:TYR:CE1	1:E:299:GLY:HA3	2.52	0.44
1:E:110:ILE:CG2	1:E:195:VAL:HG22	2.47	0.44
1:E:167:TRP:CG	1:E:174:MET:CE	3.01	0.44
1:E:286:LEU:O	1:E:289:GLN:HB2	2.18	0.44
1:E:318:PHE:CE2	1:E:398:THR:HG21	2.52	0.44
1:F:125:MET:CG	1:F:188:LEU:HD13	2.46	0.44
1:F:275:ALA:HB1	1:F:284:VAL:HG22	1.99	0.44
1:H:65:ILE:HD12	1:H:65:ILE:HA	1.61	0.44
1:H:152:THR:O	1:H:156:ASP:CG	2.55	0.44
1:H:158:PHE:O	1:H:161:PRO:HD2	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:271:VAL:HB	1:H:449:GLY:O	2.17	0.44
1:H:455:VAL:HG21	1:H:480:THR:O	2.17	0.44
1:A:38:ASP:OD2	1:A:40:ASN:CB	2.65	0.44
1:A:103:PRO:HG2	1:A:109:ASN:OD1	2.17	0.44
1:C:297:VAL:O	1:C:298:ILE:HD13	2.18	0.44
1:E:425:GLU:CD	1:E:425:GLU:N	2.70	0.44
1:F:70:LYS:CB	1:F:496:ARG:HH12	2.29	0.44
1:F:137:THR:C	1:F:148:ARG:HH12	2.20	0.44
1:F:162:TYR:O	1:F:166:VAL:CG1	2.65	0.44
1:F:310:ILE:HG22	1:F:311:GLY:N	2.32	0.44
1:F:443:TRP:HE3	1:F:443:TRP:H	1.64	0.44
1:H:223:ILE:HD13	1:H:223:ILE:N	2.33	0.44
1:H:434:LEU:HB2	1:H:435:PRO:HD3	2.00	0.44
1:A:447:ARG:HD2	2:A:601:FAD:H3'	2.00	0.44
1:B:119:VAL:HG13	1:H:193:THR:HG22	1.99	0.44
1:C:193:THR:O	1:C:197:LEU:HG	2.17	0.44
1:C:437:LEU:CD1	1:C:444:SER:HB2	2.48	0.44
1:D:346:LEU:HD13	1:D:408:VAL:HG13	1.99	0.44
1:E:104:TYR:CE1	3:E:602:GDU:C5	2.94	0.44
1:E:336:PRO:HG2	1:E:337:TYR:CE1	2.53	0.44
1:F:294:SER:CB	1:F:414:ARG:NH2	2.80	0.44
1:F:298:ILE:HG22	1:F:298:ILE:O	2.16	0.44
1:G:18:THR:CB	2:G:601:FAD:O2P	2.66	0.44
1:G:108:ASN:OD1	1:G:108:ASN:N	2.49	0.44
1:H:296:HIS:HB2	1:H:374:VAL:HB	1.98	0.44
1:A:398:THR:O	1:A:399:GLU:HB2	2.18	0.44
1:B:150:MET:HE3	1:B:159:MET:HG3	1.99	0.44
1:C:249:ASN:O	1:C:251:THR:HG23	2.17	0.44
1:D:296:HIS:CE1	1:D:382:VAL:HG21	2.52	0.44
1:D:455:VAL:O	1:D:460:HIS:CB	2.64	0.44
1:E:24:LYS:HA	1:E:24:LYS:HD3	1.73	0.44
1:E:109:ASN:N	1:E:109:ASN:HD22	2.16	0.44
1:E:306:ARG:O	1:E:306:ARG:HG2	2.18	0.44
1:F:107:GLN:NE2	1:F:108:ASN:OD1	2.51	0.44
1:F:382:VAL:HG23	1:F:383:ASN:N	2.32	0.44
1:G:204:TRP:O	1:G:208:ALA:HB3	2.18	0.44
1:G:348:THR:HB	1:G:357:PRO:HB3	2.00	0.44
1:A:183:VAL:HG22	3:A:602:GDU:C1D	2.48	0.44
1:A:425:GLU:CD	1:A:425:GLU:H	2.20	0.44
1:B:350:GLN:HE21	1:B:350:GLN:HB2	1.51	0.44
1:B:402:LYS:HB3	1:B:404:THR:HG23	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ILE:O	1:B:436:LYS:HB2	2.17	0.44
1:B:469:VAL:O	1:B:473:VAL:HG23	2.18	0.44
1:C:264:LYS:HD2	1:C:443:TRP:CH2	2.53	0.44
1:D:384:GLN:H	1:D:384:GLN:HG2	1.65	0.44
1:E:303:ARG:HH21	1:E:363:LYS:HB2	1.82	0.44
1:F:18:THR:HG23	1:F:464:LEU:HB2	1.98	0.44
1:G:5:ASP:C	1:G:6:ILE:HG12	2.37	0.44
1:G:160:ARG:HB2	1:G:161:PRO:CD	2.48	0.44
1:H:5:ASP:C	1:H:6:ILE:HG12	2.38	0.44
1:H:296:HIS:ND1	1:H:412:HIS:HE1	2.16	0.44
1:H:443:TRP:N	1:H:443:TRP:CE3	2.86	0.44
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.61	0.43
1:A:199:LYS:HD2	1:A:200:THR:H	1.83	0.43
1:A:455:VAL:O	1:A:460:HIS:CB	2.63	0.43
1:A:499:ASP:O	1:A:503:VAL:HG23	2.18	0.43
1:C:46:LEU:HB2	2:C:601:FAD:O4'	2.18	0.43
1:C:67:SER:HA	1:C:459:ASP:OD2	2.17	0.43
1:C:407:ILE:O	1:C:407:ILE:HG22	2.18	0.43
1:E:244:LYS:HB3	1:E:244:LYS:HE3	1.74	0.43
1:E:349:MET:O	1:E:350:GLN:CB	2.66	0.43
1:G:65:ILE:O	1:G:65:ILE:HG22	2.18	0.43
1:G:445:ARG:HH11	1:G:481:LEU:HD22	1.81	0.43
1:H:15:ALA:HB2	1:H:38:ASP:HB2	2.00	0.43
1:H:57:LEU:HD11	1:H:337:TYR:O	2.17	0.43
1:H:108:ASN:N	1:H:108:ASN:OD1	2.51	0.43
1:B:70:LYS:HA	1:B:70:LYS:HD2	1.53	0.43
1:B:110:ILE:CA	1:B:113:LEU:HD12	2.37	0.43
1:B:323:CYS:HB2	1:B:325:PHE:CE2	2.54	0.43
1:C:446:GLY:O	1:C:450:SER:HB2	2.19	0.43
1:F:109:ASN:HD22	1:F:109:ASN:N	2.16	0.43
1:G:89:HIS:NE2	1:G:334:TYR:O	2.51	0.43
1:G:126:ILE:HG22	1:G:127:ASP:N	2.33	0.43
1:G:167:TRP:O	1:G:169:VAL:HG12	2.18	0.43
1:G:383:ASN:O	1:G:387:ILE:HB	2.18	0.43
1:G:460:HIS:O	1:G:464:LEU:HB2	2.19	0.43
1:H:83:GLU:HA	1:H:86:TRP:HD1	1.82	0.43
1:H:336:PRO:HG2	1:H:337:TYR:HD1	1.82	0.43
1:H:351:LEU:HD21	1:H:357:PRO:HA	2.00	0.43
1:B:398:THR:CG2	1:B:400:MET:CG	2.96	0.43
1:B:411:TYR:CD2	1:B:412:HIS:N	2.87	0.43
2:C:601:FAD:C2'	2:C:601:FAD:H9	2.48	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:411:TYR:CD2	1:D:412:HIS:N	2.86	0.43
1:E:64:VAL:CG1	1:E:65:ILE:N	2.81	0.43
1:E:158:PHE:CD1	1:E:319:PRO:HG3	2.53	0.43
1:E:298:ILE:O	1:E:298:ILE:HG22	2.16	0.43
1:F:187:ASN:OD1	1:F:189:LYS:CB	2.60	0.43
1:H:47:ALA:HA	2:H:601:FAD:O2'	2.18	0.43
1:H:130:LEU:O	1:H:133:ARG:N	2.51	0.43
1:H:234:THR:HB	1:H:236:PHE:CE2	2.53	0.43
1:A:47:ALA:HB1	1:A:222:TRP:NE1	2.32	0.43
1:A:480:THR:HA	1:A:487:VAL:HG11	1.99	0.43
1:C:495:ARG:O	1:C:496:ARG:HD2	2.19	0.43
1:D:178:TRP:CB	1:D:454:GLU:CG	2.96	0.43
1:E:155:ALA:HA	1:E:159:MET:HB2	2.01	0.43
1:E:159:MET:HE3	3:E:602:GDU:N3	2.33	0.43
1:E:325:PHE:HA	1:E:374:VAL:HG13	1.99	0.43
1:E:370:ILE:HG22	1:E:372:LEU:HD23	2.00	0.43
1:F:47:ALA:HB1	1:F:222:TRP:HE1	1.83	0.43
1:G:63:HIS:CD2	1:G:63:HIS:N	2.86	0.43
1:G:185:ALA:O	1:G:186:PRO:C	2.57	0.43
1:H:85:ASP:HA	1:H:214:ALA:CB	2.48	0.43
1:H:92:ILE:O	1:H:314:CYS:HB2	2.18	0.43
1:H:372:LEU:HD21	1:H:391:CYS:HB3	1.99	0.43
1:H:420:PRO:HB2	1:H:451:TRP:CD1	2.54	0.43
1:A:467:GLU:HG2	1:A:495:ARG:HH12	1.83	0.43
1:B:286:LEU:O	1:B:289:GLN:HG3	2.19	0.43
1:B:389:ALA:HA	1:B:392:ILE:CD1	2.49	0.43
1:D:142:PHE:CE1	1:D:179:LEU:HD21	2.53	0.43
1:E:147:VAL:CG2	1:E:160:ARG:HH21	2.30	0.43
1:E:332:SER:HB3	1:E:369:SER:H	1.83	0.43
1:E:467:GLU:HG2	1:E:495:ARG:HH22	1.83	0.43
1:F:137:THR:O	1:F:148:ARG:NH1	2.51	0.43
1:F:321:ASP:OD1	1:F:321:ASP:N	2.46	0.43
1:F:376:GLU:HG2	1:F:377:SER:N	2.33	0.43
1:G:109:ASN:C	1:G:111:SER:N	2.72	0.43
1:G:244:LYS:HB3	1:G:244:LYS:HE2	1.93	0.43
1:H:77:ASP:N	1:H:77:ASP:OD1	2.49	0.43
1:H:341:GLU:CG	1:H:343:SER:H	2.29	0.43
1:H:480:THR:HG23	1:H:487:VAL:HG21	2.00	0.43
1:B:115:LYS:O	1:B:118:GLN:HB2	2.18	0.43
1:B:483:TYR:N	1:B:484:PRO:HD3	2.33	0.43
2:B:601:FAD:O4'	2:B:601:FAD:O2'	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:ASP:HB3	1:C:283:LEU:HB2	2.00	0.43
1:C:323:CYS:HB2	1:C:325:PHE:CE2	2.53	0.43
1:C:467:GLU:HG2	1:C:495:ARG:HH12	1.84	0.43
1:E:69:TYR:CD1	1:E:463:MET:HG3	2.54	0.43
1:E:126:ILE:O	1:E:130:LEU:HG	2.18	0.43
1:E:145:TRP:HE3	1:E:146:ILE:N	2.17	0.43
1:E:207:ASN:HB3	1:E:315:TRP:CZ2	2.53	0.43
1:E:368:TRP:HZ3	1:E:370:ILE:HD11	1.80	0.43
1:F:328:ALA:HB2	1:F:372:LEU:HB3	2.00	0.43
1:G:125:MET:HG2	1:G:188:LEU:CD2	2.48	0.43
1:G:163:ASN:O	1:G:167:TRP:HB2	2.18	0.43
1:G:455:VAL:HG12	1:G:460:HIS:CD2	2.54	0.43
1:H:11:LEU:HD21	1:H:252:VAL:CG1	2.49	0.43
1:H:16:GLY:O	1:H:20:LEU:HG	2.19	0.43
1:H:351:LEU:HD13	1:H:404:THR:O	2.18	0.43
1:H:352:ALA:HB2	1:H:405:ASP:HB2	2.00	0.43
1:A:315:TRP:C	1:A:316:LEU:HG	2.38	0.43
1:A:346:LEU:HD13	1:A:408:VAL:CG1	2.48	0.43
1:B:96:ARG:O	1:B:319:PRO:HD2	2.19	0.43
1:B:142:PHE:CE1	1:B:179:LEU:HD21	2.54	0.43
1:B:263:LYS:HD2	1:F:504:PHE:CE1	2.53	0.43
1:C:423:THR:HB	1:C:425:GLU:OE1	2.18	0.43
1:D:49:THR:HG22	1:D:50:ASP:N	2.34	0.43
1:E:326:TYR:C	1:E:326:TYR:CD1	2.92	0.43
1:E:359:SER:OG	1:E:361:GLU:CB	2.66	0.43
1:E:376:GLU:HB2	1:E:382:VAL:HG13	2.01	0.43
1:E:455:VAL:HA	1:E:460:HIS:ND1	2.23	0.43
3:F:602:GDU:C2	3:F:602:GDU:H5'2	2.48	0.43
1:G:100:GLN:OE1	1:G:100:GLN:HA	2.19	0.43
1:H:384:GLN:O	1:H:387:ILE:HG22	2.19	0.43
1:A:307:PRO:HB2	1:A:309:ARG:HG2	2.01	0.43
1:A:335:SER:OG	1:A:336:PRO:HD2	2.19	0.43
1:D:286:LEU:O	1:D:289:GLN:HG3	2.19	0.43
1:D:346:LEU:HD23	1:D:347:PRO:CD	2.48	0.43
1:F:6:ILE:CG2	1:F:7:SER:N	2.82	0.43
1:G:11:LEU:HB3	1:G:265:LEU:CD1	2.48	0.43
1:G:204:TRP:HB3	1:G:208:ALA:CB	2.47	0.43
1:G:419:TYR:N	1:G:448:PHE:HZ	2.16	0.43
1:H:39:SER:HA	1:H:237:GLY:O	2.18	0.43
1:H:256:ASP:OD1	1:H:256:ASP:N	2.46	0.43
1:A:114:PRO:O	1:A:118:GLN:HG3	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:O	1:B:81:PRO:HA	2.19	0.43
1:B:297:VAL:O	1:B:298:ILE:HD13	2.19	0.43
1:B:417:HIS:HB3	1:B:448:PHE:CZ	2.54	0.43
1:B:483:TYR:CE1	1:F:486:PHE:HE1	2.37	0.43
1:B:499:ASP:HB3	1:F:473:VAL:O	2.19	0.43
1:D:91:ARG:HG3	1:D:315:TRP:CZ2	2.54	0.43
1:D:346:LEU:HD23	1:D:347:PRO:HD2	2.01	0.43
1:E:69:TYR:O	1:E:72:PHE:HB3	2.18	0.43
1:E:306:ARG:HA	1:E:307:PRO:HD3	1.69	0.43
1:F:291:PHE:CE1	1:F:292:TYR:O	2.72	0.43
1:H:165:LYS:HD3	1:H:318:PHE:O	2.18	0.43
1:H:168:ALA:HB1	1:H:377:SER:OG	2.18	0.43
1:H:446:GLY:N	1:H:450:SER:N	2.64	0.43
1:C:350:GLN:NE2	1:C:351:LEU:O	2.52	0.43
1:E:12:VAL:CB	1:E:36:ILE:HG13	2.46	0.43
1:E:94:TYR:CE1	1:E:103:PRO:HG3	2.54	0.43
1:E:419:TYR:CE1	2:E:601:FAD:HM73	2.46	0.43
1:F:9:ASP:HB2	1:F:33:SER:O	2.18	0.43
1:F:58:TYR:CE1	1:F:299:GLY:HA3	2.54	0.43
1:F:179:LEU:N	1:F:179:LEU:CD2	2.80	0.43
1:F:322:ASN:HD21	1:F:398:THR:HG22	1.84	0.43
1:F:387:ILE:HG23	1:F:388:LEU:H	1.83	0.43
1:F:506:LYS:HD3	1:F:506:LYS:H	1.84	0.43
1:G:152:THR:O	1:G:156:ASP:CG	2.56	0.43
1:G:252:VAL:CG1	1:G:252:VAL:O	2.67	0.43
1:G:443:TRP:N	1:G:443:TRP:HE3	2.17	0.43
1:G:455:VAL:HB	1:G:460:HIS:HB3	2.01	0.43
1:H:270:ALA:HA	1:H:448:PHE:C	2.39	0.43
1:H:479:LEU:HA	1:H:483:TYR:CD2	2.54	0.43
1:A:138:LYS:HE3	1:A:138:LYS:HB2	1.89	0.42
1:B:175:GLN:HE21	1:B:178:TRP:HD1	1.67	0.42
1:C:125:MET:HG2	1:C:188:LEU:HD13	2.01	0.42
1:C:166:VAL:HG13	1:C:167:TRP:CD1	2.53	0.42
1:C:245:VAL:HG22	1:C:252:VAL:CG2	2.48	0.42
1:C:411:TYR:CD2	1:C:412:HIS:N	2.86	0.42
1:E:134:VAL:O	1:E:134:VAL:HG13	2.19	0.42
1:E:436:LYS:O	1:E:439:ASP:HB2	2.19	0.42
1:F:291:PHE:CG	1:F:292:TYR:N	2.87	0.42
1:G:57:LEU:CD1	1:G:57:LEU:N	2.82	0.42
1:G:387:ILE:HG23	1:G:388:LEU:N	2.34	0.42
1:H:165:LYS:NZ	1:H:325:PHE:O	2.43	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:272:ASP:O	1:H:276:GLU:OE2	2.37	0.42
1:A:204:TRP:CD2	1:A:205:GLY:N	2.85	0.42
1:C:199:LYS:HD2	1:C:200:THR:N	2.34	0.42
1:D:13:ILE:HG12	1:D:242:VAL:HG21	2.00	0.42
1:D:501:ALA:HB2	1:H:473:VAL:HG13	2.01	0.42
1:E:250:LYS:HA	1:E:262:TYR:CZ	2.55	0.42
1:E:318:PHE:CE1	1:E:325:PHE:HE1	2.37	0.42
1:F:24:LYS:HD3	1:F:24:LYS:HA	1.82	0.42
1:F:108:ASN:O	1:F:194:ASN:HB3	2.19	0.42
1:F:122:ILE:HD12	1:F:122:ILE:HA	1.87	0.42
1:F:430:LEU:HD23	1:F:430:LEU:HA	1.82	0.42
1:G:69:TYR:CG	1:G:463:MET:HG3	2.53	0.42
1:G:77:ASP:OD1	1:G:77:ASP:N	2.49	0.42
1:G:272:ASP:O	1:G:275:ALA:N	2.52	0.42
1:G:296:HIS:ND1	1:G:412:HIS:HE1	2.17	0.42
1:G:309:ARG:HG2	1:G:310:ILE:HD12	2.01	0.42
1:H:158:PHE:HE1	1:H:162:TYR:CD2	2.37	0.42
1:H:302:VAL:HA	1:H:406:GLU:O	2.18	0.42
1:H:385:GLU:CD	1:H:385:GLU:H	2.23	0.42
1:H:394:GLY:HA2	1:H:397:ASN:ND2	2.34	0.42
1:H:443:TRP:HB3	1:H:445:ARG:NE	2.33	0.42
1:C:16:GLY:HA3	2:C:601:FAD:O1P	2.20	0.42
1:C:47:ALA:CB	1:C:222:TRP:NE1	2.81	0.42
1:C:160:ARG:HB2	1:C:161:PRO:HD3	2.02	0.42
1:D:134:VAL:O	1:D:134:VAL:HG13	2.19	0.42
1:E:68:HIS:ND1	1:E:68:HIS:N	2.67	0.42
1:E:113:LEU:HB3	1:E:114:PRO:HD2	2.00	0.42
1:F:167:TRP:CG	1:F:174:MET:CE	3.02	0.42
1:F:455:VAL:HG11	1:F:480:THR:O	2.19	0.42
1:G:162:TYR:CE2	1:G:166:VAL:HG11	2.54	0.42
1:G:387:ILE:HD12	1:G:387:ILE:HA	1.72	0.42
1:G:471:ASN:HA	1:G:476:ALA:N	2.32	0.42
1:H:402:LYS:HD3	1:H:402:LYS:H	1.84	0.42
1:H:477:VAL:CG2	1:H:478:GLU:N	2.82	0.42
1:A:32:PRO:CG	1:E:504:PHE:HD2	2.33	0.42
1:A:60:VAL:O	1:A:63:HIS:CD2	2.71	0.42
1:B:204:TRP:CD2	1:B:205:GLY:N	2.86	0.42
1:B:386:THR:OG1	1:B:387:ILE:N	2.53	0.42
1:B:486:PHE:CE1	1:F:483:TYR:CD1	3.04	0.42
1:C:107:GLN:H	1:C:107:GLN:CD	2.17	0.42
1:E:122:ILE:CG2	1:E:123:ASP:N	2.81	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ALA:HB1	1:E:380:LYS:HB3	2.00	0.42
1:E:445:ARG:NE	1:E:481:LEU:HD22	2.34	0.42
1:E:467:GLU:HG2	1:E:495:ARG:HH12	1.83	0.42
2:E:601:FAD:O1P	2:E:601:FAD:O5B	2.38	0.42
1:F:422:PRO:HA	1:F:426:ARG:HD3	2.01	0.42
1:G:309:ARG:HG2	1:G:310:ILE:CD1	2.49	0.42
1:G:443:TRP:N	1:G:443:TRP:CE3	2.88	0.42
1:G:471:ASN:HB2	1:G:476:ALA:O	2.19	0.42
1:H:24:LYS:HA	1:H:24:LYS:HD3	1.69	0.42
1:H:89:HIS:NE2	1:H:334:TYR:HA	2.34	0.42
1:H:156:ASP:HA	1:H:160:ARG:HE	1.84	0.42
1:H:302:VAL:HG12	1:H:368:TRP:O	2.20	0.42
1:H:394:GLY:HA2	1:H:397:ASN:HB2	2.01	0.42
1:H:453:TYR:O	1:H:454:GLU:C	2.57	0.42
1:B:69:TYR:CD2	1:B:463:MET:HG3	2.54	0.42
1:B:458:GLN:HG3	2:B:601:FAD:N1	2.33	0.42
1:B:483:TYR:O	1:B:486:PHE:HB3	2.19	0.42
1:C:38:ASP:HA	2:C:601:FAD:C2A	2.48	0.42
1:C:175:GLN:HE22	1:C:177:ALA:HB3	1.85	0.42
1:E:16:GLY:H	2:E:601:FAD:H4B	1.84	0.42
1:E:110:ILE:HG13	1:E:113:LEU:HD12	2.02	0.42
1:E:129:ALA:O	1:E:132:ALA:HB3	2.20	0.42
1:E:396:VAL:HA	1:E:401:LEU:HB2	2.01	0.42
1:E:438:GLN:NE2	1:E:442:ILE:O	2.48	0.42
1:F:5:ASP:N	1:F:259:THR:OG1	2.30	0.42
1:F:143:ASP:OD2	1:F:171:THR:OG1	2.34	0.42
1:F:345:LYS:HG2	1:F:364:GLU:HG3	2.01	0.42
1:F:352:ALA:HB3	1:F:403:PRO:HA	2.01	0.42
1:G:303:ARG:NH2	1:G:346:LEU:O	2.52	0.42
1:H:235:ARG:HE	1:H:235:ARG:HB3	1.51	0.42
2:H:601:FAD:H9	2:H:601:FAD:H1'1	1.34	0.42
1:A:57:LEU:HD12	1:A:57:LEU:N	2.35	0.42
1:A:174:MET:HB2	1:A:422:PRO:O	2.18	0.42
1:A:175:GLN:HG3	1:A:422:PRO:O	2.19	0.42
1:A:443:TRP:CD1	1:A:445:ARG:NH2	2.88	0.42
1:B:57:LEU:HD22	1:B:338:ASN:HA	2.02	0.42
1:C:291:PHE:O	1:C:421:THR:HB	2.20	0.42
1:C:331:PHE:HD1	1:C:331:PHE:HA	1.73	0.42
1:D:182:ARG:HD2	3:D:602:GDU:O2A	2.19	0.42
1:D:244:LYS:HG2	1:D:245:VAL:H	1.84	0.42
1:D:280:ASP:HB3	1:D:283:LEU:HB2	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:SER:OG	1:D:369:SER:N	2.42	0.42
1:E:70:LYS:CB	1:E:496:ARG:HH12	2.29	0.42
1:E:205:GLY:HA2	1:E:206:PRO:HD3	1.74	0.42
1:E:231:LYS:HE2	1:E:231:LYS:HB3	1.71	0.42
1:E:303:ARG:HH22	1:E:363:LYS:HG3	1.79	0.42
1:E:427:GLU:O	1:E:428:GLY:C	2.58	0.42
1:E:437:LEU:O	1:E:442:ILE:N	2.45	0.42
1:G:11:LEU:HB3	1:G:265:LEU:HD12	2.01	0.42
1:G:85:ASP:HA	1:G:214:ALA:HB2	2.02	0.42
1:G:102:VAL:CG1	1:G:109:ASN:HB3	2.50	0.42
1:G:367:TYR:CD1	1:G:408:VAL:HG21	2.51	0.42
1:G:402:LYS:HB2	1:G:402:LYS:HE2	1.68	0.42
1:H:447:ARG:HG2	1:H:448:PHE:CE2	2.54	0.42
1:B:100:GLN:OE1	1:B:100:GLN:HA	2.19	0.42
1:B:150:MET:HG2	1:B:154:ILE:HG21	2.02	0.42
1:D:38:ASP:HA	2:D:601:FAD:C2A	2.50	0.42
1:D:63:HIS:CD2	2:D:601:FAD:C6	3.03	0.42
1:D:158:PHE:CZ	3:D:602:GDU:N3	2.87	0.42
1:D:443:TRP:N	1:D:443:TRP:CE3	2.88	0.42
1:D:473:VAL:HG12	1:H:501:ALA:CA	2.50	0.42
1:E:146:ILE:HG13	1:E:146:ILE:H	1.72	0.42
1:E:159:MET:HE1	3:E:602:GDU:C2	2.49	0.42
3:F:602:GDU:H6	3:F:602:GDU:H2D	1.85	0.42
1:G:27:ASN:O	1:G:30:ASP:HB2	2.20	0.42
1:G:70:LYS:HE2	1:G:496:ARG:NH1	2.35	0.42
1:G:92:ILE:HG22	1:G:94:TYR:HE2	1.84	0.42
1:G:102:VAL:HA	1:G:103:PRO:HD3	1.78	0.42
1:H:25:ARG:NH2	1:H:495:ARG:HG3	2.34	0.42
1:H:71:TYR:CD2	1:H:496:ARG:C	2.93	0.42
1:H:483:TYR:CD2	1:H:483:TYR:N	2.87	0.42
1:A:407:ILE:O	1:A:407:ILE:HG22	2.19	0.42
1:A:447:ARG:HB2	2:A:601:FAD:H5'2	2.02	0.42
1:B:35:MET:HE1	1:B:235:ARG:HG3	2.00	0.42
1:B:331:PHE:HB3	1:B:369:SER:HB3	2.01	0.42
1:C:296:HIS:NE2	1:C:382:VAL:HG21	2.34	0.42
1:C:306:ARG:HA	1:C:307:PRO:HD3	1.82	0.42
1:C:499:ASP:HB3	1:G:473:VAL:O	2.19	0.42
1:D:8:VAL:HG11	1:D:35:MET:HG2	2.02	0.42
1:D:27:ASN:C	1:D:27:ASN:HD22	2.23	0.42
1:E:49:THR:HG22	1:E:50:ASP:N	2.35	0.42
1:F:26:LEU:HD22	1:F:34:TRP:HB3	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:425:GLU:CD	1:G:425:GLU:H	2.22	0.42
1:H:30:ASP:O	1:H:30:ASP:OD1	2.37	0.42
1:H:156:ASP:HB2	1:H:157:LEU:HD12	2.02	0.42
1:B:106:PHE:C	1:B:106:PHE:HD2	2.23	0.42
1:C:287:THR:O	1:C:290:LEU:HD12	2.20	0.42
1:C:433:ILE:O	1:C:436:LYS:HB2	2.20	0.42
1:C:483:TYR:O	1:C:486:PHE:HB3	2.19	0.42
1:D:178:TRP:CH2	1:D:179:LEU:HD23	2.55	0.42
1:D:423:THR:O	1:D:426:ARG:HB2	2.19	0.42
1:F:7:SER:HA	1:F:261:GLY:O	2.20	0.42
1:F:413:ARG:HG2	1:F:414:ARG:N	2.35	0.42
1:G:47:ALA:HA	1:G:63:HIS:HE1	1.83	0.42
1:G:110:ILE:HG13	1:G:113:LEU:HD12	2.01	0.42
1:G:258:THR:CG2	1:G:259:THR:N	2.82	0.42
1:G:388:LEU:O	1:G:392:ILE:HG13	2.20	0.42
1:A:411:TYR:CD2	1:A:412:HIS:N	2.87	0.42
1:B:111:SER:HB2	1:B:112:MET:HE3	2.02	0.42
1:B:158:PHE:CE2	1:B:159:MET:HE1	2.55	0.42
1:B:317:TYR:HE1	3:B:602:GDU:O1B	2.03	0.42
1:B:437:LEU:HD12	1:B:444:SER:HB2	2.00	0.42
1:C:446:GLY:H	1:C:450:SER:HB2	1.85	0.42
1:C:494:GLU:OE1	1:C:494:GLU:N	2.46	0.42
1:D:199:LYS:HD2	1:D:200:THR:N	2.35	0.42
1:F:46:LEU:O	1:F:60:VAL:HG21	2.20	0.42
1:F:168:ALA:HB1	1:F:377:SER:OG	2.20	0.42
1:G:302:VAL:HG13	1:G:368:TRP:CG	2.55	0.42
1:G:387:ILE:HA	1:G:390:ASP:OD2	2.19	0.42
1:H:82:LYS:HE2	1:H:84:ASP:OD1	2.19	0.42
1:H:297:VAL:HB	1:H:415:PHE:CE2	2.47	0.42
1:H:302:VAL:HG13	1:H:368:TRP:CG	2.55	0.42
1:H:401:LEU:HA	1:H:405:ASP:OD2	2.20	0.42
1:H:402:LYS:HE2	1:H:402:LYS:HB2	1.63	0.42
1:A:139:PRO:HB2	1:A:176:CYS:SG	2.60	0.41
1:A:250:LYS:HA	1:A:262:TYR:CZ	2.55	0.41
1:B:477:VAL:CG2	1:B:478:GLU:N	2.83	0.41
1:E:271:VAL:HG13	1:E:287:THR:CG2	2.49	0.41
1:E:467:GLU:CG	1:E:495:ARG:NH1	2.83	0.41
3:E:602:GDU:O1B	3:E:602:GDU:O5'	2.37	0.41
1:F:94:TYR:CE1	1:F:103:PRO:HG3	2.55	0.41
1:F:158:PHE:CD1	1:F:158:PHE:C	2.92	0.41
1:G:61:GLY:HA2	1:G:373:GLU:OE1	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:104:TYR:CG	1:G:105:PRO:HA	2.55	0.41
1:G:210:PHE:HD2	1:G:210:PHE:H	1.66	0.41
1:G:307:PRO:HG2	1:G:368:TRP:CZ2	2.55	0.41
1:G:335:SER:HB3	1:G:338:ASN:OD1	2.19	0.41
1:H:235:ARG:O	1:H:240:GLY:HA3	2.20	0.41
1:A:175:GLN:HG3	1:A:175:GLN:H	1.55	0.41
1:A:268:THR:HA	1:A:445:ARG:O	2.20	0.41
1:B:484:PRO:HA	1:B:487:VAL:HG22	2.02	0.41
1:D:57:LEU:HD12	1:D:57:LEU:N	2.35	0.41
1:D:110:ILE:CA	1:D:113:LEU:HD12	2.43	0.41
1:E:145:TRP:HH2	1:E:183:VAL:HG21	1.81	0.41
1:E:221:ILE:H	1:E:221:ILE:HG13	1.66	0.41
1:E:469:VAL:O	1:E:472:ILE:N	2.54	0.41
1:E:510:GLN:OE1	1:E:510:GLN:N	2.53	0.41
1:F:16:GLY:O	1:F:19:GLY:N	2.53	0.41
1:F:42:THR:HA	1:F:43:PRO:HD2	1.85	0.41
1:F:153:GLY:O	1:F:157:LEU:HB2	2.20	0.41
1:G:90:GLN:O	1:G:92:ILE:HG12	2.20	0.41
1:G:130:LEU:O	1:G:133:ARG:CB	2.64	0.41
1:G:167:TRP:CZ2	1:G:178:TRP:CH2	3.08	0.41
1:H:71:TYR:HB2	1:H:495:ARG:O	2.20	0.41
1:H:122:ILE:HD13	1:H:122:ILE:HA	1.96	0.41
1:H:471:ASN:HB2	1:H:476:ALA:O	2.20	0.41
1:H:499:ASP:O	1:H:500:GLY:C	2.58	0.41
1:A:8:VAL:HA	1:A:33:SER:OG	2.19	0.41
1:A:176:CYS:HA	1:A:179:LEU:HD11	2.01	0.41
1:A:239:LYS:O	1:A:254:LEU:HD13	2.20	0.41
1:A:304:GLY:O	1:A:368:TRP:HD1	2.04	0.41
1:A:389:ALA:HA	1:A:392:ILE:CD1	2.50	0.41
1:B:16:GLY:CA	2:B:601:FAD:O1A	2.67	0.41
1:B:94:TYR:H	1:B:316:LEU:HB3	1.85	0.41
1:B:447:ARG:HB2	2:B:601:FAD:H5'2	2.00	0.41
1:C:115:LYS:O	1:C:118:GLN:HB2	2.19	0.41
1:C:146:ILE:HG23	1:C:150:MET:HE3	2.02	0.41
1:C:339:GLN:CD	1:C:339:GLN:N	2.74	0.41
1:D:150:MET:HG2	1:D:154:ILE:CG2	2.49	0.41
1:E:125:MET:CG	1:E:188:LEU:HD13	2.48	0.41
1:E:183:VAL:CG1	3:E:602:GDU:C2	2.99	0.41
1:E:213:PRO:HG2	1:E:217:GLY:O	2.21	0.41
1:E:417:HIS:HB3	1:E:448:PHE:CZ	2.54	0.41
1:F:122:ILE:O	1:F:125:MET:N	2.53	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:231:LYS:HE2	1:F:231:LYS:HB3	1.73	0.41
1:F:263:LYS:N	1:F:263:LYS:HD2	2.36	0.41
1:G:166:VAL:HG12	1:G:326:TYR:CB	2.50	0.41
1:G:453:TYR:O	1:G:454:GLU:C	2.59	0.41
1:G:499:ASP:O	1:G:500:GLY:C	2.57	0.41
1:H:107:GLN:O	1:H:110:ILE:HG22	2.21	0.41
1:H:124:GLY:HA3	1:H:153:GLY:H	1.86	0.41
1:H:164:PHE:CD1	1:H:164:PHE:C	2.92	0.41
1:H:499:ASP:O	1:H:502:GLN:N	2.52	0.41
1:B:133:ARG:NH2	1:H:134:VAL:HG21	2.35	0.41
1:B:299:GLY:HA2	1:B:370:ILE:O	2.20	0.41
1:B:443:TRP:HD1	1:B:445:ARG:HH21	1.66	0.41
1:B:446:GLY:H	1:B:450:SER:HB2	1.84	0.41
1:C:199:LYS:HB3	1:C:199:LYS:HE2	1.69	0.41
1:C:303:ARG:NH2	1:C:363:LYS:C	2.68	0.41
1:C:304:GLY:O	1:C:368:TRP:CD1	2.74	0.41
1:D:299:GLY:HA2	1:D:370:ILE:O	2.20	0.41
1:D:325:PHE:CA	1:D:374:VAL:HG22	2.50	0.41
3:D:602:GDU:H3'	3:D:602:GDU:O1B	2.19	0.41
1:E:18:THR:HG23	1:E:461:SER:O	2.20	0.41
1:F:68:HIS:ND1	1:F:68:HIS:N	2.67	0.41
1:F:142:PHE:HB3	1:F:174:MET:HB2	2.02	0.41
1:G:18:THR:HG22	1:G:19:GLY:N	2.34	0.41
1:G:175:GLN:HG2	1:G:422:PRO:O	2.21	0.41
1:G:329:THR:HG21	1:G:334:TYR:CE2	2.56	0.41
1:H:383:ASN:OD1	1:H:385:GLU:HG2	2.21	0.41
1:B:199:LYS:HB3	1:B:199:LYS:HE2	1.71	0.41
1:E:43:PRO:HG2	1:E:223:ILE:HD13	2.02	0.41
1:E:91:ARG:HB2	1:E:207:ASN:O	2.21	0.41
1:E:294:SER:CB	1:E:414:ARG:NH2	2.83	0.41
1:E:447:ARG:O	1:E:451:TRP:HA	2.20	0.41
1:F:207:ASN:HB3	1:F:315:TRP:HH2	1.83	0.41
1:G:337:TYR:N	1:G:337:TYR:HD1	2.17	0.41
1:G:387:ILE:CG2	1:G:388:LEU:N	2.83	0.41
1:H:116:GLU:OE2	1:H:117:GLU:HG2	2.21	0.41
1:H:120:LYS:HB2	1:H:120:LYS:HE3	1.82	0.41
1:D:106:PHE:C	1:D:106:PHE:CD2	2.94	0.41
1:D:166:VAL:HG13	1:D:167:TRP:CD1	2.55	0.41
1:D:331:PHE:HD1	1:D:331:PHE:HA	1.72	0.41
1:E:468:ALA:O	1:E:472:ILE:HG13	2.20	0.41
1:F:122:ILE:CG2	1:F:126:ILE:HD11	2.47	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:183:VAL:HG12	3:F:602:GDU:C2	2.50	0.41
1:F:270:ALA:HB3	1:F:273:PHE:HD2	1.83	0.41
1:F:397:ASN:C	1:F:399:GLU:N	2.74	0.41
1:G:25:ARG:HA	1:G:28:GLN:CB	2.50	0.41
1:G:28:GLN:CG	1:G:497:LEU:HD12	2.50	0.41
1:G:120:LYS:HE3	1:G:120:LYS:HB2	1.76	0.41
1:H:139:PRO:HA	1:H:144:GLU:OE2	2.21	0.41
1:H:308:GLU:HG3	1:H:309:ARG:H	1.86	0.41
1:A:6:ILE:O	1:A:260:ILE:HA	2.20	0.41
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.55	0.41
1:B:244:LYS:HG2	1:B:245:VAL:H	1.85	0.41
1:B:398:THR:O	1:B:399:GLU:HB2	2.21	0.41
1:C:63:HIS:CD2	2:C:601:FAD:C6	3.04	0.41
1:C:503:VAL:HA	1:C:506:LYS:HE2	2.03	0.41
1:D:331:PHE:HB3	1:D:369:SER:HB3	2.03	0.41
1:D:469:VAL:O	1:D:472:ILE:N	2.54	0.41
1:E:139:PRO:HA	1:E:144:GLU:CD	2.41	0.41
1:E:142:PHE:CB	1:E:174:MET:HB2	2.50	0.41
1:E:457:ASN:C	2:E:601:FAD:O3'	2.59	0.41
1:F:104:TYR:CG	1:F:105:PRO:HA	2.55	0.41
1:F:178:TRP:CD2	1:F:179:LEU:HD22	2.55	0.41
1:F:364:GLU:HA	1:F:367:TYR:OH	2.20	0.41
1:G:160:ARG:N	1:G:161:PRO:HD2	2.36	0.41
1:H:80:LEU:HA	1:H:81:PRO:HD2	1.89	0.41
1:H:92:ILE:HG22	1:H:94:TYR:HE2	1.85	0.41
1:A:329:THR:O	1:A:370:ILE:HA	2.21	0.41
1:A:420:PRO:O	1:A:422:PRO:HD3	2.20	0.41
1:B:175:GLN:HG3	1:B:175:GLN:H	1.60	0.41
1:C:150:MET:HG2	1:C:154:ILE:HG21	2.02	0.41
1:D:5:ASP:OD2	1:D:258:THR:HA	2.21	0.41
1:D:58:TYR:HE1	1:D:369:SER:HG	1.66	0.41
1:D:176:CYS:HA	1:D:179:LEU:HD11	2.02	0.41
1:D:458:GLN:CA	2:D:601:FAD:O3'	2.68	0.41
1:E:38:ASP:OD1	2:E:601:FAD:H1B	2.20	0.41
1:E:150:MET:HG3	1:E:154:ILE:HB	2.02	0.41
1:E:152:THR:O	1:E:153:GLY:C	2.57	0.41
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.92	0.41
1:F:187:ASN:CG	1:F:189:LYS:HB2	2.39	0.41
1:F:306:ARG:O	1:F:306:ARG:HG2	2.19	0.41
1:G:80:LEU:HA	1:G:81:PRO:HD2	1.90	0.41
1:A:12:VAL:HB	1:A:36:ILE:HB	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:O	1:A:134:VAL:HG13	2.21	0.41
1:A:278:MET:O	1:A:279:ASN:HB2	2.20	0.41
1:A:286:LEU:O	1:A:289:GLN:HG3	2.20	0.41
1:B:8:VAL:O	1:B:262:TYR:HA	2.21	0.41
1:B:110:ILE:CG2	1:B:118:GLN:HG2	2.51	0.41
1:B:204:TRP:CE3	1:B:205:GLY:N	2.88	0.41
1:B:328:ALA:HB2	1:B:372:LEU:HB3	2.02	0.41
1:B:339:GLN:OE1	1:B:339:GLN:N	2.54	0.41
1:B:420:PRO:O	1:B:422:PRO:HD3	2.21	0.41
1:C:35:MET:HE2	1:C:35:MET:HB2	1.88	0.41
1:C:142:PHE:CE1	1:C:179:LEU:HD21	2.56	0.41
1:C:145:TRP:HB2	1:C:176:CYS:CB	2.51	0.41
1:C:223:ILE:HD13	1:C:223:ILE:HA	1.92	0.41
1:C:256:ASP:OD2	1:C:256:ASP:N	2.51	0.41
1:C:389:ALA:HA	1:C:392:ILE:CD1	2.50	0.41
1:D:376:GLU:HA	1:D:380:LYS:O	2.21	0.41
1:D:389:ALA:HA	1:D:392:ILE:CD1	2.51	0.41
1:E:18:THR:HA	1:E:462:PHE:HA	2.02	0.41
1:E:108:ASN:O	1:E:194:ASN:HB3	2.21	0.41
1:E:178:TRP:CD2	1:E:179:LEU:HD22	2.56	0.41
1:F:26:LEU:HD13	1:F:34:TRP:CB	2.49	0.41
1:F:328:ALA:CB	1:F:372:LEU:HB3	2.51	0.41
1:F:350:GLN:HE22	1:F:407:ILE:HD12	1.84	0.41
1:F:392:ILE:O	1:F:395:LEU:HB2	2.21	0.41
1:G:103:PRO:HD2	1:G:109:ASN:CG	2.41	0.41
1:G:136:ASN:OD1	1:G:136:ASN:N	2.47	0.41
1:G:252:VAL:HG13	1:G:254:LEU:CD2	2.51	0.41
1:G:313:LYS:H	1:G:313:LYS:HG3	1.71	0.41
1:G:383:ASN:OD1	1:G:385:GLU:HG2	2.21	0.41
1:H:28:GLN:CG	1:H:497:LEU:HD12	2.51	0.41
1:H:34:TRP:HH2	1:H:229:LEU:HD22	1.85	0.41
1:H:273:PHE:CZ	1:H:417:HIS:NE2	2.89	0.41
1:H:298:ILE:HG23	1:H:411:TYR:O	2.20	0.41
1:H:480:THR:CA	1:H:487:VAL:HG11	2.51	0.41
1:A:91:ARG:HG3	1:A:315:TRP:CZ2	2.55	0.41
1:A:376:GLU:HA	1:A:380:LYS:O	2.20	0.41
1:B:250:LYS:HA	1:B:262:TYR:CZ	2.56	0.41
1:B:423:THR:HB	1:B:425:GLU:OE1	2.21	0.41
1:C:56:PHE:CE1	1:C:339:GLN:HB3	2.56	0.41
1:D:42:THR:HA	1:D:43:PRO:HD2	1.82	0.41
1:D:494:GLU:OE2	1:H:477:VAL:HB	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:ARG:HG2	1:E:414:ARG:H	1.85	0.41
1:E:506:LYS:HD3	1:E:506:LYS:H	1.85	0.41
1:F:146:ILE:HG13	1:F:146:ILE:H	1.72	0.41
1:H:66:PHE:CD1	1:H:67:SER:N	2.89	0.41
1:H:83:GLU:HA	1:H:86:TRP:CD1	2.55	0.41
1:H:128:ALA:HB2	1:H:151:GLY:HA2	2.02	0.41
1:H:351:LEU:HB2	1:H:355:SER:H	1.87	0.41
1:B:56:PHE:CE1	1:B:339:GLN:HB3	2.56	0.40
1:B:60:VAL:O	1:B:63:HIS:CD2	2.75	0.40
1:B:62:GLY:O	3:B:602:GDU:C6'	2.69	0.40
1:D:63:HIS:HB3	1:D:458:GLN:HE22	1.86	0.40
1:E:18:THR:HG23	1:E:464:LEU:HB2	2.01	0.40
1:E:192:THR:O	1:E:193:THR:C	2.59	0.40
1:F:80:LEU:HA	1:F:81:PRO:HD2	1.90	0.40
1:G:57:LEU:HD11	1:G:337:TYR:O	2.21	0.40
1:G:115:LYS:HA	1:G:118:GLN:CG	2.35	0.40
1:G:307:PRO:HG2	1:G:368:TRP:CH2	2.57	0.40
1:H:90:GLN:HA	1:H:209:THR:HG23	2.03	0.40
1:H:160:ARG:HB2	1:H:161:PRO:CD	2.51	0.40
1:H:351:LEU:CD1	1:H:404:THR:HA	2.50	0.40
1:A:60:VAL:HB	1:A:63:HIS:CE1	2.56	0.40
1:A:175:GLN:HE21	1:A:178:TRP:HD1	1.69	0.40
1:A:306:ARG:HA	1:A:307:PRO:HD3	1.81	0.40
1:B:194:ASN:HD22	1:B:194:ASN:HA	1.56	0.40
1:C:110:ILE:O	1:C:113:LEU:HB2	2.20	0.40
1:C:250:LYS:HA	1:C:262:TYR:CZ	2.56	0.40
1:D:278:MET:CE	1:D:442:ILE:HD12	2.51	0.40
1:E:77:ASP:OD1	1:E:211:ARG:NH1	2.53	0.40
1:E:104:TYR:CE1	3:E:602:GDU:O4	2.75	0.40
1:F:143:ASP:N	1:F:171:THR:O	2.53	0.40
1:F:145:TRP:HE3	1:F:146:ILE:N	2.20	0.40
1:F:414:ARG:HG2	1:F:415:PHE:N	2.36	0.40
1:G:9:ASP:HA	1:G:263:LYS:HD3	2.03	0.40
1:G:235:ARG:O	1:G:240:GLY:HA3	2.21	0.40
1:G:271:VAL:HG13	1:G:272:ASP:H	1.86	0.40
1:G:336:PRO:HG2	1:G:337:TYR:HD1	1.83	0.40
1:H:63:HIS:HA	2:H:601:FAD:C4	2.51	0.40
1:H:239:LYS:HB2	1:H:239:LYS:HE3	1.91	0.40
1:A:296:HIS:NE2	1:A:382:VAL:HG21	2.36	0.40
1:C:128:ALA:HB1	1:C:148:ARG:O	2.21	0.40
1:C:469:VAL:O	1:C:473:VAL:HG23	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ARG:HA	1:D:307:PRO:HD3	1.83	0.40
1:E:267:SER:OG	1:E:274:LEU:HD22	2.21	0.40
1:E:348:THR:HG23	1:E:407:ILE:N	2.36	0.40
1:F:139:PRO:HA	1:F:144:GLU:CD	2.42	0.40
1:G:196:ILE:HG22	1:G:197:LEU:HD23	2.03	0.40
1:G:235:ARG:O	1:G:236:PHE:CD1	2.74	0.40
1:G:237:GLY:C	1:G:239:LYS:N	2.73	0.40
1:G:270:ALA:HA	1:G:448:PHE:O	2.21	0.40
1:G:497:LEU:HD12	1:G:497:LEU:O	2.21	0.40
1:H:222:TRP:O	1:H:226:ALA:HB2	2.22	0.40
1:A:108:ASN:HB2	1:A:194:ASN:OD1	2.21	0.40
1:A:242:VAL:HA	1:A:254:LEU:HD22	2.03	0.40
1:B:91:ARG:O	1:B:92:ILE:HD13	2.21	0.40
1:B:146:ILE:HG23	1:B:150:MET:HE3	2.03	0.40
1:B:166:VAL:HG13	1:B:167:TRP:CD1	2.56	0.40
1:B:433:ILE:HG22	1:B:434:LEU:N	2.36	0.40
1:C:443:TRP:CE3	1:C:443:TRP:N	2.89	0.40
1:D:94:TYR:H	1:D:316:LEU:HB3	1.85	0.40
1:D:249:ASN:O	1:D:251:THR:HG23	2.22	0.40
1:D:335:SER:HB3	1:D:338:ASN:OD1	2.21	0.40
1:D:495:ARG:O	1:D:496:ARG:HD2	2.22	0.40
1:E:63:HIS:HB2	1:E:458:GLN:HE22	1.86	0.40
1:E:69:TYR:HB2	1:E:72:PHE:CB	2.52	0.40
1:F:66:PHE:HB3	1:F:206:PRO:O	2.21	0.40
1:F:91:ARG:HG3	1:F:315:TRP:CZ2	2.55	0.40
1:F:347:PRO:HA	1:F:361:GLU:O	2.21	0.40
1:G:421:THR:HA	1:G:422:PRO:HD3	1.71	0.40
1:G:464:LEU:HD21	1:G:481:LEU:N	2.36	0.40
1:H:70:LYS:HG3	1:H:496:ARG:NH1	2.36	0.40
1:H:95:VAL:HG22	1:H:317:TYR:CD2	2.55	0.40
1:H:283:LEU:HD13	1:H:437:LEU:HD21	2.03	0.40
1:H:384:GLN:H	1:H:384:GLN:HG2	1.56	0.40
1:C:268:THR:HA	1:C:445:ARG:O	2.21	0.40
1:C:335:SER:OG	1:C:336:PRO:HD2	2.22	0.40
1:C:443:TRP:CD1	1:C:445:ARG:NH2	2.90	0.40
1:D:46:LEU:HB2	2:D:601:FAD:O4'	2.22	0.40
1:E:65:ILE:O	1:E:210:PHE:HB3	2.22	0.40
1:E:82:LYS:HB2	1:E:85:ASP:CG	2.42	0.40
1:E:307:PRO:CB	1:E:309:ARG:HE	2.35	0.40
1:F:40:ASN:O	1:F:236:PHE:HB3	2.22	0.40
1:F:65:ILE:O	1:F:210:PHE:HB3	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:TRP:CE3	1:F:205:GLY:CA	3.05	0.40
1:F:388:LEU:HD13	1:F:388:LEU:HA	1.97	0.40
1:H:65:ILE:O	1:H:65:ILE:CG2	2.68	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	47	79
1	B	507/509 (100%)	476 (94%)	29 (6%)	2 (0%)	34	69
1	C	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	47	79
1	D	507/509 (100%)	481 (95%)	25 (5%)	1 (0%)	47	79
1	E	507/509 (100%)	456 (90%)	51 (10%)	0	100	100
1	F	507/509 (100%)	457 (90%)	49 (10%)	1 (0%)	47	79
1	G	507/509 (100%)	462 (91%)	45 (9%)	0	100	100
1	H	507/509 (100%)	460 (91%)	46 (9%)	1 (0%)	47	79
All	All	4056/4072 (100%)	3744 (92%)	305 (8%)	7 (0%)	47	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	203	ASN
1	B	61	GLY
1	A	107	GLN
1	B	107	GLN
1	C	107	GLN
1	D	107	GLN
1	F	60	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	430/430 (100%)	372 (86%)	58 (14%)	4	16
1	B	430/430 (100%)	367 (85%)	63 (15%)	3	13
1	C	430/430 (100%)	370 (86%)	60 (14%)	3	15
1	D	430/430 (100%)	366 (85%)	64 (15%)	3	13
1	E	430/430 (100%)	363 (84%)	67 (16%)	2	11
1	F	430/430 (100%)	359 (84%)	71 (16%)	2	10
1	G	430/430 (100%)	347 (81%)	83 (19%)	1	6
1	H	430/430 (100%)	351 (82%)	79 (18%)	1	7
All	All	3440/3440 (100%)	2895 (84%)	545 (16%)	2	11

All (545) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	35	MET
1	A	40	ASN
1	A	57	LEU
1	A	65	ILE
1	A	67	SER
1	A	82	LYS
1	A	88	THR
1	A	89	HIS
1	A	95	VAL
1	A	106	PHE
1	A	108	ASN
1	A	111	SER
1	A	112	MET
1	A	122	ILE
1	A	140	LYS
1	A	149	MET
1	A	150	MET
1	A	152	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	175	GLN
1	A	179	LEU
1	A	199	LYS
1	A	209	THR
1	A	232	GLU
1	A	241	LYS
1	A	252	VAL
1	A	271	VAL
1	A	274	LEU
1	A	281	GLN
1	A	286	LEU
1	A	293	SER
1	A	316	LEU
1	A	317	TYR
1	A	331	PHE
1	A	332	SER
1	A	338	ASN
1	A	339	GLN
1	A	350	GLN
1	A	351	LEU
1	A	358	GLN
1	A	359	SER
1	A	360	THR
1	A	372	LEU
1	A	384	GLN
1	A	392	ILE
1	A	393	GLN
1	A	404	THR
1	A	411	TYR
1	A	424	LEU
1	A	433	ILE
1	A	450	SER
1	A	455	VAL
1	A	473	VAL
1	A	477	VAL
1	A	478	GLU
1	A	485	ASP
1	A	506	LYS
1	A	510	GLN
1	B	6	ILE
1	B	35	MET
1	B	40	ASN

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	57	LEU
1	B	65	ILE
1	B	67	SER
1	B	68	HIS
1	B	70	LYS
1	B	82	LYS
1	B	88	THR
1	B	89	HIS
1	B	95	VAL
1	B	106	PHE
1	B	107	GLN
1	B	108	ASN
1	B	111	SER
1	B	112	MET
1	B	116	GLU
1	B	140	LYS
1	B	149	MET
1	B	150	MET
1	B	152	THR
1	B	175	GLN
1	B	179	LEU
1	B	194	ASN
1	B	199	LYS
1	B	209	THR
1	B	232	GLU
1	B	241	LYS
1	B	252	VAL
1	B	274	LEU
1	B	281	GLN
1	B	284	VAL
1	B	286	LEU
1	B	293	SER
1	B	316	LEU
1	B	317	TYR
1	B	331	PHE
1	B	332	SER
1	B	338	ASN
1	B	339	GLN
1	B	350	GLN
1	B	360	THR
1	B	369	SER
1	B	372	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	373	GLU
1	B	384	GLN
1	B	392	ILE
1	B	393	GLN
1	B	404	THR
1	B	411	TYR
1	B	424	LEU
1	B	433	ILE
1	B	444	SER
1	B	450	SER
1	B	451	TRP
1	B	455	VAL
1	B	473	VAL
1	B	477	VAL
1	B	478	GLU
1	B	485	ASP
1	B	506	LYS
1	B	510	GLN
1	C	6	ILE
1	C	35	MET
1	C	40	ASN
1	C	42	THR
1	C	57	LEU
1	C	65	ILE
1	C	67	SER
1	C	68	HIS
1	C	70	LYS
1	C	82	LYS
1	C	88	THR
1	C	89	HIS
1	C	95	VAL
1	C	106	PHE
1	C	107	GLN
1	C	108	ASN
1	C	111	SER
1	C	112	MET
1	C	116	GLU
1	C	140	LYS
1	C	149	MET
1	C	150	MET
1	C	152	THR
1	C	175	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	179	LEU
1	C	199	LYS
1	C	209	THR
1	C	232	GLU
1	C	241	LYS
1	C	252	VAL
1	C	271	VAL
1	C	274	LEU
1	C	281	GLN
1	C	284	VAL
1	C	286	LEU
1	C	293	SER
1	C	316	LEU
1	C	317	TYR
1	C	331	PHE
1	C	332	SER
1	C	338	ASN
1	C	339	GLN
1	C	350	GLN
1	C	351	LEU
1	C	360	THR
1	C	372	LEU
1	C	373	GLU
1	C	384	GLN
1	C	393	GLN
1	C	404	THR
1	C	410	THR
1	C	411	TYR
1	C	424	LEU
1	C	433	ILE
1	C	444	SER
1	C	455	VAL
1	C	473	VAL
1	C	477	VAL
1	C	485	ASP
1	C	510	GLN
1	D	6	ILE
1	D	27	ASN
1	D	35	MET
1	D	40	ASN
1	D	57	LEU
1	D	65	ILE

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	67	SER
1	D	70	LYS
1	D	82	LYS
1	D	88	THR
1	D	89	HIS
1	D	95	VAL
1	D	106	PHE
1	D	107	GLN
1	D	108	ASN
1	D	111	SER
1	D	112	MET
1	D	140	LYS
1	D	149	MET
1	D	150	MET
1	D	152	THR
1	D	175	GLN
1	D	179	LEU
1	D	199	LYS
1	D	209	THR
1	D	232	GLU
1	D	241	LYS
1	D	252	VAL
1	D	271	VAL
1	D	274	LEU
1	D	281	GLN
1	D	284	VAL
1	D	286	LEU
1	D	293	SER
1	D	316	LEU
1	D	317	TYR
1	D	331	PHE
1	D	332	SER
1	D	338	ASN
1	D	339	GLN
1	D	350	GLN
1	D	351	LEU
1	D	359	SER
1	D	360	THR
1	D	364	GLU
1	D	369	SER
1	D	372	LEU
1	D	373	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	377	SER
1	D	384	GLN
1	D	392	ILE
1	D	393	GLN
1	D	404	THR
1	D	411	TYR
1	D	424	LEU
1	D	450	SER
1	D	455	VAL
1	D	473	VAL
1	D	477	VAL
1	D	478	GLU
1	D	485	ASP
1	D	490	ARG
1	D	506	LYS
1	D	510	GLN
1	E	3	HIS
1	E	25	ARG
1	E	35	MET
1	E	39	SER
1	E	41	GLU
1	E	42	THR
1	E	65	ILE
1	E	66	PHE
1	E	68	HIS
1	E	70	LYS
1	E	78	GLU
1	E	93	SER
1	E	116	GLU
1	E	122	ILE
1	E	125	MET
1	E	133	ARG
1	E	136	ASN
1	E	141	THR
1	E	149	MET
1	E	154	ILE
1	E	157	LEU
1	E	166	VAL
1	E	175	GLN
1	E	179	LEU
1	E	200	THR
1	E	204	TRP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	209	THR
1	E	225	VAL
1	E	234	THR
1	E	243	THR
1	E	248	ASN
1	E	251	THR
1	E	263	LYS
1	E	269	MET
1	E	271	VAL
1	E	278	MET
1	E	290	LEU
1	E	298	ILE
1	E	306	ARG
1	E	308	GLU
1	E	309	ARG
1	E	326	TYR
1	E	343	SER
1	E	363	LYS
1	E	364	GLU
1	E	372	LEU
1	E	374	VAL
1	E	378	SER
1	E	385	GLU
1	E	388	LEU
1	E	405	ASP
1	E	408	VAL
1	E	410	THR
1	E	413	ARG
1	E	433	ILE
1	E	438	GLN
1	E	451	TRP
1	E	464	LEU
1	E	473	VAL
1	E	478	GLU
1	E	479	LEU
1	E	493	THR
1	E	494	GLU
1	E	496	ARG
1	E	502	GLN
1	E	506	LYS
1	E	508	LYS
1	F	3	HIS

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	13	ILE
1	F	25	ARG
1	F	35	MET
1	F	39	SER
1	F	41	GLU
1	F	42	THR
1	F	63	HIS
1	F	65	ILE
1	F	66	PHE
1	F	68	HIS
1	F	70	LYS
1	F	93	SER
1	F	109	ASN
1	F	116	GLU
1	F	121	CYS
1	F	122	ILE
1	F	125	MET
1	F	133	ARG
1	F	136	ASN
1	F	141	THR
1	F	149	MET
1	F	154	ILE
1	F	157	LEU
1	F	166	VAL
1	F	169	VAL
1	F	175	GLN
1	F	179	LEU
1	F	200	THR
1	F	204	TRP
1	F	209	THR
1	F	225	VAL
1	F	234	THR
1	F	248	ASN
1	F	251	THR
1	F	271	VAL
1	F	278	MET
1	F	281	GLN
1	F	286	LEU
1	F	290	LEU
1	F	295	THR
1	F	298	ILE
1	F	303	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	306	ARG
1	F	308	GLU
1	F	309	ARG
1	F	343	SER
1	F	363	LYS
1	F	364	GLU
1	F	372	LEU
1	F	374	VAL
1	F	382	VAL
1	F	385	GLU
1	F	388	LEU
1	F	393	GLN
1	F	405	ASP
1	F	408	VAL
1	F	410	THR
1	F	438	GLN
1	F	443	TRP
1	F	451	TRP
1	F	473	VAL
1	F	478	GLU
1	F	479	LEU
1	F	493	THR
1	F	494	GLU
1	F	496	ARG
1	F	497	LEU
1	F	502	GLN
1	F	506	LYS
1	F	508	LYS
1	G	6	ILE
1	G	10	VAL
1	G	13	ILE
1	G	18	THR
1	G	24	LYS
1	G	36	ILE
1	G	41	GLU
1	G	42	THR
1	G	57	LEU
1	G	64	VAL
1	G	65	ILE
1	G	84	ASP
1	G	87	TYR
1	G	92	ILE

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	107	GLN
1	G	108	ASN
1	G	111	SER
1	G	112	MET
1	G	116	GLU
1	G	119	VAL
1	G	142	PHE
1	G	143	ASP
1	G	147	VAL
1	G	150	MET
1	G	152	THR
1	G	158	PHE
1	G	159	MET
1	G	169	VAL
1	G	182	ARG
1	G	183	VAL
1	G	193	THR
1	G	194	ASN
1	G	200	THR
1	G	204	TRP
1	G	207	ASN
1	G	209	THR
1	G	210	PHE
1	G	222	TRP
1	G	223	ILE
1	G	248	ASN
1	G	249	ASN
1	G	252	VAL
1	G	254	LEU
1	G	256	ASP
1	G	258	THR
1	G	269	MET
1	G	271	VAL
1	G	272	ASP
1	G	279	ASN
1	G	281	GLN
1	G	286	LEU
1	G	294	SER
1	G	308	GLU
1	G	309	ARG
1	G	316	LEU
1	G	320	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	326	TYR
1	G	331	PHE
1	G	332	SER
1	G	337	TYR
1	G	341	GLU
1	G	351	LEU
1	G	361	GLU
1	G	363	LYS
1	G	364	GLU
1	G	385	GLU
1	G	387	ILE
1	G	393	GLN
1	G	398	THR
1	G	402	LYS
1	G	408	VAL
1	G	411	TYR
1	G	424	LEU
1	G	445	ARG
1	G	453	TYR
1	G	455	VAL
1	G	477	VAL
1	G	478	GLU
1	G	485	ASP
1	G	490	ARG
1	G	491	GLN
1	G	492	ASN
1	G	510	GLN
1	H	6	ILE
1	H	10	VAL
1	H	13	ILE
1	H	24	LYS
1	H	36	ILE
1	H	41	GLU
1	H	57	LEU
1	H	64	VAL
1	H	65	ILE
1	H	70	LYS
1	H	77	ASP
1	H	84	ASP
1	H	87	TYR
1	H	92	ILE
1	H	94	TYR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	107	GLN
1	H	108	ASN
1	H	111	SER
1	H	112	MET
1	H	116	GLU
1	H	118	GLN
1	H	143	ASP
1	H	147	VAL
1	H	152	THR
1	H	158	PHE
1	H	169	VAL
1	H	183	VAL
1	H	193	THR
1	H	194	ASN
1	H	200	THR
1	H	203	ASN
1	H	204	TRP
1	H	209	THR
1	H	210	PHE
1	H	223	ILE
1	H	235	ARG
1	H	248	ASN
1	H	249	ASN
1	H	252	VAL
1	H	254	LEU
1	H	256	ASP
1	H	271	VAL
1	H	272	ASP
1	H	274	LEU
1	H	279	ASN
1	H	286	LEU
1	H	294	SER
1	H	308	GLU
1	H	309	ARG
1	H	316	LEU
1	H	326	TYR
1	H	331	PHE
1	H	337	TYR
1	H	341	GLU
1	H	351	LEU
1	H	358	GLN
1	H	361	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	363	LYS
1	H	364	GLU
1	H	378	SER
1	H	385	GLU
1	H	387	ILE
1	H	393	GLN
1	H	398	THR
1	H	402	LYS
1	H	408	VAL
1	H	411	TYR
1	H	419	TYR
1	H	424	LEU
1	H	443	TRP
1	H	453	TYR
1	H	455	VAL
1	H	477	VAL
1	H	478	GLU
1	H	485	ASP
1	H	490	ARG
1	H	491	GLN
1	H	492	ASN
1	H	510	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	175	GLN
1	A	296	HIS
1	A	339	GLN
1	A	350	GLN
1	A	458	GLN
1	B	163	ASN
1	B	175	GLN
1	B	296	HIS
1	B	350	GLN
1	B	458	GLN
1	C	163	ASN
1	C	175	GLN
1	C	296	HIS
1	C	339	GLN
1	C	350	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	458	GLN
1	D	63	HIS
1	D	175	GLN
1	D	296	HIS
1	D	339	GLN
1	D	458	GLN
1	E	68	HIS
1	E	175	GLN
1	E	207	ASN
1	E	339	GLN
1	E	412	HIS
1	F	63	HIS
1	F	109	ASN
1	F	175	GLN
1	F	194	ASN
1	F	207	ASN
1	F	279	ASN
1	F	339	GLN
1	F	412	HIS
1	G	28	GLN
1	G	339	GLN
1	G	383	ASN
1	G	412	HIS
1	G	492	ASN
1	H	28	GLN
1	H	90	GLN
1	H	194	ASN
1	H	203	ASN
1	H	339	GLN
1	H	383	ASN
1	H	393	GLN
1	H	412	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FAD	H	601	-	53,58,58	2.59	18 (33%)	68,89,89	1.69	17 (25%)
3	GDU	F	602	-	35,38,38	1.95	8 (22%)	53,58,58	1.97	15 (28%)
2	FAD	A	601	-	53,58,58	2.37	15 (28%)	68,89,89	2.02	19 (27%)
2	FAD	E	601	-	53,58,58	2.48	15 (28%)	68,89,89	1.78	16 (23%)
3	GDU	B	602	-	35,38,38	1.97	10 (28%)	53,58,58	2.01	15 (28%)
2	FAD	G	601	-	53,58,58	2.44	20 (37%)	68,89,89	2.04	18 (26%)
2	FAD	D	601	-	53,58,58	2.52	14 (26%)	68,89,89	1.77	15 (22%)
3	GDU	C	602	-	35,38,38	2.00	9 (25%)	53,58,58	1.88	15 (28%)
2	FAD	F	601	-	53,58,58	2.41	14 (26%)	68,89,89	1.91	16 (23%)
3	GDU	A	602	-	35,38,38	1.96	8 (22%)	53,58,58	1.96	13 (24%)
2	FAD	C	601	-	53,58,58	2.48	14 (26%)	68,89,89	1.73	15 (22%)
3	GDU	D	602	-	35,38,38	2.03	9 (25%)	53,58,58	1.96	15 (28%)
3	GDU	E	602	-	35,38,38	1.96	8 (22%)	53,58,58	1.87	11 (20%)
2	FAD	B	601	-	53,58,58	2.44	14 (26%)	68,89,89	1.84	16 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	H	601	-	-	9/30/50/50	0/6/6/6
3	GDU	F	602	-	-	8/23/59/59	0/3/3/3

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	1/1/9/9	14/30/50/50	0/6/6/6
2	FAD	E	601	-	-	13/30/50/50	0/6/6/6
3	GDU	B	602	-	-	6/23/59/59	0/3/3/3
2	FAD	G	601	-	-	7/30/50/50	0/6/6/6
2	FAD	D	601	-	-	8/30/50/50	0/6/6/6
3	GDU	C	602	-	-	9/23/59/59	0/3/3/3
2	FAD	F	601	-	1/1/9/9	13/30/50/50	0/6/6/6
3	GDU	A	602	-	-	7/23/59/59	0/3/3/3
2	FAD	C	601	-	-	7/30/50/50	0/6/6/6
3	GDU	D	602	-	-	13/23/59/59	0/3/3/3
3	GDU	E	602	-	-	9/23/59/59	0/3/3/3
2	FAD	B	601	-	-	20/30/50/50	0/6/6/6

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FAD	O4-C4	10.41	1.43	1.23
2	A	601	FAD	O4-C4	10.41	1.43	1.23
2	F	601	FAD	O4-C4	10.40	1.43	1.23
2	C	601	FAD	O4-C4	10.37	1.43	1.23
2	E	601	FAD	O4-C4	10.36	1.43	1.23
2	H	601	FAD	O4-C4	10.34	1.43	1.23
2	B	601	FAD	O4-C4	10.24	1.43	1.23
2	E	601	FAD	O2-C2	7.58	1.38	1.24
2	C	601	FAD	O2-C2	7.56	1.38	1.24
2	D	601	FAD	O2-C2	7.54	1.38	1.24
2	F	601	FAD	O2-C2	7.54	1.38	1.24
2	B	601	FAD	O2-C2	7.53	1.38	1.24
2	H	601	FAD	O2-C2	7.51	1.38	1.24
2	A	601	FAD	O2-C2	7.40	1.38	1.24
3	C	602	GDU	O4-C4	7.13	1.38	1.24
3	D	602	GDU	O4-C4	6.99	1.38	1.24
3	B	602	GDU	O4-C4	6.94	1.38	1.24
3	E	602	GDU	O4-C4	6.90	1.37	1.24
3	A	602	GDU	O4-C4	6.84	1.37	1.24
3	F	602	GDU	O4-C4	6.82	1.37	1.24
2	G	601	FAD	C2B-C3B	-6.04	1.36	1.53
2	G	601	FAD	C9A-C5X	-5.72	1.31	1.41
2	H	601	FAD	C1'-C2'	-5.35	1.45	1.52
2	H	601	FAD	C2B-C3B	-5.00	1.39	1.53

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C2B-C3B	-4.75	1.40	1.53
2	E	601	FAD	C2B-C3B	-4.68	1.40	1.53
2	F	601	FAD	C2B-C3B	-4.66	1.40	1.53
2	G	601	FAD	C9A-N10	-4.61	1.33	1.41
2	D	601	FAD	C2B-C3B	-4.54	1.40	1.53
2	B	601	FAD	C2B-C3B	-4.51	1.41	1.53
2	A	601	FAD	C2B-C3B	-4.48	1.41	1.53
2	D	601	FAD	C1'-C2'	-4.39	1.46	1.52
2	C	601	FAD	C1'-C2'	-4.36	1.46	1.52
3	A	602	GDU	C4'-C3'	-4.21	1.41	1.52
2	E	601	FAD	C1'-C2'	-4.18	1.46	1.52
2	G	601	FAD	C5X-N5	-4.13	1.31	1.39
2	G	601	FAD	O3'-C3'	-4.08	1.33	1.43
2	G	601	FAD	C4'-C3'	-4.05	1.45	1.53
2	G	601	FAD	C1'-C2'	4.05	1.58	1.52
3	D	602	GDU	C4'-C3'	-4.03	1.42	1.52
3	C	602	GDU	C4'-C3'	-4.00	1.42	1.52
2	B	601	FAD	C1'-C2'	-3.98	1.47	1.52
2	H	601	FAD	C9A-N10	-3.95	1.34	1.41
2	G	601	FAD	C1'-N10	-3.85	1.38	1.48
2	D	601	FAD	C5'-C4'	-3.83	1.46	1.51
2	H	601	FAD	C5'-C4'	-3.83	1.46	1.51
2	B	601	FAD	C9A-N10	-3.73	1.34	1.41
2	H	601	FAD	O2'-C2'	-3.64	1.35	1.43
3	E	602	GDU	C3D-C2D	-3.59	1.43	1.53
3	F	602	GDU	C4'-C3'	-3.55	1.43	1.52
2	D	601	FAD	C9A-N10	-3.55	1.34	1.41
3	D	602	GDU	C3D-C2D	-3.49	1.43	1.53
2	G	601	FAD	O4B-C1B	-3.49	1.36	1.41
2	G	601	FAD	C10-N1	3.48	1.40	1.33
3	B	602	GDU	C4'-C3'	-3.47	1.43	1.52
2	G	601	FAD	C8-C7	-3.45	1.32	1.40
3	B	602	GDU	C3D-C2D	-3.45	1.43	1.53
2	E	601	FAD	C9A-N10	-3.43	1.35	1.41
3	E	602	GDU	C4'-C3'	-3.42	1.43	1.52
2	E	601	FAD	O2'-C2'	-3.38	1.36	1.43
2	C	601	FAD	O2'-C2'	-3.36	1.36	1.43
3	C	602	GDU	C3D-C2D	-3.33	1.44	1.53
2	D	601	FAD	O2'-C2'	-3.33	1.36	1.43
3	A	602	GDU	C3D-C2D	-3.30	1.44	1.53
2	C	601	FAD	C9A-N10	-3.30	1.35	1.41
2	A	601	FAD	O2'-C2'	-3.28	1.36	1.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FAD	C1'-C2'	-3.26	1.48	1.52
2	F	601	FAD	O2'-C2'	-3.26	1.36	1.43
2	G	601	FAD	O2-C2	-3.23	1.18	1.24
3	F	602	GDU	C3D-C2D	-3.22	1.44	1.53
2	G	601	FAD	C7M-C7	3.19	1.57	1.51
2	E	601	FAD	C5'-C4'	-3.18	1.47	1.51
3	D	602	GDU	C3D-C4D	-3.17	1.44	1.53
2	A	601	FAD	C1'-C2'	-3.15	1.48	1.52
2	F	601	FAD	C5'-C4'	-3.12	1.47	1.51
2	H	601	FAD	C2B-C1B	-3.12	1.49	1.53
2	C	601	FAD	C5'-C4'	-3.10	1.47	1.51
2	B	601	FAD	O2'-C2'	-3.10	1.36	1.43
2	G	601	FAD	C4X-C10	-3.08	1.35	1.44
2	E	601	FAD	C2B-C1B	-3.07	1.49	1.53
2	D	601	FAD	C2B-C1B	-2.98	1.49	1.53
3	C	602	GDU	C3D-C4D	-2.94	1.45	1.53
2	C	601	FAD	C2B-C1B	-2.91	1.49	1.53
3	F	602	GDU	C3D-C4D	-2.90	1.45	1.53
3	A	602	GDU	C3D-C4D	-2.87	1.45	1.53
2	B	601	FAD	C4-N3	-2.81	1.33	1.38
2	D	601	FAD	PA-O1A	-2.78	1.41	1.50
2	A	601	FAD	C2B-C1B	-2.77	1.49	1.53
2	C	601	FAD	PA-O1A	-2.76	1.41	1.50
3	E	602	GDU	C3D-C4D	-2.74	1.46	1.53
3	B	602	GDU	C3D-C4D	-2.72	1.46	1.53
2	G	601	FAD	O3B-C3B	-2.71	1.36	1.43
2	A	601	FAD	PA-O1A	-2.68	1.41	1.50
2	B	601	FAD	C2B-C1B	-2.67	1.49	1.53
2	B	601	FAD	C5'-C4'	-2.66	1.48	1.51
2	B	601	FAD	PA-O1A	-2.62	1.41	1.50
2	F	601	FAD	C9A-N10	-2.61	1.36	1.41
2	A	601	FAD	C5'-C4'	-2.59	1.48	1.51
2	F	601	FAD	PA-O1A	-2.58	1.41	1.50
3	E	602	GDU	C2-N1	-2.58	1.34	1.38
2	F	601	FAD	C7M-C7	2.57	1.56	1.51
2	A	601	FAD	C4-N3	-2.56	1.34	1.38
2	H	601	FAD	C7M-C7	2.55	1.56	1.51
2	A	601	FAD	C7M-C7	2.54	1.56	1.51
2	E	601	FAD	C7M-C7	2.53	1.56	1.51
2	H	601	FAD	C4-N3	-2.53	1.34	1.38
2	C	601	FAD	C7M-C7	2.52	1.56	1.51
2	C	601	FAD	C4-N3	-2.50	1.34	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	FAD	PA-O1A	-2.49	1.42	1.50
2	D	601	FAD	C7M-C7	2.48	1.56	1.51
3	E	602	GDU	O5'-C5'	2.48	1.50	1.44
2	E	601	FAD	C4-N3	-2.47	1.34	1.38
3	F	602	GDU	C2-N3	-2.46	1.33	1.38
3	D	602	GDU	O5'-C5'	2.46	1.50	1.44
2	F	601	FAD	C2B-C1B	-2.45	1.50	1.53
3	F	602	GDU	O5'-C5'	2.45	1.50	1.44
2	H	601	FAD	PA-O1A	-2.44	1.42	1.50
3	E	602	GDU	C2-N3	-2.44	1.33	1.38
3	D	602	GDU	C2-N1	-2.43	1.34	1.38
2	B	601	FAD	C7M-C7	2.43	1.55	1.51
2	F	601	FAD	C4-N3	-2.41	1.34	1.38
2	D	601	FAD	C4-N3	-2.37	1.34	1.38
3	C	602	GDU	O5'-C5'	2.35	1.50	1.44
3	B	602	GDU	C2-N3	-2.34	1.33	1.38
2	H	601	FAD	C4X-N5	2.33	1.35	1.30
2	C	601	FAD	O4B-C4B	-2.33	1.39	1.45
3	F	602	GDU	C2-N1	-2.31	1.34	1.38
2	E	601	FAD	O4B-C4B	-2.29	1.39	1.45
3	D	602	GDU	C2-N3	-2.29	1.33	1.38
2	F	601	FAD	O4B-C4B	-2.27	1.39	1.45
3	B	602	GDU	O5'-C5'	2.27	1.49	1.44
2	A	601	FAD	O4B-C4B	-2.27	1.39	1.45
2	D	601	FAD	O4B-C4B	-2.25	1.40	1.45
2	B	601	FAD	C5X-N5	-2.24	1.35	1.39
3	B	602	GDU	C2-N1	-2.23	1.34	1.38
3	A	602	GDU	C2-N1	-2.23	1.34	1.38
3	C	602	GDU	C2-N1	-2.22	1.34	1.38
2	A	601	FAD	C9A-N10	-2.20	1.37	1.41
3	E	602	GDU	C4-N3	-2.20	1.34	1.38
3	A	602	GDU	C4-N3	-2.19	1.34	1.38
3	F	602	GDU	C4-N3	-2.18	1.34	1.38
2	G	601	FAD	P-O5'	-2.17	1.50	1.59
3	A	602	GDU	C2-N3	-2.17	1.34	1.38
3	B	602	GDU	PB-O3B	-2.17	1.54	1.60
3	D	602	GDU	C6-C5	2.16	1.40	1.35
2	B	601	FAD	O4B-C4B	-2.16	1.40	1.45
2	D	601	FAD	C6A-N6A	2.16	1.41	1.34
2	E	601	FAD	C3B-C4B	-2.15	1.47	1.53
2	B	601	FAD	C6A-N6A	2.15	1.41	1.34
2	A	601	FAD	C6A-N6A	2.15	1.41	1.34

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FAD	C5X-N5	-2.15	1.35	1.39
2	F	601	FAD	C6A-N6A	2.14	1.41	1.34
3	C	602	GDU	C6-C5	2.14	1.40	1.35
2	G	601	FAD	C2-N1	2.14	1.41	1.36
2	C	601	FAD	C6A-N6A	2.12	1.41	1.34
3	C	602	GDU	C2-N3	-2.12	1.34	1.38
3	A	602	GDU	O5'-C5'	2.12	1.49	1.44
2	A	601	FAD	C5X-N5	-2.11	1.35	1.39
3	D	602	GDU	C4-N3	-2.11	1.34	1.38
2	G	601	FAD	C10-N10	-2.10	1.32	1.37
2	H	601	FAD	C2A-N3A	2.10	1.35	1.32
2	D	601	FAD	C2'-C3'	-2.10	1.49	1.53
2	H	601	FAD	O4B-C4B	-2.09	1.40	1.45
3	C	602	GDU	C4-N3	-2.08	1.34	1.38
2	H	601	FAD	C6A-N6A	2.08	1.41	1.34
2	G	601	FAD	C3B-C4B	-2.08	1.47	1.53
2	H	601	FAD	C2'-C3'	-2.07	1.49	1.53
2	E	601	FAD	C6A-N6A	2.07	1.41	1.34
2	C	601	FAD	O4B-C1B	-2.06	1.38	1.41
2	A	601	FAD	O4B-C1B	-2.06	1.38	1.41
3	B	602	GDU	C6-C5	2.06	1.39	1.35
2	H	601	FAD	C9A-C5X	-2.05	1.37	1.41
3	B	602	GDU	C4-N3	-2.04	1.34	1.38
2	H	601	FAD	C3B-C4B	-2.03	1.47	1.53
2	G	601	FAD	C5A-N7A	-2.03	1.32	1.39
2	E	601	FAD	C5X-N5	-2.02	1.35	1.39

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	GDU	N3-C2-N1	6.55	123.58	114.89
3	C	602	GDU	N3-C2-N1	6.50	123.52	114.89
3	D	602	GDU	N3-C2-N1	6.32	123.28	114.89
2	B	601	FAD	C1'-N10-C9A	-6.24	110.11	120.51
2	C	601	FAD	C1B-N9A-C4A	-6.17	115.81	126.64
3	E	602	GDU	N3-C2-N1	6.12	123.01	114.89
3	B	602	GDU	O5'-C1'-O3B	-6.06	103.44	111.36
3	F	602	GDU	N3-C2-N1	5.93	122.77	114.89
3	B	602	GDU	N3-C2-N1	5.68	122.44	114.89
2	D	601	FAD	C1B-N9A-C4A	-5.56	116.87	126.64
2	F	601	FAD	O2'-C2'-C1'	5.30	122.61	109.80
2	G	601	FAD	N3A-C2A-N1A	-5.26	120.45	128.68

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	O5'-C5'-C4'	5.25	123.38	109.36
2	G	601	FAD	O4B-C1B-C2B	-5.23	99.28	106.93
3	A	602	GDU	C4-N3-C2	-5.20	119.72	126.58
3	E	602	GDU	C4-N3-C2	-5.18	119.74	126.58
2	F	601	FAD	O5'-C5'-C4'	5.16	123.12	109.36
3	F	602	GDU	C4-N3-C2	-4.98	120.01	126.58
2	E	601	FAD	O5'-C5'-C4'	4.89	122.41	109.36
2	A	601	FAD	O2'-C2'-C1'	4.80	121.40	109.80
2	A	601	FAD	C1'-N10-C9A	4.77	128.46	120.51
2	C	601	FAD	N3A-C2A-N1A	-4.76	121.24	128.68
3	E	602	GDU	C3'-C4'-C5'	4.76	118.73	110.24
3	D	602	GDU	C4-N3-C2	-4.76	120.30	126.58
2	A	601	FAD	O2'-C2'-C3'	4.74	120.61	109.10
2	F	601	FAD	N3A-C2A-N1A	-4.71	121.31	128.68
2	G	601	FAD	O5B-PA-O1A	-4.71	90.65	109.07
2	A	601	FAD	N3A-C2A-N1A	-4.69	121.36	128.68
3	A	602	GDU	O3A-PB-O3B	4.68	111.91	102.48
3	C	602	GDU	C4-N3-C2	-4.67	120.42	126.58
2	E	601	FAD	N3A-C2A-N1A	-4.66	121.40	128.68
2	E	601	FAD	O2'-C2'-C1'	4.55	120.80	109.80
2	H	601	FAD	N3A-C2A-N1A	-4.54	121.58	128.68
2	D	601	FAD	N3A-C2A-N1A	-4.52	121.61	128.68
2	G	601	FAD	O5B-C5B-C4B	4.51	124.53	108.99
2	B	601	FAD	N3A-C2A-N1A	-4.51	121.62	128.68
2	D	601	FAD	O2'-C2'-C1'	4.44	120.53	109.80
2	F	601	FAD	O2'-C2'-C3'	4.42	119.85	109.10
2	G	601	FAD	C4-N3-C2	-4.42	117.48	125.64
3	F	602	GDU	O5'-C5'-C4'	4.37	117.63	109.69
3	D	602	GDU	O5'-C5'-C4'	4.34	117.58	109.69
2	B	601	FAD	O5'-C5'-C4'	4.31	120.87	109.36
2	D	601	FAD	O2'-C2'-C3'	4.31	119.58	109.10
2	A	601	FAD	C1B-N9A-C4A	-4.27	119.15	126.64
3	F	602	GDU	C3'-C4'-C5'	4.19	117.71	110.24
3	B	602	GDU	C4-N3-C2	-4.11	121.15	126.58
3	E	602	GDU	O3A-PB-O3B	4.11	110.77	102.48
2	H	601	FAD	C1'-N10-C9A	-4.09	113.70	120.51
3	B	602	GDU	C3'-C4'-C5'	4.00	117.38	110.24
2	F	601	FAD	C1B-N9A-C4A	-3.99	119.64	126.64
2	G	601	FAD	O2P-P-O5'	3.94	126.05	107.75
2	E	601	FAD	O2'-C2'-C3'	3.93	118.65	109.10
3	C	602	GDU	O3A-PB-O3B	3.92	110.39	102.48
2	B	601	FAD	O5B-C5B-C4B	3.91	122.44	108.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	FAD	O5'-C5'-C4'	3.91	119.79	109.36
2	A	601	FAD	C4X-C10-N10	3.88	122.16	116.48
3	F	602	GDU	O3A-PB-O3B	3.88	110.31	102.48
3	F	602	GDU	PB-O3A-PA	-3.86	119.60	132.83
2	C	601	FAD	O2'-C2'-C3'	3.84	118.44	109.10
3	D	602	GDU	PB-O3A-PA	-3.79	119.83	132.83
2	D	601	FAD	O5'-C5'-C4'	3.71	119.27	109.36
2	A	601	FAD	O5B-C5B-C4B	3.67	121.63	108.99
2	B	601	FAD	C1B-N9A-C4A	-3.67	120.20	126.64
3	E	602	GDU	O5'-C5'-C4'	3.66	116.34	109.69
2	B	601	FAD	C5X-C9A-N10	3.61	121.69	117.95
2	H	601	FAD	P-O3P-PA	-3.56	120.63	132.83
2	H	601	FAD	C1B-N9A-C4A	-3.54	120.42	126.64
2	G	601	FAD	O5'-P-O1P	-3.53	95.26	109.07
2	C	601	FAD	O5'-C5'-C4'	3.52	118.76	109.36
3	D	602	GDU	O3A-PB-O3B	3.52	109.58	102.48
3	A	602	GDU	PB-O3A-PA	-3.38	121.22	132.83
2	A	601	FAD	C4'-C3'-C2'	3.37	120.37	113.36
2	B	601	FAD	C4-N3-C2	-3.35	119.45	125.64
2	D	601	FAD	C4-C4X-N5	3.35	123.00	118.23
2	D	601	FAD	C4A-C5A-N7A	-3.33	105.93	109.40
3	C	602	GDU	O5'-C5'-C4'	3.32	115.72	109.69
2	H	601	FAD	O2'-C2'-C1'	3.30	117.78	109.80
2	F	601	FAD	C3B-C2B-C1B	3.29	105.93	100.98
3	D	602	GDU	C1'-O5'-C5'	3.27	120.10	113.69
3	D	602	GDU	C3'-C4'-C5'	3.26	116.06	110.24
2	F	601	FAD	C1'-N10-C9A	3.26	125.94	120.51
3	C	602	GDU	C3D-C2D-C1D	3.21	107.52	101.43
2	F	601	FAD	C4-N3-C2	-3.21	119.71	125.64
2	H	601	FAD	C4-N3-C2	-3.20	119.72	125.64
2	C	601	FAD	O2'-C2'-C1'	3.20	117.53	109.80
3	C	602	GDU	PB-O3A-PA	-3.20	121.86	132.83
3	B	602	GDU	O5'-C5'-C4'	3.19	115.50	109.69
3	E	602	GDU	PB-O3A-PA	-3.18	121.91	132.83
2	H	601	FAD	C4-C4X-N5	3.17	122.74	118.23
2	E	601	FAD	C1B-N9A-C4A	-3.14	121.13	126.64
2	A	601	FAD	C4-N3-C2	-3.13	119.85	125.64
2	H	601	FAD	O2'-C2'-C3'	3.13	116.71	109.10
2	F	601	FAD	O4-C4-C4X	-3.12	118.32	126.60
3	B	602	GDU	C1'-O5'-C5'	-3.10	107.60	113.69
3	A	602	GDU	C1'-C2'-C3'	3.09	116.43	110.00
2	C	601	FAD	C4-C4X-N5	3.09	122.63	118.23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	FAD	C4X-C10-N10	3.08	120.98	116.48
2	C	601	FAD	C1'-C2'-C3'	3.08	118.38	109.79
2	E	601	FAD	C4'-C3'-C2'	3.07	119.75	113.36
2	B	601	FAD	C4X-C4-N3	3.06	120.97	113.19
3	F	602	GDU	C5-C4-N3	3.06	119.41	114.84
2	D	601	FAD	P-O3P-PA	-3.05	122.35	132.83
3	E	602	GDU	O2-C2-N1	-3.04	118.74	122.79
2	E	601	FAD	C4-N3-C2	-3.04	120.02	125.64
3	A	602	GDU	O2-C2-N1	-2.99	118.81	122.79
2	G	601	FAD	C4X-C4-N3	2.99	120.79	113.19
2	C	601	FAD	C4-N3-C2	-2.98	120.13	125.64
3	C	602	GDU	C3'-C4'-C5'	2.98	115.56	110.24
2	H	601	FAD	C4X-C4-N3	2.98	120.75	113.19
3	D	602	GDU	O2-C2-N1	-2.98	118.83	122.79
2	H	601	FAD	O4B-C1B-C2B	-2.97	102.58	106.93
3	B	602	GDU	O5D-C5D-C4D	2.95	119.15	108.99
2	G	601	FAD	C8M-C8-C9	2.94	124.93	119.49
2	E	601	FAD	P-O3P-PA	-2.94	122.73	132.83
2	G	601	FAD	O4-C4-C4X	-2.94	118.81	126.60
3	C	602	GDU	O2-C2-N1	-2.93	118.89	122.79
3	F	602	GDU	O5D-C5D-C4D	2.93	119.07	108.99
2	G	601	FAD	O3B-C3B-C2B	-2.93	102.36	111.82
2	B	601	FAD	C9-C9A-N10	-2.91	117.90	121.84
2	E	601	FAD	C4X-C10-N10	2.91	120.73	116.48
2	E	601	FAD	C4-C4X-N5	2.88	122.33	118.23
2	F	601	FAD	C4X-C4-N3	2.88	120.50	113.19
3	A	602	GDU	O5D-C5D-C4D	2.88	118.89	108.99
2	F	601	FAD	P-O3P-PA	-2.86	123.00	132.83
2	E	601	FAD	C3B-C2B-C1B	2.86	105.29	100.98
2	C	601	FAD	C4X-C4-N3	2.85	120.43	113.19
3	E	602	GDU	C5-C4-N3	2.84	119.09	114.84
2	E	601	FAD	C4X-C4-N3	2.83	120.38	113.19
3	B	602	GDU	O5'-C1'-C2'	-2.78	104.45	110.35
2	D	601	FAD	C4X-C4-N3	2.78	120.25	113.19
3	A	602	GDU	O4-C4-C5	-2.78	120.28	125.16
2	C	601	FAD	O5B-C5B-C4B	2.78	118.54	108.99
2	A	601	FAD	C4A-C5A-N7A	-2.77	106.51	109.40
2	G	601	FAD	C8M-C8-C7	-2.76	115.07	120.74
2	E	601	FAD	O4-C4-C4X	-2.75	119.30	126.60
2	A	601	FAD	C1'-C2'-C3'	2.73	117.43	109.79
2	B	601	FAD	O2'-C2'-C3'	2.72	115.71	109.10
2	D	601	FAD	O4-C4-C4X	-2.72	119.39	126.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	GDU	O5'-C1'-C2'	2.71	116.09	110.35
2	A	601	FAD	C4X-C4-N3	2.70	120.06	113.19
2	F	601	FAD	O5B-C5B-C4B	2.70	118.30	108.99
3	A	602	GDU	C3D-C2D-C1D	2.70	106.56	101.43
2	D	601	FAD	C4-N3-C2	-2.70	120.66	125.64
2	H	601	FAD	O5B-C5B-C4B	2.70	118.28	108.99
2	E	601	FAD	O5B-C5B-C4B	2.69	118.26	108.99
2	C	601	FAD	C4A-C5A-N7A	-2.68	106.60	109.40
2	B	601	FAD	C3B-C2B-C1B	2.68	105.02	100.98
3	E	602	GDU	O5D-C5D-C4D	2.68	118.22	108.99
2	A	601	FAD	O4-C4-C4X	-2.67	119.52	126.60
3	B	602	GDU	O3A-PB-O3B	2.66	107.84	102.48
2	C	601	FAD	C4X-C10-N10	2.60	120.29	116.48
3	A	602	GDU	C5-C4-N3	2.57	118.69	114.84
2	A	601	FAD	C4-C4X-N5	2.56	121.88	118.23
3	D	602	GDU	O4D-C1D-N1	2.56	114.21	108.36
2	B	601	FAD	C4X-C10-N1	-2.55	118.81	124.73
2	C	601	FAD	O4-C4-C4X	-2.55	119.83	126.60
2	B	601	FAD	O4-C4-C4X	-2.54	119.87	126.60
2	E	601	FAD	O4B-C1B-C2B	-2.53	103.23	106.93
2	F	601	FAD	C1'-C2'-C3'	2.51	116.81	109.79
3	D	602	GDU	C5-C4-N3	2.51	118.59	114.84
2	D	601	FAD	C1'-C2'-C3'	2.49	116.75	109.79
3	F	602	GDU	C3D-C2D-C1D	2.48	106.14	101.43
2	D	601	FAD	C4X-C10-N10	2.47	120.09	116.48
3	B	602	GDU	O4-C4-C5	-2.45	120.84	125.16
3	A	602	GDU	O5'-C1'-C2'	2.45	115.54	110.35
3	B	602	GDU	C5-C4-N3	2.45	118.50	114.84
2	G	601	FAD	P-O3P-PA	-2.45	124.42	132.83
3	B	602	GDU	C1D-N1-C2	2.44	121.99	117.57
3	F	602	GDU	O4-C4-C5	-2.43	120.89	125.16
3	C	602	GDU	O5D-C5D-C4D	2.43	117.36	108.99
3	B	602	GDU	PB-O3A-PA	-2.42	124.51	132.83
3	E	602	GDU	O4-C4-C5	-2.42	120.91	125.16
2	G	601	FAD	C4X-C10-N1	-2.38	119.21	124.73
2	D	601	FAD	O4B-C1B-C2B	-2.38	103.45	106.93
2	H	601	FAD	O5'-C5'-C4'	2.36	115.66	109.36
3	F	602	GDU	C1D-N1-C2	2.35	121.82	117.57
2	A	601	FAD	P-O3P-PA	-2.35	124.78	132.83
2	C	601	FAD	O4B-C1B-C2B	-2.34	103.51	106.93
3	D	602	GDU	O4-C4-C5	-2.29	121.13	125.16
3	A	602	GDU	C1D-N1-C2	2.29	121.71	117.57

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	GDU	C3D-C2D-C1D	2.28	105.75	101.43
3	B	602	GDU	O2-C2-N1	-2.28	119.76	122.79
2	B	601	FAD	O2'-C2'-C1'	2.27	115.28	109.80
2	A	601	FAD	C10-C4X-N5	-2.26	120.07	124.86
2	H	601	FAD	O4-C4-C4X	-2.26	120.62	126.60
2	H	601	FAD	C10-C4X-N5	-2.26	120.07	124.86
2	F	601	FAD	C4A-C5A-N7A	-2.25	107.05	109.40
2	H	601	FAD	C9-C9A-N10	-2.25	118.80	121.84
2	F	601	FAD	C4-C4X-N5	2.25	121.43	118.23
3	C	602	GDU	C5-C4-N3	2.23	118.18	114.84
2	H	601	FAD	C4A-C5A-N7A	-2.23	107.07	109.40
3	F	602	GDU	O2-C2-N1	-2.23	119.83	122.79
2	G	601	FAD	C10-C4X-N5	-2.21	120.17	124.86
3	C	602	GDU	O4-C4-C5	-2.20	121.29	125.16
2	C	601	FAD	C10-C4X-N5	-2.20	120.19	124.86
3	F	602	GDU	O2-C2-N3	-2.20	117.40	121.50
3	C	602	GDU	C6-N1-C2	-2.19	118.19	120.99
2	B	601	FAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	A	601	FAD	C4X-C10-N1	-2.17	119.70	124.73
2	G	601	FAD	O2A-PA-O1A	2.17	122.96	112.24
2	E	601	FAD	C10-C4X-N5	-2.14	120.32	124.86
2	G	601	FAD	C4-C4X-C10	2.12	120.36	116.79
3	D	602	GDU	O5D-C5D-C4D	2.12	116.28	108.99
3	F	602	GDU	C2D-C3D-C4D	2.12	106.76	102.64
2	B	601	FAD	C4'-C3'-C2'	2.11	117.76	113.36
3	C	602	GDU	O2-C2-N3	-2.10	117.59	121.50
2	D	601	FAD	C10-C4X-N5	-2.09	120.42	124.86
3	F	602	GDU	C1'-O5'-C5'	2.09	117.79	113.69
3	A	602	GDU	O2-C2-N3	-2.09	117.61	121.50
3	C	602	GDU	C1D-N1-C2	2.07	121.31	117.57
2	A	601	FAD	O4B-C1B-C2B	-2.07	103.91	106.93
3	B	602	GDU	O4D-C1D-N1	2.06	113.08	108.36
3	C	602	GDU	O4D-C1D-N1	2.06	113.07	108.36
3	E	602	GDU	C4'-C3'-C2'	2.02	114.36	110.82
2	H	601	FAD	C4X-C10-N1	-2.01	120.07	124.73
3	D	602	GDU	C5D-C4D-C3D	-2.01	107.67	115.18

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	601	FAD	C2'
2	F	601	FAD	C2'



All (143) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	C2'-C1'-N10-C9A
2	A	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	C1'-C2'-C3'-O3'
2	A	601	FAD	C1'-C2'-C3'-C4'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	N10-C1'-C2'-C3'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	O2'-C2'-C3'-O3'
2	D	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	C3'-C4'-C5'-O5'
2	D	601	FAD	O4'-C4'-C5'-O5'
2	E	601	FAD	C5B-O5B-PA-O2A
2	E	601	FAD	N10-C1'-C2'-O2'
2	F	601	FAD	C5B-O5B-PA-O1A
2	F	601	FAD	C5B-O5B-PA-O2A
2	F	601	FAD	C2'-C1'-N10-C9A
2	F	601	FAD	C2'-C1'-N10-C10
2	F	601	FAD	N10-C1'-C2'-O2'
2	F	601	FAD	C1'-C2'-C3'-O3'
2	F	601	FAD	C1'-C2'-C3'-C4'
2	G	601	FAD	C1'-C2'-C3'-O3'
2	G	601	FAD	C1'-C2'-C3'-C4'
2	G	601	FAD	O2'-C2'-C3'-O3'
2	G	601	FAD	O2'-C2'-C3'-C4'
2	G	601	FAD	C5'-O5'-P-O1P
2	H	601	FAD	C1'-C2'-C3'-O3'
2	H	601	FAD	C1'-C2'-C3'-C4'
2	H	601	FAD	O2'-C2'-C3'-O3'
2	H	601	FAD	O2'-C2'-C3'-C4'
3	A	602	GDU	C3D-C4D-C5D-O5D

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	A	602	GDU	C4D-C5D-O5D-PA
3	A	602	GDU	C5D-O5D-PA-O3A
3	B	602	GDU	C3D-C4D-C5D-O5D
3	B	602	GDU	C5D-O5D-PA-O3A
3	B	602	GDU	O5'-C1'-O3B-PB
3	C	602	GDU	C4D-C5D-O5D-PA
3	C	602	GDU	C1'-O3B-PB-O1B
3	C	602	GDU	C1'-O3B-PB-O2B
3	D	602	GDU	C3D-C4D-C5D-O5D
3	D	602	GDU	O4D-C4D-C5D-O5D
3	D	602	GDU	C4D-C5D-O5D-PA
3	D	602	GDU	C5D-O5D-PA-O1A
3	D	602	GDU	C5D-O5D-PA-O2A
3	D	602	GDU	O5'-C1'-O3B-PB
3	E	602	GDU	C5D-O5D-PA-O1A
3	E	602	GDU	C5D-O5D-PA-O2A
3	E	602	GDU	O5'-C1'-O3B-PB
3	F	602	GDU	O4D-C1D-N1-C2
3	F	602	GDU	O4D-C1D-N1-C6
3	F	602	GDU	C4'-C5'-C6'-O6'
2	B	601	FAD	O2'-C2'-C3'-O3'
3	E	602	GDU	O4D-C4D-C5D-O5D
3	F	602	GDU	O4D-C4D-C5D-O5D
2	B	601	FAD	C2'-C3'-C4'-O4'
2	E	601	FAD	O2'-C2'-C3'-C4'
3	F	602	GDU	O5'-C5'-C6'-O6'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	C2'-C3'-C4'-C5'
3	D	602	GDU	C1'-O3B-PB-O3A
3	E	602	GDU	C1'-O3B-PB-O3A
2	E	601	FAD	O2'-C2'-C3'-O3'
2	B	601	FAD	C3B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
3	A	602	GDU	O4D-C4D-C5D-O5D
3	B	602	GDU	O4D-C4D-C5D-O5D
2	B	601	FAD	O3'-C3'-C4'-C5'
2	E	601	FAD	O4'-C4'-C5'-O5'
2	B	601	FAD	O3'-C3'-C4'-O4'
3	C	602	GDU	C1'-O3B-PB-O3A
2	D	601	FAD	O4B-C4B-C5B-O5B
2	E	601	FAD	C3'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	H	601	FAD	C3'-C4'-C5'-O5'
3	D	602	GDU	O5'-C5'-C6'-O6'
2	D	601	FAD	C3B-C4B-C5B-O5B
3	F	602	GDU	C3D-C4D-C5D-O5D
3	A	602	GDU	O5'-C5'-C6'-O6'
3	C	602	GDU	O5'-C5'-C6'-O6'
3	E	602	GDU	C3D-C4D-C5D-O5D
2	B	601	FAD	C4B-C5B-O5B-PA
3	E	602	GDU	C4D-C5D-O5D-PA
2	B	601	FAD	P-O3P-PA-O5B
2	C	601	FAD	PA-O3P-P-O5'
2	E	601	FAD	P-O3P-PA-O5B
2	F	601	FAD	P-O3P-PA-O5B
2	G	601	FAD	PA-O3P-P-O5'
2	H	601	FAD	PA-O3P-P-O5'
3	A	602	GDU	PA-O3A-PB-O3B
3	C	602	GDU	PB-O3A-PA-O5D
3	C	602	GDU	PA-O3A-PB-O3B
3	D	602	GDU	PB-O3A-PA-O5D
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C5'-O5'-P-O3P
2	E	601	FAD	C5B-O5B-PA-O3P
2	E	601	FAD	C5'-O5'-P-O3P
2	A	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5'-O5'-P-O2P
2	C	601	FAD	C3'-C4'-C5'-O5'
2	E	601	FAD	C5B-O5B-PA-O1A
3	A	602	GDU	C5D-O5D-PA-O2A
3	B	602	GDU	C5D-O5D-PA-O2A
3	C	602	GDU	O5'-C1'-O3B-PB
2	F	601	FAD	P-O3P-PA-O1A
2	F	601	FAD	C4B-C5B-O5B-PA
2	E	601	FAD	O4B-C4B-C5B-O5B
3	D	602	GDU	C1'-O3B-PB-O2B
2	H	601	FAD	C2'-C1'-N10-C10
2	H	601	FAD	O4'-C4'-C5'-O5'
3	F	602	GDU	C2D-C1D-N1-C6
2	H	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	P-O3P-PA-O1A
2	A	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	C5B-O5B-PA-O3P
2	F	601	FAD	C5B-O5B-PA-O3P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	602	GDU	C5D-O5D-PA-O3A
3	E	602	GDU	C5D-O5D-PA-O3A
3	C	602	GDU	C3D-C4D-C5D-O5D
2	E	601	FAD	PA-O3P-P-O2P
3	D	602	GDU	PB-O3A-PA-O2A
3	D	602	GDU	C2D-C1D-N1-C2
2	A	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	C5'-O5'-P-O1P
2	E	601	FAD	C5'-O5'-P-O2P
3	F	602	GDU	C5D-O5D-PA-O1A
2	F	601	FAD	O4B-C4B-C5B-O5B
2	G	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C1'-C2'-C3'-O3'
3	E	602	GDU	C1'-O3B-PB-O2B
3	B	602	GDU	C2D-C1D-N1-C2
2	F	601	FAD	O2'-C2'-C3'-C4'
2	C	601	FAD	C4B-C5B-O5B-PA

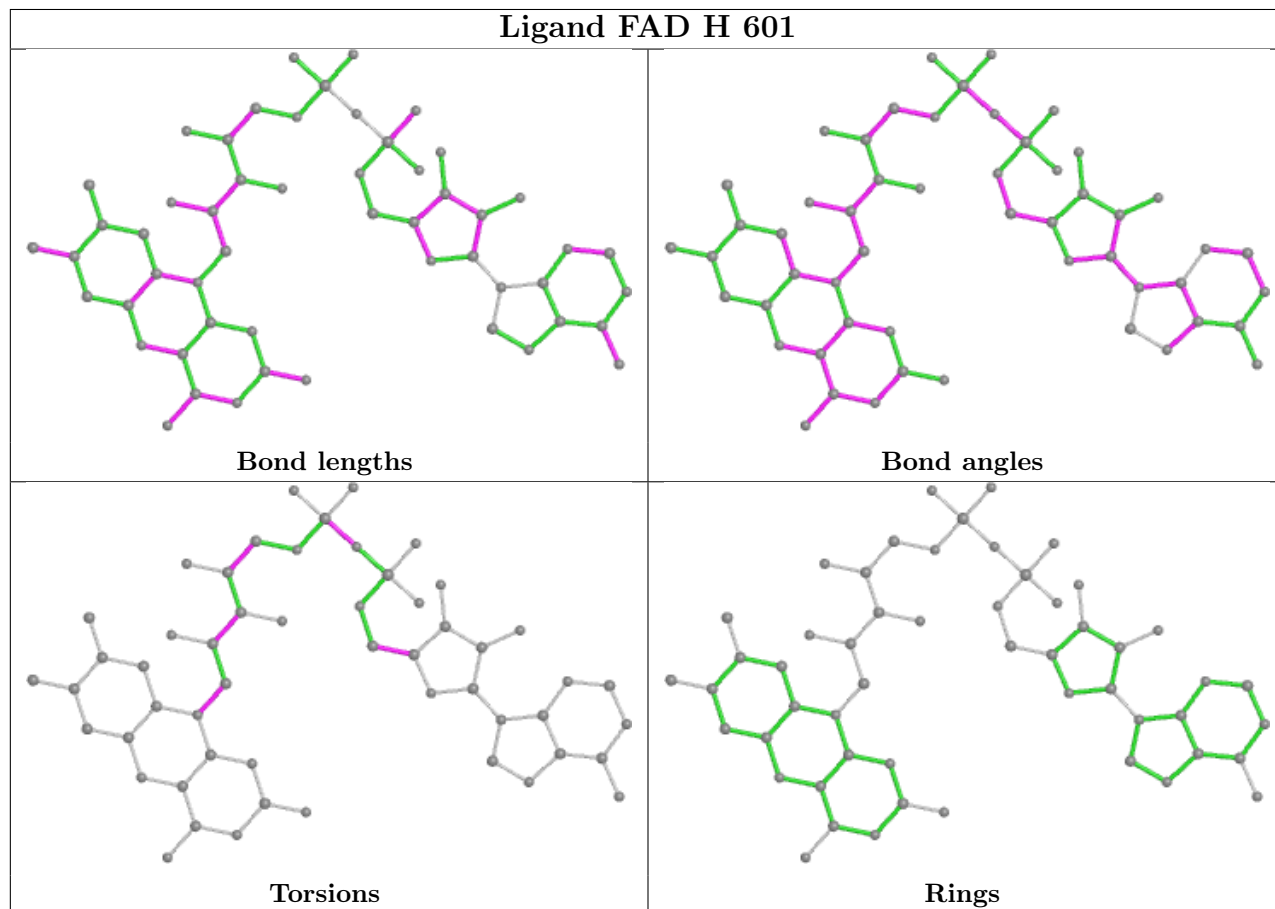
There are no ring outliers.

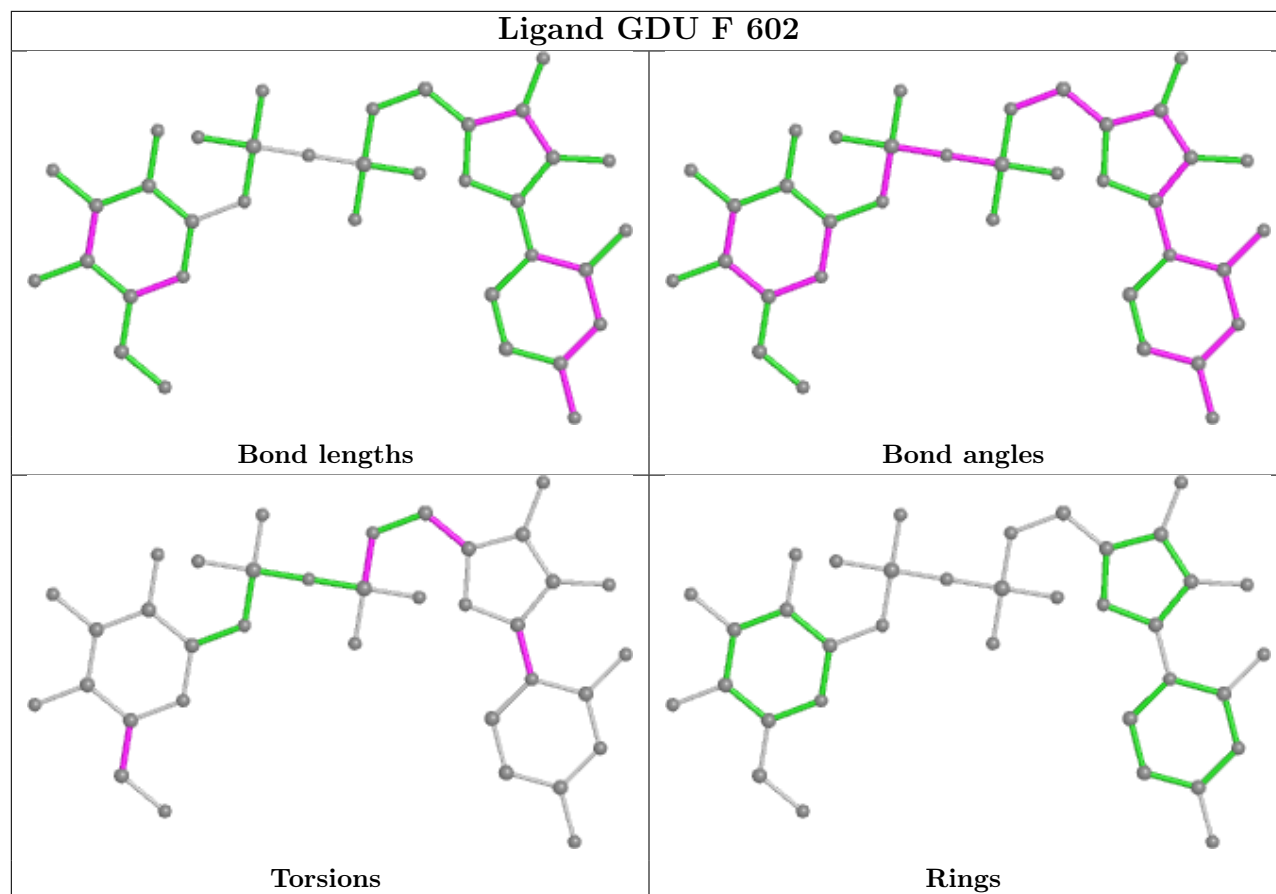
14 monomers are involved in 171 short contacts:

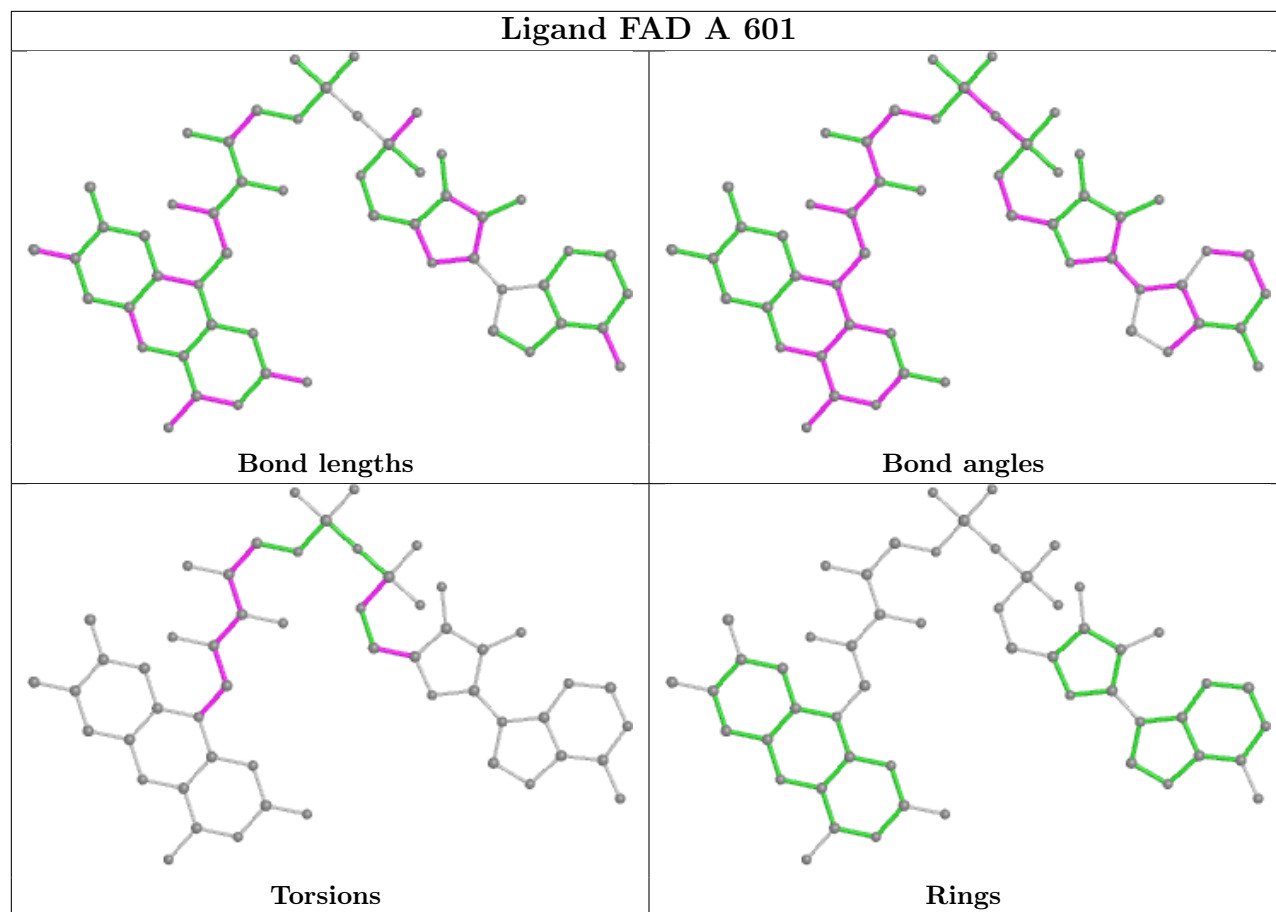
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	601	FAD	10	0
3	F	602	GDU	8	0
2	A	601	FAD	10	0
2	E	601	FAD	20	0
3	B	602	GDU	15	0
2	G	601	FAD	13	0
2	D	601	FAD	22	0
3	C	602	GDU	9	0
2	F	601	FAD	14	0
3	A	602	GDU	9	0
2	C	601	FAD	12	0
3	D	602	GDU	4	0
3	E	602	GDU	14	0
2	B	601	FAD	14	0

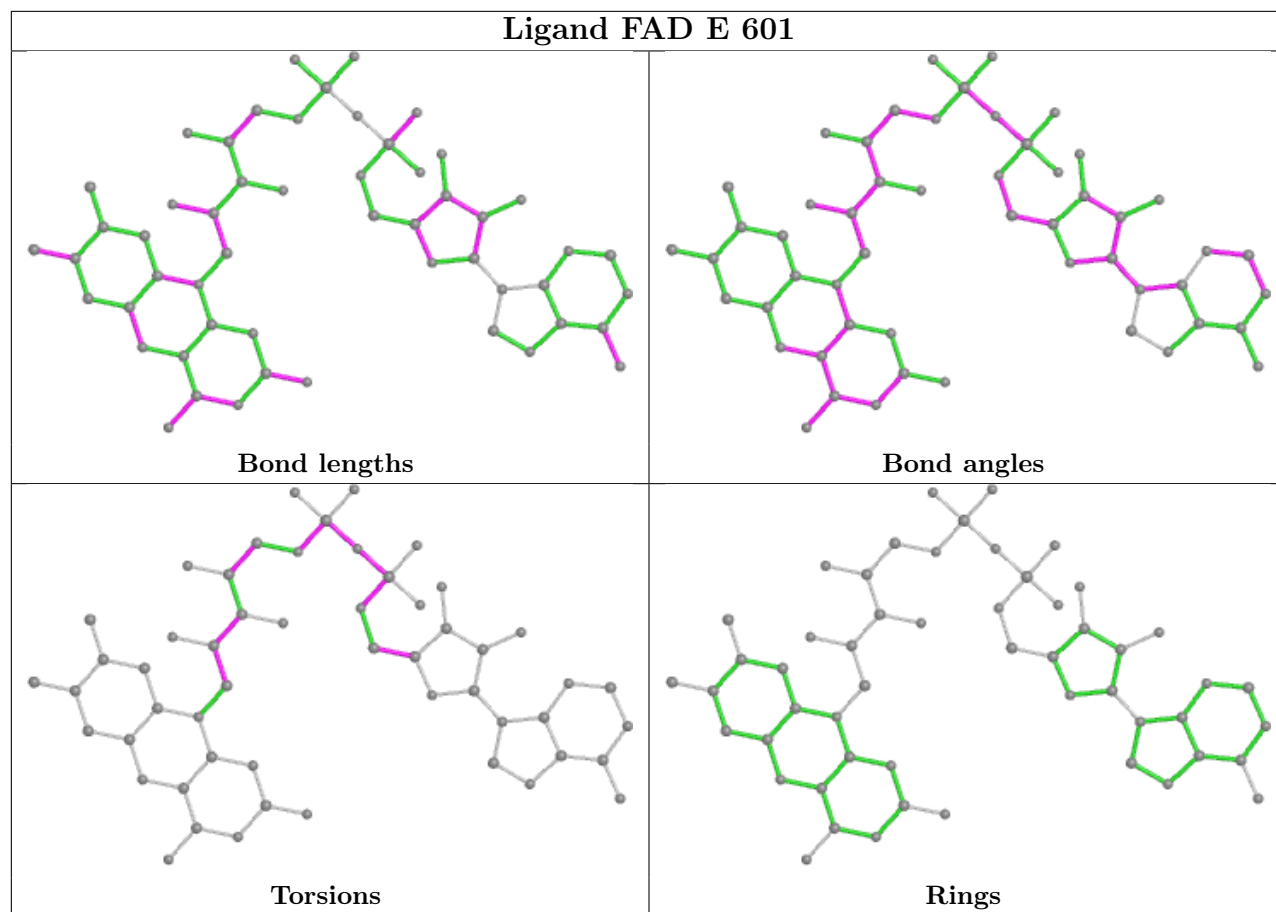
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

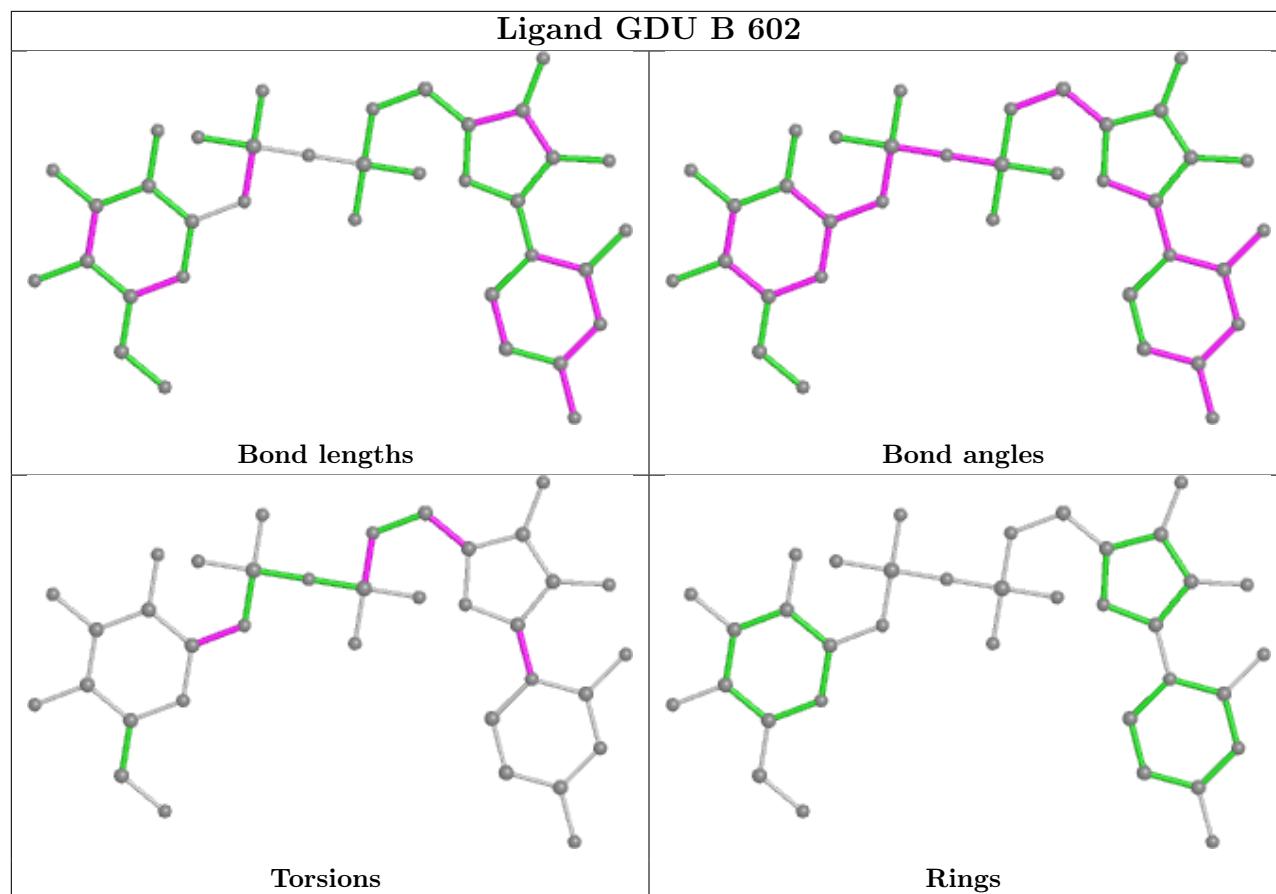


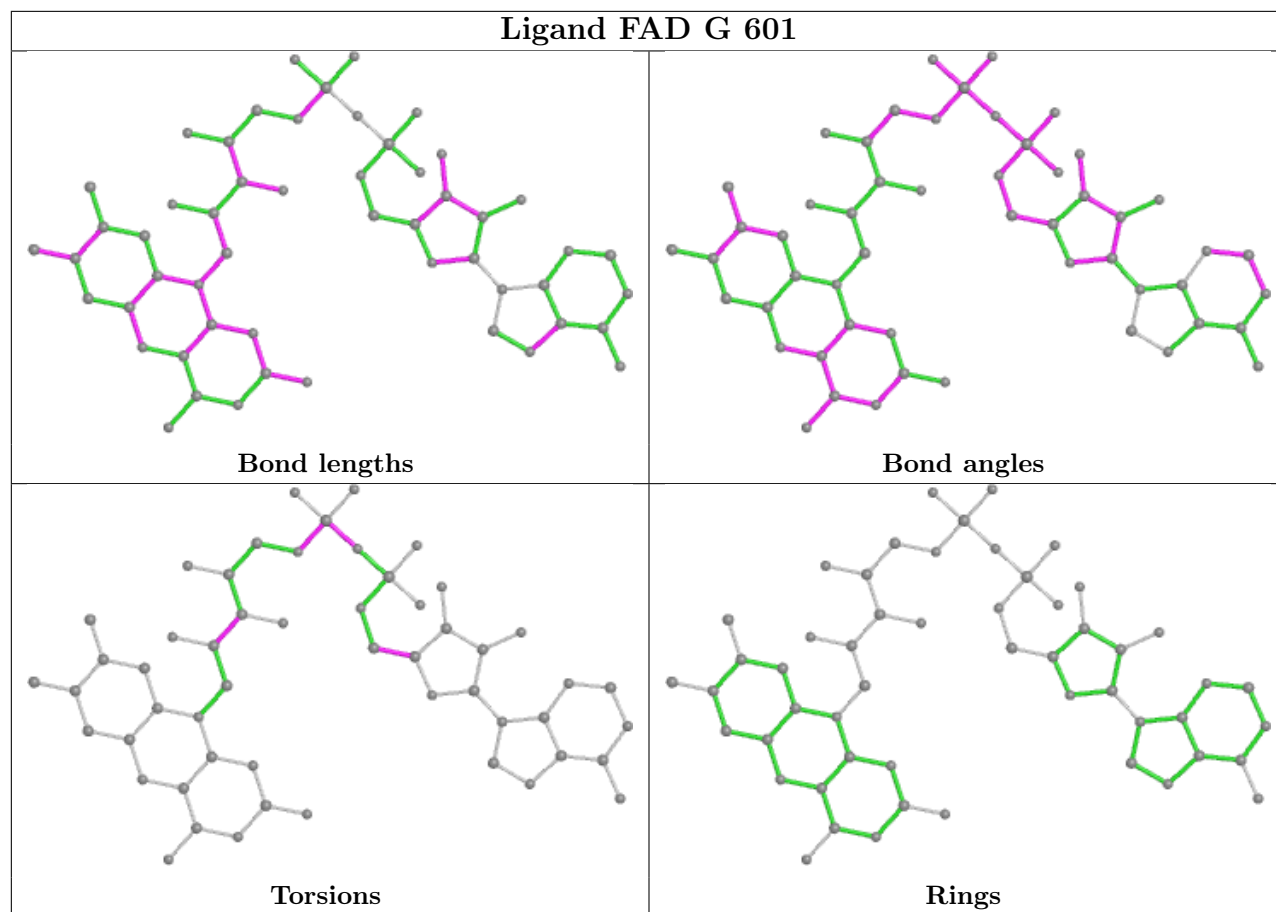


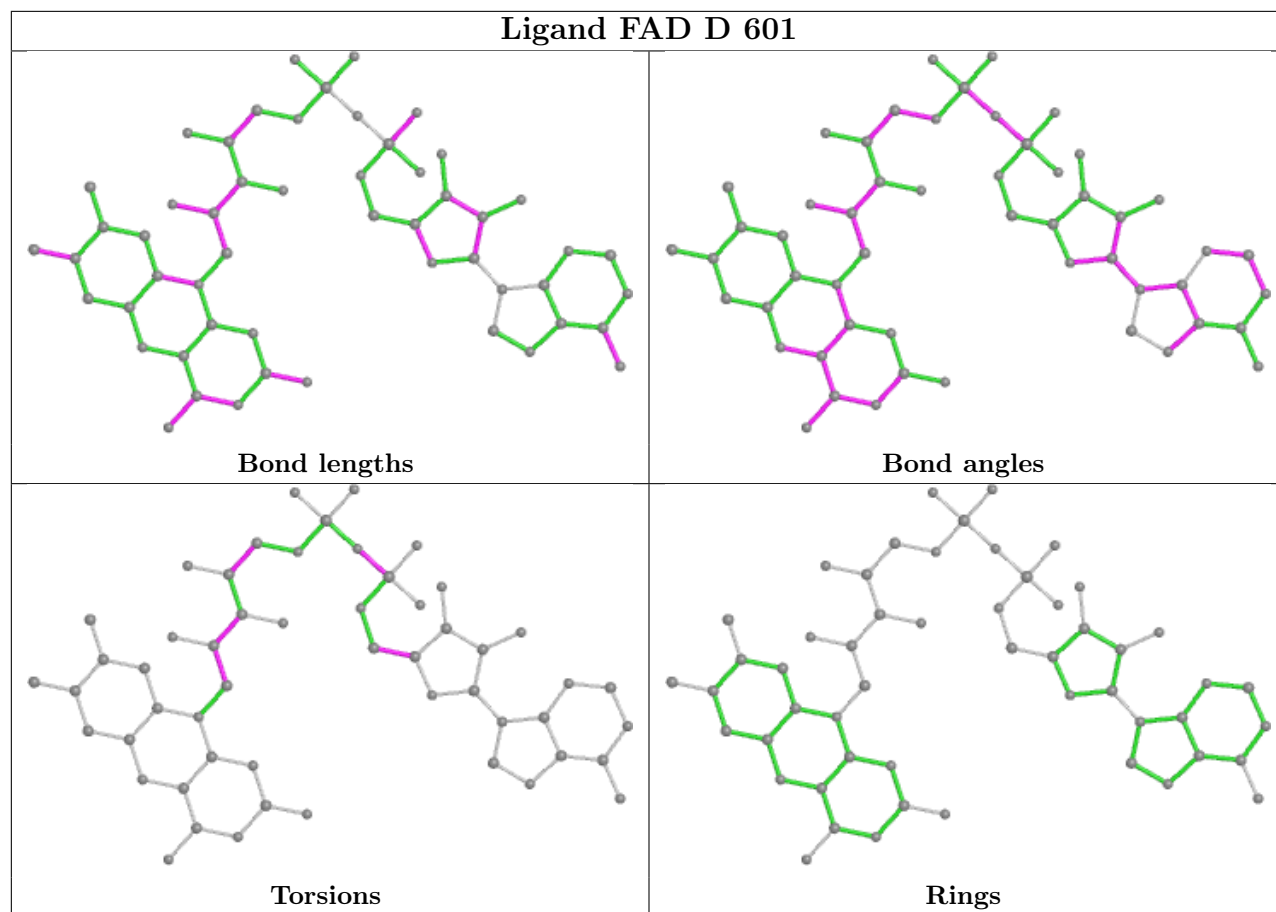


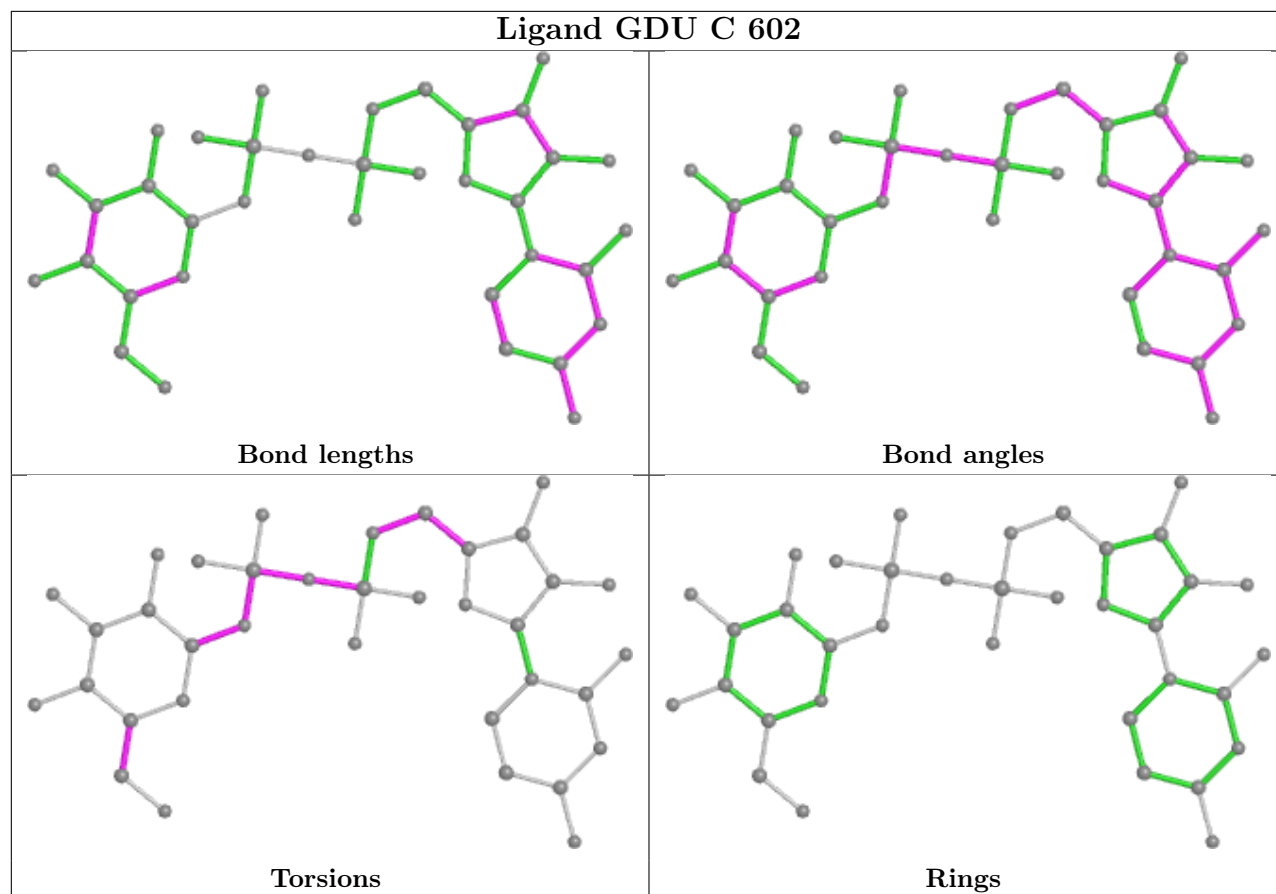


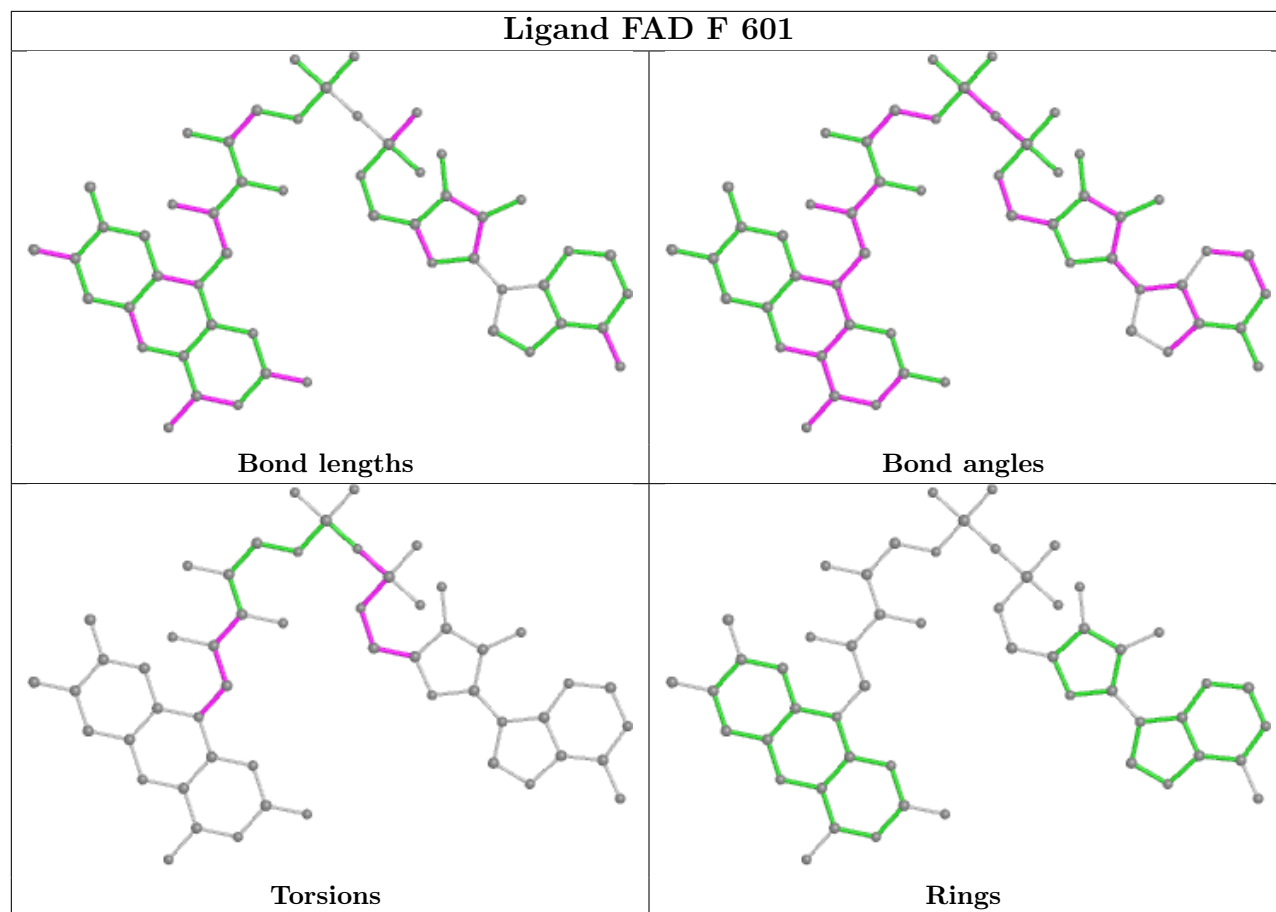


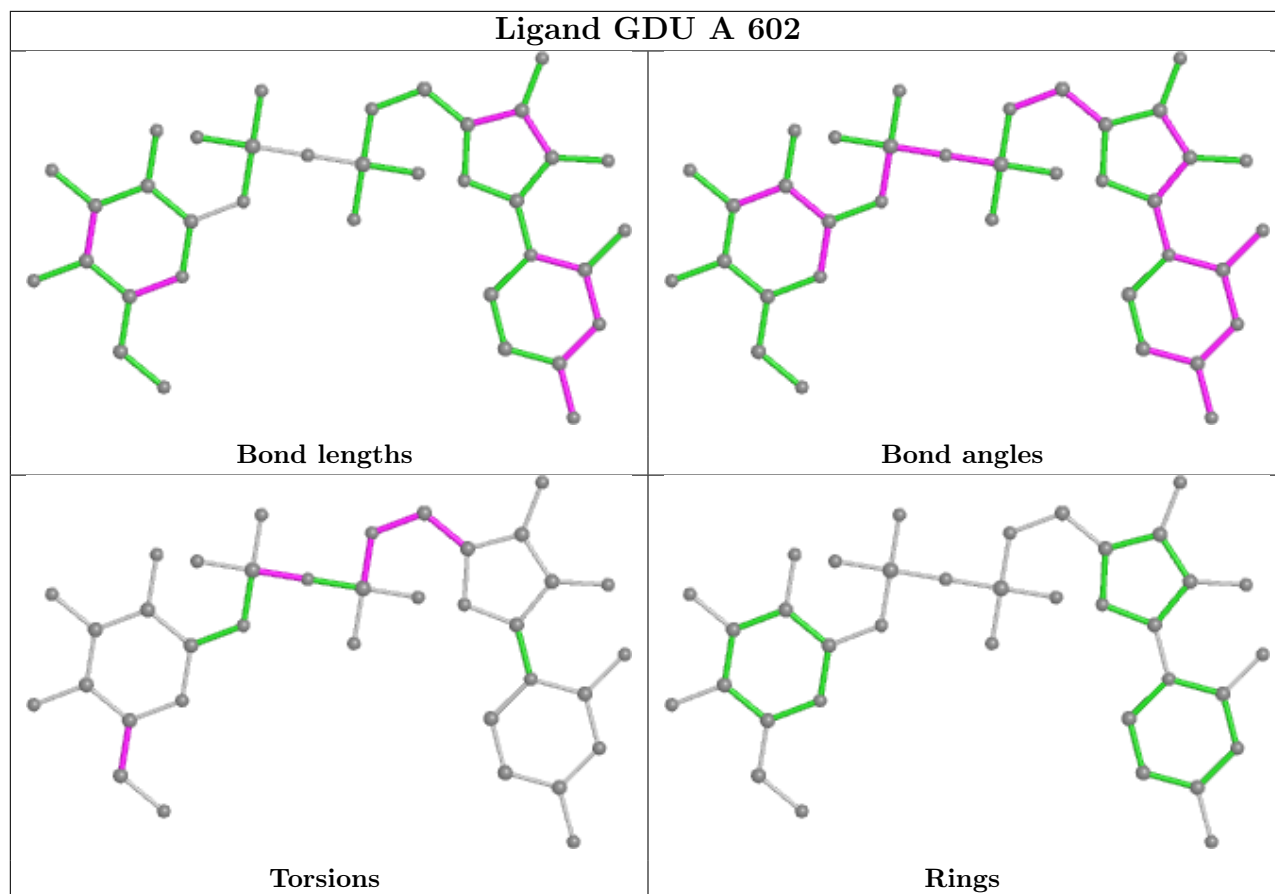


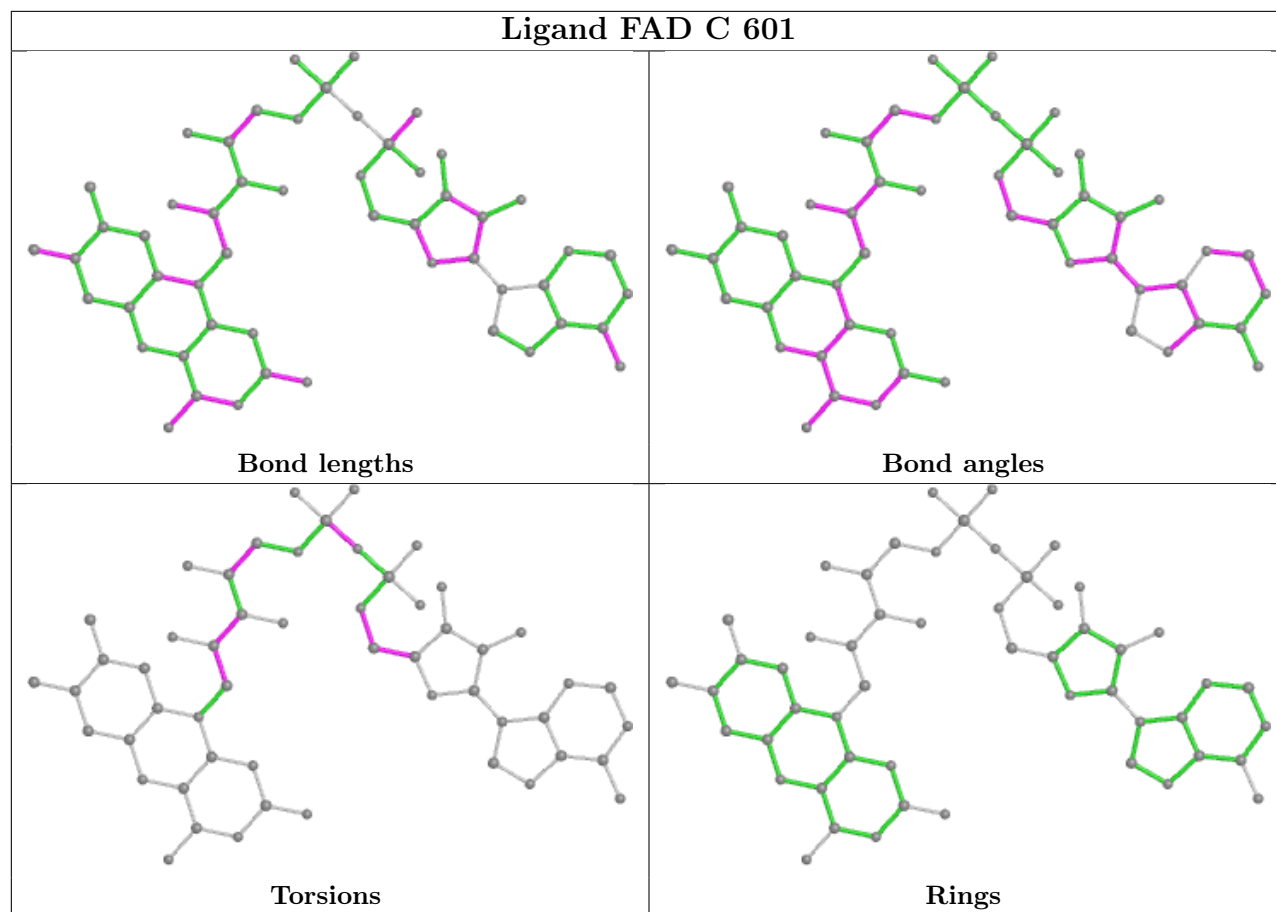


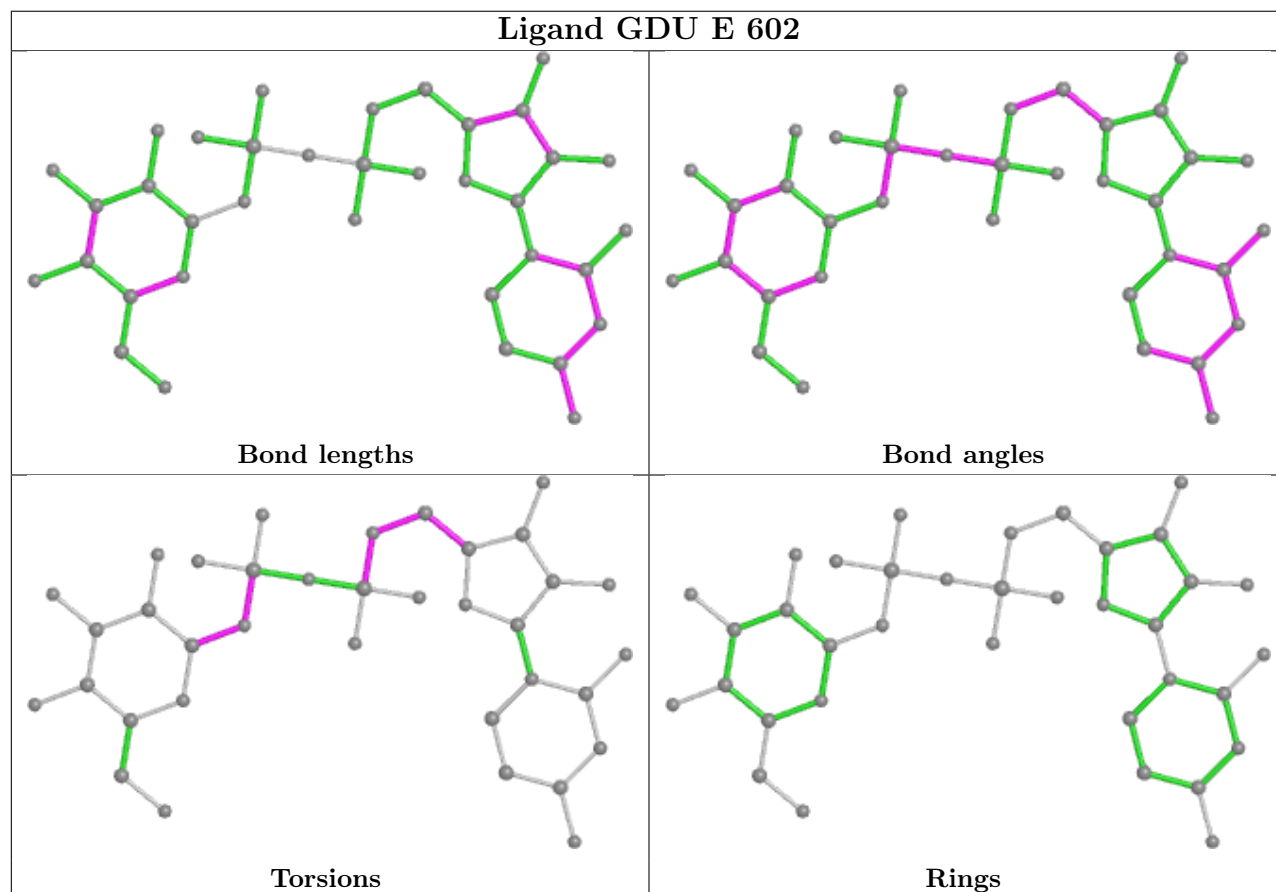
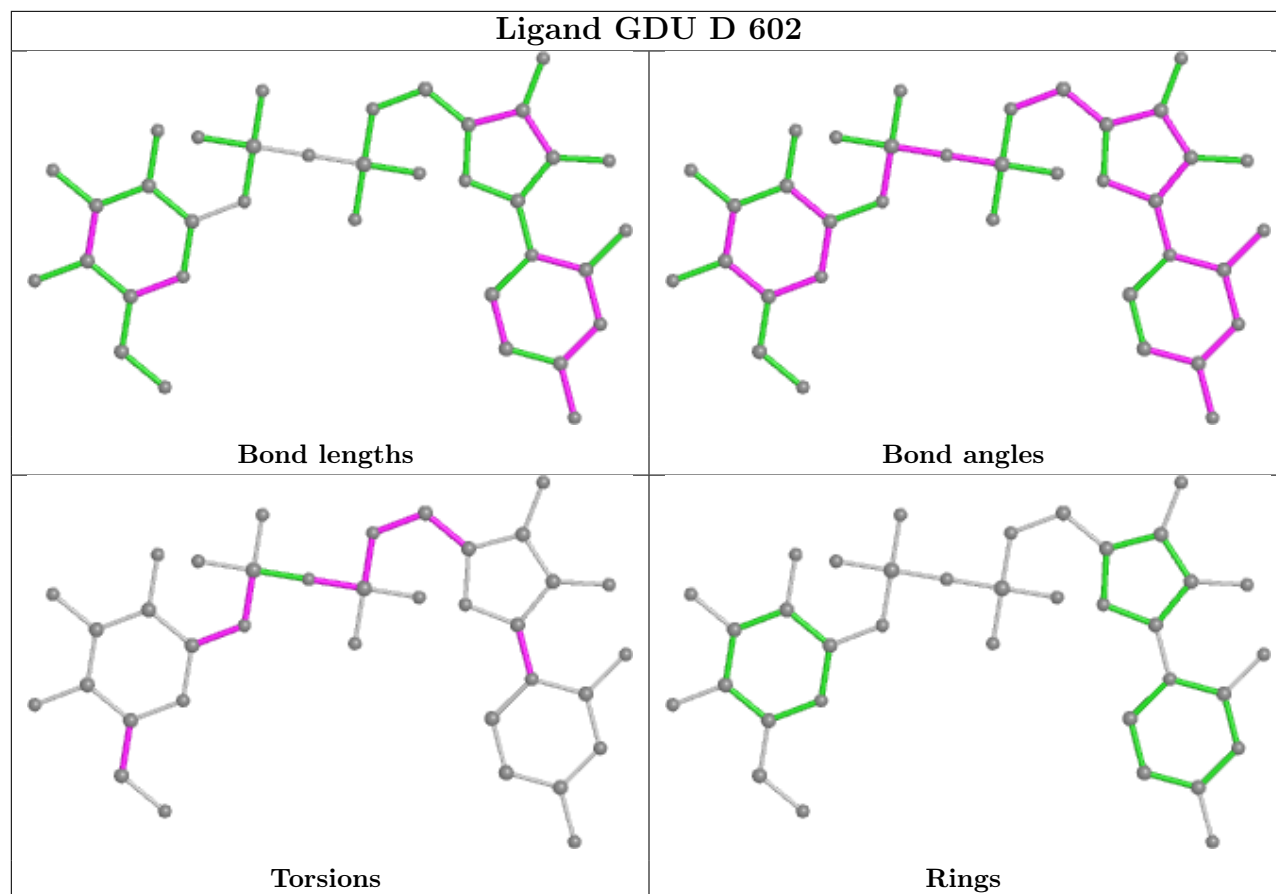




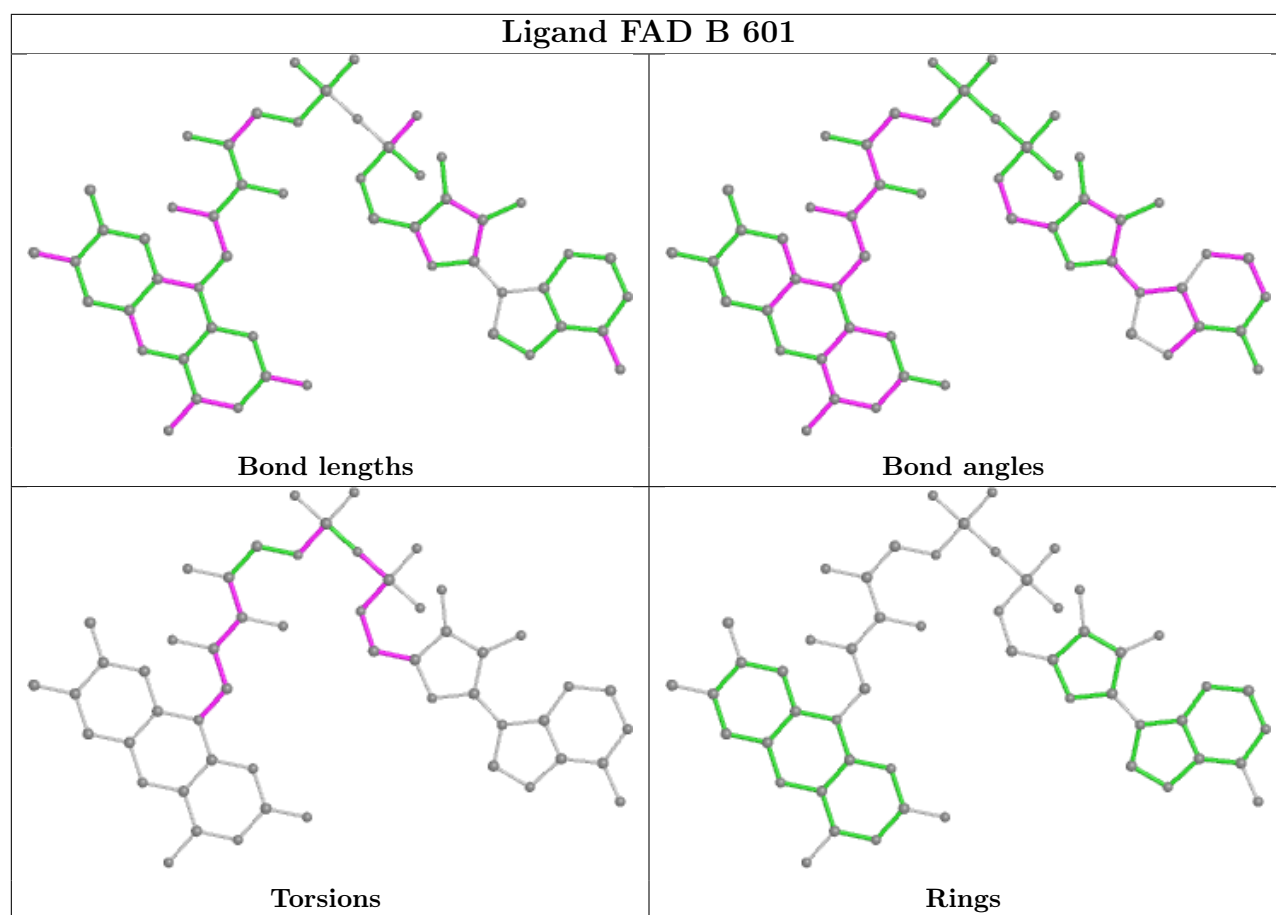












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	509/509 (100%)	-0.30	3 (0%) 89 78	22, 64, 110, 167	0
1	B	509/509 (100%)	-0.31	7 (1%) 75 56	24, 64, 106, 166	0
1	C	509/509 (100%)	-0.30	6 (1%) 79 61	29, 65, 108, 170	0
1	D	509/509 (100%)	-0.29	6 (1%) 79 61	27, 65, 109, 172	0
1	E	509/509 (100%)	-0.40	1 (0%) 95 90	22, 62, 99, 156	0
1	F	509/509 (100%)	-0.36	3 (0%) 89 78	23, 59, 99, 151	0
1	G	509/509 (100%)	-0.45	0 100 100	14, 61, 93, 126	0
1	H	509/509 (100%)	-0.43	1 (0%) 95 90	22, 63, 94, 132	1 (0%)
All	All	4072/4072 (100%)	-0.36	27 (0%) 87 75	14, 63, 104, 172	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	TRP	5.2
1	C	183	VAL	4.7
1	B	183	VAL	4.4
1	F	207	ASN	4.3
1	B	204	TRP	4.2
1	A	204	TRP	4.1
1	C	184	ALA	3.9
1	D	205	GLY	3.6
1	D	186	PRO	3.6
1	D	204	TRP	3.3
1	A	205	GLY	3.3
1	C	201	ALA	3.1
1	C	202	GLY	2.8
1	D	206	PRO	2.8
1	A	184	ALA	2.7
1	F	206	PRO	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	182	ARG	2.4
1	B	186	PRO	2.3
1	H	206	PRO	2.3
1	B	205	GLY	2.2
1	B	184	ALA	2.1
1	C	185	ALA	2.1
1	E	200	THR	2.1
1	F	185	ALA	2.1
1	D	184	ALA	2.0
1	B	180	GLY	2.0
1	D	207	ASN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

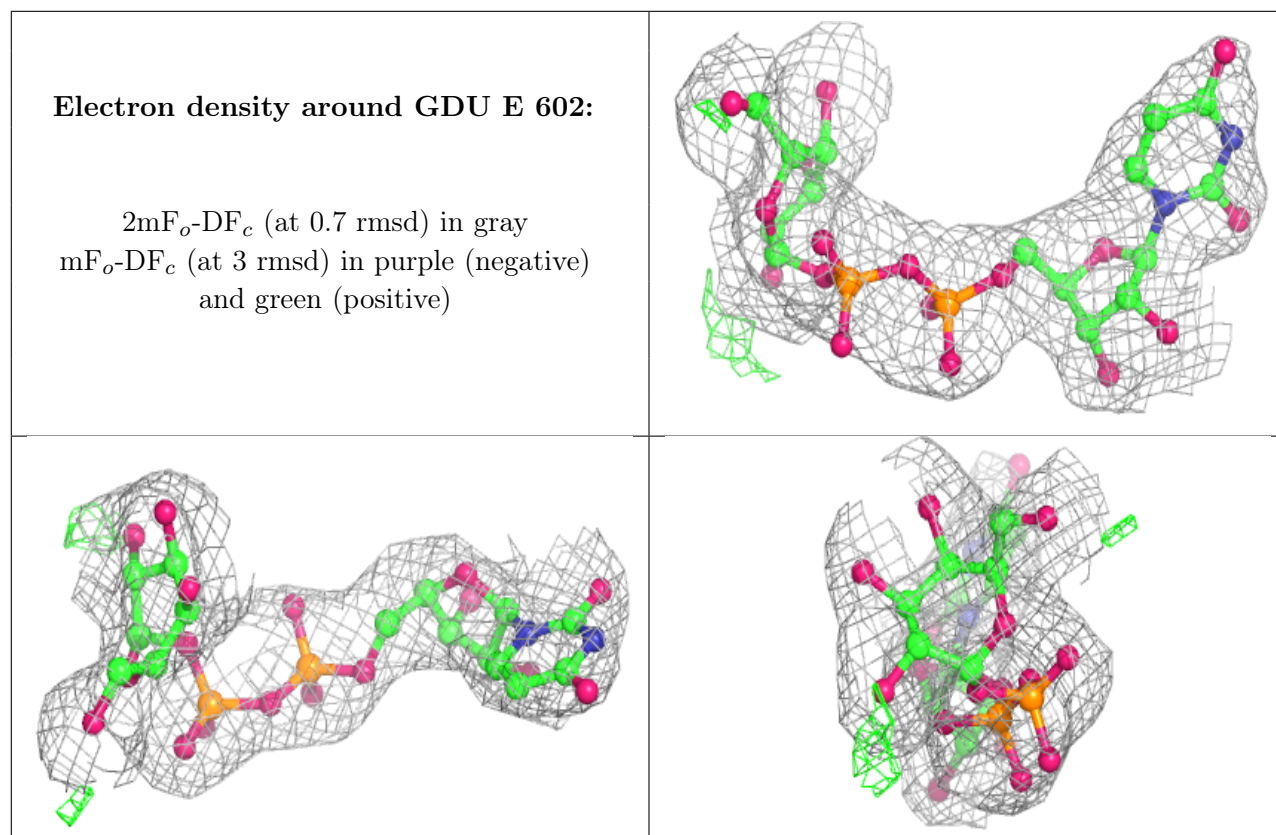
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	GDU	E	602	36/36	0.94	0.18	22,92,139,142	0
3	GDU	D	602	36/36	0.95	0.15	35,99,135,179	0
3	GDU	A	602	36/36	0.95	0.23	30,108,162,203	0
3	GDU	F	602	36/36	0.95	0.17	28,101,153,194	0
3	GDU	C	602	36/36	0.96	0.18	25,103,142,180	0
3	GDU	B	602	36/36	0.96	0.21	42,114,153,160	0
2	FAD	B	601	53/53	0.97	0.20	18,64,87,92	0
2	FAD	H	601	53/53	0.97	0.16	20,79,102,111	0
2	FAD	E	601	53/53	0.98	0.17	14,57,97,102	0
2	FAD	F	601	53/53	0.98	0.18	12,67,90,107	0
2	FAD	G	601	53/53	0.98	0.15	0,57,86,102	0
2	FAD	A	601	53/53	0.98	0.17	6,57,87,95	0

*Continued on next page...*

Continued from previous page...

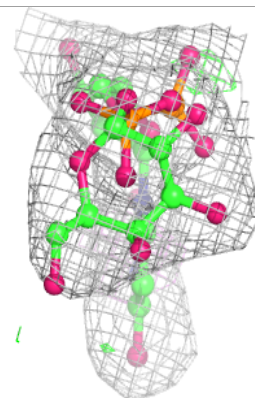
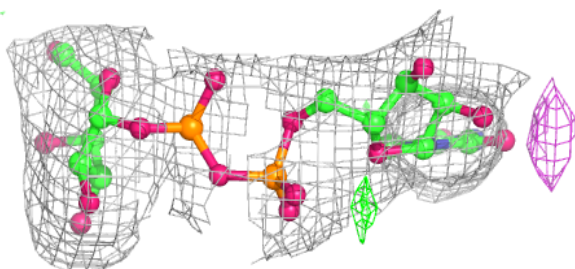
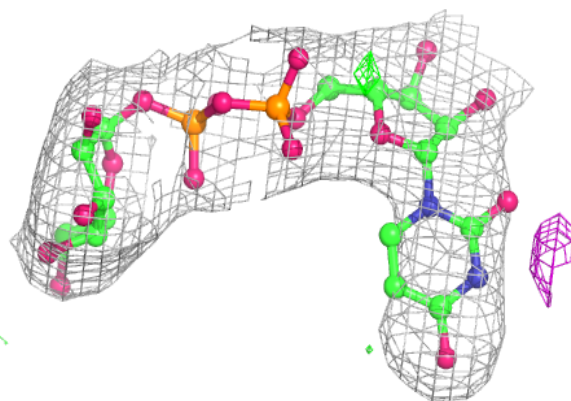
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	C	601	53/53	0.98	0.18	0,49,83,94	0
2	FAD	D	601	53/53	0.99	0.18	0,57,88,102	0

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

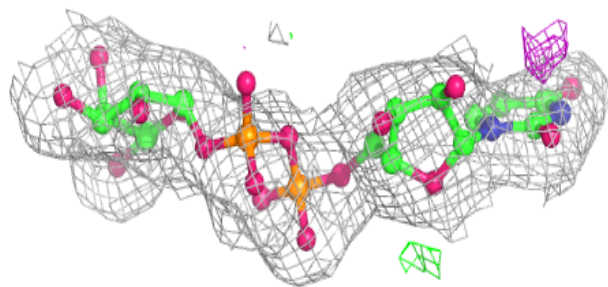
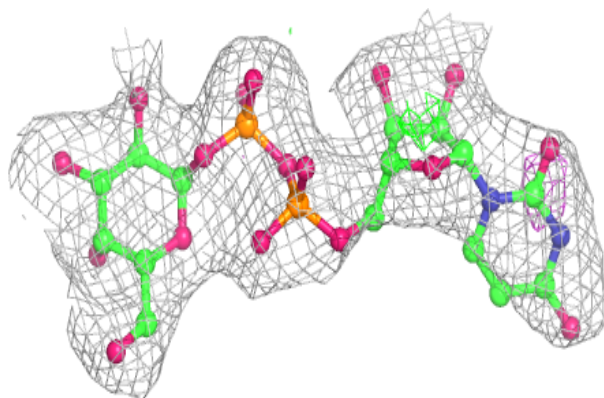


**Electron density around GDU D 602:**

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

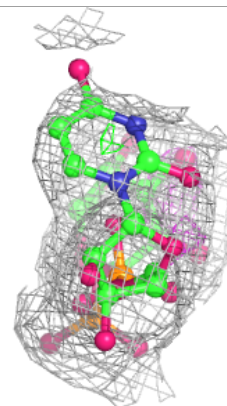
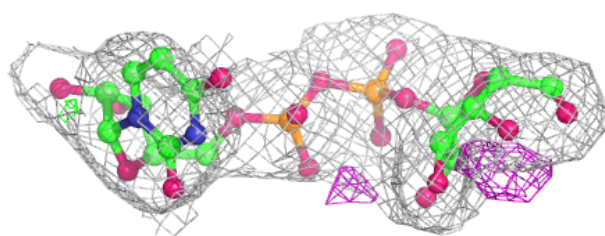
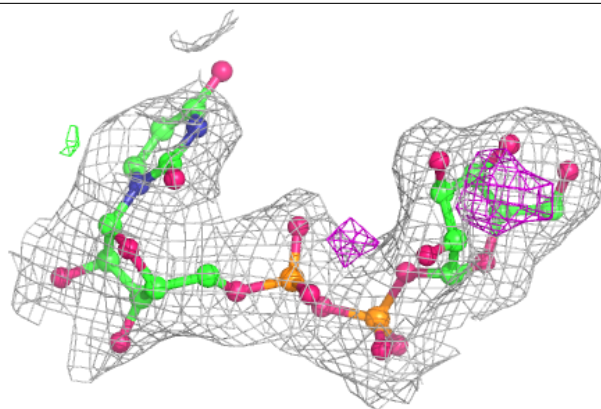
**Electron density around GDU A 602:**

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

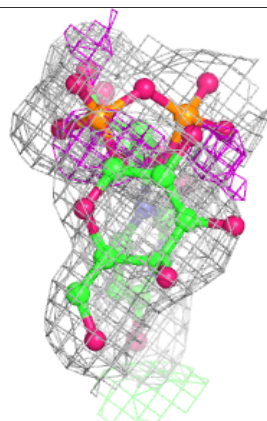
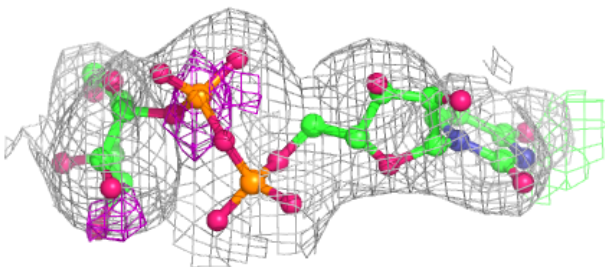
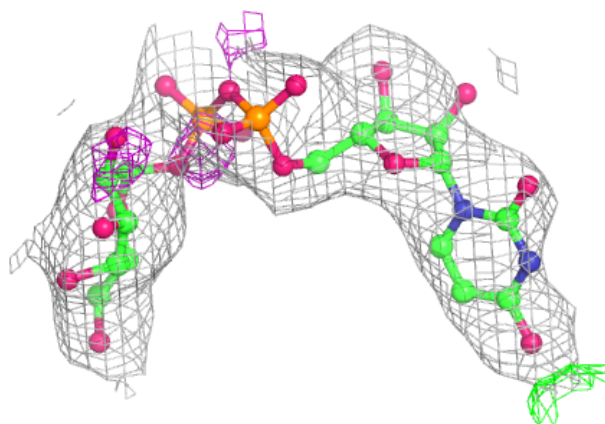


**Electron density around GDU F 602:**

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

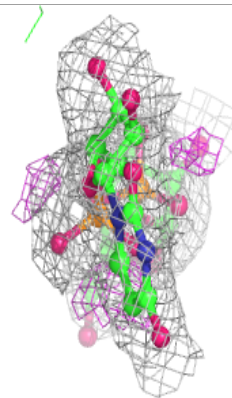
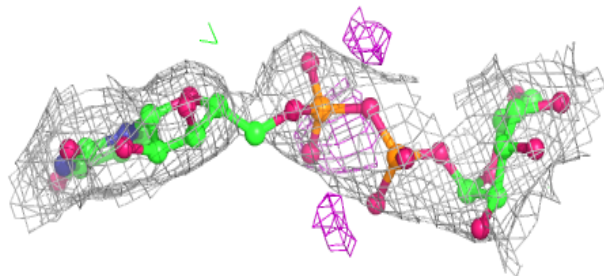
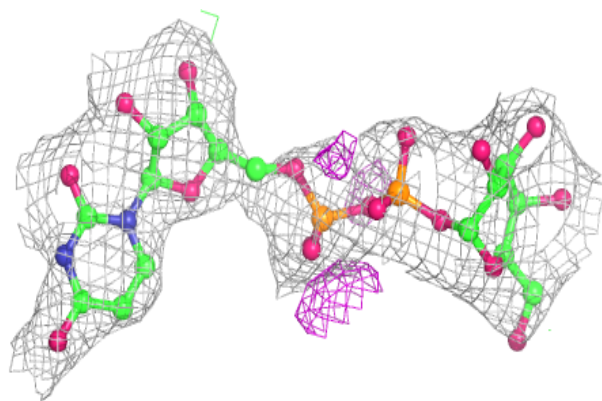
**Electron density around GDU C 602:**

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

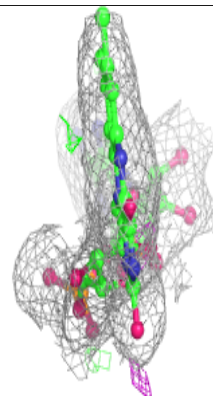
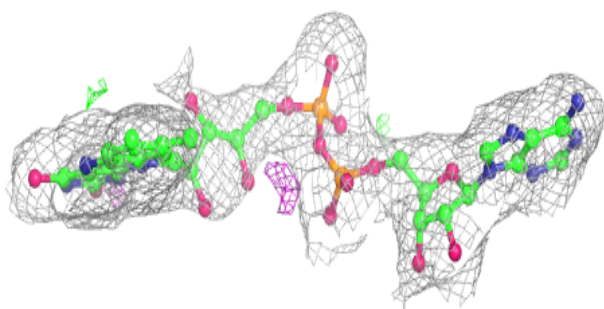
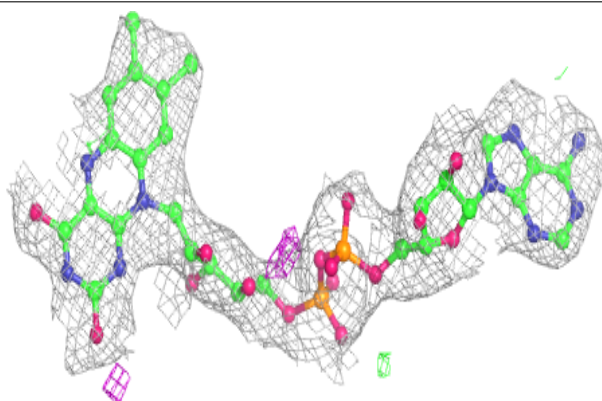


**Electron density around GDU B 602:**

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

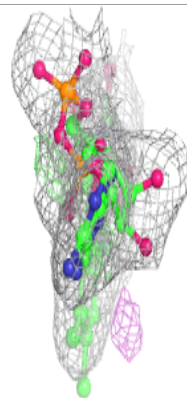
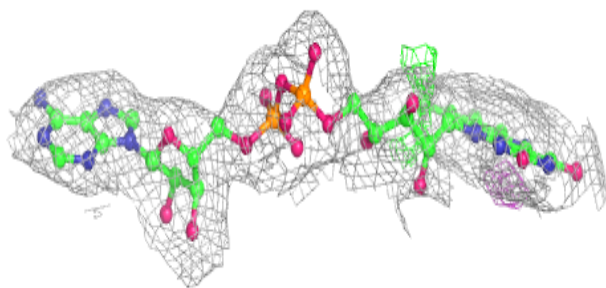
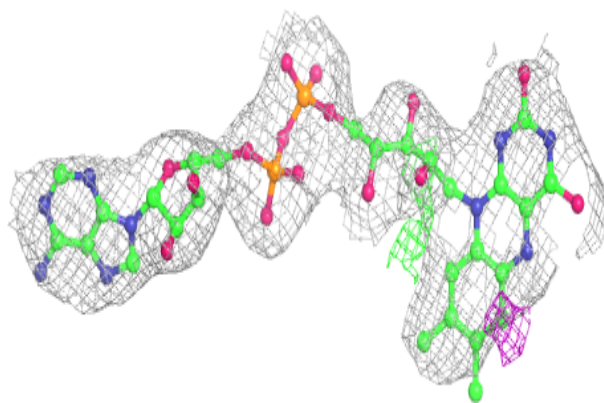
**Electron density around FAD B 601:**

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

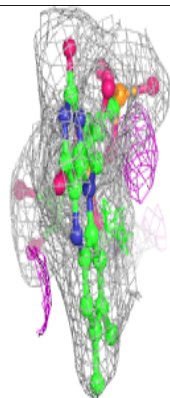
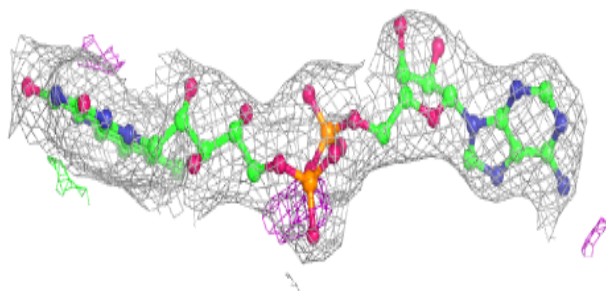
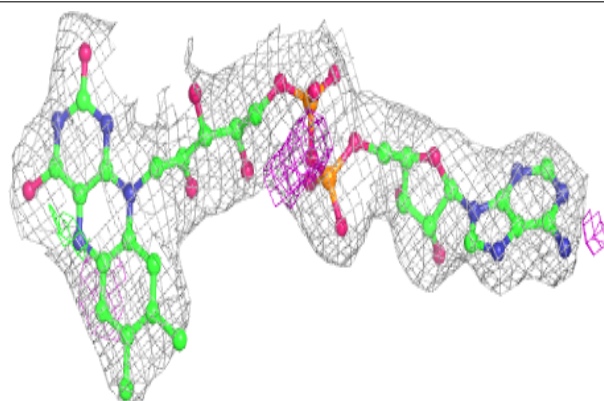


**Electron density around FAD H 601:**

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

**Electron density around FAD E 601:**

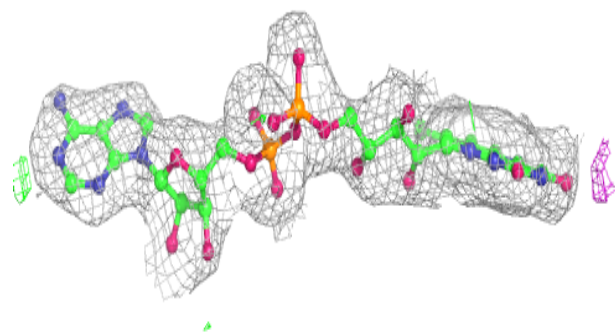
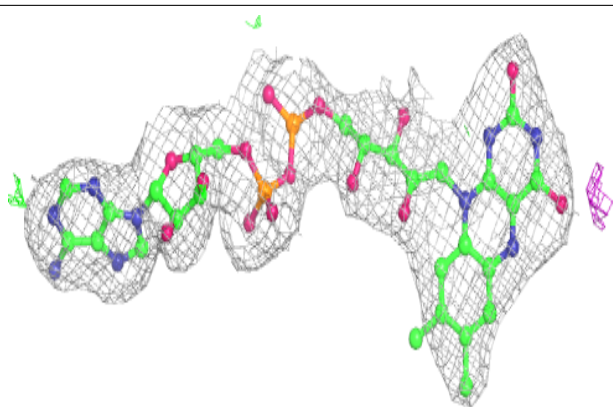
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



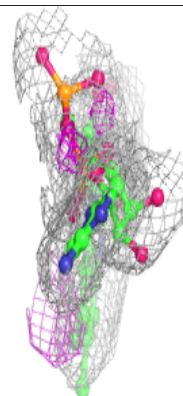
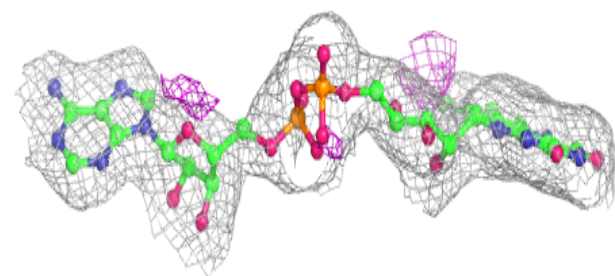
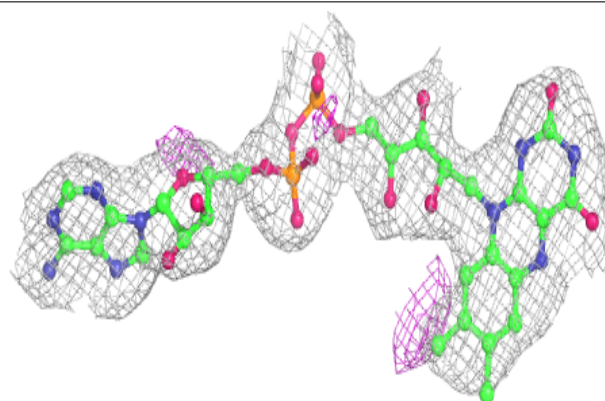


**Electron density around FAD F 601:**

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

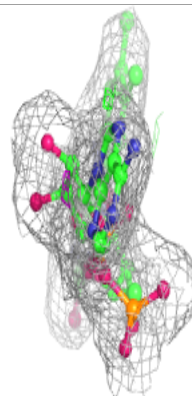
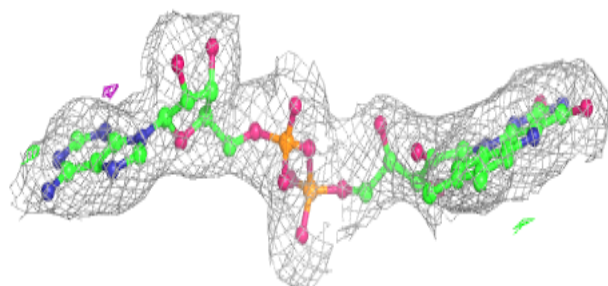
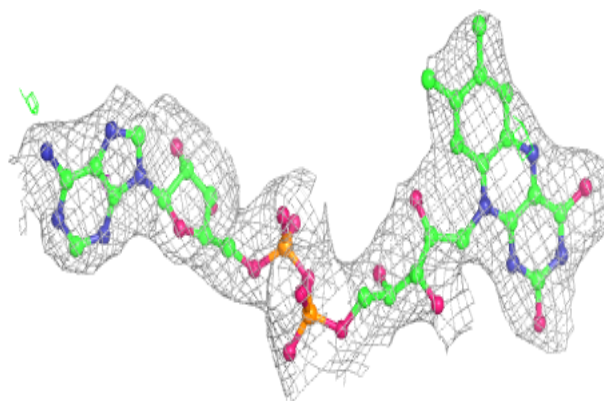
**Electron density around FAD G 601:**

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

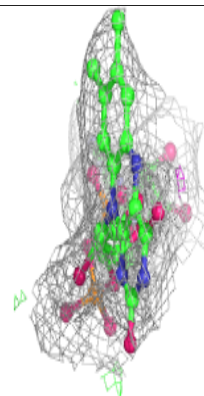
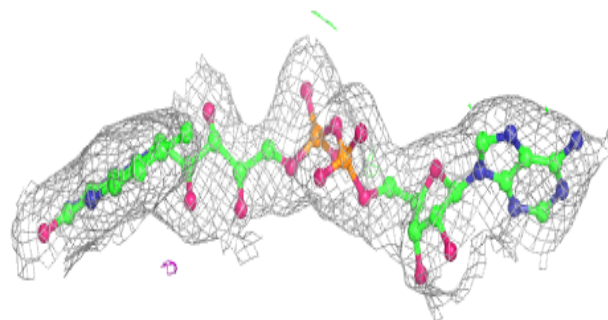
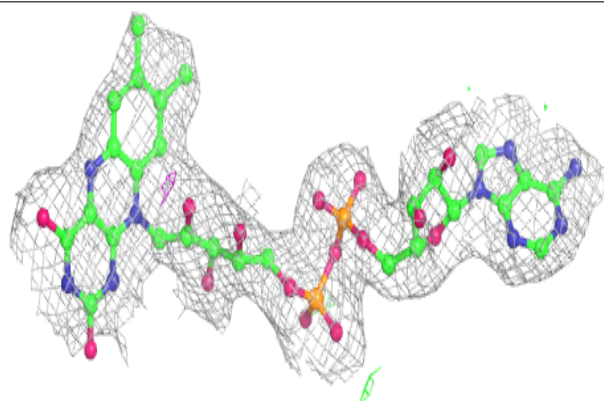


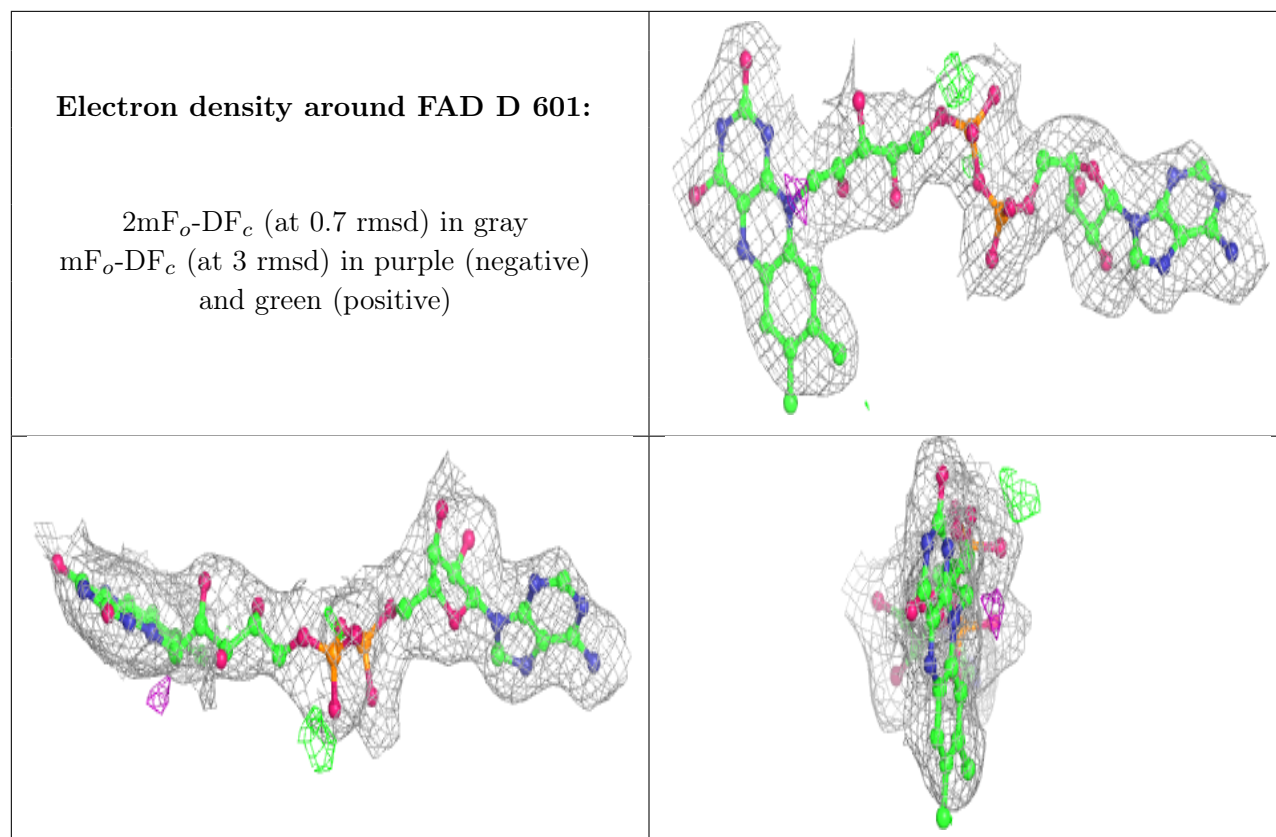
**Electron density around FAD A 601:**

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

**Electron density around FAD C 601:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.