



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 04:27 am BST

PDB ID : 3S1A  
Title : Crystal structure of the phosphorylation-site double mutant S431E/T432E of the KaiC circadian clock protein  
Authors : Pattanayek, R.; Williams, D.W.; Rossi, G.; Weigand, S.; Mori, T.; Johnson, C.H.; Stewart, P.L.; Egli, M.  
Deposited on : 2011-05-14  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

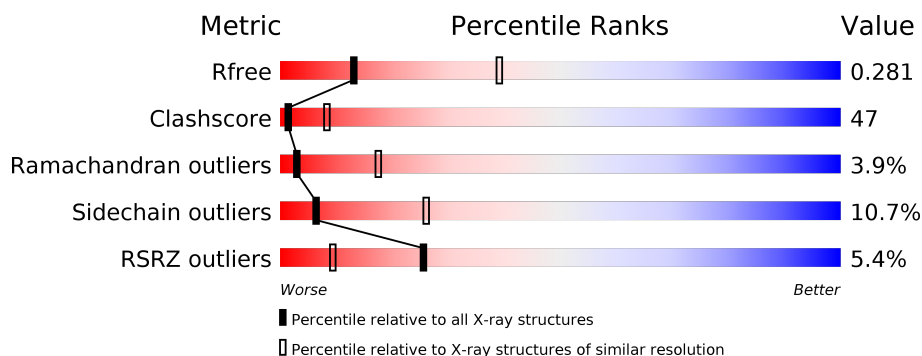
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	525	<div> <div>9%</div> <div>37% 50% 9%</div> </div>
1	F	525	<div> <div>6%</div> <div>39% 48% 9%</div> </div>
2	B	525	<div> <div>6%</div> <div>31% 53% 9% 6%</div> </div>
2	C	525	<div> <div>4%</div> <div>35% 49% 9% 7%</div> </div>
2	D	525	<div> <div>2%</div> <div>39% 46% 6% 8%</div> </div>
2	E	525	<div> <div>3%</div> <div>39% 46% 9% 6%</div> </div>

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
1	SEP	A	320	-	-	X	X
1	SEP	F	320	-	-	X	-
4	MG	A	526	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 23898 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 Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	506	Total	C	N	O	P	S	0	0	0
			3994	2512	701	765	1	15			
1	F	506	Total	C	N	O	P	S	0	0	0
			3994	2512	701	765	1	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
A	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
A	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
A	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
F	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
F	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
F	525	HIS	-	EXPRESSION TAG	UNP Q79PF4

- Molecule 2 is a protein called Circadian clock protein kinase kaiC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	491	Total	C	N	O	S		0	0	0
			3875	2442	678	740	15				
2	C	488	Total	C	N	O	S		0	0	0
			3851	2428	674	734	15				

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	485	Total	C	N	O	S	0	0	0
			3827	2414	671	727	15			
2	E	492	Total	C	N	O	S	0	0	0
			3883	2448	679	741	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
B	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
B	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
B	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
C	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
C	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
C	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
D	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
D	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
D	525	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	431	GLU	SER	ENGINEERED MUTATION	UNP Q79PF4
E	432	GLU	THR	ENGINEERED MUTATION	UNP Q79PF4
E	520	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	521	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	522	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	523	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	524	HIS	-	EXPRESSION TAG	UNP Q79PF4
E	525	HIS	-	EXPRESSION TAG	UNP Q79PF4

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	4	Total Mg 4 4	0	0
4	E	2	Total Mg 2 2	0	0
4	B	4	Total Mg 4 4	0	0
4	C	4	Total Mg 4 4	0	0
4	A	4	Total Mg 4 4	0	0
4	F	3	Total Mg 3 3	0	0

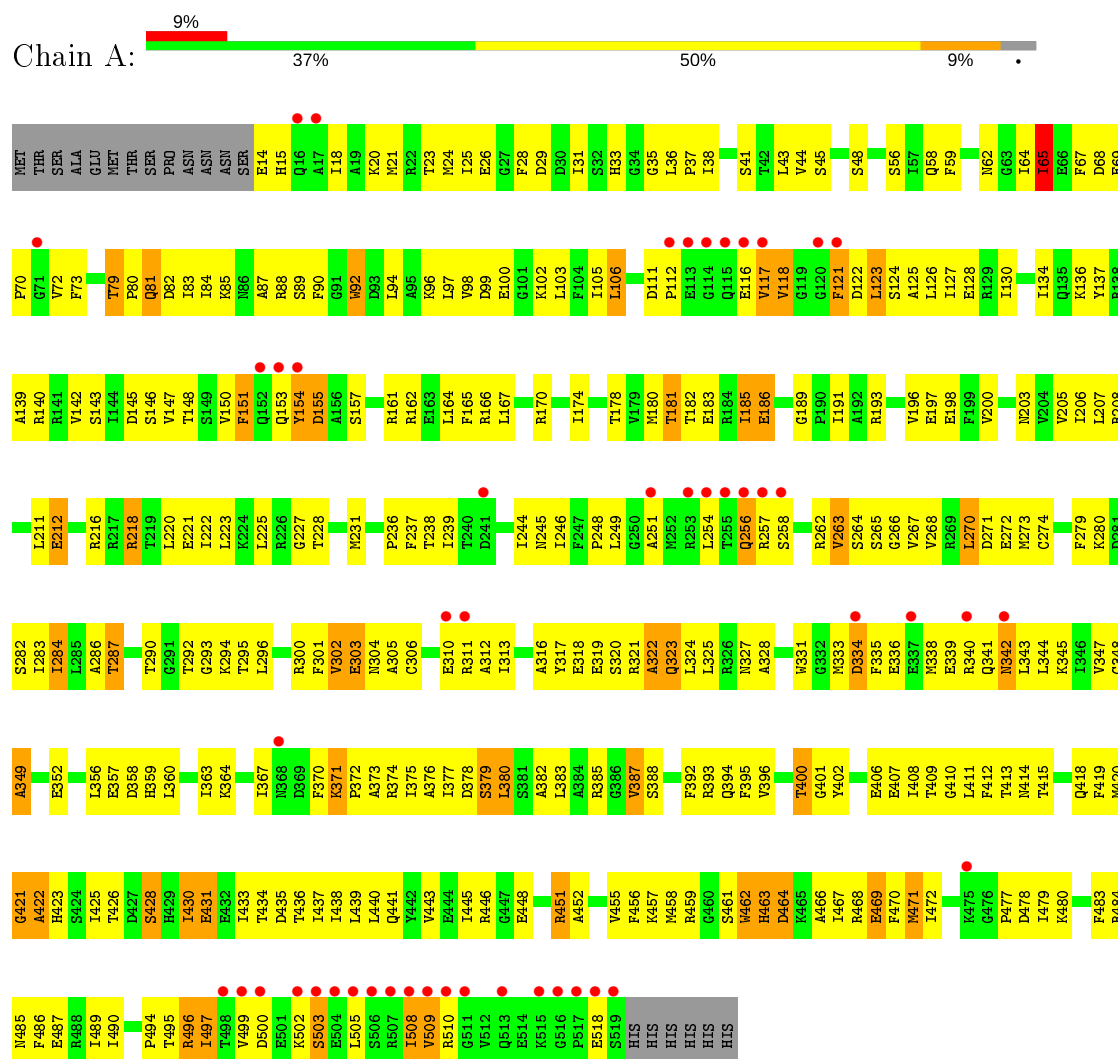
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	B	6	Total O 6 6	0	0
5	C	10	Total O 10 10	0	0
5	D	32	Total O 32 32	0	0
5	E	16	Total O 16 16	0	0
5	F	12	Total O 12 12	0	0

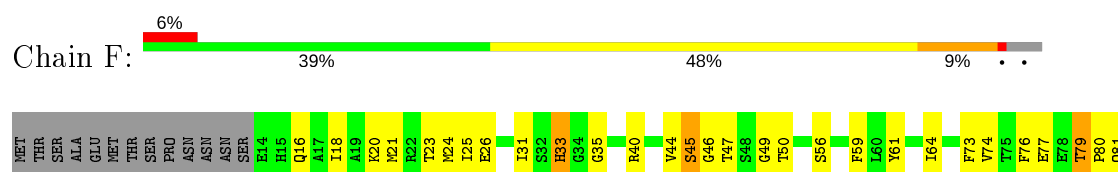
### 3 Residue-property plots

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

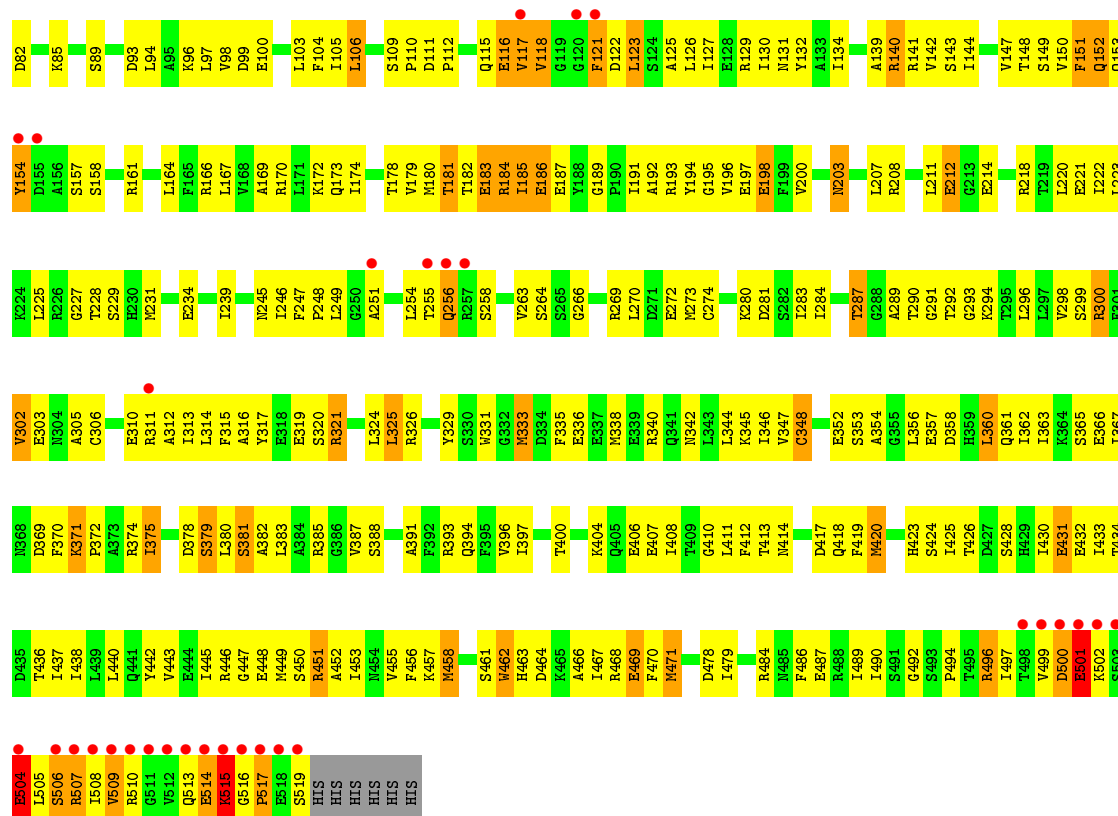
- Molecule 1: Circadian clock protein kinase kaiC

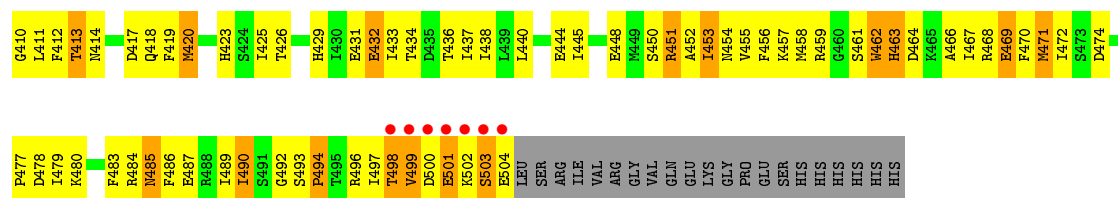


- Molecule 1: Circadian clock protein kinase kaiC

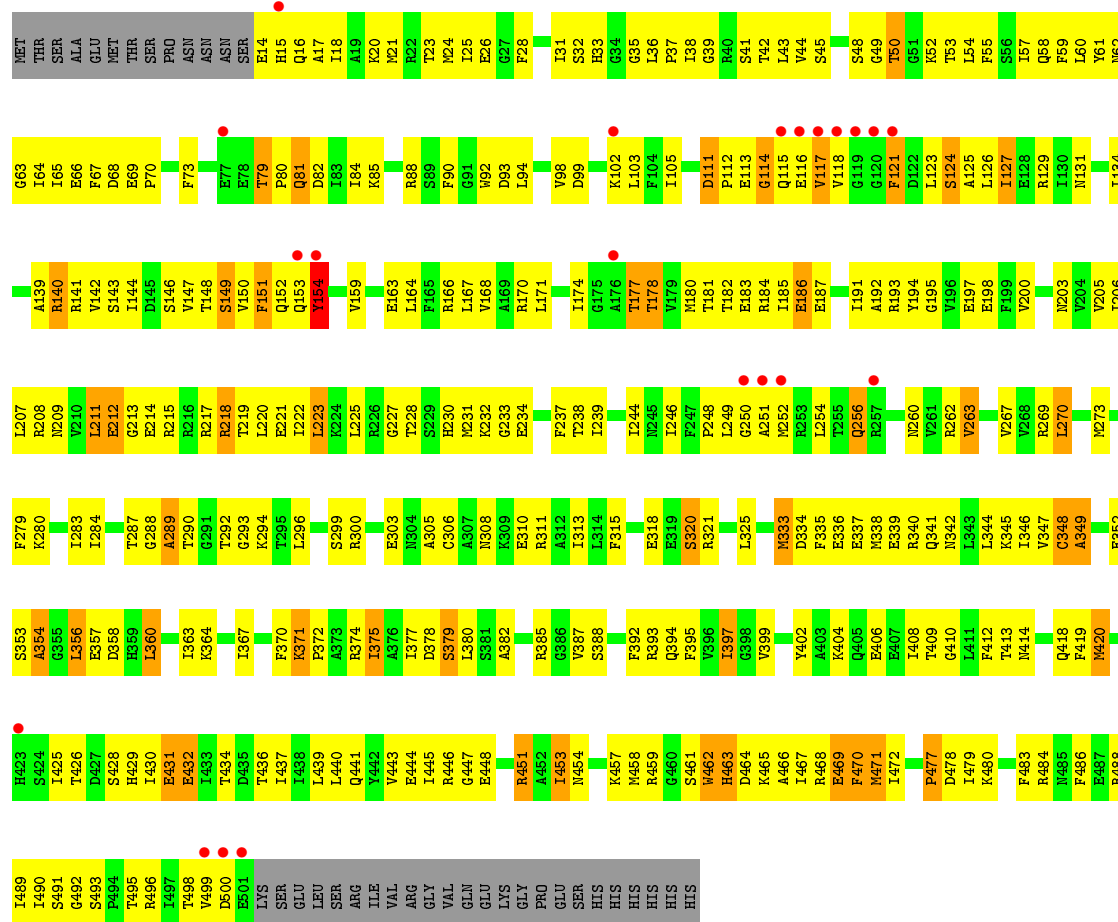




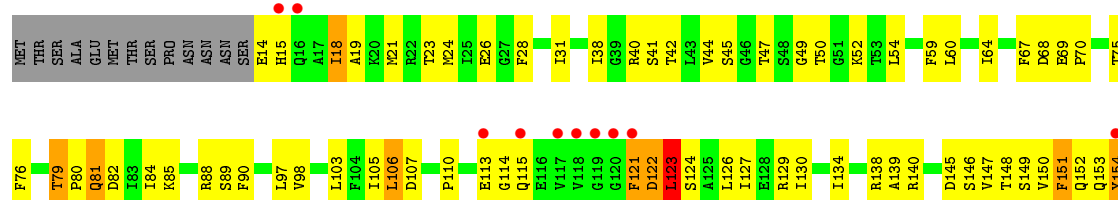


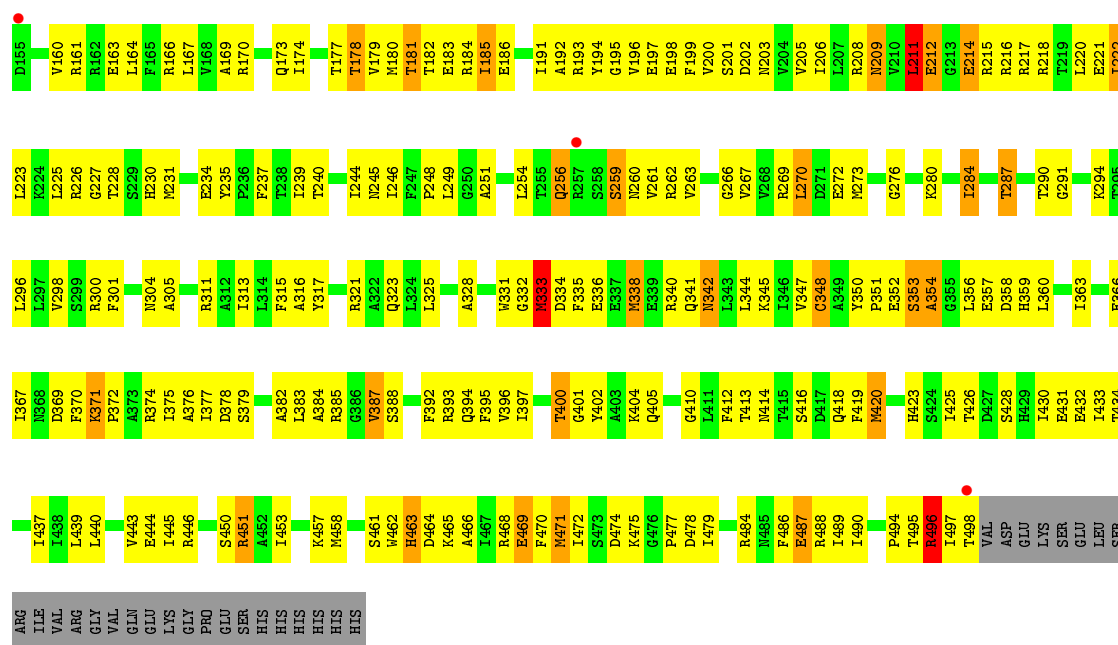


• Molecule 2: Circadian clock protein kinase kaiC

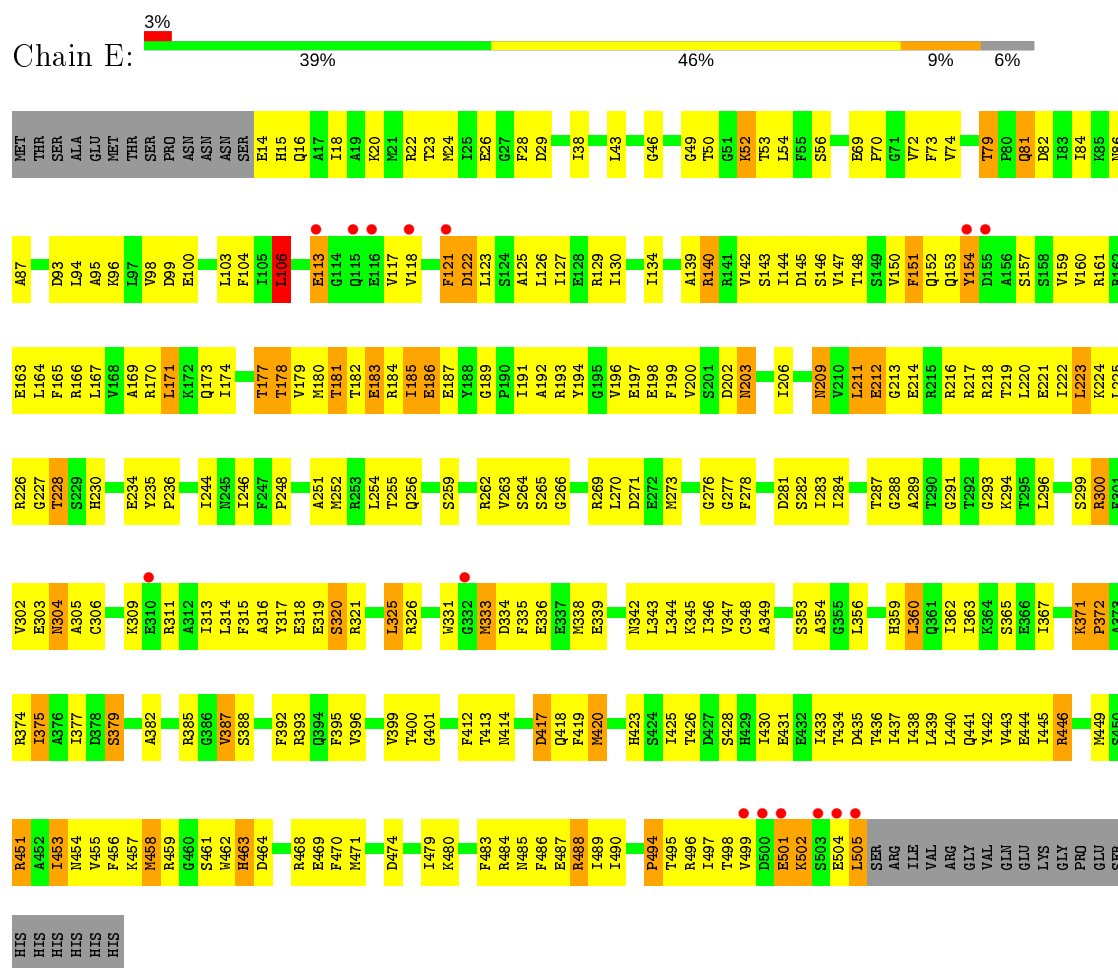


• Molecule 2: Circadian clock protein kinase kaiC





### • Molecule 2: Circadian clock protein kinase kaiC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.67Å 135.49Å 204.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 3.00 16.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	(Not available) (17.00-3.00) 92.3 (16.96-2.89)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.75 (at 2.87Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.242 , 0.288 0.239 , 0.281	Depositor DCC
$R_{free}$ test set	6459 reflections (7.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ATP, SEP

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	0.43	0/4049	0.72	1/5453 (0.0%)
1	F	0.46	0/4049	0.73	0/5453
2	B	0.40	0/3940	0.67	0/5309
2	C	0.41	0/3916	0.69	1/5278 (0.0%)
2	D	0.50	0/3892	0.73	0/5245
2	E	0.49	0/3948	0.75	2/5320 (0.0%)
All	All	0.45	0/23794	0.72	4/32058 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	213	GLY	N-CA-C	-5.96	98.21	113.10
2	E	106	LEU	CA-CB-CG	5.81	128.67	115.30
2	C	213	GLY	N-CA-C	-5.28	99.90	113.10
1	A	380	LEU	N-CA-C	-5.23	96.88	111.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3994	0	3985	444	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3994	0	3983	405	0
2	B	3875	0	3863	437	0
2	C	3851	0	3839	382	0
2	D	3827	0	3819	358	0
2	E	3883	0	3875	351	0
3	A	62	0	24	7	0
3	B	62	0	24	8	0
3	C	62	0	24	5	0
3	D	62	0	24	6	0
3	E	62	0	24	11	0
3	F	62	0	24	6	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	2	0	0	0	0
4	F	3	0	0	0	0
5	A	5	0	0	0	0
5	B	6	0	0	1	0
5	C	10	0	0	2	0
5	D	32	0	0	13	0
5	E	16	0	0	0	0
5	F	12	0	0	1	0
All	All	23898	0	23508	2227	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 47.

All (2227) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:VAL:HG12	1:A:463:HIS:CD2	1.63	1.30
1:A:320:SEP:HB2	2:B:254:LEU:O	1.42	1.17
1:A:254:LEU:CD2	1:F:320:SEP:HA	1.74	1.16
1:A:321:ARG:O	1:A:324:LEU:HB2	1.45	1.14
1:F:263:VAL:HG12	1:F:374:ARG:HH21	1.10	1.14
1:A:455:VAL:CG1	1:A:463:HIS:HD2	1.61	1.13
1:A:254:LEU:HD21	1:F:320:SEP:HA	1.15	1.13
2:D:123:LEU:HG	2:D:163:GLU:OE2	1.49	1.13
1:F:305:ALA:HB2	1:F:374:ARG:HD2	1.21	1.13
1:F:509:VAL:HG12	1:F:510:ARG:H	1.07	1.12

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:ALA:HB2	2:B:374:ARG:HD2	1.33	1.11
2:E:305:ALA:HB2	2:E:374:ARG:HD2	1.26	1.11
1:A:320:SEP:CA	2:B:254:LEU:HG	1.83	1.08
2:E:263:VAL:HG12	2:E:374:ARG:HH21	1.12	1.07
1:A:14:GLU:HG3	1:A:15:HIS:H	1.19	1.07
2:B:269:ARG:HB3	2:B:479:ILE:HD13	1.37	1.06
1:A:320:SEP:HA	2:B:254:LEU:HG	1.30	1.06
2:D:123:LEU:O	2:D:127:ILE:HD13	1.54	1.05
2:B:263:VAL:HG12	2:B:374:ARG:HH21	1.20	1.05
1:A:455:VAL:HG12	1:A:463:HIS:HD2	0.88	1.04
2:C:205:VAL:HG22	2:C:222:ILE:HD13	1.38	1.04
2:B:497:ILE:HD12	2:B:499:VAL:H	1.22	1.03
1:A:455:VAL:CG1	1:A:463:HIS:CD2	2.39	1.02
2:D:445:ILE:HD13	2:D:450:SER:OG	1.58	1.02
2:D:123:LEU:HD12	2:D:166:ARG:HD2	1.41	1.02
1:A:305:ALA:HB2	1:A:374:ARG:HD2	1.39	1.02
2:D:371:LYS:HD2	2:D:371:LYS:O	1.60	1.02
1:F:18:ILE:HD12	1:F:227:GLY:HA3	1.44	0.99
2:D:311:ARG:HD2	2:D:371:LYS:HE3	1.42	0.99
2:E:313:ILE:HD12	2:E:367:ILE:HD13	1.45	0.98
1:A:41:SER:HB3	1:A:178:THR:HB	1.46	0.97
1:F:263:VAL:CG1	1:F:374:ARG:HH21	1.76	0.97
2:D:335:PHE:HA	2:D:338:MET:HG3	1.45	0.96
1:F:79:THR:HG22	1:F:82:ASP:H	1.30	0.96
2:B:325:LEU:HD23	2:B:335:PHE:CB	1.94	0.96
2:B:147:VAL:HG11	2:B:180:MET:HE3	1.47	0.96
2:B:434:THR:HG21	2:B:437:ILE:HD11	1.48	0.95
1:A:31:ILE:HD11	1:A:246:ILE:HG21	1.45	0.95
2:B:385:ARG:HG2	2:C:393:ARG:NH1	1.80	0.95
2:C:305:ALA:HB2	2:C:374:ARG:HD2	1.48	0.95
2:E:356:LEU:HD22	2:E:387:VAL:HG11	1.48	0.94
2:C:371:LYS:HD2	2:C:371:LYS:O	1.67	0.94
2:E:311:ARG:HD2	2:E:371:LYS:HE3	1.50	0.94
1:F:509:VAL:HG12	1:F:510:ARG:N	1.83	0.93
2:C:434:THR:HG23	2:C:437:ILE:HD11	1.47	0.93
2:B:285:LEU:HD23	2:B:437:ILE:HD12	1.51	0.93
2:D:146:SER:H	2:D:181:THR:HG22	1.34	0.93
2:B:73:PHE:HB3	2:B:105:ILE:HD13	1.50	0.93
2:C:367:ILE:HG12	2:C:375:ILE:HD11	1.51	0.93
2:B:170:ARG:O	2:B:174:ILE:HG12	1.69	0.92
2:B:325:LEU:HD23	2:B:335:PHE:HB2	1.47	0.92

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:21:MET:HE3	2:C:141:ARG:NE	1.84	0.92
2:B:54:LEU:HD23	2:B:244:ILE:HD11	1.51	0.92
1:F:263:VAL:HG12	1:F:374:ARG:NH2	1.85	0.92
1:F:508:ILE:O	1:F:509:VAL:HG23	1.69	0.91
2:D:333:MET:HA	5:D:913:HOH:O	1.70	0.91
2:C:437:ILE:CD1	2:C:457:LYS:HE2	2.01	0.91
2:E:79:THR:HG23	2:E:81:GLN:HG2	1.52	0.91
1:F:18:ILE:CD1	1:F:227:GLY:HA3	2.01	0.90
1:A:25:ILE:HD12	1:A:58:GLN:HG2	1.51	0.90
2:B:483:PHE:HB3	2:B:486:PHE:HD1	1.36	0.90
2:C:123:LEU:HD23	2:C:127:ILE:HD11	1.54	0.89
2:C:287:THR:HG23	2:C:414:ASN:HD22	1.36	0.89
2:E:313:ILE:HB	2:E:375:ILE:HD11	1.54	0.89
1:A:462:TRP:O	1:A:463:HIS:HB3	1.73	0.89
2:B:45:SER:HB3	2:B:182:THR:HB	1.54	0.89
1:A:79:THR:CG2	1:A:81:GLN:HG2	2.02	0.89
2:C:344:LEU:HD22	2:C:345:LYS:H	1.37	0.89
1:A:79:THR:HG23	1:A:81:GLN:HE21	1.36	0.88
2:D:79:THR:HG22	2:D:82:ASP:H	1.36	0.88
1:A:203:ASN:HB3	1:A:225:LEU:HD23	1.55	0.88
2:D:60:LEU:O	2:D:64:ILE:HD13	1.74	0.88
2:C:206:ILE:HD11	2:C:223:LEU:HB2	1.54	0.88
2:B:147:VAL:HG11	2:B:180:MET:CE	2.05	0.87
2:E:287:THR:HG23	2:E:414:ASN:HD22	1.36	0.87
2:B:148:THR:HG21	2:B:193:ARG:HD2	1.57	0.87
1:F:509:VAL:CG1	1:F:510:ARG:H	1.86	0.87
1:A:396:VAL:HG11	1:A:430:ILE:HG21	1.56	0.87
2:E:79:THR:CG2	2:E:81:GLN:HG2	2.05	0.87
2:C:182:THR:HG21	2:C:192:ALA:HB1	1.56	0.86
2:E:303:GLU:OE2	2:E:333:MET:HB3	1.76	0.86
2:C:493:SER:HB3	2:D:488:ARG:HG2	1.56	0.86
1:F:299:SER:C	1:F:333:MET:HE1	1.95	0.86
2:C:45:SER:HB3	2:C:182:THR:HB	1.56	0.85
2:C:287:THR:HG21	2:C:425:ILE:O	1.76	0.85
2:E:269:ARG:HG2	2:E:479:ILE:HB	1.55	0.85
2:C:437:ILE:HD13	2:C:457:LYS:HE2	1.58	0.85
1:A:318:GLU:OE1	2:B:432:GLU:HG2	1.76	0.85
1:F:18:ILE:HD13	1:F:40:ARG:NH1	1.91	0.85
1:A:14:GLU:CG	1:A:15:HIS:H	1.88	0.85
1:A:451:ARG:HH11	1:A:451:ARG:HG2	1.41	0.85
2:E:293:GLY:HA2	3:E:901:ATP:O1A	1.77	0.85

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:ILE:O	1:F:367:ILE:HG12	1.76	0.85
1:F:287:THR:HG23	1:F:414:ASN:HD22	1.39	0.85
1:F:123:LEU:O	1:F:127:ILE:HD13	1.76	0.85
2:B:426:THR:HB	2:B:431:GLU:OE2	1.77	0.84
2:B:140:ARG:NH1	2:B:140:ARG:HB3	1.91	0.84
2:C:25:ILE:HG23	2:C:58:GLN:NE2	1.90	0.84
2:C:140:ARG:HB3	2:C:140:ARG:NH1	1.93	0.84
2:C:269:ARG:HB3	2:C:479:ILE:HD12	1.59	0.84
2:B:503:SER:O	2:B:504:GLU:HB2	1.74	0.84
2:E:435:ASP:HA	2:E:459:ARG:HD2	1.58	0.84
1:F:293:GLY:HA2	3:F:901:ATP:O1A	1.78	0.84
1:A:257:ARG:NH2	1:A:407:GLU:HG2	1.93	0.84
2:B:263:VAL:HG12	2:B:374:ARG:NH2	1.93	0.84
2:B:263:VAL:CG1	2:B:374:ARG:HH21	1.90	0.84
2:B:300:ARG:HA	2:B:333:MET:CE	2.07	0.83
1:F:191:ILE:HB	1:F:198:GLU:CG	2.08	0.83
2:B:116:GLU:HG2	2:B:117:VAL:H	1.44	0.83
2:C:147:VAL:O	2:C:150:VAL:HG12	1.78	0.83
1:F:313:ILE:HB	1:F:375:ILE:HD11	1.61	0.83
2:C:25:ILE:HG12	2:C:58:GLN:HE21	1.43	0.83
2:D:287:THR:HG23	2:D:414:ASN:HD22	1.41	0.83
1:A:396:VAL:HG11	1:A:430:ILE:CG2	2.08	0.82
1:F:269:ARG:HG2	1:F:479:ILE:HB	1.60	0.82
2:D:248:PRO:HB2	2:D:251:ALA:HB3	1.61	0.82
2:E:125:ALA:O	2:E:129:ARG:HG3	1.79	0.82
1:A:320:SEP:C	1:A:348:CYS:SG	2.68	0.82
2:B:451:ARG:HH11	2:B:451:ARG:HG2	1.43	0.82
1:A:21:MET:HB2	1:A:38:ILE:HD11	1.62	0.82
2:B:300:ARG:HA	2:B:333:MET:HE3	1.59	0.82
2:C:31:ILE:HD11	2:C:246:ILE:HG21	1.62	0.82
2:B:300:ARG:N	2:B:333:MET:HE1	1.95	0.81
2:E:313:ILE:HB	2:E:375:ILE:CD1	2.10	0.81
1:F:283:ILE:HG23	1:F:412:PHE:CE1	2.15	0.81
2:B:285:LEU:HB3	2:B:437:ILE:HD13	1.62	0.81
2:B:296:LEU:HD21	2:B:477:PRO:HD3	1.62	0.81
1:F:455:VAL:HG11	1:F:463:HIS:HB2	1.62	0.81
1:A:254:LEU:HD22	1:F:348:CYS:HB3	1.62	0.81
2:C:140:ARG:HB3	2:C:140:ARG:HH11	1.45	0.81
1:A:254:LEU:HD21	1:F:320:SEP:CA	2.04	0.81
2:D:147:VAL:HG11	2:D:180:MET:HE3	1.62	0.81
2:E:263:VAL:HG12	2:E:374:ARG:NH2	1.95	0.81

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:ALA:O	2:B:173:GLN:HG3	1.81	0.81
2:B:334:ASP:OD1	2:B:336:GLU:HB2	1.80	0.81
1:A:462:TRP:O	1:A:463:HIS:CB	2.30	0.80
2:B:46:GLY:HA3	2:B:50:THR:HG21	1.64	0.80
2:E:263:VAL:CG1	2:E:374:ARG:HH21	1.94	0.80
2:E:446:ARG:NH2	2:E:496:ARG:NH2	2.29	0.80
2:B:311:ARG:HD2	2:B:371:LYS:HE3	1.63	0.80
1:A:462:TRP:CE3	1:A:463:HIS:N	2.49	0.80
2:B:479:ILE:HD12	2:B:479:ILE:H	1.44	0.80
1:A:273:MET:O	1:A:274:CYS:HB2	1.79	0.80
2:C:28:PHE:CE1	2:C:222:ILE:HD11	2.17	0.79
2:D:315:PHE:HB2	2:D:377:ILE:HD13	1.64	0.79
1:F:313:ILE:O	1:F:375:ILE:HD13	1.82	0.79
2:B:299:SER:C	2:B:333:MET:HE1	2.02	0.79
2:E:426:THR:HG21	2:E:430:ILE:HG12	1.65	0.79
1:A:318:GLU:CD	2:B:432:GLU:HG2	2.02	0.79
2:B:379:SER:HA	2:B:413:THR:HG22	1.65	0.79
1:F:471:MET:HG3	1:F:478:ASP:HB3	1.61	0.79
1:A:320:SEP:HA	2:B:254:LEU:CG	2.12	0.79
2:C:123:LEU:HD13	2:C:166:ARG:HD2	1.65	0.79
2:D:44:VAL:HG22	2:D:205:VAL:HB	1.64	0.79
2:E:379:SER:H	2:E:413:THR:HB	1.47	0.79
2:D:140:ARG:NH1	2:D:140:ARG:HB3	1.98	0.78
1:F:453:ILE:HG21	1:F:479:ILE:HD12	1.64	0.78
2:D:445:ILE:HD13	2:D:450:SER:HG	1.48	0.78
1:A:164:LEU:HD11	1:A:197:GLU:HG3	1.63	0.78
2:E:371:LYS:HD2	2:E:371:LYS:O	1.83	0.78
2:E:18:ILE:HD11	2:E:228:THR:OG1	1.83	0.78
2:E:382:ALA:O	2:E:385:ARG:HG3	1.83	0.78
1:F:508:ILE:C	1:F:509:VAL:HG23	2.00	0.78
1:A:205:VAL:HG22	1:A:222:ILE:HD13	1.63	0.78
2:B:191:ILE:HB	2:B:198:GLU:CG	2.14	0.78
2:D:267:VAL:HG23	2:D:300:ARG:HG2	1.65	0.78
2:E:38:ILE:HA	2:E:177:THR:HG23	1.66	0.78
1:A:147:VAL:O	1:A:150:VAL:HG12	1.83	0.77
1:A:471:MET:SD	1:A:478:ASP:HB3	2.24	0.77
1:F:122:ASP:HA	1:F:125:ALA:HB3	1.66	0.77
1:A:227:GLY:O	1:F:89:SER:HB2	1.84	0.77
2:B:182:THR:HG21	2:B:192:ALA:HB1	1.66	0.77
2:C:262:ARG:HH22	2:C:461:SER:HB2	1.49	0.77
2:D:70:PRO:HB2	2:D:139:ALA:HA	1.67	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:313:ILE:HB	2:D:375:ILE:CD1	2.14	0.77
2:D:496:ARG:HG2	2:E:487:GLU:OE1	1.85	0.77
1:F:203:ASN:HB3	1:F:225:LEU:HD23	1.66	0.77
2:B:140:ARG:HH11	2:B:140:ARG:HB3	1.49	0.77
1:A:256:GLN:HG3	1:F:320:SEP:O1P	1.85	0.77
1:A:370:PHE:HD2	1:A:372:PRO:HG3	1.49	0.76
2:E:14:GLU:HG3	2:E:16:GLN:H	1.49	0.76
2:D:451:ARG:HH11	2:D:451:ARG:HG2	1.50	0.76
1:F:287:THR:CG2	1:F:414:ASN:HD22	1.98	0.76
1:F:486:PHE:CE2	1:F:496:ARG:HD2	2.19	0.76
1:A:263:VAL:HG12	1:A:374:ARG:HH21	1.49	0.76
2:E:356:LEU:CD2	2:E:387:VAL:HG11	2.16	0.76
1:A:375:ILE:HD13	1:A:408:ILE:HG21	1.68	0.76
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.00	0.76
2:C:170:ARG:O	2:C:174:ILE:HG12	1.86	0.76
1:F:508:ILE:O	1:F:509:VAL:CG2	2.33	0.76
2:C:205:VAL:CG2	2:C:222:ILE:HD13	2.16	0.75
2:D:182:THR:HG22	2:D:183:GLU:N	2.01	0.75
2:D:18:ILE:CD1	2:D:227:GLY:HA3	2.16	0.75
1:A:14:GLU:HG3	1:A:15:HIS:N	1.99	0.75
2:B:492:GLY:O	2:B:494:PRO:HD3	1.86	0.75
2:D:444:GLU:OE2	2:E:489:ILE:HD13	1.87	0.75
1:A:318:GLU:OE2	2:B:432:GLU:HG2	1.86	0.75
2:D:311:ARG:HD2	2:D:371:LYS:CE	2.17	0.75
1:A:325:LEU:HD23	1:A:335:PHE:HB2	1.69	0.75
2:C:299:SER:C	2:C:333:MET:HE1	2.06	0.75
2:D:148:THR:OG1	2:D:182:THR:HG23	1.86	0.75
2:E:79:THR:HG22	2:E:82:ASP:H	1.51	0.75
2:B:325:LEU:HD23	2:B:335:PHE:HB3	1.68	0.75
2:B:25:ILE:HG12	2:B:58:GLN:HE21	1.50	0.75
2:D:212:GLU:O	2:D:212:GLU:HG2	1.86	0.75
2:E:453:ILE:HG21	2:E:479:ILE:HD12	1.68	0.75
2:B:356:LEU:HD13	2:B:387:VAL:HG21	1.69	0.74
3:B:901:ATP:H3'	2:C:458:MET:O	1.87	0.74
2:E:273:MET:O	2:E:463:HIS:HA	1.87	0.74
2:D:18:ILE:HD12	2:D:227:GLY:HA3	1.68	0.74
1:A:25:ILE:CD1	1:A:58:GLN:HG2	2.17	0.74
2:D:443:VAL:O	2:D:445:ILE:HD12	1.88	0.74
2:E:148:THR:OG1	2:E:182:THR:HG23	1.86	0.74
2:E:93:ASP:OD2	2:E:96:LYS:HB2	1.87	0.74
2:E:123:LEU:HD23	2:E:127:ILE:HD11	1.69	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:MET:HB2	1:A:38:ILE:CD1	2.17	0.74
1:F:500:ASP:O	1:F:501:GLU:HB3	1.87	0.74
1:A:321:ARG:O	1:A:324:LEU:CB	2.32	0.74
2:C:335:PHE:HA	2:C:338:MET:HG3	1.68	0.74
1:A:254:LEU:HD21	1:F:319:GLU:O	1.87	0.74
1:A:508:ILE:H	1:A:508:ILE:HD13	1.51	0.74
1:F:170:ARG:O	1:F:174:ILE:HG12	1.88	0.74
2:B:148:THR:CG2	2:B:193:ARG:HD2	2.18	0.73
1:A:96:LYS:O	1:A:100:GLU:HG3	1.88	0.73
2:C:344:LEU:HD22	2:C:345:LYS:N	2.03	0.73
2:C:495:THR:HA	2:D:487:GLU:OE2	1.88	0.73
2:E:377:ILE:HD11	2:E:399:VAL:HG11	1.69	0.73
2:B:295:THR:HG21	2:B:319:GLU:OE2	1.87	0.73
2:B:21:MET:HB2	2:B:38:ILE:HG12	1.70	0.73
1:A:290:THR:HG21	2:B:425:ILE:HD12	1.69	0.73
2:B:61:TYR:CE1	2:B:92:TRP:HB2	2.24	0.73
2:D:431:GLU:O	2:D:434:THR:HG22	1.87	0.73
1:A:254:LEU:O	1:A:254:LEU:HD23	1.89	0.73
2:D:344:LEU:HD22	2:D:345:LYS:H	1.53	0.73
2:B:127:ILE:HG21	2:B:170:ARG:HG3	1.69	0.73
2:E:304:ASN:HB3	2:E:374:ARG:HH12	1.53	0.73
1:A:371:LYS:O	1:A:371:LYS:HD2	1.87	0.73
1:A:266:GLY:HA3	1:A:300:ARG:O	1.88	0.73
2:C:262:ARG:NH2	2:C:461:SER:HB2	2.04	0.73
2:C:36:LEU:HD12	2:C:59:PHE:CE1	2.23	0.73
2:E:319:GLU:O	1:F:254:LEU:HD21	1.89	0.73
1:F:283:ILE:HG23	1:F:412:PHE:HE1	1.53	0.73
2:B:25:ILE:HG12	2:B:58:GLN:NE2	2.04	0.73
2:D:478:ASP:HB2	5:D:555:HOH:O	1.89	0.73
1:F:489:ILE:HA	1:F:494:PRO:HG3	1.70	0.73
1:A:89:SER:HB2	2:B:227:GLY:O	1.89	0.73
1:A:320:SEP:O	1:A:348:CYS:SG	2.47	0.72
2:C:28:PHE:CZ	2:C:222:ILE:HD11	2.24	0.72
2:C:182:THR:HG22	2:C:183:GLU:N	2.04	0.72
2:B:493:SER:HB3	2:C:488:ARG:HG2	1.71	0.72
1:F:347:VAL:O	1:F:348:CYS:HB2	1.88	0.72
2:E:191:ILE:HD12	2:E:206:ILE:CD1	2.19	0.72
1:F:514:GLU:O	1:F:515:LYS:HB3	1.89	0.72
1:A:147:VAL:HG11	1:A:180:MET:HE3	1.71	0.72
1:F:305:ALA:CB	1:F:374:ARG:HD2	2.11	0.72
1:A:462:TRP:CD2	1:A:463:HIS:N	2.52	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:ARG:HH11	2:D:140:ARG:HB3	1.55	0.72
2:E:191:ILE:HB	2:E:198:GLU:CG	2.20	0.72
2:B:285:LEU:HB3	2:B:437:ILE:CD1	2.18	0.72
2:B:287:THR:HG23	2:B:414:ASN:HD22	1.55	0.72
2:E:159:VAL:O	2:E:163:GLU:HG2	1.90	0.72
2:D:332:GLY:C	2:D:333:MET:HG2	2.09	0.72
1:F:379:SER:H	1:F:413:THR:HB	1.55	0.72
1:A:248:PRO:HB2	1:A:251:ALA:HB3	1.72	0.71
2:D:446:ARG:N	2:D:496:ARG:HH12	1.87	0.71
1:F:111:ASP:OD1	1:F:112:PRO:HD2	1.90	0.71
2:C:269:ARG:HG2	2:C:479:ILE:HB	1.72	0.71
1:F:31:ILE:HG21	1:F:222:ILE:HD13	1.73	0.71
1:F:248:PRO:HB2	1:F:251:ALA:HB3	1.71	0.71
2:B:191:ILE:HB	2:B:198:GLU:HG3	1.71	0.71
2:B:54:LEU:HD23	2:B:244:ILE:CD1	2.20	0.71
2:E:248:PRO:HB2	2:E:251:ALA:HB3	1.70	0.71
2:C:123:LEU:HD21	2:C:167:LEU:HB2	1.73	0.71
2:D:191:ILE:HB	2:D:198:GLU:CG	2.20	0.71
2:B:178:THR:HG22	2:B:179:VAL:H	1.55	0.71
2:C:191:ILE:HB	2:C:198:GLU:CG	2.21	0.71
2:E:436:THR:HG23	2:E:458:MET:HG2	1.73	0.71
2:B:284:ILE:HG23	2:B:436:THR:HB	1.71	0.71
2:C:50:THR:HG21	2:C:207:LEU:O	1.91	0.71
2:E:313:ILE:HG13	2:E:372:PRO:CG	2.20	0.71
2:E:426:THR:HG22	2:E:428:SER:H	1.55	0.71
1:A:116:GLU:C	1:A:117:VAL:HG23	2.09	0.71
2:B:453:ILE:HD13	2:B:454:ASN:N	2.06	0.71
2:D:344:LEU:HD22	2:D:345:LYS:N	2.06	0.71
2:D:439:LEU:HD12	2:D:440:LEU:N	2.06	0.71
2:D:446:ARG:H	2:D:496:ARG:HH12	1.39	0.71
2:E:462:TRP:CE2	2:E:463:HIS:O	2.44	0.71
1:F:379:SER:OG	1:F:382:ALA:HB2	1.91	0.71
1:A:263:VAL:CG1	1:A:374:ARG:HH21	2.03	0.71
2:C:140:ARG:HH11	2:C:140:ARG:CB	2.04	0.70
2:C:377:ILE:HD12	2:C:412:PHE:CE2	2.26	0.70
1:F:96:LYS:O	1:F:100:GLU:HG3	1.91	0.70
2:B:425:ILE:HD11	2:B:456:PHE:CE2	2.26	0.70
1:F:515:LYS:HG3	1:F:516:GLY:H	1.56	0.70
2:C:393:ARG:O	2:C:397:ILE:HD13	1.90	0.70
2:C:25:ILE:HG23	2:C:58:GLN:HE22	1.54	0.70
1:F:31:ILE:CG2	1:F:222:ILE:HD13	2.21	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:HIS:O	2:D:363:ILE:HG12	1.91	0.70
2:E:446:ARG:NH2	2:E:496:ARG:HH22	1.88	0.70
2:E:317:TYR:OH	2:E:363:ILE:HD11	1.90	0.70
1:A:318:GLU:OE1	2:B:432:GLU:HB3	1.91	0.70
2:E:453:ILE:HB	2:E:470:PHE:CD2	2.27	0.70
1:A:321:ARG:HA	1:A:324:LEU:HD12	1.71	0.70
2:E:266:GLY:HA2	2:E:304:ASN:HD22	1.55	0.70
1:A:458:MET:O	3:F:901:ATP:H3'	1.91	0.70
1:F:147:VAL:O	1:F:150:VAL:HG12	1.92	0.70
2:C:283:ILE:HD11	2:C:404:LYS:HG3	1.74	0.70
2:C:379:SER:H	2:C:413:THR:HB	1.56	0.70
2:E:418:GLN:HB2	1:F:423:HIS:O	1.91	0.70
2:B:434:THR:CG2	2:B:437:ILE:HD11	2.21	0.69
1:F:18:ILE:HD13	1:F:40:ARG:HH12	1.53	0.69
2:D:478:ASP:CB	5:D:555:HOH:O	2.40	0.69
2:E:300:ARG:HA	2:E:333:MET:HE1	1.72	0.69
1:A:154:TYR:O	1:A:155:ASP:CG	2.30	0.69
2:E:43:LEU:HD11	2:E:182:THR:OG1	1.92	0.69
1:F:208:ARG:NH2	1:F:221:GLU:OE2	2.24	0.69
1:F:338:MET:HB3	1:F:344:LEU:HB3	1.74	0.69
1:F:317:TYR:OH	1:F:363:ILE:HD11	1.92	0.69
2:C:221:GLU:HG3	2:C:233:GLY:O	1.92	0.69
2:D:147:VAL:O	2:D:150:VAL:HG12	1.92	0.69
2:D:161:ARG:HB2	2:D:196:VAL:HG11	1.74	0.69
2:D:284:ILE:HD12	2:D:410:GLY:O	1.92	0.69
1:F:515:LYS:HG3	1:F:516:GLY:N	2.08	0.69
2:B:218:ARG:CZ	2:B:239:ILE:HD12	2.22	0.69
2:D:387:VAL:HG12	2:D:388:SER:N	2.08	0.69
2:D:269:ARG:HG2	2:D:479:ILE:HB	1.74	0.69
1:F:462:TRP:O	1:F:463:HIS:CD2	2.46	0.69
1:A:484:ARG:NH1	1:A:484:ARG:HB3	2.07	0.69
2:B:84:ILE:HD12	2:B:94:LEU:HB2	1.74	0.69
2:E:126:LEU:O	2:E:130:ILE:HG12	1.92	0.69
2:E:294:LYS:HG2	2:E:413:THR:HG23	1.75	0.69
1:A:451:ARG:HD2	1:A:451:ARG:N	2.08	0.69
1:A:425:ILE:HD12	1:F:290:THR:HG21	1.73	0.69
2:C:94:LEU:O	2:C:98:VAL:HG23	1.92	0.69
2:D:147:VAL:HG11	2:D:180:MET:CE	2.23	0.69
2:D:220:LEU:HD13	2:D:246:ILE:HD11	1.73	0.69
1:F:264:SER:O	1:F:374:ARG:NH2	2.25	0.69
1:A:287:THR:HG23	1:A:414:ASN:HD22	1.58	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SEP:HB2	2:B:254:LEU:C	2.13	0.69
2:C:218:ARG:CZ	2:C:239:ILE:HD12	2.23	0.69
2:C:287:THR:HG23	2:C:414:ASN:ND2	2.07	0.69
2:C:419:PHE:O	2:C:420:MET:HB2	1.92	0.69
2:C:393:ARG:HH21	2:C:429:HIS:HB2	1.58	0.69
1:A:320:SEP:O1P	2:B:256:GLN:HG3	1.92	0.68
1:A:396:VAL:O	1:A:400:THR:HB	1.94	0.68
2:B:51:GLY:O	2:B:54:LEU:N	2.26	0.68
1:A:254:LEU:HD23	1:F:320:SEP:HA	1.74	0.68
1:A:318:GLU:OE1	2:B:432:GLU:CG	2.42	0.68
2:B:225:LEU:HD12	2:B:230:HIS:HB3	1.74	0.68
2:C:159:VAL:O	2:C:163:GLU:HG2	1.93	0.68
2:C:453:ILE:HD13	2:C:454:ASN:N	2.07	0.68
2:E:320:SER:HA	1:F:254:LEU:HG	1.75	0.68
1:A:264:SER:HA	1:A:271:ASP:OD1	1.94	0.68
2:B:315:PHE:CE2	2:B:347:VAL:HG21	2.29	0.68
2:E:74:VAL:HG21	2:E:130:ILE:HD12	1.76	0.68
2:B:325:LEU:CD2	2:B:335:PHE:HB3	2.23	0.68
2:C:45:SER:CB	2:C:182:THR:HB	2.23	0.68
2:E:377:ILE:HD12	2:E:412:PHE:CE2	2.28	0.68
1:A:191:ILE:HB	1:A:198:GLU:CG	2.24	0.68
1:A:372:PRO:O	1:A:408:ILE:HD12	1.94	0.68
1:A:88:ARG:HH11	1:A:88:ARG:HG2	1.58	0.68
2:C:111:ASP:OD1	2:C:113:GLU:HG2	1.92	0.68
2:D:122:ASP:O	2:D:123:LEU:HB2	1.92	0.68
2:D:301:PHE:CZ	2:D:374:ARG:HD3	2.28	0.68
1:F:508:ILE:O	1:F:509:VAL:CB	2.42	0.68
2:C:447:GLY:HA2	2:D:489:ILE:HD12	1.76	0.68
2:E:287:THR:HG23	2:E:414:ASN:ND2	2.08	0.68
2:D:347:VAL:O	2:D:348:CYS:HB2	1.94	0.68
2:E:123:LEU:O	2:E:127:ILE:HG12	1.93	0.68
1:A:84:ILE:HG23	1:A:94:LEU:HB2	1.76	0.68
2:B:502:LYS:HG3	2:B:504:GLU:O	1.94	0.68
1:A:266:GLY:HA3	1:A:300:ARG:HG3	1.74	0.68
2:D:478:ASP:CA	5:D:555:HOH:O	2.41	0.68
2:B:140:ARG:CB	2:B:140:ARG:HH11	2.07	0.67
2:C:470:PHE:HB2	2:C:478:ASP:O	1.94	0.67
2:D:475:LYS:HA	5:D:553:HOH:O	1.93	0.67
2:E:140:ARG:NH1	2:E:140:ARG:HB3	2.09	0.67
2:E:344:LEU:HD11	2:E:346:ILE:HG13	1.76	0.67
1:F:471:MET:CG	1:F:478:ASP:HB3	2.24	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:PHE:CB	1:F:489:ILE:HD11	2.24	0.67
2:C:431:GLU:HG2	2:C:431:GLU:O	1.94	0.67
2:E:363:ILE:O	2:E:367:ILE:HG12	1.93	0.67
1:A:211:LEU:HB2	1:A:216:ARG:NE	2.09	0.67
2:E:171:LEU:HA	2:E:174:ILE:HD12	1.76	0.67
1:A:208:ARG:NH2	1:A:221:GLU:OE2	2.28	0.67
1:A:79:THR:HG21	1:A:81:GLN:HG2	1.74	0.67
2:B:56:SER:O	2:B:59:PHE:HB3	1.94	0.67
2:C:451:ARG:HH11	2:C:451:ARG:HG2	1.59	0.67
2:D:222:ILE:HD12	2:D:222:ILE:N	2.09	0.67
2:E:377:ILE:HD12	2:E:412:PHE:HE2	1.57	0.67
2:E:445:ILE:O	2:E:446:ARG:HB2	1.93	0.67
1:A:311:ARG:HA	1:A:343:LEU:O	1.95	0.67
1:A:323:GLN:HG3	1:A:324:LEU:N	2.10	0.67
2:D:400:THR:HG22	2:D:401:GLY:N	2.08	0.67
2:D:287:THR:CG2	2:D:414:ASN:HD22	2.06	0.67
2:D:81:GLN:NE2	2:D:81:GLN:H	1.93	0.67
1:F:191:ILE:HB	1:F:198:GLU:CD	2.14	0.67
1:A:484:ARG:HB3	1:A:484:ARG:HH11	1.58	0.66
2:B:497:ILE:HD12	2:B:499:VAL:N	2.03	0.66
2:C:54:LEU:HD23	2:C:244:ILE:HG12	1.77	0.66
2:C:151:PHE:C	2:C:153:GLN:H	1.95	0.66
2:E:496:ARG:O	2:E:497:ILE:HD13	1.95	0.66
1:F:426:THR:HG22	1:F:428:SER:H	1.61	0.66
2:B:79:THR:CG2	2:B:81:GLN:HG2	2.25	0.66
2:B:287:THR:HG21	2:B:425:ILE:O	1.95	0.66
2:D:313:ILE:HB	2:D:375:ILE:HD13	1.76	0.66
2:E:289:ALA:HB2	2:E:419:PHE:HA	1.77	0.66
2:B:325:LEU:CD2	2:B:335:PHE:CB	2.72	0.66
2:B:52:LYS:N	3:B:903:ATP:O1B	2.28	0.66
2:C:436:THR:C	2:C:437:ILE:HD12	2.16	0.66
1:A:73:PHE:HB3	1:A:105:ILE:HD13	1.77	0.66
1:A:359:HIS:O	1:A:363:ILE:HG12	1.95	0.66
1:A:421:GLY:O	1:A:422:ALA:C	2.34	0.66
1:A:487:GLU:HG3	1:A:497:ILE:HD11	1.77	0.66
2:B:246:ILE:O	2:B:248:PRO:HD3	1.95	0.66
2:B:425:ILE:HD11	2:B:456:PHE:CD2	2.31	0.66
2:C:28:PHE:HA	2:C:246:ILE:HD12	1.78	0.66
2:C:31:ILE:CD1	2:C:246:ILE:HG21	2.24	0.66
2:E:487:GLU:O	2:E:488:ARG:HB2	1.96	0.66
1:F:18:ILE:CD1	1:F:40:ARG:HH12	2.08	0.66

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:345:LYS:HE2	1:F:366:GLU:OE1	1.95	0.66
1:F:46:GLY:HA2	1:F:184:ARG:HD2	1.76	0.66
2:D:31:ILE:HG21	2:D:222:ILE:CD1	2.25	0.66
2:B:44:VAL:HG22	2:B:205:VAL:CG1	2.26	0.66
2:E:170:ARG:O	2:E:174:ILE:HG13	1.94	0.66
1:F:49:GLY:HA2	3:F:903:ATP:O2B	1.96	0.66
2:C:79:THR:CG2	2:C:82:ASP:H	2.08	0.66
1:A:406:GLU:HB3	1:A:408:ILE:HG12	1.78	0.65
2:B:462:TRP:O	2:B:463:HIS:CG	2.49	0.65
2:C:439:LEU:HD12	2:C:440:LEU:N	2.10	0.65
2:D:21:MET:HE1	2:D:177:THR:HB	1.78	0.65
2:D:379:SER:H	2:D:413:THR:HB	1.61	0.65
2:E:121:PHE:CD1	2:E:121:PHE:N	2.63	0.65
2:B:145:ASP:OD2	2:B:181:THR:HG21	1.96	0.65
2:C:121:PHE:H	2:C:121:PHE:HD1	1.44	0.65
2:C:25:ILE:HG12	2:C:58:GLN:NE2	2.12	0.65
2:C:437:ILE:HD13	2:C:457:LYS:HG2	1.79	0.65
2:E:451:ARG:HD2	2:E:451:ARG:H	1.62	0.65
2:B:43:LEU:HD11	2:B:182:THR:OG1	1.97	0.65
2:B:79:THR:HG23	2:B:81:GLN:HG2	1.78	0.65
1:F:505:LEU:O	1:F:506:SER:HB3	1.96	0.65
2:B:20:LYS:HE3	2:B:228:THR:HG21	1.78	0.65
2:B:311:ARG:HD2	2:B:371:LYS:CE	2.26	0.65
2:B:65:ILE:HG22	2:B:65:ILE:O	1.94	0.65
2:C:182:THR:HG22	2:C:183:GLU:H	1.59	0.65
2:D:18:ILE:HD13	2:D:40:ARG:NH1	2.12	0.65
2:E:147:VAL:O	2:E:150:VAL:HG12	1.97	0.65
2:D:194:TYR:O	2:D:196:VAL:HG23	1.97	0.65
2:E:191:ILE:HB	2:E:198:GLU:HG2	1.78	0.65
1:F:151:PHE:C	1:F:153:GLN:H	2.00	0.65
2:C:335:PHE:O	2:C:339:GLU:HG3	1.96	0.65
2:D:49:GLY:O	2:D:218:ARG:NH2	2.30	0.65
2:E:334:ASP:OD1	2:E:336:GLU:HB2	1.97	0.65
1:F:378:ASP:OD1	1:F:413:THR:HG21	1.97	0.65
2:D:170:ARG:O	2:D:174:ILE:HG13	1.97	0.65
1:F:20:LYS:HD3	1:F:35:GLY:O	1.96	0.65
2:C:367:ILE:HG12	2:C:375:ILE:CD1	2.26	0.64
2:E:106:LEU:HD21	2:E:130:ILE:HD13	1.79	0.64
2:E:359:HIS:HA	2:E:362:ILE:HD12	1.78	0.64
1:A:338:MET:HB3	1:A:344:LEU:HB3	1.79	0.64
1:A:436:THR:CG2	1:A:458:MET:HG2	2.28	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:41:SER:CB	2:D:178:THR:HB	2.26	0.64
2:E:449:MET:HE3	1:F:490:ILE:HD11	1.78	0.64
2:D:81:GLN:H	2:D:81:GLN:CD	1.98	0.64
2:E:311:ARG:HD2	2:E:371:LYS:CE	2.26	0.64
3:E:901:ATP:H3'	1:F:458:MET:O	1.96	0.64
1:F:504:GLU:HA	1:F:507:ARG:NE	2.13	0.64
1:F:79:THR:HG23	1:F:81:GLN:H	1.61	0.64
1:A:320:SEP:N	2:B:254:LEU:HG	2.12	0.64
2:C:284:ILE:HD12	2:C:410:GLY:O	1.98	0.64
2:D:383:LEU:HD13	2:D:395:PHE:CE2	2.31	0.64
2:C:448:GLU:HG2	2:D:466:ALA:HA	1.79	0.64
1:A:321:ARG:O	1:A:324:LEU:N	2.30	0.64
2:C:123:LEU:CD2	2:C:127:ILE:HD11	2.27	0.64
2:C:61:TYR:CE1	2:C:92:TRP:HB2	2.32	0.64
2:D:146:SER:N	2:D:181:THR:HG22	2.11	0.64
1:A:379:SER:H	1:A:413:THR:HB	1.62	0.64
2:B:497:ILE:CD1	2:B:499:VAL:H	2.06	0.64
2:D:383:LEU:HD13	2:D:395:PHE:HE2	1.63	0.64
2:E:23:THR:O	2:E:24:MET:HB2	1.98	0.64
2:D:197:GLU:CD	2:D:197:GLU:H	1.99	0.64
2:B:283:ILE:CD1	2:B:404:LYS:HG3	2.28	0.64
2:C:123:LEU:HD11	2:C:163:GLU:O	1.98	0.64
1:A:328:ALA:O	1:A:333:MET:CG	2.46	0.63
2:B:294:LYS:HB3	2:B:413:THR:OG1	1.98	0.63
2:B:62:ASN:O	2:B:66:GLU:HB2	1.98	0.63
2:E:455:VAL:HG11	2:E:463:HIS:HB2	1.80	0.63
2:E:94:LEU:O	2:E:98:VAL:HG23	1.98	0.63
1:F:104:PHE:CE2	1:F:106:LEU:HB2	2.33	0.63
1:F:140:ARG:HB3	1:F:140:ARG:HH11	1.61	0.63
2:C:344:LEU:HD11	2:C:346:ILE:HG13	1.79	0.63
2:D:328:ALA:HB2	5:D:552:HOH:O	1.97	0.63
2:E:344:LEU:HD22	2:E:345:LYS:H	1.63	0.63
2:D:208:ARG:NH2	2:D:221:GLU:OE2	2.31	0.63
2:D:446:ARG:H	2:D:496:ARG:NH1	1.97	0.63
1:F:382:ALA:O	1:F:385:ARG:HG3	1.97	0.63
1:A:147:VAL:HG11	1:A:180:MET:CE	2.27	0.63
1:A:25:ILE:HD12	1:A:58:GLN:CG	2.28	0.63
2:C:293:GLY:HA2	3:C:901:ATP:O1A	1.98	0.63
2:E:38:ILE:HA	2:E:177:THR:CG2	2.28	0.63
1:F:356:LEU:HD13	1:F:387:VAL:HG21	1.79	0.63
1:A:218:ARG:CZ	1:A:239:ILE:HD12	2.29	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:447:GLY:HA2	2:D:489:ILE:CD1	2.29	0.63
1:F:372:PRO:O	1:F:408:ILE:HD12	1.99	0.63
2:B:147:VAL:O	2:B:150:VAL:HG12	1.98	0.63
2:B:239:ILE:HG12	2:B:244:ILE:HD13	1.81	0.63
2:B:273:MET:O	2:B:463:HIS:HA	1.98	0.63
2:D:353:SER:O	2:D:354:ALA:HB2	1.98	0.63
2:E:202:ASP:HA	2:E:226:ARG:HD2	1.80	0.63
2:E:84:ILE:HG21	2:E:95:ALA:HB2	1.81	0.63
1:F:182:THR:HG21	1:F:192:ALA:HB1	1.80	0.63
2:B:387:VAL:HG12	2:B:388:SER:N	2.13	0.63
2:B:80:PRO:O	2:B:84:ILE:HG12	1.99	0.63
2:B:360:LEU:HD22	2:B:360:LEU:O	1.97	0.63
2:C:146:SER:H	2:C:181:THR:HB	1.64	0.63
2:C:313:ILE:HG12	2:C:345:LYS:HB3	1.81	0.63
2:D:123:LEU:CD1	2:D:166:ARG:HD2	2.24	0.63
1:F:311:ARG:HD2	1:F:371:LYS:CE	2.29	0.63
1:A:45:SER:HB3	1:A:182:THR:HB	1.80	0.62
2:B:203:ASN:HB3	2:B:225:LEU:HD23	1.81	0.62
2:C:43:LEU:HD11	2:C:182:THR:OG1	1.98	0.62
2:D:114:GLY:O	2:D:115:GLN:HG3	1.98	0.62
1:F:191:ILE:HB	1:F:198:GLU:HG3	1.80	0.62
1:A:254:LEU:HD22	1:F:348:CYS:CB	2.29	0.62
2:C:81:GLN:NE2	2:C:81:GLN:H	1.96	0.62
2:D:393:ARG:O	2:D:397:ILE:HG13	1.99	0.62
2:E:313:ILE:HG13	2:E:372:PRO:HG3	1.81	0.62
1:A:24:MET:HB2	1:A:62:ASN:HD22	1.63	0.62
2:B:45:SER:CB	2:B:182:THR:HB	2.29	0.62
2:C:80:PRO:O	2:C:84:ILE:HG12	1.99	0.62
2:E:461:SER:OG	2:E:462:TRP:N	2.32	0.62
1:A:433:ILE:HG22	1:A:433:ILE:O	1.99	0.62
2:C:206:ILE:CD1	2:C:223:LEU:HB2	2.27	0.62
2:E:150:VAL:HG13	2:E:151:PHE:N	2.13	0.62
2:E:431:GLU:O	2:E:434:THR:HG22	2.00	0.62
1:F:486:PHE:HB3	1:F:489:ILE:HD11	1.79	0.62
1:A:335:PHE:O	1:A:338:MET:N	2.32	0.62
1:A:451:ARG:NH1	1:A:451:ARG:HG2	2.13	0.62
1:A:273:MET:HG2	1:A:464:ASP:OD2	1.99	0.62
2:C:441:GLN:HE22	2:C:490:ILE:HD13	1.64	0.62
2:D:231:MET:CE	2:D:251:ALA:HB2	2.30	0.62
2:D:453:ILE:HG21	2:D:479:ILE:HD12	1.79	0.62
1:F:287:THR:HG21	1:F:425:ILE:O	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:MET:CB	2:B:62:ASN:HD22	2.12	0.62
2:B:305:ALA:CB	2:B:374:ARG:HD2	2.21	0.62
2:D:356:LEU:HD22	2:D:387:VAL:HG11	1.80	0.62
1:F:320:SEP:N	1:F:320:SEP:O2P	2.33	0.62
1:F:186:GLU:OE2	1:F:187:GLU:N	2.32	0.62
1:A:379:SER:OG	1:A:382:ALA:CB	2.48	0.62
2:B:356:LEU:HD22	2:B:387:VAL:HG11	1.81	0.62
2:B:471:MET:HE2	2:B:478:ASP:HB3	1.81	0.62
2:D:148:THR:CG2	2:D:193:ARG:HD2	2.29	0.62
2:D:18:ILE:HD13	2:D:40:ARG:HH12	1.64	0.62
2:E:437:ILE:CD1	2:E:457:LYS:HE2	2.29	0.62
1:A:499:VAL:O	1:A:499:VAL:HG12	1.99	0.62
2:E:287:THR:HG22	2:E:288:GLY:H	1.63	0.62
1:A:258:SER:OG	1:F:326:ARG:HD3	1.99	0.62
2:C:148:THR:CG2	2:C:193:ARG:HD2	2.29	0.62
2:D:344:LEU:HD13	2:D:344:LEU:C	2.20	0.62
2:E:182:THR:HG21	2:E:192:ALA:HB1	1.82	0.62
2:E:439:LEU:HD12	2:E:440:LEU:N	2.14	0.62
1:A:256:GLN:HG3	1:F:320:SEP:P	2.40	0.62
2:C:232:LYS:N	2:C:232:LYS:HD2	2.14	0.61
1:F:134:ILE:HD11	1:F:142:VAL:CG2	2.29	0.61
1:F:315:PHE:CE1	1:F:375:ILE:HD11	2.35	0.61
1:F:298:VAL:HG22	1:F:411:LEU:HD23	1.80	0.61
2:B:300:ARG:CA	2:B:333:MET:HE1	2.30	0.61
2:C:371:LYS:CD	2:C:371:LYS:O	2.47	0.61
2:E:444:GLU:OE1	1:F:490:ILE:HG12	1.99	0.61
2:E:296:LEU:HD13	2:E:331:TRP:CD2	2.36	0.61
2:E:304:ASN:HB3	2:E:374:ARG:NH1	2.14	0.61
1:A:356:LEU:HD13	1:A:387:VAL:HG21	1.81	0.61
1:A:274:CYS:N	1:A:463:HIS:O	2.31	0.61
2:B:31:ILE:HA	2:B:231:MET:SD	2.41	0.61
2:E:485:ASN:ND2	2:E:496:ARG:HH11	1.99	0.61
1:F:344:LEU:HD22	1:F:345:LYS:N	2.15	0.61
1:A:89:SER:CB	2:B:227:GLY:O	2.48	0.61
2:D:41:SER:HB3	2:D:178:THR:HB	1.83	0.61
2:D:222:ILE:N	2:D:222:ILE:CD1	2.63	0.61
2:D:445:ILE:HA	2:D:496:ARG:HH12	1.65	0.61
2:E:356:LEU:HD13	2:E:387:VAL:HG21	1.81	0.61
2:E:451:ARG:HD2	2:E:451:ARG:N	2.16	0.61
1:A:148:THR:HG21	1:A:183:GLU:HG3	1.81	0.61
1:A:327:ASN:ND2	1:A:331:TRP:CH2	2.69	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:HG2	1:A:402:TYR:CE2	2.35	0.61
2:D:426:THR:HG21	2:D:430:ILE:HG12	1.82	0.61
1:A:183:GLU:HB2	2:B:199:PHE:CE1	2.35	0.61
1:A:377:ILE:HD13	1:A:412:PHE:CE2	2.36	0.61
2:B:117:VAL:O	2:B:117:VAL:HG12	2.01	0.61
2:C:20:LYS:HE3	2:C:228:THR:HG21	1.82	0.61
1:F:311:ARG:HD2	1:F:371:LYS:HE3	1.83	0.61
2:B:379:SER:CA	2:B:413:THR:HG22	2.31	0.61
2:D:79:THR:CG2	2:D:82:ASP:H	2.12	0.61
1:F:106:LEU:C	1:F:106:LEU:HD12	2.21	0.61
1:F:200:VAL:O	1:F:200:VAL:HG12	2.00	0.61
1:F:296:LEU:HD13	1:F:331:TRP:CD2	2.35	0.61
1:F:499:VAL:HG13	1:F:500:ASP:OD1	2.01	0.61
1:A:441:GLN:HE22	1:A:490:ILE:HD13	1.65	0.61
2:C:28:PHE:CA	2:C:246:ILE:HD12	2.31	0.61
2:C:469:GLU:HG3	2:C:480:LYS:HE3	1.81	0.61
2:E:496:ARG:HG3	2:E:497:ILE:N	2.14	0.61
2:B:335:PHE:O	2:B:339:GLU:HG3	2.01	0.60
2:B:221:GLU:HG3	2:B:233:GLY:O	2.01	0.60
2:B:284:ILE:HD12	2:B:410:GLY:O	2.01	0.60
2:C:269:ARG:O	2:C:273:MET:HG3	2.01	0.60
1:F:170:ARG:HB3	1:F:170:ARG:NH1	2.16	0.60
1:F:300:ARG:N	1:F:333:MET:HE1	2.17	0.60
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.64	0.60
1:A:316:ALA:O	1:A:348:CYS:HA	2.01	0.60
2:B:80:PRO:HB3	2:B:105:ILE:HG21	1.82	0.60
2:D:433:ILE:HG22	2:D:433:ILE:O	2.00	0.60
2:E:287:THR:CG2	2:E:414:ASN:HD22	2.10	0.60
1:F:451:ARG:HH11	1:F:451:ARG:HG2	1.66	0.60
1:A:462:TRP:O	1:A:463:HIS:ND1	2.34	0.60
2:C:418:GLN:HB2	2:D:423:HIS:O	2.01	0.60
1:A:161:ARG:NH2	1:F:149:SER:HB3	2.17	0.60
2:C:164:LEU:HB3	2:C:200:VAL:HG11	1.83	0.60
2:B:195:GLY:HA2	2:B:198:GLU:OE1	2.00	0.60
2:C:24:MET:HB2	2:C:62:ASN:HD22	1.66	0.60
2:E:344:LEU:C	2:E:344:LEU:HD13	2.22	0.60
2:D:151:PHE:C	2:D:153:GLN:H	2.05	0.60
2:E:441:GLN:HE22	2:E:490:ILE:HD13	1.66	0.60
2:B:344:LEU:HD11	2:B:346:ILE:HD11	1.83	0.60
2:B:283:ILE:HD11	2:B:404:LYS:HG3	1.84	0.60
2:C:24:MET:HB2	2:C:62:ASN:ND2	2.17	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:HD3	2:D:15:HIS:O	2.01	0.60
1:A:471:MET:HB3	1:A:480:LYS:NZ	2.15	0.60
2:B:237:PHE:CB	2:B:246:ILE:HG12	2.32	0.60
1:A:31:ILE:CD1	1:A:246:ILE:HG21	2.26	0.59
2:C:287:THR:CG2	2:C:414:ASN:HD22	2.12	0.59
2:E:164:LEU:HB3	2:E:200:VAL:HG11	1.84	0.59
2:E:284:ILE:HD12	2:E:284:ILE:N	2.17	0.59
2:E:499:VAL:HG12	2:E:499:VAL:O	2.02	0.59
2:B:219:THR:HB	2:B:234:GLU:HB3	1.84	0.59
2:B:382:ALA:O	2:B:385:ARG:HB2	2.02	0.59
2:C:239:ILE:HG12	2:C:244:ILE:HD13	1.84	0.59
2:D:169:ALA:O	2:D:173:GLN:HG3	2.02	0.59
2:D:267:VAL:CG2	2:D:300:ARG:HG2	2.30	0.59
2:D:47:THR:O	2:D:50:THR:HG23	2.02	0.59
2:E:426:THR:HG22	2:E:428:SER:N	2.17	0.59
1:A:98:VAL:HA	1:A:103:LEU:O	2.01	0.59
2:B:448:GLU:HG2	2:C:466:ALA:HA	1.84	0.59
2:C:182:THR:HG21	2:C:192:ALA:CB	2.31	0.59
2:D:130:ILE:O	2:D:134:ILE:HG12	2.02	0.59
2:D:356:LEU:CD2	2:D:387:VAL:HG11	2.33	0.59
1:A:164:LEU:CD1	1:A:197:GLU:HG3	2.32	0.59
1:A:495:THR:HG22	1:A:497:ILE:HG23	1.84	0.59
2:C:454:ASN:HB2	2:C:467:ILE:HD13	1.84	0.59
1:A:392:PHE:HE2	1:A:430:ILE:HD11	1.67	0.59
2:B:377:ILE:HD13	2:B:412:PHE:CE2	2.37	0.59
2:C:395:PHE:O	2:C:399:VAL:HG23	2.02	0.59
2:D:122:ASP:O	2:D:123:LEU:CB	2.51	0.59
2:E:294:LYS:HB2	3:E:901:ATP:O1B	2.02	0.59
1:A:370:PHE:CD2	1:A:372:PRO:HG3	2.34	0.59
2:C:437:ILE:HD11	2:C:457:LYS:HE2	1.84	0.59
2:C:471:MET:HG3	2:C:478:ASP:HB3	1.85	0.59
1:F:461:SER:OG	1:F:462:TRP:N	2.34	0.59
1:A:161:ARG:HB2	1:A:196:VAL:HG11	1.83	0.59
2:D:317:TYR:OH	2:D:363:ILE:HD11	2.02	0.59
1:A:203:ASN:HB3	1:A:225:LEU:CD2	2.28	0.59
1:A:318:GLU:OE1	2:B:432:GLU:CB	2.50	0.59
2:D:220:LEU:HD13	2:D:246:ILE:CD1	2.32	0.59
2:D:287:THR:HG21	2:D:425:ILE:O	2.03	0.59
2:D:478:ASP:HA	5:D:555:HOH:O	2.01	0.59
2:E:269:ARG:O	2:E:273:MET:HG3	2.03	0.59
2:C:387:VAL:HG12	2:C:388:SER:N	2.18	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:ASP:HB3	2:C:429:HIS:CE1	2.38	0.58
2:C:262:ARG:HH22	2:C:461:SER:CB	2.15	0.58
2:C:340:ARG:O	2:C:342:ASN:N	2.36	0.58
2:D:182:THR:HG21	2:D:192:ALA:HB1	1.84	0.58
1:A:325:LEU:HD23	1:A:335:PHE:CB	2.32	0.58
1:A:311:ARG:HB3	1:A:370:PHE:CE2	2.39	0.58
2:C:21:MET:HE3	2:C:141:ARG:CZ	2.31	0.58
1:F:313:ILE:HD12	1:F:367:ILE:HD13	1.85	0.58
1:A:257:ARG:HH22	1:A:407:GLU:HG2	1.66	0.58
1:A:402:TYR:O	1:A:406:GLU:HB2	2.03	0.58
1:A:287:THR:CG2	1:A:414:ASN:HD22	2.16	0.58
2:D:161:ARG:HD2	2:D:196:VAL:HG13	1.85	0.58
2:D:31:ILE:HG21	2:D:222:ILE:HD13	1.86	0.58
2:D:363:ILE:O	2:D:367:ILE:HG12	2.03	0.58
1:F:31:ILE:CD1	1:F:246:ILE:HG21	2.33	0.58
1:A:371:LYS:N	1:A:372:PRO:HD3	2.17	0.58
2:C:70:PRO:HD2	2:C:140:ARG:HG2	1.85	0.58
2:C:79:THR:HG22	2:C:82:ASP:HB2	1.86	0.58
2:E:184:ARG:C	2:E:185:ILE:HD13	2.24	0.58
1:A:265:SER:O	1:A:301:PHE:HA	2.04	0.58
1:A:284:ILE:HD12	1:A:284:ILE:H	1.67	0.58
2:B:300:ARG:HA	2:B:333:MET:HE1	1.84	0.58
2:B:451:ARG:NH1	2:B:451:ARG:HG2	2.12	0.58
2:C:311:ARG:HD2	2:C:371:LYS:HE3	1.86	0.58
2:C:313:ILE:HD11	2:C:370:PHE:HB3	1.84	0.58
2:D:79:THR:CG2	2:D:81:GLN:HG2	2.33	0.58
2:E:344:LEU:HD22	2:E:345:LYS:N	2.18	0.58
1:F:375:ILE:O	1:F:410:GLY:HA2	2.04	0.58
1:F:484:ARG:HH11	1:F:484:ARG:HB3	1.68	0.58
2:D:396:VAL:O	2:D:400:THR:HB	2.04	0.58
1:F:148:THR:HG21	1:F:193:ARG:HD2	1.84	0.58
2:C:451:ARG:NH1	2:C:451:ARG:HG2	2.18	0.58
2:D:182:THR:HG22	2:D:183:GLU:H	1.67	0.58
1:A:127:ILE:HD11	1:A:167:LEU:CD1	2.33	0.58
1:A:305:ALA:CB	1:A:374:ARG:HD2	2.25	0.58
2:B:151:PHE:C	2:B:153:GLN:H	2.07	0.58
2:D:418:GLN:HB2	2:E:423:HIS:O	2.04	0.58
2:E:140:ARG:HB3	2:E:140:ARG:HH11	1.68	0.58
1:F:426:THR:HB	1:F:431:GLU:OE2	2.03	0.58
2:B:51:GLY:N	3:B:903:ATP:O1B	2.36	0.58
2:E:377:ILE:CD1	2:E:399:VAL:HG11	2.33	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:LYS:NZ	1:F:407:GLU:HB3	2.19	0.58
1:F:352:GLU:CD	1:F:352:GLU:H	2.07	0.58
1:F:357:GLU:HG3	1:F:358:ASP:N	2.18	0.58
1:A:64:ILE:HG22	1:A:65:ILE:HD13	1.86	0.58
2:B:496:ARG:HG2	2:B:498:THR:HG23	1.86	0.58
2:D:192:ALA:HB3	2:D:197:GLU:OE2	2.04	0.58
2:D:266:GLY:O	2:D:300:ARG:HG3	2.04	0.58
1:F:287:THR:HG23	1:F:414:ASN:ND2	2.14	0.58
1:A:272:GLU:C	1:A:273:MET:O	2.36	0.57
2:B:305:ALA:HB2	2:B:374:ARG:CD	2.21	0.57
2:E:123:LEU:CD2	2:E:127:ILE:HD11	2.33	0.57
2:E:50:THR:HG22	2:E:209:ASN:HB2	1.86	0.57
1:A:371:LYS:O	1:A:371:LYS:CD	2.52	0.57
1:A:379:SER:OG	1:A:382:ALA:HB2	2.04	0.57
2:B:285:LEU:HD23	2:B:437:ILE:CD1	2.31	0.57
2:C:147:VAL:HG11	2:C:180:MET:HE3	1.85	0.57
2:D:218:ARG:CZ	2:D:239:ILE:HD12	2.34	0.57
1:F:306:CYS:SG	1:F:344:LEU:HB2	2.44	0.57
2:B:194:TYR:O	2:B:196:VAL:HG23	2.05	0.57
2:C:353:SER:O	2:C:354:ALA:HB2	2.04	0.57
2:C:79:THR:HG23	2:C:82:ASP:H	1.69	0.57
2:D:191:ILE:HB	2:D:198:GLU:HG3	1.85	0.57
2:E:140:ARG:HH11	2:E:140:ARG:CB	2.17	0.57
2:E:283:ILE:HG23	2:E:412:PHE:CE1	2.39	0.57
1:A:150:VAL:HG13	1:A:151:PHE:N	2.18	0.57
1:A:483:PHE:HB3	1:A:486:PHE:CD1	2.40	0.57
2:B:191:ILE:HB	2:B:198:GLU:CD	2.25	0.57
2:C:486:PHE:CB	2:C:489:ILE:HD11	2.34	0.57
2:D:47:THR:HG22	2:D:184:ARG:O	2.03	0.57
1:F:118:VAL:O	1:F:118:VAL:HG13	2.03	0.57
1:A:254:LEU:HD22	1:F:348:CYS:SG	2.45	0.57
1:A:363:ILE:O	1:A:367:ILE:HG12	2.05	0.57
2:C:14:GLU:HG3	2:C:16:GLN:H	1.69	0.57
2:C:334:ASP:OD1	2:C:336:GLU:HB2	2.05	0.57
2:D:31:ILE:HD11	2:D:246:ILE:HG21	1.85	0.57
2:D:79:THR:HG22	2:D:82:ASP:N	2.15	0.57
2:D:183:GLU:HB2	2:E:199:PHE:CE1	2.39	0.57
1:F:74:VAL:HB	1:F:144:ILE:HD13	1.86	0.57
2:D:296:LEU:HD12	2:D:296:LEU:O	2.05	0.57
2:D:79:THR:HG23	2:D:81:GLN:HG2	1.86	0.57
1:F:76:PHE:O	1:F:109:SER:HA	2.04	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:THR:OG1	1:F:182:THR:HG23	2.04	0.57
1:F:321:ARG:O	1:F:325:LEU:HD12	2.05	0.57
1:A:311:ARG:HD2	1:A:371:LYS:CE	2.35	0.57
1:A:469:GLU:HB2	1:A:483:PHE:CZ	2.39	0.57
2:D:182:THR:CG2	2:D:183:GLU:N	2.67	0.57
1:A:266:GLY:CA	1:A:300:ARG:HG3	2.35	0.57
1:A:302:VAL:HG12	1:A:303:GLU:N	2.20	0.57
1:A:311:ARG:HD2	1:A:371:LYS:HE3	1.86	0.57
2:B:81:GLN:CD	2:B:81:GLN:H	2.08	0.57
2:C:353:SER:O	2:C:354:ALA:CB	2.53	0.57
2:C:377:ILE:HD12	2:C:412:PHE:HE2	1.68	0.57
1:A:313:ILE:CD1	1:A:372:PRO:HG2	2.34	0.57
2:B:334:ASP:O	2:B:338:MET:HG2	2.04	0.57
2:B:294:LYS:N	3:B:901:ATP:O1B	2.37	0.57
2:E:441:GLN:NE2	2:E:490:ILE:HD13	2.20	0.57
2:E:214:GLU:HB3	1:F:234:GLU:HB2	1.86	0.57
2:B:264:SER:HA	2:B:271:ASP:OD1	2.05	0.57
2:C:397:ILE:H	2:C:397:ILE:HD13	1.69	0.57
2:D:296:LEU:HA	2:D:331:TRP:CZ3	2.40	0.57
2:E:379:SER:N	2:E:413:THR:HB	2.17	0.57
1:A:439:LEU:HD12	1:A:440:LEU:N	2.20	0.56
2:B:150:VAL:O	2:B:153:GLN:HG3	2.05	0.56
1:F:16:GLN:HE22	1:F:33:HIS:HB3	1.70	0.56
1:A:263:VAL:HG12	1:A:374:ARG:NH2	2.18	0.56
1:A:479:ILE:H	1:A:479:ILE:HD12	1.69	0.56
2:E:287:THR:HG21	2:E:425:ILE:O	2.06	0.56
1:A:487:GLU:HG3	1:A:497:ILE:CD1	2.34	0.56
2:C:33:HIS:CD2	2:C:230:HIS:HA	2.41	0.56
2:C:325:LEU:HD23	2:C:335:PHE:HB2	1.87	0.56
2:D:31:ILE:CG2	2:D:222:ILE:CD1	2.84	0.56
2:E:163:GLU:HA	2:E:163:GLU:OE2	2.05	0.56
2:E:302:VAL:CG1	2:E:344:LEU:HD23	2.35	0.56
2:E:441:GLN:HE22	2:E:490:ILE:HA	1.70	0.56
1:F:371:LYS:CD	1:F:371:LYS:O	2.54	0.56
2:B:264:SER:HB3	2:B:304:ASN:HD21	1.70	0.56
2:C:431:GLU:HA	2:C:434:THR:HG22	1.87	0.56
2:D:487:GLU:OE1	2:D:497:ILE:HD13	2.05	0.56
2:E:23:THR:OG1	2:E:29:ASP:OD1	2.24	0.56
1:F:273:MET:O	1:F:463:HIS:HA	2.05	0.56
1:A:271:ASP:C	1:A:273:MET:O	2.44	0.56
1:A:328:ALA:O	1:A:333:MET:HG2	2.05	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:SER:HA	1:A:178:THR:O	2.06	0.56
2:B:248:PRO:HB2	2:B:251:ALA:HB3	1.87	0.56
2:B:88:ARG:HG2	2:B:88:ARG:HH11	1.70	0.56
2:E:148:THR:CG2	2:E:193:ARG:HD2	2.35	0.56
1:F:352:GLU:N	1:F:352:GLU:CD	2.59	0.56
1:F:484:ARG:CB	1:F:484:ARG:NH1	2.68	0.56
1:F:504:GLU:O	1:F:505:LEU:HB2	2.03	0.56
1:A:463:HIS:O	1:A:464:ASP:HB3	2.06	0.56
2:B:205:VAL:CG2	2:B:222:ILE:HD13	2.35	0.56
2:B:41:SER:OG	2:B:168:VAL:HG13	2.05	0.56
2:B:444:GLU:OE2	2:C:489:ILE:HG12	2.05	0.56
2:C:444:GLU:OE2	2:D:489:ILE:HG13	2.06	0.56
1:A:14:GLU:CG	1:A:15:HIS:N	2.60	0.56
1:A:153:GLN:O	1:A:154:TYR:HD2	1.87	0.56
2:B:418:GLN:HG3	2:B:418:GLN:O	2.06	0.56
2:C:18:ILE:HB	2:C:228:THR:HG23	1.88	0.56
2:E:497:ILE:HG22	2:E:498:THR:H	1.70	0.56
2:B:185:ILE:H	2:B:185:ILE:HD12	1.71	0.56
2:C:283:ILE:HD13	2:C:404:LYS:HE3	1.87	0.56
2:E:70:PRO:HB2	2:E:139:ALA:HA	1.88	0.56
2:E:356:LEU:CD1	2:E:387:VAL:HG21	2.36	0.56
1:F:134:ILE:HD13	1:F:139:ALA:HB3	1.88	0.56
1:A:88:ARG:NH1	1:A:88:ARG:HG2	2.20	0.56
2:C:393:ARG:NH2	2:C:429:HIS:HB2	2.21	0.56
2:D:347:VAL:HG12	2:D:348:CYS:N	2.20	0.56
2:E:462:TRP:CD2	2:E:463:HIS:O	2.59	0.56
1:F:144:ILE:CG2	1:F:147:VAL:HG12	2.36	0.56
2:B:196:VAL:O	2:B:200:VAL:HG23	2.06	0.55
2:C:54:LEU:CD2	2:C:244:ILE:HG12	2.36	0.55
2:D:76:PHE:CZ	2:D:126:LEU:HD21	2.41	0.55
1:A:347:VAL:O	1:A:348:CYS:HB2	2.06	0.55
2:B:462:TRP:O	2:B:463:HIS:CD2	2.60	0.55
2:B:64:ILE:HG21	2:B:97:LEU:HD13	1.88	0.55
2:C:238:THR:HG22	2:C:239:ILE:N	2.21	0.55
1:F:344:LEU:HD13	1:F:344:LEU:C	2.27	0.55
1:A:121:PHE:O	1:A:125:ALA:HB2	2.05	0.55
1:A:333:MET:O	1:A:334:ASP:HB2	2.06	0.55
1:A:471:MET:CE	1:A:478:ASP:HB3	2.36	0.55
2:C:21:MET:O	2:C:35:GLY:HA3	2.07	0.55
2:D:340:ARG:O	2:D:342:ASN:N	2.38	0.55
2:E:191:ILE:HD12	2:E:206:ILE:HD11	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:291:GLY:HA3	1:F:442:TYR:OH	2.07	0.55
1:A:323:GLN:CB	2:B:258:SER:OG	2.54	0.55
2:B:90:PHE:HB2	2:B:92:TRP:CE2	2.41	0.55
2:C:238:THR:HG22	2:C:239:ILE:H	1.70	0.55
2:D:191:ILE:CD1	2:D:198:GLU:HG2	2.36	0.55
2:D:76:PHE:HZ	2:D:126:LEU:HD21	1.70	0.55
2:D:89:SER:HB2	2:E:227:GLY:O	2.07	0.55
2:E:396:VAL:HG11	2:E:430:ILE:HG21	1.89	0.55
1:F:191:ILE:CB	1:F:198:GLU:CG	2.84	0.55
2:B:150:VAL:HG13	2:B:151:PHE:N	2.22	0.55
2:C:144:ILE:CG2	2:C:147:VAL:HG12	2.36	0.55
2:C:471:MET:CG	2:C:478:ASP:HB3	2.37	0.55
2:C:67:PHE:HB2	2:C:69:GLU:HG3	1.88	0.55
2:E:150:VAL:CG1	2:E:151:PHE:N	2.69	0.55
2:E:193:ARG:NH2	1:F:195:GLY:O	2.32	0.55
1:A:18:ILE:CD1	1:F:85:LYS:HG3	2.36	0.55
1:A:317:TYR:OH	1:A:363:ILE:HD11	2.07	0.55
2:C:225:LEU:HD12	2:C:230:HIS:HB3	1.89	0.55
2:E:348:CYS:HB3	1:F:254:LEU:HD23	1.89	0.55
1:F:443:VAL:CG1	1:F:445:ILE:HD11	2.37	0.55
2:C:336:GLU:OE1	2:C:336:GLU:HA	2.07	0.55
1:F:316:ALA:O	1:F:348:CYS:HA	2.06	0.55
1:F:486:PHE:HE2	1:F:496:ARG:HD2	1.68	0.55
1:F:508:ILE:O	1:F:509:VAL:HB	2.06	0.55
1:A:505:LEU:O	1:A:508:ILE:HD11	2.06	0.55
2:B:313:ILE:HG13	2:B:372:PRO:CG	2.37	0.55
2:C:340:ARG:C	2:C:342:ASN:H	2.09	0.55
2:E:20:LYS:HE3	2:E:228:THR:HG21	1.88	0.55
2:E:313:ILE:HG13	2:E:372:PRO:HG2	1.89	0.55
1:F:371:LYS:HD2	1:F:371:LYS:O	2.07	0.55
1:A:287:THR:HG23	1:A:414:ASN:HB3	1.89	0.55
1:A:400:THR:HG22	1:A:401:GLY:N	2.22	0.55
2:E:294:LYS:N	3:E:901:ATP:O1B	2.39	0.55
1:F:336:GLU:HB3	1:F:340:ARG:NH2	2.21	0.55
1:F:501:GLU:HG3	1:F:502:LYS:N	2.22	0.55
1:A:448:GLU:HG2	2:B:466:ALA:HB2	1.89	0.55
2:C:397:ILE:N	2:C:397:ILE:CD1	2.69	0.55
2:E:145:ASP:OD2	2:E:181:THR:HG21	2.06	0.55
2:E:336:GLU:HA	2:E:336:GLU:OE1	2.05	0.55
2:E:451:ARG:HH11	2:E:451:ARG:HG2	1.72	0.55
1:A:200:VAL:HG12	1:A:200:VAL:O	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:HD22	1:A:472:ILE:HD12	1.87	0.54
2:B:205:VAL:HG23	2:B:222:ILE:HD13	1.89	0.54
1:A:322:ALA:HB3	2:B:256:GLN:O	2.06	0.54
2:B:265:SER:HB2	2:B:270:LEU:HD13	1.90	0.54
2:B:81:GLN:H	2:B:81:GLN:NE2	2.04	0.54
2:D:215:ARG:HA	2:D:215:ARG:NE	2.22	0.54
2:D:387:VAL:CG1	2:D:388:SER:N	2.70	0.54
2:D:443:VAL:HG12	2:D:445:ILE:HD11	1.89	0.54
2:E:86:ASN:OD1	1:F:18:ILE:HD11	2.06	0.54
1:F:280:LYS:HZ3	1:F:407:GLU:HB3	1.73	0.54
1:F:486:PHE:HB2	1:F:489:ILE:HD11	1.89	0.54
1:A:43:LEU:HD11	1:A:182:THR:OG1	2.07	0.54
2:B:129:ARG:O	2:B:132:TYR:HB3	2.07	0.54
2:B:202:ASP:HA	2:B:226:ARG:HD2	1.89	0.54
2:B:93:ASP:OD1	2:B:95:ALA:HB3	2.07	0.54
2:C:206:ILE:N	2:C:206:ILE:HD12	2.22	0.54
2:D:484:ARG:HH11	2:D:484:ARG:HB3	1.72	0.54
2:E:347:VAL:HG12	2:E:348:CYS:N	2.21	0.54
2:E:79:THR:HG21	2:E:81:GLN:HG2	1.88	0.54
1:F:169:ALA:O	1:F:173:GLN:HG3	2.07	0.54
1:F:23:THR:HB	1:F:25:ILE:HG12	1.88	0.54
2:B:479:ILE:N	2:B:479:ILE:HD12	2.20	0.54
2:E:169:ALA:O	2:E:173:GLN:HG3	2.07	0.54
2:B:286:ALA:HA	2:B:438:ILE:O	2.08	0.54
2:C:464:ASP:OD1	2:C:465:LYS:N	2.40	0.54
2:D:323:GLN:NE2	2:E:459:ARG:HD3	2.22	0.54
2:D:426:THR:HG22	2:D:428:SER:H	1.72	0.54
1:A:56:SER:HB2	1:A:143:SER:HB3	1.89	0.54
2:B:178:THR:HG22	2:B:179:VAL:N	2.22	0.54
2:C:111:ASP:O	2:C:113:GLU:N	2.34	0.54
2:C:127:ILE:CD1	2:C:167:LEU:HD13	2.37	0.54
2:C:426:THR:HG22	2:C:428:SER:H	1.72	0.54
2:C:437:ILE:HD12	2:C:437:ILE:N	2.22	0.54
2:C:461:SER:OG	2:C:462:TRP:N	2.39	0.54
2:D:443:VAL:CG1	2:D:445:ILE:HD11	2.38	0.54
1:F:117:VAL:O	1:F:118:VAL:HB	2.07	0.54
2:B:273:MET:O	2:B:464:ASP:N	2.36	0.54
2:C:127:ILE:HD13	2:C:127:ILE:N	2.23	0.54
2:D:195:GLY:HA2	2:D:198:GLU:OE1	2.08	0.54
2:D:263:VAL:HG12	2:D:374:ARG:NH2	2.22	0.54
2:E:54:LEU:HD23	2:E:244:ILE:HD11	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ILE:HD13	1:A:508:ILE:N	2.19	0.54
2:B:24:MET:HB2	2:B:62:ASN:HD22	1.72	0.54
2:B:256:GLN:HE21	2:B:404:LYS:HB3	1.72	0.54
1:F:126:LEU:O	1:F:130:ILE:HG12	2.06	0.54
1:F:45:SER:HB2	1:F:182:THR:HB	1.89	0.54
1:A:455:VAL:HG11	1:A:463:HIS:CD2	2.40	0.54
1:A:502:LYS:O	1:A:503:SER:HB3	2.08	0.54
2:B:38:ILE:HA	2:B:177:THR:CG2	2.38	0.54
2:B:21:MET:CB	2:B:38:ILE:HG12	2.37	0.54
2:B:46:GLY:CA	2:B:50:THR:HG21	2.35	0.54
2:D:31:ILE:CG2	2:D:222:ILE:HD13	2.38	0.54
2:D:394:GLN:HA	2:D:397:ILE:HD12	1.88	0.54
1:F:469:GLU:HG3	1:F:470:PHE:N	2.23	0.54
2:B:31:ILE:HD13	2:B:231:MET:SD	2.47	0.54
2:B:372:PRO:O	2:B:408:ILE:HD12	2.08	0.54
1:F:197:GLU:H	1:F:197:GLU:CD	2.11	0.54
1:F:313:ILE:HB	1:F:375:ILE:CD1	2.35	0.54
1:A:296:LEU:HD13	1:A:331:TRP:CE2	2.42	0.54
1:A:470:PHE:HE1	1:A:472:ILE:HD11	1.73	0.54
2:B:264:SER:HB3	2:B:304:ASN:ND2	2.22	0.54
2:B:67:PHE:HB2	2:B:69:GLU:HG3	1.89	0.54
2:D:443:VAL:O	2:D:445:ILE:CD1	2.54	0.54
1:A:20:LYS:HD3	1:A:35:GLY:O	2.07	0.53
2:D:225:LEU:HD12	2:D:230:HIS:HB3	1.90	0.53
2:E:127:ILE:CD1	2:E:167:LEU:HD13	2.38	0.53
2:E:325:LEU:CD2	2:E:335:PHE:HB2	2.38	0.53
1:F:294:LYS:N	3:F:901:ATP:O1B	2.41	0.53
1:A:378:ASP:O	1:A:379:SER:CB	2.57	0.53
2:C:31:ILE:HA	2:C:231:MET:SD	2.48	0.53
2:D:317:TYR:CE2	2:D:383:LEU:HD21	2.43	0.53
2:E:152:GLN:HG3	1:F:161:ARG:HH11	1.73	0.53
1:A:123:LEU:O	1:A:127:ILE:HG12	2.09	0.53
1:A:372:PRO:HB2	1:A:375:ILE:CD1	2.38	0.53
2:C:283:ILE:CD1	2:C:404:LYS:HG3	2.37	0.53
2:D:106:LEU:CD1	2:D:129:ARG:NH2	2.72	0.53
2:D:256:GLN:HG3	2:D:404:LYS:HD3	1.90	0.53
2:D:419:PHE:O	2:D:420:MET:HB2	2.08	0.53
2:E:347:VAL:O	2:E:348:CYS:HB2	2.08	0.53
1:A:41:SER:CB	1:A:178:THR:HB	2.29	0.53
1:A:336:GLU:O	1:A:339:GLU:HB2	2.08	0.53
1:A:462:TRP:O	1:A:463:HIS:CG	2.61	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ILE:N	2:B:206:ILE:HD12	2.24	0.53
2:D:151:PHE:O	2:D:153:GLN:N	2.38	0.53
2:D:80:PRO:O	2:D:84:ILE:HG12	2.08	0.53
2:E:79:THR:CG2	2:E:82:ASP:H	2.21	0.53
1:F:178:THR:HG22	1:F:179:VAL:N	2.23	0.53
1:F:414:ASN:ND2	1:F:426:THR:HG23	2.23	0.53
2:E:449:MET:HE3	1:F:467:ILE:HD11	1.90	0.53
1:A:183:GLU:CB	2:B:199:PHE:CE1	2.91	0.53
2:B:469:GLU:HG3	2:B:470:PHE:N	2.23	0.53
2:B:483:PHE:HB3	2:B:486:PHE:CD1	2.29	0.53
2:B:84:ILE:HA	2:B:94:LEU:HD12	1.89	0.53
2:C:248:PRO:HB2	2:C:251:ALA:HB3	1.90	0.53
1:A:374:ARG:O	1:A:375:ILE:HD12	2.08	0.53
2:B:191:ILE:CB	2:B:198:GLU:HG3	2.39	0.53
2:C:356:LEU:HD22	2:C:387:VAL:HG11	1.91	0.53
2:D:178:THR:HG22	2:D:179:VAL:N	2.23	0.53
2:D:468:ARG:HH11	2:D:468:ARG:HG2	1.74	0.53
2:E:287:THR:HG22	2:E:288:GLY:N	2.23	0.53
1:F:125:ALA:O	1:F:129:ARG:HG3	2.07	0.53
1:F:443:VAL:O	1:F:445:ILE:HD12	2.07	0.53
1:F:56:SER:HB2	1:F:143:SER:HB3	1.90	0.53
1:A:170:ARG:O	1:A:174:ILE:HG12	2.09	0.53
1:A:327:ASN:OD1	2:B:459:ARG:O	2.27	0.53
1:A:376:ALA:HA	1:A:411:LEU:O	2.09	0.53
2:B:18:ILE:HB	2:B:228:THR:CG2	2.38	0.53
2:C:308:ASN:O	2:C:310:GLU:HG3	2.08	0.53
2:D:446:ARG:H	2:D:496:ARG:HH22	1.57	0.53
2:C:123:LEU:HA	2:C:127:ILE:CD1	2.39	0.53
2:D:150:VAL:O	2:D:153:GLN:HG3	2.09	0.53
2:D:21:MET:HE3	2:D:59:PHE:CZ	2.44	0.53
2:B:123:LEU:O	2:B:123:LEU:HD13	2.09	0.53
2:C:347:VAL:O	2:C:348:CYS:HB2	2.08	0.53
2:D:31:ILE:HG21	2:D:222:ILE:HD11	1.90	0.53
1:A:280:LYS:O	1:A:409:THR:OG1	2.23	0.53
1:A:31:ILE:HD11	1:A:246:ILE:CG2	2.30	0.53
1:A:296:LEU:CD2	1:A:472:ILE:HD12	2.39	0.53
2:C:378:ASP:O	2:C:379:SER:HB3	2.09	0.53
2:D:140:ARG:HH11	2:D:140:ARG:CB	2.20	0.53
2:D:150:VAL:HG13	2:D:151:PHE:N	2.23	0.53
2:D:315:PHE:HE1	2:D:375:ILE:HD12	1.73	0.53
2:E:259:SER:N	2:E:281:ASP:OD2	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:LEU:HD11	1:F:346:ILE:HG13	1.89	0.53
1:F:504:GLU:HA	1:F:507:ARG:HG3	1.90	0.53
2:B:220:LEU:HD13	2:B:246:ILE:HD13	1.91	0.52
2:B:64:ILE:HG22	2:B:65:ILE:HD13	1.90	0.52
2:C:123:LEU:HD12	2:C:163:GLU:OE2	2.09	0.52
2:C:126:LEU:O	2:C:129:ARG:HB2	2.10	0.52
2:C:182:THR:CG2	2:C:183:GLU:N	2.72	0.52
2:C:42:THR:HA	2:C:203:ASN:HB2	1.91	0.52
1:A:320:SEP:O1P	2:B:256:GLN:CG	2.57	0.52
2:B:318:GLU:OE2	2:C:432:GLU:HG2	2.10	0.52
2:C:146:SER:HA	2:C:181:THR:O	2.08	0.52
2:C:18:ILE:HD12	2:C:18:ILE:N	2.24	0.52
2:C:486:PHE:CE2	2:C:496:ARG:HG2	2.44	0.52
1:F:115:GLN:HG3	1:F:116:GLU:N	2.23	0.52
1:F:338:MET:HB3	1:F:344:LEU:CB	2.37	0.52
1:F:467:ILE:HG22	1:F:467:ILE:O	2.09	0.52
1:A:306:CYS:SG	1:A:338:MET:SD	3.08	0.52
2:B:298:VAL:HG11	2:B:314:LEU:HD11	1.89	0.52
2:B:320:SER:HA	2:C:254:LEU:HG	1.91	0.52
2:C:267:VAL:HB	2:C:270:LEU:HB2	1.92	0.52
2:D:266:GLY:HA3	2:D:300:ARG:O	2.08	0.52
2:D:451:ARG:HH11	2:D:451:ARG:CG	2.19	0.52
2:D:468:ARG:NH1	2:D:468:ARG:HG2	2.25	0.52
2:E:72:VAL:HG21	2:E:134:ILE:HD13	1.91	0.52
1:A:153:GLN:O	1:A:154:TYR:HB3	2.10	0.52
2:B:379:SER:N	2:B:413:THR:HG22	2.24	0.52
2:B:89:SER:HB2	2:C:227:GLY:O	2.09	0.52
2:C:73:PHE:HD1	2:C:143:SER:HB2	1.74	0.52
2:C:262:ARG:NE	2:C:279:PHE:CE2	2.77	0.52
2:D:470:PHE:CE1	2:D:472:ILE:HD11	2.44	0.52
3:D:903:ATP:O3'	2:E:224:LYS:HB2	2.09	0.52
1:F:170:ARG:HD2	1:F:173:GLN:OE1	2.10	0.52
1:F:291:GLY:HA3	1:F:442:TYR:HH	1.75	0.52
1:F:303:GLU:OE2	1:F:333:MET:HB3	2.10	0.52
1:F:468:ARG:NH1	1:F:468:ARG:HG2	2.25	0.52
1:A:379:SER:OG	1:A:382:ALA:N	2.43	0.52
1:A:510:ARG:HA	1:A:510:ARG:NE	2.25	0.52
2:C:356:LEU:CD2	2:C:387:VAL:HG11	2.39	0.52
2:B:38:ILE:HA	2:B:177:THR:HG23	1.92	0.52
2:B:220:LEU:HD13	2:B:246:ILE:CD1	2.40	0.52
2:C:111:ASP:CG	2:C:113:GLU:HG2	2.30	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:VAL:O	2:C:178:THR:HA	2.09	0.52
2:C:144:ILE:HG21	2:C:147:VAL:HG12	1.92	0.52
2:C:348:CYS:HB3	2:D:254:LEU:HB3	1.89	0.52
2:C:79:THR:HG22	2:C:82:ASP:CB	2.39	0.52
2:E:439:LEU:HD12	2:E:440:LEU:H	1.74	0.52
2:E:437:ILE:HD11	2:E:457:LYS:HE2	1.92	0.52
1:F:161:ARG:HB2	1:F:196:VAL:HG11	1.92	0.52
1:F:445:ILE:HD13	1:F:450:SER:OG	2.08	0.52
1:A:45:SER:CB	1:A:182:THR:HB	2.40	0.52
1:A:479:ILE:HD12	1:A:479:ILE:N	2.25	0.52
1:A:82:ASP:O	1:A:85:LYS:HB3	2.10	0.52
2:B:471:MET:HB3	2:B:480:LYS:HZ1	1.75	0.52
2:D:301:PHE:CE1	2:D:374:ARG:HD3	2.44	0.52
2:E:203:ASN:HB3	2:E:225:LEU:HD23	1.91	0.52
1:F:23:THR:CB	1:F:25:ILE:HG12	2.39	0.52
1:A:206:ILE:N	1:A:206:ILE:HD12	2.24	0.52
1:A:320:SEP:O	1:A:324:LEU:HD12	2.10	0.52
1:A:456:PHE:HE2	1:F:290:THR:HG23	1.73	0.52
1:A:471:MET:HB3	1:A:480:LYS:HZ1	1.73	0.52
2:B:209:ASN:HD21	2:B:216:ARG:HB3	1.74	0.52
2:B:289:ALA:HB2	2:B:419:PHE:HA	1.92	0.52
2:B:51:GLY:O	2:B:52:LYS:C	2.47	0.52
2:E:184:ARG:HD2	2:E:191:ILE:O	2.10	0.52
2:E:469:GLU:HB3	2:E:483:PHE:CZ	2.44	0.52
1:F:500:ASP:O	1:F:501:GLU:CB	2.57	0.52
2:B:145:ASP:HA	2:B:181:THR:HB	1.92	0.52
2:B:232:LYS:N	2:B:232:LYS:HD2	2.24	0.52
2:C:148:THR:HG21	2:C:193:ARG:HD2	1.92	0.52
2:E:160:VAL:HG21	2:E:194:TYR:CD2	2.44	0.52
2:E:299:SER:O	2:E:333:MET:HE2	2.09	0.52
1:A:151:PHE:C	1:A:153:GLN:H	2.14	0.52
1:A:218:ARG:NH1	1:A:239:ILE:HD12	2.25	0.52
2:C:150:VAL:HG13	2:C:151:PHE:N	2.24	0.52
2:C:65:ILE:N	2:C:65:ILE:HD12	2.25	0.52
2:E:313:ILE:HG22	2:E:314:LEU:N	2.25	0.52
1:F:74:VAL:HG21	1:F:130:ILE:HD12	1.91	0.52
1:F:191:ILE:CB	1:F:198:GLU:HG3	2.39	0.52
1:A:284:ILE:HB	1:A:411:LEU:HD12	1.91	0.51
1:A:455:VAL:HG11	1:A:463:HIS:HB2	1.91	0.51
2:C:182:THR:CG2	2:C:183:GLU:H	2.23	0.51
2:C:61:TYR:CD2	2:C:65:ILE:HD13	2.46	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:153:GLN:C	1:F:158:SER:HB2	2.30	0.51
1:F:516:GLY:N	1:F:517:PRO:HD2	2.24	0.51
1:A:254:LEU:O	1:A:254:LEU:CD2	2.57	0.51
1:A:377:ILE:N	1:A:377:ILE:HD12	2.25	0.51
2:B:316:ALA:O	2:B:348:CYS:HA	2.11	0.51
1:A:415:THR:HB	2:B:432:GLU:OE1	2.11	0.51
2:C:495:THR:HG22	2:D:487:GLU:OE2	2.10	0.51
2:C:48:SER:HB2	2:D:199:PHE:CE1	2.46	0.51
2:E:98:VAL:HA	2:E:103:LEU:O	2.10	0.51
2:E:413:THR:HG22	2:E:414:ASN:N	2.25	0.51
2:E:454:ASN:HD21	2:E:456:PHE:HA	1.75	0.51
1:F:220:LEU:C	1:F:220:LEU:HD23	2.30	0.51
1:F:462:TRP:CE3	1:F:463:HIS:N	2.73	0.51
1:A:446:ARG:HA	1:A:496:ARG:NH2	2.25	0.51
1:F:360:LEU:O	1:F:360:LEU:HD22	2.10	0.51
1:A:161:ARG:CB	1:A:196:VAL:HG11	2.40	0.51
1:A:425:ILE:HD13	1:A:437:ILE:HD13	1.92	0.51
1:A:467:ILE:N	1:A:467:ILE:HD12	2.25	0.51
1:A:87:ALA:O	1:A:92:TRP:CD1	2.62	0.51
2:B:315:PHE:CD2	2:B:347:VAL:HG21	2.46	0.51
2:C:123:LEU:CD2	2:C:167:LEU:HB2	2.38	0.51
2:D:203:ASN:HB3	2:D:225:LEU:HD23	1.92	0.51
2:E:496:ARG:C	2:E:497:ILE:HD13	2.31	0.51
1:F:104:PHE:HE2	1:F:106:LEU:HB2	1.76	0.51
1:A:296:LEU:HD13	1:A:331:TRP:CD2	2.46	0.51
2:B:371:LYS:N	2:B:372:PRO:HD3	2.25	0.51
2:D:145:ASP:OD2	2:D:181:THR:HG21	2.11	0.51
2:E:151:PHE:C	2:E:153:GLN:H	2.14	0.51
1:F:270:LEU:O	1:F:273:MET:HB2	2.10	0.51
1:F:315:PHE:HE1	1:F:375:ILE:HD11	1.74	0.51
1:A:279:PHE:HB2	1:A:282:SER:HB3	1.93	0.51
2:B:240:THR:HG21	2:B:361:GLN:HE22	1.76	0.51
2:C:206:ILE:H	2:C:206:ILE:HD12	1.76	0.51
2:C:21:MET:HB2	2:C:38:ILE:HG12	1.93	0.51
2:C:220:LEU:C	2:C:220:LEU:HD23	2.31	0.51
2:C:54:LEU:O	2:C:57:ILE:N	2.44	0.51
2:D:185:ILE:HD12	2:D:185:ILE:H	1.76	0.51
2:D:461:SER:OG	2:D:462:TRP:N	2.43	0.51
2:E:127:ILE:HD12	2:E:167:LEU:CD1	2.41	0.51
1:F:73:PHE:HB3	1:F:105:ILE:HD13	1.91	0.51
1:F:380:LEU:O	1:F:382:ALA:N	2.43	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ILE:HB	2:B:228:THR:HG23	1.93	0.51
2:B:80:PRO:CB	2:B:105:ILE:HG21	2.41	0.51
2:C:121:PHE:N	2:C:121:PHE:CD1	2.79	0.51
2:D:31:ILE:HA	2:D:231:MET:SD	2.51	0.51
2:D:445:ILE:HD12	2:D:445:ILE:N	2.26	0.51
1:F:468:ARG:HH11	1:F:468:ARG:HG2	1.75	0.51
2:B:187:GLU:O	2:B:208:ARG:HD3	2.11	0.51
2:B:161:ARG:NH2	2:B:199:PHE:HB2	2.26	0.51
2:B:469:GLU:HB2	2:B:483:PHE:CZ	2.46	0.51
2:C:85:LYS:NZ	2:D:14:GLU:HB3	2.25	0.51
2:E:52:LYS:HD3	2:E:182:THR:O	2.10	0.51
1:F:451:ARG:HB3	1:F:470:PHE:CE2	2.46	0.51
1:A:433:ILE:CG2	1:A:433:ILE:O	2.59	0.51
1:A:463:HIS:O	1:A:464:ASP:CB	2.59	0.51
1:A:470:PHE:CE1	1:A:472:ILE:HD11	2.45	0.51
2:B:381:SER:HB3	2:B:414:ASN:OD1	2.10	0.51
2:C:151:PHE:C	2:C:153:GLN:N	2.63	0.51
2:C:184:ARG:HG2	2:C:191:ILE:O	2.11	0.51
2:C:431:GLU:O	2:C:432:GLU:HB2	2.09	0.51
2:E:359:HIS:O	2:E:363:ILE:HG12	2.10	0.51
1:A:254:LEU:HD11	1:F:319:GLU:O	2.11	0.51
1:A:70:PRO:HB2	1:A:139:ALA:HA	1.93	0.51
2:B:451:ARG:CG	2:B:451:ARG:NH1	2.74	0.51
2:C:214:GLU:OE2	2:D:217:ARG:NH1	2.44	0.51
2:C:252:MET:HE3	2:C:397:ILE:HG22	1.92	0.51
2:D:437:ILE:CD1	2:D:457:LYS:HE2	2.41	0.51
1:F:320:SEP:O	1:F:324:LEU:HB2	2.10	0.51
1:F:284:ILE:HD12	1:F:410:GLY:O	2.11	0.51
1:A:140:ARG:HH11	1:A:140:ARG:CB	2.23	0.50
2:E:123:LEU:HD23	2:E:127:ILE:CD1	2.37	0.50
2:E:28:PHE:N	2:E:246:ILE:HD12	2.26	0.50
1:F:148:THR:HG21	1:F:183:GLU:HG3	1.93	0.50
1:A:67:PHE:HB2	1:A:69:GLU:HG3	1.93	0.50
2:D:214:GLU:HA	2:E:234:GLU:OE1	2.12	0.50
1:F:312:ALA:HA	1:F:374:ARG:O	2.12	0.50
2:B:147:VAL:HG11	2:B:180:MET:HE2	1.90	0.50
1:A:320:SEP:CB	2:B:254:LEU:O	2.36	0.50
2:B:280:LYS:NZ	2:B:407:GLU:HB3	2.26	0.50
2:B:440:LEU:CD2	2:B:453:ILE:HG12	2.40	0.50
2:C:38:ILE:HA	2:C:177:THR:HG23	1.94	0.50
2:C:28:PHE:HE1	2:C:222:ILE:HD11	1.71	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:150:VAL:CG1	2:D:151:PHE:N	2.75	0.50
2:D:446:ARG:HB3	2:E:484:ARG:HG3	1.93	0.50
2:D:451:ARG:HB3	2:D:470:PHE:CE2	2.45	0.50
2:D:385:ARG:HG2	2:E:393:ARG:NH1	2.26	0.50
1:F:203:ASN:HB3	1:F:225:LEU:CD2	2.40	0.50
1:F:79:THR:HG23	1:F:81:GLN:HG2	1.92	0.50
1:A:116:GLU:O	1:A:117:VAL:HG23	2.10	0.50
1:A:79:THR:HG22	1:A:82:ASP:H	1.76	0.50
2:C:360:LEU:HA	2:C:363:ILE:HD12	1.93	0.50
2:D:211:LEU:HA	2:D:216:ARG:HD3	1.93	0.50
2:D:323:GLN:HE22	2:E:459:ARG:HD3	1.75	0.50
2:D:371:LYS:CD	2:D:371:LYS:O	2.48	0.50
2:E:191:ILE:HD12	2:E:206:ILE:HG13	1.93	0.50
1:A:118:VAL:HG23	1:A:153:GLN:OE1	2.11	0.50
1:A:148:THR:HG21	1:A:183:GLU:CG	2.41	0.50
2:B:485:ASN:N	2:B:485:ASN:OD1	2.44	0.50
2:D:161:ARG:HB2	2:D:196:VAL:CG1	2.41	0.50
2:D:402:TYR:O	2:D:405:GLN:HG2	2.12	0.50
1:F:140:ARG:CB	1:F:140:ARG:HH11	2.24	0.50
1:A:271:ASP:O	1:A:273:MET:O	2.30	0.50
1:A:335:PHE:O	1:A:336:GLU:C	2.48	0.50
2:B:249:LEU:CD1	2:B:394:GLN:HG2	2.42	0.50
2:E:118:VAL:O	2:E:118:VAL:HG12	2.12	0.50
2:E:255:THR:O	2:E:255:THR:HG22	2.11	0.50
1:F:123:LEU:O	1:F:123:LEU:HD13	2.10	0.50
1:F:151:PHE:O	1:F:153:GLN:N	2.42	0.50
1:A:456:PHE:CE2	1:F:290:THR:HG23	2.46	0.50
1:F:313:ILE:HG13	1:F:372:PRO:CG	2.41	0.50
1:A:435:ASP:HA	1:A:459:ARG:HD2	1.93	0.50
2:D:446:ARG:H	2:D:496:ARG:NH2	2.10	0.50
2:E:148:THR:HG21	2:E:183:GLU:CG	2.42	0.50
1:F:18:ILE:HD11	1:F:227:GLY:HA3	1.87	0.50
1:F:462:TRP:CD2	1:F:463:HIS:N	2.80	0.50
1:A:64:ILE:HD12	1:A:102:LYS:HB3	1.94	0.50
1:A:267:VAL:HB	1:A:270:LEU:HB2	1.94	0.50
2:B:68:ASP:OD1	2:B:102:LYS:NZ	2.44	0.50
2:B:106:LEU:HD12	2:B:106:LEU:C	2.32	0.50
2:B:237:PHE:HB2	2:B:246:ILE:HG12	1.93	0.50
2:B:248:PRO:O	2:B:251:ALA:N	2.45	0.50
2:B:433:ILE:O	2:B:433:ILE:HG22	2.12	0.50
2:C:393:ARG:HH21	2:C:429:HIS:CB	2.22	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ASP:OD1	2:D:336:GLU:HB2	2.11	0.50
2:E:440:LEU:CD2	2:E:453:ILE:HG12	2.41	0.50
2:E:54:LEU:HD23	2:E:244:ILE:CD1	2.42	0.50
1:F:425:ILE:HD11	1:F:456:PHE:CD2	2.46	0.50
1:F:79:THR:CG2	1:F:81:GLN:HG2	2.42	0.50
1:A:153:GLN:O	1:A:154:TYR:CD2	2.64	0.50
2:B:358:ASP:O	2:B:362:ILE:HG12	2.11	0.50
2:C:127:ILE:HD13	2:C:127:ILE:H	1.77	0.50
2:C:41:SER:OG	2:C:168:VAL:HG13	2.11	0.50
2:C:54:LEU:HD13	2:C:90:PHE:CZ	2.47	0.50
1:F:151:PHE:C	1:F:153:GLN:N	2.65	0.50
1:F:353:SER:O	1:F:354:ALA:HB2	2.11	0.50
1:F:317:TYR:CD2	1:F:383:LEU:HD21	2.47	0.50
1:A:136:LYS:HD3	1:A:137:TYR:CE1	2.47	0.49
1:A:45:SER:HA	1:A:182:THR:O	2.12	0.49
1:A:467:ILE:HD13	1:F:447:GLY:C	2.32	0.49
2:C:116:GLU:O	2:C:117:VAL:HB	2.11	0.49
2:C:214:GLU:C	2:C:215:ARG:HE	2.15	0.49
2:D:127:ILE:HD11	2:D:167:LEU:HD13	1.94	0.49
2:D:81:GLN:N	2:D:81:GLN:CD	2.66	0.49
2:E:385:ARG:HA	1:F:393:ARG:NH1	2.27	0.49
1:F:504:GLU:HA	1:F:507:ARG:CG	2.41	0.49
1:A:419:PHE:O	1:A:420:MET:HB2	2.12	0.49
1:A:484:ARG:NH1	1:A:484:ARG:CB	2.74	0.49
2:C:117:VAL:HG12	2:C:117:VAL:O	2.11	0.49
2:C:313:ILE:HD12	2:C:372:PRO:HG2	1.93	0.49
2:C:52:LYS:HD2	2:C:182:THR:O	2.12	0.49
2:E:396:VAL:HG11	2:E:430:ILE:CG2	2.42	0.49
1:F:49:GLY:CA	3:F:903:ATP:O2B	2.59	0.49
1:A:377:ILE:HG22	1:A:379:SER:O	2.13	0.49
1:A:426:THR:HG22	1:A:428:SER:H	1.77	0.49
1:A:436:THR:HG23	1:A:457:LYS:O	2.12	0.49
2:C:289:ALA:HB2	2:C:419:PHE:HA	1.93	0.49
2:C:18:ILE:HG21	2:C:37:PRO:HB3	1.95	0.49
2:C:252:MET:CE	2:C:397:ILE:HG22	2.42	0.49
2:C:52:LYS:N	3:C:903:ATP:O1B	2.45	0.49
2:D:121:PHE:O	2:D:124:SER:OG	2.26	0.49
2:E:309:LYS:HA	2:E:343:LEU:HD13	1.94	0.49
1:F:33:HIS:CD2	1:F:229:SER:OG	2.65	0.49
1:F:287:THR:HG23	1:F:414:ASN:HB3	1.93	0.49
1:F:514:GLU:HG2	1:F:519:SER:HB3	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:O	1:A:236:PRO:HA	2.12	0.49
1:A:448:GLU:HG2	2:B:466:ALA:CB	2.43	0.49
2:B:126:LEU:HD12	2:B:129:ARG:HD3	1.95	0.49
2:B:162:ARG:HB2	2:B:162:ARG:NH1	2.27	0.49
2:B:340:ARG:C	2:B:342:ASN:H	2.15	0.49
2:C:191:ILE:HB	2:C:198:GLU:HG3	1.91	0.49
2:C:486:PHE:HB2	2:C:489:ILE:HD11	1.94	0.49
2:D:333:MET:CG	5:D:910:HOH:O	2.60	0.49
2:E:140:ARG:HH11	2:E:140:ARG:CA	2.25	0.49
1:F:144:ILE:HG22	1:F:147:VAL:HG12	1.94	0.49
1:F:148:THR:CG2	1:F:193:ARG:HD2	2.43	0.49
1:A:284:ILE:N	1:A:284:ILE:HD12	2.26	0.49
1:A:344:LEU:HD13	1:A:344:LEU:C	2.33	0.49
1:A:436:THR:HG23	1:A:458:MET:HG2	1.93	0.49
2:B:318:GLU:HG3	5:B:528:HOH:O	2.13	0.49
2:B:376:ALA:HA	2:B:411:LEU:O	2.13	0.49
2:C:225:LEU:HB2	2:C:230:HIS:HD2	1.77	0.49
2:C:149:SER:HB3	2:D:161:ARG:NH2	2.26	0.49
2:D:179:VAL:HG12	2:D:179:VAL:O	2.12	0.49
2:D:191:ILE:HG12	2:D:206:ILE:HD11	1.95	0.49
2:D:273:MET:CE	2:D:468:ARG:HD2	2.41	0.49
1:A:441:GLN:NE2	1:A:490:ILE:HD13	2.27	0.49
2:B:23:THR:O	2:B:24:MET:HB2	2.12	0.49
2:B:273:MET:CE	2:B:468:ARG:HD2	2.42	0.49
2:B:344:LEU:HD11	2:B:346:ILE:CD1	2.42	0.49
2:B:377:ILE:N	2:B:377:ILE:HD12	2.28	0.49
2:C:147:VAL:HG11	2:C:180:MET:CE	2.41	0.49
2:C:163:GLU:HA	2:C:163:GLU:OE2	2.13	0.49
2:C:397:ILE:H	2:C:397:ILE:CD1	2.25	0.49
2:D:446:ARG:N	2:D:496:ARG:NH1	2.57	0.49
2:D:67:PHE:HB2	2:D:69:GLU:HG3	1.93	0.49
2:E:262:ARG:NH2	2:E:461:SER:HB2	2.28	0.49
2:E:79:THR:HG23	2:E:81:GLN:H	1.77	0.49
2:B:486:PHE:CE2	2:B:496:ARG:HB2	2.48	0.49
2:C:121:PHE:HB3	2:C:125:ALA:HB3	1.94	0.49
2:C:334:ASP:O	2:C:338:MET:HG2	2.13	0.49
2:C:340:ARG:C	2:C:342:ASN:N	2.65	0.49
2:D:60:LEU:O	2:D:64:ILE:CD1	2.55	0.49
2:E:315:PHE:CE2	2:E:363:ILE:HD13	2.48	0.49
1:A:284:ILE:HD12	1:A:410:GLY:O	2.13	0.49
2:B:194:TYR:O	2:B:196:VAL:N	2.46	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:ASN:ND2	2:B:216:ARG:HD2	2.28	0.49
2:C:98:VAL:HA	2:C:103:LEU:O	2.12	0.49
2:C:211:LEU:HD12	2:C:215:ARG:O	2.13	0.49
2:C:218:ARG:NH1	2:C:239:ILE:HD12	2.27	0.49
2:D:335:PHE:HA	2:D:338:MET:CG	2.30	0.49
2:D:412:PHE:N	2:D:412:PHE:CD1	2.80	0.49
1:F:289:ALA:HB2	1:F:419:PHE:HA	1.95	0.49
1:A:244:ILE:HG22	1:A:246:ILE:CD1	2.43	0.49
1:A:82:ASP:O	1:A:83:ILE:C	2.51	0.49
2:D:79:THR:HG22	2:D:82:ASP:HB2	1.94	0.49
2:E:273:MET:O	2:E:463:HIS:CA	2.60	0.49
1:F:218:ARG:CZ	1:F:239:ILE:HD12	2.43	0.49
2:E:123:LEU:HD23	2:E:127:ILE:CG1	2.43	0.49
1:F:21:MET:HE3	1:F:141:ARG:CZ	2.43	0.49
1:F:245:ASN:HD22	1:F:361:GLN:HE21	1.60	0.49
1:F:507:ARG:CD	1:F:507:ARG:O	2.61	0.49
1:A:205:VAL:HG22	1:A:222:ILE:CD1	2.37	0.48
2:B:436:THR:HG23	2:B:458:MET:HG3	1.95	0.48
2:C:93:ASP:OD1	2:C:93:ASP:C	2.50	0.48
2:D:237:PHE:HB3	2:D:246:ILE:HG12	1.95	0.48
2:D:85:LYS:NZ	2:E:14:GLU:HB3	2.27	0.48
2:E:302:VAL:HG13	2:E:344:LEU:HD23	1.94	0.48
2:E:387:VAL:HG12	2:E:388:SER:N	2.28	0.48
1:F:393:ARG:O	1:F:397:ILE:HG13	2.12	0.48
1:A:237:PHE:HB3	1:A:246:ILE:HG13	1.95	0.48
1:A:338:MET:HB3	1:A:344:LEU:CB	2.42	0.48
2:D:21:MET:CE	2:D:177:THR:HB	2.42	0.48
2:D:231:MET:HB3	2:D:235:TYR:OH	2.13	0.48
2:D:385:ARG:NH2	2:E:433:ILE:HD11	2.27	0.48
2:E:96:LYS:O	2:E:100:GLU:HG3	2.12	0.48
2:E:271:ASP:OD1	2:E:277:GLY:HA2	2.13	0.48
2:E:486:PHE:HA	2:E:495:THR:O	2.13	0.48
2:E:93:ASP:OD2	2:E:96:LYS:CB	2.59	0.48
2:C:239:ILE:CG1	2:C:244:ILE:HD13	2.44	0.48
2:D:121:PHE:N	2:D:121:PHE:CD1	2.81	0.48
2:D:336:GLU:OE1	2:D:336:GLU:HA	2.13	0.48
2:D:445:ILE:CA	2:D:496:ARG:HH12	2.27	0.48
2:E:299:SER:C	2:E:333:MET:HE2	2.33	0.48
2:E:53:THR:OG1	3:E:903:ATP:O2G	2.31	0.48
1:F:115:GLN:CG	1:F:116:GLU:N	2.74	0.48
1:F:182:THR:HG22	1:F:183:GLU:N	2.28	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:197:GLU:N	1:F:197:GLU:OE2	2.41	0.48
1:F:284:ILE:N	1:F:284:ILE:HD12	2.28	0.48
1:F:325:LEU:HD23	1:F:335:PHE:HB2	1.96	0.48
1:A:186:GLU:HB3	1:A:189:GLY:HA3	1.94	0.48
2:C:123:LEU:O	2:C:124:SER:C	2.51	0.48
2:C:214:GLU:HB3	2:D:234:GLU:HB2	1.95	0.48
2:D:433:ILE:CG2	2:D:433:ILE:O	2.60	0.48
2:D:486:PHE:CE2	2:D:496:ARG:HB3	2.49	0.48
1:F:220:LEU:HD21	1:F:222:ILE:CD1	2.43	0.48
1:A:106:LEU:HD12	1:A:106:LEU:C	2.34	0.48
2:C:123:LEU:O	2:C:126:LEU:N	2.46	0.48
2:C:364:LYS:HE2	2:C:402:TYR:CD1	2.49	0.48
2:C:454:ASN:CB	2:C:467:ILE:HD13	2.43	0.48
2:C:54:LEU:O	2:C:55:PHE:C	2.52	0.48
2:D:149:SER:HA	2:D:152:GLN:HB2	1.95	0.48
2:E:49:GLY:O	2:E:218:ARG:NH2	2.47	0.48
2:E:303:GLU:HB2	2:E:333:MET:CE	2.43	0.48
2:E:316:ALA:O	2:E:348:CYS:HA	2.14	0.48
2:E:81:GLN:NE2	2:E:81:GLN:H	2.10	0.48
1:F:305:ALA:O	1:F:310:GLU:HB2	2.13	0.48
1:F:484:ARG:NH1	1:F:484:ARG:HB3	2.27	0.48
2:B:56:SER:HB2	2:B:143:SER:HB3	1.96	0.48
2:B:222:ILE:HG22	2:B:230:HIS:CE1	2.49	0.48
2:D:451:ARG:N	2:D:451:ARG:HD2	2.28	0.48
2:E:148:THR:HG21	2:E:193:ARG:HD2	1.94	0.48
1:F:182:THR:CG2	1:F:192:ALA:HB1	2.44	0.48
1:F:23:THR:O	1:F:24:MET:HB2	2.14	0.48
1:F:380:LEU:C	1:F:382:ALA:H	2.16	0.48
2:B:237:PHE:HB3	2:B:246:ILE:HG12	1.94	0.48
2:B:438:ILE:HG23	2:B:453:ILE:HD11	1.94	0.48
2:C:218:ARG:HB3	5:C:528:HOH:O	2.13	0.48
2:D:262:ARG:HD2	2:D:276:GLY:O	2.14	0.48
1:A:256:GLN:CG	1:F:320:SEP:P	3.01	0.48
1:F:431:GLU:O	1:F:434:THR:HG22	2.13	0.48
1:A:313:ILE:HD12	1:A:367:ILE:HD13	1.94	0.48
2:B:503:SER:O	2:B:504:GLU:CB	2.55	0.48
2:D:197:GLU:OE2	2:D:197:GLU:N	2.35	0.48
2:D:270:LEU:O	2:D:270:LEU:HD23	2.13	0.48
2:D:443:VAL:C	2:D:445:ILE:HD12	2.34	0.48
2:E:148:THR:HG21	2:E:183:GLU:HG3	1.96	0.48
1:F:446:ARG:H	1:F:496:ARG:NH2	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:509:VAL:CG1	1:F:510:ARG:N	2.54	0.48
2:B:215:ARG:NH2	2:C:234:GLU:O	2.47	0.48
2:C:284:ILE:H	2:C:284:ILE:HD12	1.79	0.48
2:C:371:LYS:N	2:C:372:PRO:HD3	2.28	0.48
2:C:431:GLU:CG	2:C:431:GLU:O	2.61	0.48
2:D:212:GLU:CG	2:D:212:GLU:O	2.60	0.48
2:E:273:MET:CE	2:E:468:ARG:HD2	2.44	0.48
1:A:317:TYR:CD2	1:A:383:LEU:HD21	2.49	0.48
2:B:72:VAL:HG23	2:B:139:ALA:CB	2.44	0.48
2:C:434:THR:CG2	2:C:437:ILE:HD11	2.31	0.48
2:C:464:ASP:OD1	2:C:464:ASP:C	2.52	0.48
2:D:182:THR:CG2	2:D:183:GLU:H	2.24	0.48
2:D:352:GLU:C	2:D:354:ALA:H	2.18	0.48
3:E:901:ATP:O3'	1:F:457:LYS:HB2	2.14	0.48
1:A:150:VAL:CG1	1:A:151:PHE:N	2.76	0.47
1:A:344:LEU:HD13	1:A:345:LYS:N	2.29	0.47
2:B:184:ARG:NH2	2:B:186:GLU:O	2.47	0.47
2:B:296:LEU:HD21	2:B:477:PRO:CD	2.38	0.47
2:C:249:LEU:HD13	2:C:394:GLN:O	2.14	0.47
2:D:151:PHE:C	2:D:153:GLN:N	2.67	0.47
2:D:68:ASP:O	2:D:68:ASP:OD1	2.31	0.47
2:E:203:ASN:ND2	2:E:203:ASN:N	2.61	0.47
2:E:336:GLU:O	2:E:339:GLU:HB2	2.14	0.47
2:E:485:ASN:OD1	2:E:485:ASN:N	2.47	0.47
1:F:20:LYS:HB3	1:F:35:GLY:O	2.13	0.47
1:F:302:VAL:HG12	1:F:303:GLU:N	2.28	0.47
1:F:283:ILE:HD11	1:F:404:LYS:HG3	1.96	0.47
1:F:452:ALA:HA	1:F:469:GLU:HA	1.96	0.47
1:A:162:ARG:NH1	1:F:116:GLU:HG2	2.29	0.47
1:A:320:SEP:O	1:A:324:LEU:CD1	2.63	0.47
1:A:294:LYS:N	3:A:901:ATP:O1B	2.47	0.47
2:B:125:ALA:O	2:B:129:ARG:HG3	2.13	0.47
1:A:425:ILE:CD1	1:F:290:THR:HG21	2.42	0.47
1:A:118:VAL:HG12	1:A:122:ASP:HB3	1.95	0.47
1:A:249:LEU:HD12	1:A:394:GLN:OE1	2.15	0.47
2:B:284:ILE:N	2:B:284:ILE:HD12	2.29	0.47
2:C:197:GLU:CD	2:C:197:GLU:H	2.14	0.47
2:C:462:TRP:CE2	2:C:463:HIS:O	2.68	0.47
2:D:266:GLY:O	2:D:300:ARG:CG	2.62	0.47
2:D:315:PHE:CE1	2:D:375:ILE:HD12	2.50	0.47
2:D:334:ASP:O	2:D:338:MET:HG2	2.14	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:451:ARG:HG2	2:D:451:ARG:NH1	2.23	0.47
2:D:471:MET:HG3	2:D:478:ASP:HB3	1.96	0.47
2:E:167:LEU:HG	2:E:171:LEU:HD12	1.96	0.47
2:E:344:LEU:HD11	2:E:346:ILE:CG1	2.42	0.47
2:E:49:GLY:N	3:E:903:ATP:O2B	2.48	0.47
1:F:338:MET:CB	1:F:344:LEU:HB3	2.43	0.47
1:A:111:ASP:CG	1:A:112:PRO:HD2	2.34	0.47
1:A:451:ARG:CG	1:A:451:ARG:NH1	2.76	0.47
1:A:90:PHE:HB2	1:A:92:TRP:CE2	2.49	0.47
2:B:104:PHE:HD2	2:B:133:ALA:HB1	1.79	0.47
2:B:419:PHE:O	2:B:420:MET:HB2	2.14	0.47
2:D:304:ASN:OD1	2:D:374:ARG:NH2	2.47	0.47
2:D:332:GLY:O	2:D:333:MET:O	2.31	0.47
2:D:370:PHE:O	2:D:371:LYS:HG3	2.13	0.47
2:D:64:ILE:HD12	2:D:64:ILE:N	2.29	0.47
2:D:385:ARG:HH22	2:E:433:ILE:CD1	2.28	0.47
1:F:106:LEU:HD13	1:F:129:ARG:CZ	2.44	0.47
1:F:336:GLU:OE1	1:F:336:GLU:HA	2.14	0.47
1:F:370:PHE:C	1:F:372:PRO:HD3	2.34	0.47
1:A:457:LYS:HB2	3:F:901:ATP:O3'	2.14	0.47
2:B:371:LYS:O	2:B:371:LYS:HD2	2.14	0.47
2:C:191:ILE:HB	2:C:198:GLU:HG2	1.96	0.47
2:D:425:ILE:CD1	2:D:439:LEU:HD22	2.45	0.47
2:E:142:VAL:HB	2:E:178:THR:HG23	1.96	0.47
2:D:110:PRO:HD2	2:E:165:PHE:CE2	2.49	0.47
2:E:52:LYS:HE3	3:E:903:ATP:O1B	2.14	0.47
1:A:467:ILE:HD11	1:F:449:MET:HG2	1.95	0.47
1:A:154:TYR:O	1:A:155:ASP:CB	2.62	0.47
1:A:421:GLY:O	1:A:422:ALA:O	2.32	0.47
1:A:462:TRP:CG	1:A:463:HIS:N	2.76	0.47
2:B:22:ARG:NH2	2:B:24:MET:SD	2.87	0.47
2:B:25:ILE:HG23	2:B:58:GLN:NE2	2.29	0.47
3:A:901:ATP:O3'	2:B:457:LYS:HB2	2.14	0.47
2:B:73:PHE:HD2	2:B:105:ILE:HD12	1.80	0.47
2:C:334:ASP:OD1	2:C:336:GLU:N	2.48	0.47
2:C:419:PHE:O	2:C:420:MET:CB	2.61	0.47
2:D:42:THR:HA	2:D:203:ASN:HB2	1.97	0.47
2:D:225:LEU:HB2	2:D:230:HIS:HD2	1.79	0.47
2:D:231:MET:HE1	2:D:251:ALA:HB2	1.96	0.47
2:D:98:VAL:HA	2:D:103:LEU:O	2.15	0.47
2:E:123:LEU:HD13	2:E:166:ARG:HD2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:147:VAL:HG23	2:E:148:THR:N	2.30	0.47
2:E:127:ILE:HD12	2:E:167:LEU:HD13	1.96	0.47
1:F:31:ILE:HD11	1:F:246:ILE:HG21	1.95	0.47
1:A:370:PHE:C	1:A:372:PRO:HD3	2.35	0.47
2:B:150:VAL:CG1	2:B:151:PHE:N	2.77	0.47
2:C:419:PHE:CG	2:C:419:PHE:O	2.67	0.47
2:C:437:ILE:HD13	2:C:457:LYS:CE	2.38	0.47
2:D:328:ALA:CA	5:D:552:HOH:O	2.62	0.47
2:E:417:ASP:O	1:F:424:SER:HB3	2.15	0.47
1:F:430:ILE:O	1:F:432:GLU:N	2.47	0.47
1:A:262:ARG:O	1:A:263:VAL:HG22	2.15	0.47
2:B:118:VAL:HG12	2:B:121:PHE:HB2	1.96	0.47
2:B:184:ARG:HG2	2:B:191:ILE:O	2.14	0.47
2:B:313:ILE:CD1	2:B:372:PRO:HG2	2.45	0.47
2:C:263:VAL:HG21	2:C:280:LYS:HA	1.96	0.47
2:C:294:LYS:HB2	3:C:901:ATP:O1B	2.15	0.47
2:E:371:LYS:N	2:E:372:PRO:HD3	2.29	0.47
1:A:256:GLN:CG	1:F:320:SEP:O1P	2.60	0.47
1:A:244:ILE:HG22	1:A:246:ILE:HD11	1.96	0.47
2:B:269:ARG:O	2:B:273:MET:HG3	2.15	0.47
2:B:350:TYR:HE1	2:C:252:MET:HG2	1.80	0.47
2:B:80:PRO:HG3	2:B:105:ILE:CG2	2.44	0.47
2:C:294:LYS:N	3:C:901:ATP:O1B	2.46	0.47
2:D:18:ILE:CD1	2:D:40:ARG:HH12	2.27	0.47
2:D:451:ARG:NH1	2:D:451:ARG:CG	2.75	0.47
2:E:150:VAL:CG1	2:E:151:PHE:H	2.28	0.47
1:F:380:LEU:C	1:F:382:ALA:N	2.68	0.47
1:F:269:ARG:CG	1:F:479:ILE:HB	2.40	0.47
1:F:61:TYR:O	1:F:64:ILE:N	2.48	0.47
1:A:452:ALA:HA	1:A:468:ARG:O	2.15	0.47
2:B:217:ARG:HG3	2:B:357:GLU:OE2	2.15	0.47
2:E:344:LEU:HD13	2:E:345:LYS:N	2.29	0.47
1:F:98:VAL:HA	1:F:103:LEU:O	2.15	0.47
1:F:115:GLN:CG	1:F:116:GLU:H	2.27	0.47
1:F:504:GLU:OE2	1:F:505:LEU:HD13	2.15	0.47
1:F:507:ARG:O	1:F:507:ARG:HD3	2.15	0.47
1:A:134:ILE:HA	1:A:139:ALA:HB3	1.97	0.47
1:A:270:LEU:O	1:A:273:MET:O	2.33	0.47
2:B:74:VAL:HG13	2:B:106:LEU:HG	1.97	0.47
2:B:501:GLU:HB2	2:B:502:LYS:H	1.36	0.47
2:C:313:ILE:HD11	2:C:370:PHE:CB	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:LEU:HD11	1:F:197:GLU:HG3	1.96	0.47
1:F:287:THR:CG2	1:F:414:ASN:ND2	2.74	0.47
1:F:458:MET:SD	1:F:461:SER:HB3	2.55	0.47
1:A:237:PHE:CB	1:A:246:ILE:HG13	2.44	0.46
1:A:28:PHE:CE1	1:A:222:ILE:HD11	2.50	0.46
1:A:313:ILE:HG13	1:A:372:PRO:CG	2.45	0.46
1:A:65:ILE:HD11	1:A:97:LEU:HD21	1.97	0.46
1:A:79:THR:HB	1:A:82:ASP:OD2	2.14	0.46
2:B:170:ARG:HH12	2:B:174:ILE:HD11	1.80	0.46
2:B:222:ILE:O	2:B:230:HIS:CE1	2.69	0.46
2:C:144:ILE:HD11	2:C:171:LEU:HD11	1.96	0.46
2:C:144:ILE:HD13	2:C:167:LEU:HD21	1.97	0.46
2:B:193:ARG:NH2	2:C:195:GLY:O	2.42	0.46
2:E:468:ARG:HH11	2:E:468:ARG:HG2	1.80	0.46
1:F:315:PHE:CE1	1:F:375:ILE:CD1	2.97	0.46
1:A:153:GLN:O	1:A:154:TYR:CB	2.63	0.46
1:A:357:GLU:HG3	1:A:358:ASP:N	2.29	0.46
1:A:356:LEU:CD1	1:A:387:VAL:HG21	2.45	0.46
2:B:327:ASN:HD21	2:C:459:ARG:HB3	1.79	0.46
2:B:463:HIS:ND1	2:B:463:HIS:C	2.68	0.46
2:B:52:LYS:HE2	3:B:903:ATP:O1B	2.16	0.46
2:C:315:PHE:CE2	2:C:363:ILE:HA	2.50	0.46
2:C:249:LEU:HD12	2:C:394:GLN:OE1	2.15	0.46
2:D:147:VAL:CG2	2:D:148:THR:N	2.77	0.46
2:D:211:LEU:HD12	2:D:215:ARG:O	2.15	0.46
2:D:486:PHE:CE2	2:D:496:ARG:HD3	2.51	0.46
2:E:318:GLU:OE2	1:F:432:GLU:HB3	2.15	0.46
2:E:453:ILE:HB	2:E:470:PHE:HD2	1.80	0.46
1:A:340:ARG:C	1:A:342:ASN:H	2.18	0.46
2:C:215:ARG:NE	2:C:215:ARG:HA	2.30	0.46
2:C:49:GLY:O	2:C:218:ARG:NH2	2.48	0.46
2:C:64:ILE:CD1	2:C:103:LEU:HB2	2.46	0.46
2:D:181:THR:HG22	2:D:181:THR:O	2.14	0.46
2:E:219:THR:HA	2:E:235:TYR:O	2.15	0.46
2:D:348:CYS:HB3	2:E:254:LEU:HB3	1.98	0.46
1:F:255:THR:O	1:F:255:THR:HG22	2.15	0.46
1:F:436:THR:OG1	1:F:458:MET:HG2	2.15	0.46
1:A:68:ASP:CG	1:A:102:LYS:HZ2	2.18	0.46
2:B:127:ILE:HG22	2:B:127:ILE:O	2.16	0.46
2:B:184:ARG:HH22	2:B:187:GLU:C	2.19	0.46
2:B:208:ARG:O	2:B:218:ARG:HA	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ARG:HG2	2:B:479:ILE:HB	1.96	0.46
2:B:313:ILE:HG13	2:B:372:PRO:HG3	1.97	0.46
2:B:454:ASN:HB2	2:B:467:ILE:HD13	1.96	0.46
2:C:333:MET:H	2:C:333:MET:HG2	1.42	0.46
2:C:49:GLY:CA	3:C:903:ATP:O2B	2.63	0.46
2:D:28:PHE:HA	2:D:31:ILE:HD12	1.98	0.46
2:E:191:ILE:HG23	2:E:206:ILE:CD1	2.45	0.46
2:E:221:GLU:HG3	2:E:222:ILE:N	2.31	0.46
2:E:281:ASP:O	2:E:282:SER:HB3	2.16	0.46
1:F:147:VAL:HG11	1:F:180:MET:HE3	1.97	0.46
1:F:471:MET:O	1:F:471:MET:HE2	2.16	0.46
1:A:145:ASP:OD2	1:A:181:THR:HG21	2.15	0.46
1:A:292:THR:HB	1:A:440:LEU:HB3	1.96	0.46
1:A:423:HIS:O	1:F:418:GLN:HB2	2.16	0.46
1:A:440:LEU:HD22	1:A:470:PHE:CE2	2.51	0.46
2:B:387:VAL:CG1	2:B:388:SER:N	2.78	0.46
2:B:469:GLU:HG2	2:B:480:LYS:HB2	1.97	0.46
2:C:232:LYS:N	2:C:232:LYS:CD	2.79	0.46
2:B:353:SER:HA	2:C:250:GLY:O	2.16	0.46
2:C:357:GLU:HG3	2:C:358:ASP:N	2.30	0.46
2:D:185:ILE:N	2:D:185:ILE:HD12	2.31	0.46
2:E:191:ILE:HD12	2:E:206:ILE:CG1	2.45	0.46
1:F:207:LEU:HD21	1:F:220:LEU:HD12	1.96	0.46
1:F:414:ASN:HD21	1:F:426:THR:HG23	1.80	0.46
1:F:455:VAL:HG12	1:F:463:HIS:ND1	2.31	0.46
1:F:505:LEU:O	1:F:506:SER:CB	2.63	0.46
2:B:122:ASP:C	2:B:124:SER:H	2.19	0.46
2:B:489:ILE:O	2:B:492:GLY:N	2.49	0.46
2:C:31:ILE:HD11	2:C:246:ILE:CG2	2.41	0.46
2:C:426:THR:HG21	2:C:430:ILE:HG12	1.97	0.46
2:E:283:ILE:HG13	2:E:400:THR:HG23	1.98	0.46
2:E:396:VAL:O	2:E:400:THR:HB	2.16	0.46
2:E:453:ILE:O	2:E:453:ILE:HG23	2.15	0.46
2:E:454:ASN:ND2	2:E:456:PHE:HA	2.30	0.46
1:F:149:SER:HA	1:F:152:GLN:HB2	1.96	0.46
1:F:319:GLU:HA	1:F:320:SEP:O2P	2.16	0.46
1:A:333:MET:O	1:A:334:ASP:CB	2.63	0.46
1:A:392:PHE:HE2	1:A:430:ILE:CD1	2.29	0.46
2:B:213:GLY:O	2:B:214:GLU:HB2	2.16	0.46
2:B:265:SER:CB	2:B:270:LEU:HD13	2.46	0.46
2:B:363:ILE:HG22	2:B:367:ILE:HD11	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:THR:HG23	2:B:82:ASP:H	1.80	0.46
3:B:901:ATP:O3'	2:C:457:LYS:HB2	2.15	0.46
2:C:38:ILE:HG22	2:C:39:GLY:N	2.31	0.46
1:F:315:PHE:CE2	1:F:347:VAL:HG21	2.50	0.46
1:A:466:ALA:HA	1:F:448:GLU:HG2	1.98	0.46
1:F:514:GLU:CB	1:F:519:SER:HB3	2.46	0.46
2:B:360:LEU:HD23	2:B:399:VAL:CG2	2.46	0.46
2:B:57:ILE:C	2:B:59:PHE:N	2.69	0.46
2:C:283:ILE:N	2:C:283:ILE:HD12	2.31	0.46
2:C:430:ILE:O	2:C:432:GLU:N	2.48	0.46
2:D:123:LEU:HA	2:D:123:LEU:HD22	1.83	0.46
2:D:356:LEU:HD13	2:D:387:VAL:HG21	1.98	0.46
2:D:294:LYS:N	3:D:901:ATP:O1B	2.46	0.46
2:E:223:LEU:HD22	2:E:223:LEU:O	2.16	0.46
2:E:269:ARG:NH2	2:E:468:ARG:NH2	2.64	0.46
1:F:270:LEU:CD2	1:F:274:CYS:SG	3.04	0.46
1:F:484:ARG:CZ	1:F:484:ARG:HB2	2.46	0.46
1:A:191:ILE:CG2	1:A:198:GLU:HG3	2.46	0.46
1:A:207:LEU:HD22	1:A:237:PHE:HE2	1.81	0.46
1:A:231:MET:CE	1:A:251:ALA:HB2	2.45	0.46
2:B:20:LYS:HG2	2:B:35:GLY:O	2.16	0.46
2:B:462:TRP:CE3	2:B:463:HIS:N	2.84	0.46
2:C:249:LEU:HD12	2:C:394:GLN:HG2	1.97	0.46
2:D:211:LEU:O	2:D:215:ARG:O	2.34	0.46
2:E:46:GLY:HA2	2:E:184:ARG:HD3	1.97	0.46
2:E:501:GLU:O	2:E:502:LYS:HG3	2.16	0.46
1:F:122:ASP:O	1:F:126:LEU:HB2	2.16	0.46
1:F:191:ILE:CG2	1:F:198:GLU:HG3	2.46	0.46
1:A:393:ARG:NH1	1:F:385:ARG:HA	2.31	0.46
1:A:375:ILE:O	1:A:410:GLY:HA2	2.15	0.46
2:C:150:VAL:O	2:C:153:GLN:HG3	2.16	0.46
2:C:197:GLU:N	2:C:197:GLU:OE2	2.39	0.46
2:D:287:THR:HG23	2:D:414:ASN:ND2	2.22	0.46
2:D:382:ALA:O	2:D:385:ARG:HG3	2.16	0.46
2:E:123:LEU:HD22	2:E:166:ARG:HD2	1.98	0.46
1:A:116:GLU:O	1:A:117:VAL:CB	2.63	0.45
1:A:185:ILE:HD12	1:A:185:ILE:N	2.31	0.45
1:A:364:LYS:HG2	1:A:402:TYR:CD2	2.50	0.45
2:C:50:THR:HA	5:C:528:HOH:O	2.15	0.45
2:C:88:ARG:HD3	2:D:15:HIS:C	2.36	0.45
2:D:191:ILE:HD12	2:D:198:GLU:HG2	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:262:ARG:HH22	2:E:461:SER:HB2	1.81	0.45
1:F:387:VAL:CG1	1:F:388:SER:N	2.79	0.45
1:F:420:MET:HE3	1:F:492:GLY:HA3	1.98	0.45
1:F:292:THR:HB	1:F:440:LEU:HB3	1.98	0.45
2:B:123:LEU:HD12	2:B:166:ARG:HD2	1.98	0.45
2:B:84:ILE:HG23	2:B:94:LEU:HB2	1.97	0.45
2:E:385:ARG:HA	1:F:393:ARG:HH12	1.81	0.45
2:E:495:THR:HA	1:F:487:GLU:OE1	2.17	0.45
2:E:504:GLU:HG2	2:E:505:LEU:N	2.30	0.45
1:A:420:MET:O	1:A:422:ALA:N	2.41	0.45
2:C:334:ASP:C	2:C:334:ASP:OD1	2.55	0.45
2:C:462:TRP:CD2	2:C:463:HIS:O	2.69	0.45
2:D:313:ILE:HG21	2:D:315:PHE:CZ	2.50	0.45
2:D:305:ALA:HB2	2:D:374:ARG:HD2	1.98	0.45
2:D:471:MET:HE2	2:D:478:ASP:HB2	1.98	0.45
1:F:222:ILE:HD12	1:F:222:ILE:N	2.31	0.45
1:F:356:LEU:CD1	1:F:387:VAL:HG21	2.44	0.45
1:F:284:ILE:HB	1:F:411:LEU:HD12	1.97	0.45
1:A:262:ARG:NH2	1:A:461:SER:HB2	2.31	0.45
1:A:496:ARG:HG3	2:B:487:GLU:OE1	2.16	0.45
1:A:295:THR:HB	3:A:901:ATP:PA	2.57	0.45
2:B:140:ARG:CB	2:B:140:ARG:NH1	2.69	0.45
2:B:379:SER:H	2:B:413:THR:HG22	1.81	0.45
2:C:150:VAL:CG1	2:C:151:PHE:N	2.80	0.45
2:D:218:ARG:NH1	2:D:239:ILE:HD12	2.31	0.45
2:D:298:VAL:HG13	2:D:376:ALA:HB1	1.98	0.45
2:E:74:VAL:CG2	2:E:130:ILE:HD12	2.46	0.45
2:E:315:PHE:CE2	2:E:347:VAL:HG21	2.51	0.45
2:E:392:PHE:O	2:E:395:PHE:N	2.49	0.45
2:E:56:SER:OG	2:E:73:PHE:HE1	1.99	0.45
1:F:134:ILE:HD11	1:F:142:VAL:HG22	1.97	0.45
1:A:293:GLY:HA2	3:A:901:ATP:O1A	2.16	0.45
1:A:311:ARG:O	1:A:373:ALA:N	2.40	0.45
1:A:387:VAL:HG12	1:A:388:SER:N	2.31	0.45
1:A:380:LEU:N	1:A:413:THR:O	2.48	0.45
1:A:286:ALA:HA	1:A:438:ILE:O	2.16	0.45
2:B:218:ARG:NH2	2:B:239:ILE:HD12	2.31	0.45
2:C:73:PHE:HB3	2:C:105:ILE:HD13	1.97	0.45
2:C:127:ILE:HD12	2:C:167:LEU:HD13	1.98	0.45
2:C:127:ILE:HG21	2:C:170:ARG:HG3	1.97	0.45
2:C:60:LEU:O	2:C:61:TYR:C	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:445:ILE:HA	2:D:496:ARG:NH1	2.32	0.45
2:E:140:ARG:HH11	2:E:140:ARG:HA	1.81	0.45
2:E:145:ASP:O	2:E:146:SER:OG	2.32	0.45
1:F:122:ASP:O	1:F:126:LEU:N	2.50	0.45
1:F:299:SER:CB	1:F:333:MET:HE1	2.46	0.45
1:F:296:LEU:HD13	1:F:331:TRP:CE2	2.51	0.45
1:A:164:LEU:HD11	1:A:197:GLU:CG	2.41	0.45
1:A:287:THR:HG21	1:A:425:ILE:O	2.16	0.45
2:C:287:THR:HG22	2:C:288:GLY:N	2.31	0.45
2:C:311:ARG:HD2	2:C:371:LYS:CE	2.46	0.45
2:D:263:VAL:HG21	2:D:280:LYS:HA	1.98	0.45
2:E:14:GLU:HG3	2:E:16:GLN:N	2.26	0.45
2:E:193:ARG:HH11	2:E:193:ARG:HG2	1.82	0.45
2:E:400:THR:HG22	2:E:401:GLY:N	2.30	0.45
2:E:283:ILE:HG23	2:E:412:PHE:HE1	1.79	0.45
1:F:31:ILE:HG22	1:F:222:ILE:HD13	1.97	0.45
1:F:387:VAL:HG12	1:F:388:SER:N	2.32	0.45
1:A:246:ILE:O	1:A:248:PRO:HD3	2.17	0.45
1:A:296:LEU:HA	1:A:331:TRP:CZ3	2.51	0.45
2:B:314:LEU:HB3	2:B:346:ILE:HD13	1.98	0.45
2:B:356:LEU:HD21	2:B:392:PHE:HA	1.99	0.45
2:C:300:ARG:N	2:C:333:MET:HE1	2.31	0.45
2:D:259:SER:OG	2:D:261:VAL:HG23	2.17	0.45
2:D:316:ALA:O	2:D:348:CYS:HA	2.16	0.45
2:E:121:PHE:O	2:E:122:ASP:C	2.55	0.45
1:F:497:ILE:HG13	1:F:497:ILE:O	2.14	0.45
1:A:18:ILE:HD11	1:F:85:LYS:HG3	1.99	0.45
1:A:211:LEU:HB2	1:A:216:ARG:CD	2.46	0.45
2:B:122:ASP:C	2:B:124:SER:N	2.70	0.45
2:B:147:VAL:CG2	2:B:148:THR:N	2.79	0.45
2:B:284:ILE:H	2:B:284:ILE:HD12	1.81	0.45
2:B:445:ILE:HD12	2:B:486:PHE:CZ	2.52	0.45
2:C:406:GLU:O	2:C:408:ILE:HG13	2.17	0.45
2:D:325:LEU:HD23	2:D:335:PHE:HB2	1.98	0.45
1:F:178:THR:CG2	1:F:179:VAL:N	2.79	0.45
1:F:256:GLN:HG2	1:F:256:GLN:H	1.50	0.45
1:A:127:ILE:HD11	1:A:167:LEU:HD13	1.98	0.45
1:A:268:VAL:O	1:A:271:ASP:HB2	2.17	0.45
1:A:352:GLU:CD	1:A:352:GLU:N	2.70	0.45
1:A:489:ILE:HD13	1:A:494:PRO:HB3	1.99	0.45
2:B:116:GLU:HG2	2:B:117:VAL:N	2.23	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:ARG:CA	2:B:140:ARG:HH11	2.30	0.45
2:B:212:GLU:HG2	2:B:212:GLU:O	2.16	0.45
2:B:88:ARG:HG2	2:B:88:ARG:NH1	2.32	0.45
2:C:79:THR:HG22	2:C:82:ASP:H	1.79	0.45
2:D:202:ASP:HA	2:D:226:ARG:HD2	1.99	0.45
2:D:333:MET:HG2	5:D:910:HOH:O	2.17	0.45
2:D:315:PHE:CD2	2:D:347:VAL:HG21	2.52	0.45
1:F:129:ARG:O	1:F:132:TYR:HB3	2.17	0.45
1:F:471:MET:SD	1:F:478:ASP:HB3	2.56	0.45
1:A:183:GLU:OE2	2:B:161:ARG:NH1	2.49	0.45
2:B:298:VAL:HG12	2:B:299:SER:N	2.32	0.45
2:D:23:THR:O	2:D:24:MET:HB2	2.17	0.45
2:E:144:ILE:HD11	2:E:171:LEU:HD11	1.98	0.45
1:F:131:ASN:OD1	1:F:174:ILE:HD12	2.16	0.45
1:F:504:GLU:HB2	1:F:505:LEU:H	1.48	0.45
1:A:207:LEU:HD22	1:A:237:PHE:CE2	2.52	0.44
1:A:428:SER:OG	1:A:430:ILE:HD11	2.17	0.44
2:B:302:VAL:HG13	2:B:344:LEU:HD23	1.98	0.44
2:B:492:GLY:C	2:B:494:PRO:HD3	2.36	0.44
2:D:67:PHE:CB	2:D:69:GLU:HG3	2.47	0.44
1:F:231:MET:SD	1:F:251:ALA:HB2	2.56	0.44
1:F:379:SER:HA	1:F:413:THR:HG22	1.99	0.44
1:F:514:GLU:O	1:F:515:LYS:CB	2.60	0.44
1:A:146:SER:H	1:A:181:THR:HG22	1.81	0.44
1:A:182:THR:HG22	1:A:183:GLU:N	2.32	0.44
1:A:24:MET:N	1:A:29:ASP:OD2	2.44	0.44
1:A:311:ARG:NH1	1:A:371:LYS:HE3	2.32	0.44
3:A:901:ATP:H3'	2:B:458:MET:O	2.17	0.44
2:B:105:ILE:O	2:B:105:ILE:HG22	2.16	0.44
2:B:295:THR:HG23	2:B:378:ASP:OD2	2.18	0.44
2:B:57:ILE:C	2:B:59:PHE:H	2.20	0.44
2:C:337:GLU:OE1	2:C:340:ARG:NH1	2.50	0.44
2:C:68:ASP:CG	2:C:102:LYS:HZ1	2.20	0.44
2:D:191:ILE:HB	2:D:198:GLU:HG2	1.97	0.44
2:E:161:ARG:CA	2:E:196:VAL:HG11	2.47	0.44
2:E:191:ILE:CB	2:E:198:GLU:HG2	2.46	0.44
2:E:315:PHE:CD2	2:E:363:ILE:HD13	2.52	0.44
1:F:121:PHE:HD2	1:F:121:PHE:HA	1.69	0.44
1:F:315:PHE:HE1	1:F:375:ILE:CD1	2.30	0.44
1:F:515:LYS:HG3	1:F:517:PRO:HD2	1.98	0.44
1:A:44:VAL:HG22	1:A:205:VAL:HB	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:HG13	1:A:372:PRO:HG2	1.98	0.44
1:A:441:GLN:O	1:A:441:GLN:HG3	2.18	0.44
2:B:44:VAL:HA	2:B:205:VAL:O	2.17	0.44
2:B:360:LEU:HD23	2:B:399:VAL:HG23	1.99	0.44
2:B:371:LYS:O	2:B:371:LYS:CD	2.66	0.44
2:D:47:THR:HG22	2:D:184:ARG:C	2.36	0.44
1:F:116:GLU:O	1:F:117:VAL:HB	2.16	0.44
1:A:462:TRP:C	1:A:463:HIS:HD1	2.21	0.44
2:B:126:LEU:C	2:B:128:GLU:H	2.19	0.44
2:B:79:THR:HG22	2:B:82:ASP:OD2	2.17	0.44
2:C:263:VAL:CG2	2:C:280:LYS:HA	2.47	0.44
2:C:469:GLU:CG	2:C:480:LYS:HE3	2.47	0.44
2:D:340:ARG:C	2:D:342:ASN:N	2.71	0.44
2:D:378:ASP:O	2:D:379:SER:HB3	2.18	0.44
2:D:464:ASP:OD1	2:D:465:LYS:N	2.50	0.44
2:E:130:ILE:O	2:E:134:ILE:HG12	2.17	0.44
2:E:443:VAL:HG12	2:E:445:ILE:HG13	2.00	0.44
2:E:489:ILE:HD12	2:E:489:ILE:N	2.32	0.44
1:F:123:LEU:HD12	1:F:166:ARG:HD2	1.99	0.44
1:F:80:PRO:HB2	1:F:81:GLN:NE2	2.32	0.44
1:A:31:ILE:HD13	1:A:220:LEU:HD22	1.98	0.44
1:A:320:SEP:C	1:A:348:CYS:HG	2.27	0.44
1:A:420:MET:CE	2:B:490:ILE:HG21	2.48	0.44
2:C:126:LEU:O	2:C:129:ARG:N	2.50	0.44
2:C:284:ILE:HD11	2:C:409:THR:HG22	2.00	0.44
2:D:41:SER:HB2	2:D:178:THR:HB	1.98	0.44
2:E:104:PHE:CE2	2:E:106:LEU:HB2	2.53	0.44
1:F:106:LEU:HD13	1:F:129:ARG:NH2	2.32	0.44
1:F:504:GLU:HB3	1:F:507:ARG:NH2	2.32	0.44
1:A:127:ILE:HD11	1:A:167:LEU:HD12	1.99	0.44
2:B:47:THR:O	2:B:50:THR:HB	2.17	0.44
2:B:497:ILE:HD12	2:B:498:THR:N	2.33	0.44
2:C:41:SER:HA	2:C:178:THR:O	2.18	0.44
2:D:353:SER:O	2:D:354:ALA:CB	2.61	0.44
2:D:311:ARG:CD	2:D:371:LYS:HE3	2.29	0.44
2:D:385:ARG:NH2	2:E:433:ILE:CD1	2.80	0.44
1:F:191:ILE:HD13	1:F:198:GLU:HG2	1.99	0.44
1:A:418:GLN:HB2	2:B:423:HIS:O	2.17	0.44
2:B:280:LYS:HZ3	2:B:407:GLU:HB3	1.83	0.44
2:B:461:SER:OG	2:B:462:TRP:N	2.50	0.44
2:D:148:THR:HG21	2:D:193:ARG:HD2	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:GLY:CA	3:D:901:ATP:O2B	2.65	0.44
2:D:458:MET:HB2	2:D:463:HIS:HD2	1.83	0.44
2:E:202:ASP:HB2	2:E:203:ASN:ND2	2.33	0.44
2:E:212:GLU:HG2	2:E:212:GLU:O	2.17	0.44
2:E:451:ARG:HH11	2:E:451:ARG:CG	2.30	0.44
2:E:469:GLU:CB	2:E:483:PHE:CZ	3.01	0.44
1:F:21:MET:HE3	1:F:141:ARG:NE	2.33	0.44
1:F:468:ARG:HD3	1:F:479:ILE:HG22	1.99	0.44
1:F:504:GLU:HA	1:F:507:ARG:HE	1.81	0.44
1:A:79:THR:HG23	1:A:81:GLN:HG2	1.92	0.44
2:B:194:TYR:C	2:B:196:VAL:N	2.67	0.44
2:B:266:GLY:O	2:B:300:ARG:CG	2.66	0.44
2:B:327:ASN:ND2	2:C:459:ARG:HB3	2.33	0.44
2:C:239:ILE:HG12	2:C:244:ILE:CD1	2.48	0.44
2:C:284:ILE:N	2:C:284:ILE:HD12	2.33	0.44
2:C:325:LEU:CD2	2:C:335:PHE:HB2	2.47	0.44
2:E:451:ARG:HB3	2:E:470:PHE:CE2	2.53	0.44
2:D:495:THR:HA	2:E:487:GLU:OE2	2.18	0.44
1:F:462:TRP:O	1:F:463:HIS:CG	2.70	0.44
1:A:448:GLU:HG2	2:B:466:ALA:HA	2.00	0.44
2:B:353:SER:O	2:B:354:ALA:HB2	2.17	0.44
2:B:44:VAL:HG22	2:B:205:VAL:HG12	1.99	0.44
2:B:500:ASP:C	2:B:501:GLU:HG3	2.38	0.44
2:B:84:ILE:HD12	2:B:94:LEU:CB	2.44	0.44
2:C:140:ARG:CA	2:C:140:ARG:HH11	2.31	0.44
2:C:420:MET:HE3	2:C:492:GLY:HA3	2.00	0.44
2:D:333:MET:CA	5:D:913:HOH:O	2.44	0.44
2:D:426:THR:HB	2:D:431:GLU:OE2	2.18	0.44
2:E:192:ALA:HB3	2:E:197:GLU:OE2	2.18	0.44
2:E:489:ILE:HA	2:E:494:PRO:HG3	1.99	0.44
2:E:504:GLU:CG	2:E:505:LEU:H	2.30	0.44
1:F:44:VAL:O	1:F:181:THR:HA	2.18	0.44
1:F:313:ILE:HG13	1:F:372:PRO:HG2	2.00	0.44
1:A:124:SER:O	1:A:128:GLU:HG3	2.18	0.43
2:B:199:PHE:CD2	2:B:199:PHE:N	2.86	0.43
2:B:93:ASP:OD2	2:B:96:LYS:HB2	2.18	0.43
2:D:19:ALA:HB1	2:D:38:ILE:HD12	1.99	0.43
2:E:148:THR:HG1	2:E:182:THR:HG23	1.83	0.43
1:F:231:MET:CE	1:F:251:ALA:HB2	2.48	0.43
1:F:445:ILE:HG22	1:F:446:ARG:HD2	2.00	0.43
1:F:513:GLN:HA	1:F:513:GLN:OE1	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:CB	1:A:489:ILE:HD11	2.48	0.43
2:B:126:LEU:C	2:B:128:GLU:N	2.71	0.43
2:B:283:ILE:HG12	2:B:400:THR:HG23	2.00	0.43
2:C:134:ILE:HG23	2:C:139:ALA:HB3	1.99	0.43
2:C:164:LEU:HD11	2:C:197:GLU:HG3	2.00	0.43
2:D:123:LEU:HD21	2:D:163:GLU:HB3	2.00	0.43
2:D:273:MET:O	2:D:463:HIS:HA	2.17	0.43
2:E:419:PHE:O	2:E:420:MET:HB2	2.18	0.43
1:F:111:ASP:HA	1:F:112:PRO:HD3	1.92	0.43
1:F:127:ILE:CD1	1:F:167:LEU:HD13	2.48	0.43
1:F:185:ILE:N	1:F:185:ILE:HD13	2.33	0.43
1:A:377:ILE:HD13	1:A:412:PHE:CD2	2.53	0.43
2:B:146:SER:H	2:B:181:THR:CG2	2.31	0.43
2:B:87:ALA:HB1	2:B:92:TRP:CD1	2.53	0.43
2:C:292:THR:HB	2:C:440:LEU:HB3	1.99	0.43
2:C:453:ILE:HD13	2:C:453:ILE:C	2.38	0.43
2:C:81:GLN:CD	2:C:81:GLN:H	2.20	0.43
2:D:350:TYR:CE1	2:E:252:MET:HE2	2.53	0.43
2:E:313:ILE:HB	2:E:375:ILE:HD13	1.94	0.43
2:E:438:ILE:N	2:E:438:ILE:HD12	2.33	0.43
1:F:406:GLU:HB3	1:F:408:ILE:HG12	1.99	0.43
2:B:131:ASN:OD1	2:B:174:ILE:HD12	2.18	0.43
2:B:377:ILE:HB	2:B:412:PHE:HD2	1.82	0.43
2:B:426:THR:HG22	2:B:429:HIS:H	1.83	0.43
2:C:131:ASN:OD1	2:C:174:ILE:HD12	2.17	0.43
2:C:387:VAL:CG1	2:C:388:SER:N	2.82	0.43
2:D:350:TYR:O	2:D:351:PRO:C	2.56	0.43
2:E:444:GLU:O	2:E:494:PRO:HD2	2.17	0.43
1:F:496:ARG:HD3	1:F:496:ARG:N	2.33	0.43
1:A:136:LYS:HD3	1:A:137:TYR:HE1	1.83	0.43
1:A:153:GLN:C	1:A:154:TYR:CD2	2.92	0.43
1:A:305:ALA:O	1:A:310:GLU:HB2	2.19	0.43
1:A:312:ALA:HA	1:A:374:ARG:O	2.19	0.43
1:A:378:ASP:OD1	1:A:413:THR:HG21	2.19	0.43
1:A:274:CYS:HA	1:A:463:HIS:HB2	1.99	0.43
1:A:471:MET:HE2	1:A:471:MET:O	2.18	0.43
1:A:72:VAL:HB	1:A:142:VAL:HG22	2.00	0.43
1:A:211:LEU:HD21	2:B:188:TYR:HE2	1.84	0.43
2:C:121:PHE:O	2:C:125:ALA:HB3	2.18	0.43
2:C:392:PHE:CE2	2:C:430:ILE:HD11	2.54	0.43
2:C:66:GLU:C	2:C:67:PHE:CD1	2.92	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:79:THR:HG23	2:C:81:GLN:HG2	2.01	0.43
2:C:318:GLU:OE2	2:D:432:GLU:HG2	2.19	0.43
2:E:184:ARG:CD	2:E:191:ILE:O	2.66	0.43
2:E:22:ARG:HB3	2:E:29:ASP:OD2	2.19	0.43
1:F:281:ASP:OD1	1:F:407:GLU:OE1	2.37	0.43
1:F:284:ILE:HD12	1:F:284:ILE:H	1.83	0.43
2:B:123:LEU:O	2:B:127:ILE:HG13	2.19	0.43
2:B:164:LEU:HD11	2:B:197:GLU:HG3	2.00	0.43
2:B:52:LYS:HD2	2:B:182:THR:O	2.19	0.43
2:C:256:GLN:HG2	2:C:256:GLN:H	1.54	0.43
2:D:203:ASN:HB3	2:D:225:LEU:CD2	2.48	0.43
2:D:387:VAL:CG1	2:D:388:SER:H	2.32	0.43
2:E:313:ILE:CD1	2:E:372:PRO:HG2	2.48	0.43
2:B:51:GLY:H	3:B:903:ATP:PB	2.42	0.43
2:B:79:THR:HG21	2:B:81:GLN:HG2	1.99	0.43
2:C:471:MET:HB3	2:C:480:LYS:NZ	2.34	0.43
2:D:148:THR:HG23	2:D:193:ARG:HD2	1.99	0.43
2:D:203:ASN:CB	2:D:225:LEU:HD23	2.49	0.43
2:D:296:LEU:HD11	2:D:477:PRO:HD3	2.01	0.43
1:F:464:ASP:OD2	1:F:466:ALA:HB3	2.19	0.43
1:A:18:ILE:HG21	1:A:37:PRO:HB3	2.00	0.43
1:A:65:ILE:HG12	1:A:65:ILE:H	1.62	0.43
2:B:136:LYS:HE2	2:B:137:TYR:CE1	2.54	0.43
2:B:142:VAL:HG23	2:B:176:ALA:HB1	2.01	0.43
2:B:333:MET:HG2	2:B:333:MET:H	1.34	0.43
2:B:455:VAL:HG11	2:B:463:HIS:HB2	2.01	0.43
2:B:92:TRP:HD1	2:B:92:TRP:O	2.02	0.43
2:B:89:SER:CB	2:C:227:GLY:O	2.67	0.43
2:D:230:HIS:C	2:D:230:HIS:HD1	2.22	0.43
2:D:446:ARG:H	2:D:496:ARG:CZ	2.31	0.43
2:E:486:PHE:CB	2:E:489:ILE:HD11	2.49	0.43
1:F:109:SER:HA	1:F:110:PRO:HD3	1.84	0.43
1:F:126:LEU:HD11	1:F:130:ILE:HD11	2.01	0.43
1:F:455:VAL:HG11	1:F:463:HIS:CB	2.40	0.43
2:B:21:MET:HB2	2:B:38:ILE:CG1	2.43	0.43
2:C:44:VAL:HA	2:C:205:VAL:O	2.18	0.43
2:D:469:GLU:HG3	2:D:470:PHE:N	2.31	0.43
1:F:247:PHE:HB3	1:F:249:LEU:HD21	2.01	0.43
1:F:248:PRO:HB2	1:F:251:ALA:CB	2.45	0.43
1:F:94:LEU:O	1:F:97:LEU:N	2.51	0.43
1:A:126:LEU:HG	1:A:130:ILE:CD1	2.49	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:TYR:N	1:A:137:TYR:CD1	2.86	0.43
1:A:148:THR:CG2	1:A:193:ARG:HD2	2.49	0.43
1:A:317:TYR:CE2	1:A:383:LEU:HD21	2.54	0.43
1:A:471:MET:HG3	1:A:471:MET:H	1.67	0.43
2:B:127:ILE:HD13	2:B:170:ARG:HG3	2.01	0.43
2:C:113:GLU:O	2:C:114:GLY:C	2.58	0.43
2:C:127:ILE:N	2:C:127:ILE:CD1	2.82	0.43
2:C:446:ARG:HG2	2:C:496:ARG:CZ	2.49	0.43
2:C:61:TYR:CG	2:C:65:ILE:HD13	2.53	0.43
2:D:209:ASN:HD22	2:D:209:ASN:HA	1.61	0.43
1:F:329:TYR:C	1:F:331:TRP:N	2.72	0.43
1:F:515:LYS:CG	1:F:517:PRO:HD2	2.49	0.43
1:F:93:ASP:OD2	1:F:96:LYS:HB2	2.18	0.43
1:A:267:VAL:CG1	1:A:270:LEU:HB2	2.48	0.42
1:A:356:LEU:HD23	1:A:395:PHE:HB2	2.01	0.42
2:B:162:ARG:HH11	2:B:162:ARG:CB	2.31	0.42
2:C:348:CYS:O	2:C:349:ALA:HB2	2.19	0.42
2:C:483:PHE:N	2:C:483:PHE:CD1	2.87	0.42
2:E:147:VAL:CG2	2:E:148:THR:N	2.82	0.42
1:F:380:LEU:O	1:F:383:LEU:N	2.50	0.42
1:A:340:ARG:O	1:A:342:ASN:N	2.53	0.42
1:A:379:SER:H	1:A:413:THR:CB	2.32	0.42
2:C:425:ILE:HD12	2:C:425:ILE:H	1.84	0.42
2:C:44:VAL:HG12	2:C:44:VAL:O	2.19	0.42
2:D:394:GLN:NE2	5:D:530:HOH:O	2.51	0.42
2:D:471:MET:HE2	2:D:478:ASP:CB	2.49	0.42
2:E:296:LEU:HD13	2:E:331:TRP:CE3	2.54	0.42
2:E:371:LYS:CD	2:E:371:LYS:O	2.62	0.42
1:F:134:ILE:CD1	1:F:139:ALA:HB3	2.50	0.42
1:F:289:ALA:O	1:F:292:THR:HG23	2.18	0.42
1:F:375:ILE:HA	1:F:375:ILE:HD13	1.87	0.42
1:F:387:VAL:CG1	1:F:391:ALA:HB3	2.49	0.42
1:A:304:ASN:OD1	1:A:304:ASN:O	2.38	0.42
1:A:82:ASP:O	1:A:85:LYS:N	2.52	0.42
2:B:451:ARG:HB3	2:B:470:PHE:CE2	2.54	0.42
2:C:378:ASP:O	2:C:379:SER:CB	2.66	0.42
2:C:443:VAL:HG12	2:C:445:ILE:HG12	2.02	0.42
2:C:472:ILE:HD12	2:C:472:ILE:N	2.34	0.42
2:D:18:ILE:HD12	2:D:227:GLY:CA	2.42	0.42
2:D:385:ARG:HG2	2:E:393:ARG:CZ	2.48	0.42
2:E:69:GLU:HA	2:E:70:PRO:HD3	1.89	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:LEU:O	1:F:167:LEU:N	2.52	0.42
1:F:212:GLU:OE2	1:F:212:GLU:O	2.36	0.42
1:A:212:GLU:CG	1:A:212:GLU:O	2.68	0.42
1:A:266:GLY:C	1:A:300:ARG:HG3	2.39	0.42
1:A:36:LEU:HA	1:A:37:PRO:HD3	1.87	0.42
1:A:64:ILE:CD1	1:A:70:PRO:HA	2.48	0.42
2:B:98:VAL:HA	2:B:103:LEU:O	2.19	0.42
2:B:393:ARG:O	2:B:397:ILE:HG13	2.19	0.42
2:B:451:ARG:HD2	2:B:451:ARG:N	2.34	0.42
2:C:486:PHE:HE2	2:C:496:ARG:HG2	1.84	0.42
2:D:244:ILE:HG22	2:D:245:ASN:N	2.34	0.42
2:D:64:ILE:HG21	2:D:97:LEU:HD13	2.00	0.42
2:E:348:CYS:O	2:E:349:ALA:HB2	2.19	0.42
2:E:289:ALA:CB	2:E:419:PHE:HA	2.46	0.42
2:E:462:TRP:O	2:E:463:HIS:CD2	2.72	0.42
2:E:331:TRP:NE1	3:E:901:ATP:N7	2.59	0.42
1:F:18:ILE:HB	1:F:228:THR:CG2	2.48	0.42
1:F:313:ILE:CD1	1:F:372:PRO:HG2	2.49	0.42
1:A:320:SEP:O2P	2:B:256:GLN:O	2.37	0.42
1:A:336:GLU:OE1	1:A:336:GLU:HA	2.19	0.42
2:D:420:MET:HE3	2:D:420:MET:HB3	1.83	0.42
2:D:52:LYS:N	3:D:903:ATP:O1B	2.43	0.42
2:E:223:LEU:HD23	2:E:223:LEU:HA	1.45	0.42
2:E:315:PHE:CD2	2:E:347:VAL:HG21	2.54	0.42
2:E:445:ILE:HD11	2:E:483:PHE:CE2	2.54	0.42
1:F:484:ARG:CB	1:F:484:ARG:HH11	2.29	0.42
1:F:47:THR:O	1:F:50:THR:HG23	2.20	0.42
3:A:901:ATP:O2G	2:B:459:ARG:NH2	2.51	0.42
2:B:73:PHE:CD2	2:B:105:ILE:HD12	2.54	0.42
2:B:204:VAL:HG23	2:B:224:LYS:HG2	2.00	0.42
2:B:36:LEU:HD12	2:B:59:PHE:CE1	2.54	0.42
2:B:24:MET:HB3	2:B:62:ASN:HD22	1.84	0.42
2:C:486:PHE:HB3	2:C:489:ILE:HD11	2.01	0.42
2:D:160:VAL:O	2:D:164:LEU:HB2	2.19	0.42
2:D:127:ILE:CD1	2:D:167:LEU:HD13	2.50	0.42
2:D:52:LYS:HB2	2:D:52:LYS:HE3	1.85	0.42
1:F:191:ILE:HG21	1:F:198:GLU:HG3	2.02	0.42
1:F:484:ARG:HB2	1:F:484:ARG:NH1	2.34	0.42
1:A:148:THR:OG1	1:A:182:THR:HG23	2.20	0.42
1:A:325:LEU:HD22	1:A:336:GLU:HG2	2.02	0.42
1:A:485:ASN:N	1:A:485:ASN:OD1	2.48	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:LEU:HB3	2:B:200:VAL:HG11	2.02	0.42
2:B:453:ILE:HD13	2:B:454:ASN:H	1.83	0.42
2:C:186:GLU:OE2	2:C:187:GLU:N	2.53	0.42
2:C:208:ARG:NH2	2:C:221:GLU:OE2	2.52	0.42
2:C:363:ILE:HG22	2:C:367:ILE:HD11	2.02	0.42
2:D:367:ILE:HG23	2:D:372:PRO:HD2	2.01	0.42
2:D:384:ALA:HB2	2:D:392:PHE:CE1	2.54	0.42
2:E:413:THR:CG2	2:E:414:ASN:N	2.83	0.42
1:F:269:ARG:O	1:F:272:GLU:HB2	2.20	0.42
1:F:367:ILE:HD11	1:F:375:ILE:HG13	2.00	0.42
1:A:393:ARG:HH12	1:F:385:ARG:HA	1.85	0.42
1:A:306:CYS:HB2	1:A:338:MET:SD	2.59	0.42
1:A:311:ARG:CZ	1:A:371:LYS:HE3	2.50	0.42
1:A:382:ALA:O	1:A:385:ARG:HG3	2.20	0.42
1:A:81:GLN:H	1:A:81:GLN:NE2	2.18	0.42
1:A:348:CYS:HB3	2:B:254:LEU:HD23	2.02	0.42
2:B:445:ILE:HD11	2:B:494:PRO:HG2	2.01	0.42
2:C:439:LEU:HD12	2:C:439:LEU:C	2.40	0.42
2:E:220:LEU:C	2:E:220:LEU:HD23	2.40	0.42
2:E:225:LEU:HD12	2:E:230:HIS:HB3	2.00	0.42
2:E:23:THR:O	2:E:24:MET:CB	2.68	0.42
1:A:166:ARG:HG3	1:F:112:PRO:O	2.20	0.42
2:B:436:THR:HG23	2:B:458:MET:CG	2.50	0.42
2:C:62:ASN:O	2:C:66:GLU:N	2.47	0.42
2:D:332:GLY:O	2:D:333:MET:HG2	2.19	0.42
2:D:325:LEU:CD2	2:D:335:PHE:HB2	2.50	0.42
2:E:106:LEU:HD13	2:E:129:ARG:NH2	2.34	0.42
2:E:164:LEU:HD23	2:E:164:LEU:HA	1.81	0.42
2:E:217:ARG:HH21	2:E:236:PRO:HB3	1.85	0.42
2:E:344:LEU:CD1	2:E:346:ILE:HG13	2.48	0.42
2:E:360:LEU:HD22	2:E:360:LEU:O	2.20	0.42
2:E:445:ILE:HG22	2:E:445:ILE:O	2.20	0.42
2:E:486:PHE:HB2	2:E:489:ILE:HD11	2.00	0.42
2:E:326:ARG:HD3	1:F:258:SER:OG	2.20	0.42
1:F:433:ILE:N	1:F:433:ILE:HD12	2.34	0.42
1:A:319:GLU:O	2:B:254:LEU:HD21	2.20	0.42
1:A:348:CYS:O	1:A:349:ALA:HB2	2.20	0.42
1:A:426:THR:HB	1:A:431:GLU:OE1	2.20	0.42
1:A:451:ARG:CD	1:A:451:ARG:N	2.81	0.42
2:B:350:TYR:CE1	2:C:252:MET:HE2	2.55	0.42
2:C:54:LEU:HD23	2:C:244:ILE:CG1	2.47	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:O	1:F:118:VAL:CB	2.67	0.42
1:F:451:ARG:NH1	1:F:451:ARG:HG2	2.33	0.42
1:A:323:GLN:HA	2:B:258:SER:OG	2.19	0.41
1:A:367:ILE:HD12	1:A:375:ILE:HD11	2.01	0.41
2:B:125:ALA:O	2:B:128:GLU:HB2	2.20	0.41
2:B:282:SER:C	2:B:283:ILE:HD12	2.41	0.41
2:B:471:MET:HB3	2:B:480:LYS:NZ	2.34	0.41
2:B:50:THR:HG22	2:B:52:LYS:HE2	2.02	0.41
2:B:61:TYR:CZ	2:B:92:TRP:HB2	2.55	0.41
2:C:142:VAL:HG12	2:C:178:THR:HG23	2.02	0.41
2:D:70:PRO:HG2	2:D:138:ARG:O	2.20	0.41
2:D:19:ALA:CB	2:D:38:ILE:HD12	2.49	0.41
2:D:439:LEU:HD12	2:D:439:LEU:C	2.40	0.41
2:D:54:LEU:HD13	2:D:90:PHE:CZ	2.55	0.41
2:E:489:ILE:H	2:E:489:ILE:HD12	1.85	0.41
1:F:150:VAL:O	1:F:153:GLN:HG3	2.20	0.41
1:F:249:LEU:HD12	1:F:394:GLN:CD	2.39	0.41
1:F:344:LEU:HD13	1:F:344:LEU:O	2.20	0.41
1:F:371:LYS:N	1:F:372:PRO:HD3	2.35	0.41
1:F:438:ILE:O	1:F:438:ILE:HG22	2.19	0.41
1:F:49:GLY:O	1:F:218:ARG:NH2	2.52	0.41
1:A:283:ILE:HD12	1:A:412:PHE:CE1	2.55	0.41
3:A:903:ATP:O3'	2:B:224:LYS:HB2	2.21	0.41
2:B:73:PHE:HE2	2:B:83:ILE:HD13	1.85	0.41
2:C:290:THR:HG23	2:C:290:THR:O	2.21	0.41
2:E:180:MET:HB3	2:E:180:MET:HE2	1.82	0.41
2:E:200:VAL:O	2:E:200:VAL:CG1	2.67	0.41
1:F:161:ARG:HB2	1:F:196:VAL:CG1	2.49	0.41
1:F:486:PHE:HD2	1:F:494:PRO:HB2	1.84	0.41
1:A:244:ILE:CG2	1:A:246:ILE:HD11	2.50	0.41
1:A:79:THR:HG23	1:A:81:GLN:NE2	2.17	0.41
2:B:336:GLU:OE1	2:B:336:GLU:HA	2.21	0.41
2:B:249:LEU:HD13	2:B:394:GLN:HG2	2.02	0.41
2:C:42:THR:HG23	2:C:203:ASN:HB2	2.01	0.41
2:D:106:LEU:HD11	2:D:129:ARG:CZ	2.50	0.41
2:E:443:VAL:HG11	2:E:445:ILE:HD11	2.02	0.41
1:F:21:MET:HE1	1:F:141:ARG:HG2	2.02	0.41
1:F:433:ILE:HG22	1:F:433:ILE:O	2.19	0.41
1:A:20:LYS:HE3	1:A:228:THR:HG21	2.01	0.41
2:B:51:GLY:C	3:B:903:ATP:O1B	2.59	0.41
2:C:219:THR:O	2:C:237:PHE:HE2	2.04	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:32:SER:OG	2:C:35:GLY:HA2	2.20	0.41
2:C:380:LEU:HA	2:C:380:LEU:HD23	1.90	0.41
2:C:25:ILE:CG1	2:C:58:GLN:HE21	2.24	0.41
2:D:45:SER:HB3	2:D:182:THR:HB	2.02	0.41
2:E:49:GLY:HA2	3:E:903:ATP:O2B	2.21	0.41
1:F:220:LEU:HD21	1:F:222:ILE:HD11	2.03	0.41
1:A:489:ILE:HD13	1:A:494:PRO:CG	2.50	0.41
2:B:182:THR:HG21	2:B:192:ALA:CB	2.41	0.41
2:B:194:TYR:O	2:B:195:GLY:C	2.57	0.41
2:B:452:ALA:O	2:B:470:PHE:HE2	2.03	0.41
2:B:499:VAL:C	2:B:501:GLU:H	2.23	0.41
2:C:382:ALA:O	2:C:385:ARG:HG3	2.19	0.41
2:C:70:PRO:HB2	2:C:139:ALA:HA	2.02	0.41
2:D:344:LEU:HD13	2:D:345:LYS:N	2.36	0.41
1:F:396:VAL:O	1:F:400:THR:HB	2.19	0.41
1:A:396:VAL:O	1:A:400:THR:CB	2.67	0.41
2:B:347:VAL:O	2:B:348:CYS:HB2	2.21	0.41
2:B:36:LEU:HD12	2:B:59:PHE:CZ	2.56	0.41
2:B:471:MET:HG2	2:B:480:LYS:HZ3	1.84	0.41
2:B:73:PHE:HB3	2:B:105:ILE:CD1	2.36	0.41
2:B:326:ARG:HG3	2:C:260:ASN:ND2	2.35	0.41
2:C:63:GLY:CA	2:C:141:ARG:CZ	2.98	0.41
2:D:328:ALA:N	5:D:552:HOH:O	2.53	0.41
2:D:88:ARG:HD3	2:E:15:HIS:O	2.20	0.41
2:E:18:ILE:HD12	2:E:18:ILE:O	2.21	0.41
2:E:353:SER:O	2:E:354:ALA:HB2	2.20	0.41
2:E:468:ARG:NH1	2:E:468:ARG:HG2	2.36	0.41
1:F:266:GLY:HA3	1:F:300:ARG:HG3	2.02	0.41
1:F:312:ALA:HB2	1:F:374:ARG:HB2	2.01	0.41
1:A:94:LEU:HD22	1:A:103:LEU:CD2	2.51	0.41
1:A:323:GLN:HA	2:B:258:SER:CB	2.51	0.41
1:A:319:GLU:OE1	1:A:324:LEU:HD23	2.21	0.41
1:A:36:LEU:HD12	1:A:59:PHE:CE1	2.56	0.41
2:B:151:PHE:C	2:B:153:GLN:N	2.74	0.41
2:B:182:THR:HG22	2:B:183:GLU:H	1.86	0.41
2:B:311:ARG:CD	2:B:371:LYS:HE3	2.41	0.41
1:A:448:GLU:HG2	2:B:466:ALA:CA	2.50	0.41
2:B:80:PRO:HA	2:B:83:ILE:HD12	2.03	0.41
2:C:468:ARG:HG2	2:C:468:ARG:NH1	2.35	0.41
2:C:61:TYR:CZ	2:C:92:TRP:HB2	2.56	0.41
2:D:84:ILE:HD11	2:D:105:ILE:CD1	2.51	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:GLY:CA	3:D:903:ATP:O2B	2.68	0.41
2:E:152:GLN:HG3	1:F:161:ARG:NH1	2.34	0.41
2:E:211:LEU:HD12	2:E:211:LEU:HA	1.88	0.41
1:F:299:SER:HB3	1:F:333:MET:HE1	2.01	0.41
1:A:304:ASN:HB3	1:A:374:ARG:HH12	1.86	0.41
1:A:461:SER:OG	1:A:462:TRP:N	2.54	0.41
1:A:64:ILE:HG21	1:A:97:LEU:HD22	2.02	0.41
1:A:320:SEP:CB	2:B:254:LEU:HG	2.46	0.41
2:B:51:GLY:O	2:B:54:LEU:HB3	2.21	0.41
2:C:127:ILE:HD11	2:C:167:LEU:HD13	2.02	0.41
2:C:23:THR:O	2:C:24:MET:HB2	2.21	0.41
2:C:306:CYS:SG	2:C:344:LEU:HB2	2.61	0.41
2:D:106:LEU:C	2:D:106:LEU:HD12	2.41	0.41
2:E:269:ARG:HH22	2:E:468:ARG:NH2	2.18	0.41
2:E:291:GLY:C	2:E:442:TYR:OH	2.59	0.41
2:E:325:LEU:HD23	2:E:335:PHE:HB2	2.03	0.41
1:A:467:ILE:HD13	1:F:447:GLY:O	2.20	0.41
2:B:161:ARG:HB2	2:B:196:VAL:HG11	2.01	0.41
2:B:479:ILE:CD1	2:B:479:ILE:H	2.21	0.41
2:B:76:PHE:CZ	2:B:126:LEU:HD21	2.56	0.41
2:B:92:TRP:CD1	2:B:92:TRP:O	2.74	0.41
2:C:448:GLU:HG2	2:D:466:ALA:CA	2.48	0.41
2:D:21:MET:CE	2:D:59:PHE:HZ	2.33	0.41
2:D:246:ILE:O	2:D:248:PRO:HD3	2.20	0.41
2:D:54:LEU:CD2	2:D:239:ILE:HG23	2.51	0.41
2:E:419:PHE:O	2:E:420:MET:O	2.39	0.41
2:E:445:ILE:O	2:E:446:ARG:CB	2.65	0.41
1:F:299:SER:C	1:F:333:MET:CE	2.79	0.41
1:A:162:ARG:O	1:A:165:PHE:HB3	2.20	0.41
1:A:284:ILE:HG22	1:A:438:ILE:HD13	2.03	0.41
2:B:111:ASP:O	2:B:113:GLU:N	2.54	0.41
2:B:45:SER:HB3	2:B:182:THR:CB	2.39	0.41
2:B:96:LYS:O	2:B:100:GLU:HG3	2.21	0.41
2:C:118:VAL:O	2:C:118:VAL:HG12	2.21	0.41
2:C:20:LYS:HE2	2:C:228:THR:OG1	2.21	0.41
2:C:231:MET:CE	2:C:251:ALA:HB2	2.51	0.41
2:D:294:LYS:O	2:D:298:VAL:HG23	2.20	0.41
2:D:387:VAL:HG12	2:D:388:SER:H	1.83	0.41
2:E:264:SER:O	2:E:374:ARG:NH2	2.53	0.41
2:E:265:SER:HB3	2:E:278:PHE:CZ	2.55	0.41
2:E:362:ILE:O	2:E:365:SER:HB3	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:269:ARG:CG	2:E:479:ILE:HB	2.40	0.41
2:E:84:ILE:O	2:E:87:ALA:HB3	2.20	0.41
1:A:116:GLU:O	1:A:117:VAL:HB	2.21	0.41
1:A:23:THR:OG1	1:A:25:ILE:HG12	2.21	0.41
2:B:116:GLU:HG2	2:B:154:TYR:HE2	1.86	0.41
2:B:213:GLY:O	2:B:214:GLU:CB	2.68	0.41
2:B:211:LEU:O	2:B:215:ARG:O	2.39	0.41
2:B:451:ARG:NH1	2:B:472:ILE:HD12	2.35	0.41
2:C:53:THR:O	2:C:57:ILE:HG12	2.20	0.41
2:E:443:VAL:CG1	2:E:494:PRO:HG2	2.50	0.41
1:F:126:LEU:O	1:F:127:ILE:C	2.58	0.41
1:F:194:TYR:O	1:F:195:GLY:C	2.58	0.41
1:F:443:VAL:HG12	1:F:445:ILE:HD11	2.03	0.41
1:A:116:GLU:C	1:A:117:VAL:CG2	2.79	0.40
1:A:443:VAL:CG1	1:A:445:ILE:HD11	2.51	0.40
1:A:296:LEU:HD21	1:A:477:PRO:HD3	2.03	0.40
1:A:496:ARG:O	1:A:497:ILE:HG23	2.21	0.40
1:A:80:PRO:HD2	1:A:81:GLN:NE2	2.36	0.40
2:B:429:HIS:HA	2:B:431:GLU:OE2	2.20	0.40
2:B:81:GLN:CD	2:B:81:GLN:N	2.73	0.40
2:C:194:TYR:CD1	2:C:194:TYR:N	2.89	0.40
2:C:21:MET:HE3	2:C:141:ARG:CD	2.51	0.40
2:C:352:GLU:N	2:C:352:GLU:CD	2.74	0.40
2:C:296:LEU:HD21	2:C:477:PRO:HB3	2.03	0.40
2:D:443:VAL:HG12	2:D:445:ILE:CD1	2.51	0.40
2:D:484:ARG:NH1	2:D:484:ARG:CB	2.84	0.40
2:E:148:THR:HG23	2:E:193:ARG:HD2	2.03	0.40
2:E:306:CYS:SG	2:E:338:MET:SD	3.20	0.40
2:E:392:PHE:O	2:E:395:PHE:HB3	2.20	0.40
2:E:451:ARG:CG	2:E:451:ARG:NH1	2.84	0.40
1:F:21:MET:CE	1:F:59:PHE:CE1	3.04	0.40
1:A:112:PRO:O	2:B:166:ARG:HG3	2.21	0.40
1:A:237:PHE:HA	1:A:245:ASN:O	2.21	0.40
1:A:24:MET:CB	1:A:62:ASN:HD22	2.31	0.40
2:B:161:ARG:HB2	2:B:196:VAL:CG1	2.50	0.40
1:A:420:MET:HE1	2:B:490:ILE:HG21	2.02	0.40
2:B:497:ILE:O	2:B:498:THR:C	2.59	0.40
2:C:153:GLN:O	2:C:154:TYR:CB	2.69	0.40
2:C:320:SER:HA	2:D:254:LEU:HG	2.02	0.40
2:D:200:VAL:O	2:D:200:VAL:HG12	2.20	0.40
2:D:64:ILE:HD12	2:D:69:GLU:O	2.20	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:GLY:HA2	3:D:903:ATP:O2B	2.21	0.40
2:E:143:SER:HA	2:E:179:VAL:O	2.20	0.40
1:F:393:ARG:NH2	5:F:527:HOH:O	2.45	0.40
1:A:237:PHE:C	1:A:237:PHE:CD1	2.94	0.40
1:A:340:ARG:C	1:A:342:ASN:N	2.75	0.40
1:A:489:ILE:HD13	1:A:494:PRO:HG3	2.04	0.40
2:B:47:THR:HG23	2:B:187:GLU:OE2	2.21	0.40
2:B:267:VAL:HB	2:B:270:LEU:HB2	2.04	0.40
2:B:326:ARG:HG3	2:C:260:ASN:HD21	1.87	0.40
2:B:249:LEU:HD12	2:B:394:GLN:HG2	2.02	0.40
2:B:25:ILE:HG23	2:B:58:GLN:HE22	1.86	0.40
2:C:123:LEU:HA	2:C:127:ILE:HD13	2.02	0.40
2:C:28:PHE:N	2:C:246:ILE:HD12	2.36	0.40
2:C:468:ARG:HG2	2:C:468:ARG:HH11	1.85	0.40
2:C:484:ARG:HB3	2:C:484:ARG:NH1	2.35	0.40
2:D:396:VAL:HG11	2:D:430:ILE:CG2	2.51	0.40
2:D:472:ILE:N	2:D:472:ILE:HD12	2.37	0.40
2:D:75:THR:HG22	2:D:107:ASP:HA	2.04	0.40
1:F:18:ILE:HD12	1:F:227:GLY:CA	2.33	0.40
1:F:362:ILE:O	1:F:365:SER:HB3	2.21	0.40
1:A:487:GLU:OE1	1:F:496:ARG:HG2	2.22	0.40
2:B:134:ILE:HA	2:B:139:ALA:HB3	2.02	0.40
1:A:290:THR:CG2	2:B:425:ILE:HD12	2.44	0.40
2:C:149:SER:HA	2:C:152:GLN:HB2	2.03	0.40
2:D:315:PHE:HA	2:D:347:VAL:HB	2.04	0.40
2:E:186:GLU:OE2	2:E:187:GLU:N	2.54	0.40
2:E:262:ARG:HD2	2:E:276:GLY:O	2.21	0.40
2:E:436:THR:HG23	2:E:458:MET:CG	2.47	0.40
1:F:357:GLU:CG	1:F:358:ASP:N	2.84	0.40
1:F:425:ILE:HD13	1:F:437:ILE:HG21	2.03	0.40
2:B:119:GLY:C	2:B:121:PHE:N	2.75	0.40
2:B:363:ILE:O	2:B:367:ILE:HG13	2.21	0.40
2:C:111:ASP:OD2	2:C:113:GLU:HG2	2.21	0.40
2:C:121:PHE:HB3	2:C:125:ALA:CB	2.51	0.40
2:C:65:ILE:HG22	2:C:65:ILE:O	2.21	0.40
2:D:249:LEU:CD1	2:D:394:GLN:HG2	2.51	0.40
2:D:269:ARG:O	2:D:272:GLU:HB2	2.20	0.40
2:D:357:GLU:HG3	2:D:358:ASP:N	2.36	0.40
2:D:44:VAL:O	2:D:44:VAL:HG12	2.21	0.40
2:E:333:MET:HB2	2:E:333:MET:HE3	1.96	0.40
2:E:428:SER:CB	2:E:430:ILE:HD11	2.51	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:428:SER:OG	2:E:430:ILE:HD11	2.22	0.40
2:E:49:GLY:CA	3:E:903:ATP:O2B	2.70	0.40
1:F:172:LYS:HE3	1:F:172:LYS:HB2	1.92	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	503/525 (96%)	406 (81%)	76 (15%)	21 (4%)	3	16
1	F	503/525 (96%)	422 (84%)	61 (12%)	20 (4%)	3	17
2	B	489/525 (93%)	389 (80%)	82 (17%)	18 (4%)	3	19
2	C	486/525 (93%)	419 (86%)	45 (9%)	22 (4%)	2	14
2	D	483/525 (92%)	415 (86%)	52 (11%)	16 (3%)	4	21
2	E	490/525 (93%)	402 (82%)	69 (14%)	19 (4%)	3	17
All	All	2954/3150 (94%)	2453 (83%)	385 (13%)	116 (4%)	3	17

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	TYR
1	A	334	ASP
1	A	462	TRP
1	A	463	HIS
1	A	503	SER
2	B	52	LYS
2	B	154	TYR
2	B	211	LEU
2	C	17	ALA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	117	VAL
2	C	154	TYR
2	C	354	ALA
2	C	432	GLU
2	C	463	HIS
2	D	113	GLU
2	D	154	TYR
2	D	211	LEU
2	D	463	HIS
2	E	122	ASP
2	E	154	TYR
2	E	157	SER
2	E	211	LEU
2	E	387	VAL
1	F	118	VAL
1	F	154	TYR
1	F	211	LEU
1	F	431	GLU
1	F	504	GLU
1	F	506	SER
1	F	509	VAL
1	A	117	VAL
1	A	155	ASP
1	A	322	ALA
1	A	422	ALA
2	B	119	GLY
2	B	341	GLN
2	B	484	ARG
2	C	112	PRO
2	C	124	SER
2	C	211	LEU
2	C	341	GLN
2	C	431	GLU
2	D	123	LEU
2	D	333	MET
2	D	341	GLN
2	D	354	ALA
2	D	494	PRO
2	E	420	MET
2	E	463	HIS
2	E	494	PRO
2	E	502	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	117	VAL
1	F	214	GLU
1	F	420	MET
1	F	500	ASP
1	F	501	GLU
1	A	341	GLN
1	A	387	VAL
1	A	464	ASP
1	A	500	ASP
2	B	420	MET
2	C	379	SER
2	D	214	GLU
2	E	304	ASN
2	E	446	ARG
1	F	189	GLY
1	F	379	SER
1	F	381	SER
1	A	157	SER
1	A	379	SER
2	B	149	SER
2	B	348	CYS
2	B	379	SER
2	B	498	THR
2	C	289	ALA
2	C	349	ALA
2	D	353	SER
2	D	387	VAL
2	D	420	MET
2	D	496	ARG
2	E	52	LYS
2	E	189	GLY
2	E	379	SER
1	F	152	GLN
1	F	515	LYS
2	B	17	ALA
2	B	87	ALA
2	B	112	PRO
2	B	167	LEU
2	C	114	GLY
2	C	115	GLN
2	C	149	SER
2	C	348	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	348	CYS
2	E	372	PRO
2	E	480	LYS
2	E	488	ARG
1	F	157	SER
1	F	348	CYS
1	F	517	PRO
1	A	48	SER
1	A	349	ALA
1	A	421	GLY
1	A	509	VAL
2	B	494	PRO
2	C	212	GLU
2	C	420	MET
2	E	113	GLU
2	C	477	PRO
2	E	117	VAL
2	B	117	VAL
1	A	65	ILE
1	A	497	ILE
2	B	195	GLY
2	C	499	VAL
2	D	18	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	431/449 (96%)	389 (90%)	42 (10%)	8	31
1	F	431/449 (96%)	383 (89%)	48 (11%)	6	25
2	B	419/450 (93%)	370 (88%)	49 (12%)	5	22
2	C	416/450 (92%)	374 (90%)	42 (10%)	7	29
2	D	413/450 (92%)	367 (89%)	46 (11%)	6	25
2	E	420/450 (93%)	377 (90%)	43 (10%)	7	28

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2530/2698 (94%)	2260 (89%)	270 (11%)	6 26

All (270) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	33	HIS
1	A	65	ILE
1	A	79	THR
1	A	81	GLN
1	A	92	TRP
1	A	99	ASP
1	A	106	LEU
1	A	118	VAL
1	A	121	PHE
1	A	123	LEU
1	A	151	PHE
1	A	181	THR
1	A	185	ILE
1	A	186	GLU
1	A	212	GLU
1	A	218	ARG
1	A	223	LEU
1	A	238	THR
1	A	256	GLN
1	A	263	VAL
1	A	270	LEU
1	A	284	ILE
1	A	287	THR
1	A	302	VAL
1	A	303	GLU
1	A	323	GLN
1	A	342	ASN
1	A	360	LEU
1	A	371	LYS
1	A	400	THR
1	A	428	SER
1	A	430	ILE
1	A	431	GLU
1	A	434	THR
1	A	451	ARG
1	A	469	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	471	MET
1	A	496	ARG
1	A	508	ILE
1	A	509	VAL
1	A	518	GLU
2	B	26	GLU
2	B	52	LYS
2	B	81	GLN
2	B	92	TRP
2	B	99	ASP
2	B	106	LEU
2	B	111	ASP
2	B	112	PRO
2	B	123	LEU
2	B	128	GLU
2	B	140	ARG
2	B	151	PHE
2	B	154	TYR
2	B	178	THR
2	B	181	THR
2	B	183	GLU
2	B	185	ILE
2	B	186	GLU
2	B	198	GLU
2	B	209	ASN
2	B	212	GLU
2	B	223	LEU
2	B	256	GLN
2	B	270	LEU
2	B	284	ILE
2	B	303	GLU
2	B	320	SER
2	B	333	MET
2	B	360	LEU
2	B	366	GLU
2	B	369	ASP
2	B	371	LYS
2	B	375	ILE
2	B	380	LEU
2	B	413	THR
2	B	432	GLU
2	B	450	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	451	ARG
2	B	453	ILE
2	B	462	TRP
2	B	463	HIS
2	B	469	GLU
2	B	471	MET
2	B	474	ASP
2	B	485	ASN
2	B	490	ILE
2	B	499	VAL
2	B	501	GLU
2	B	503	SER
2	C	15	HIS
2	C	26	GLU
2	C	50	THR
2	C	79	THR
2	C	81	GLN
2	C	99	ASP
2	C	111	ASP
2	C	121	PHE
2	C	127	ILE
2	C	140	ARG
2	C	151	PHE
2	C	154	TYR
2	C	177	THR
2	C	178	THR
2	C	185	ILE
2	C	186	GLU
2	C	209	ASN
2	C	212	GLU
2	C	217	ARG
2	C	218	ARG
2	C	223	LEU
2	C	256	GLN
2	C	263	VAL
2	C	270	LEU
2	C	303	GLU
2	C	320	SER
2	C	321	ARG
2	C	333	MET
2	C	356	LEU
2	C	360	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	C	371	LYS
2	C	375	ILE
2	C	397	ILE
2	C	451	ARG
2	C	453	ILE
2	C	462	TRP
2	C	469	GLU
2	C	470	PHE
2	C	471	MET
2	C	491	SER
2	C	498	THR
2	C	500	ASP
2	D	26	GLU
2	D	79	THR
2	D	81	GLN
2	D	106	LEU
2	D	121	PHE
2	D	122	ASP
2	D	123	LEU
2	D	151	PHE
2	D	154	TYR
2	D	178	THR
2	D	181	THR
2	D	185	ILE
2	D	186	GLU
2	D	201	SER
2	D	209	ASN
2	D	211	LEU
2	D	212	GLU
2	D	222	ILE
2	D	223	LEU
2	D	228	THR
2	D	240	THR
2	D	256	GLN
2	D	259	SER
2	D	260	ASN
2	D	270	LEU
2	D	284	ILE
2	D	287	THR
2	D	290	THR
2	D	321	ARG
2	D	333	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	338	MET
2	D	342	ASN
2	D	360	LEU
2	D	366	GLU
2	D	369	ASP
2	D	371	LYS
2	D	400	THR
2	D	416	SER
2	D	451	ARG
2	D	469	GLU
2	D	471	MET
2	D	474	ASP
2	D	487	GLU
2	D	490	ILE
2	D	496	ARG
2	D	498	THR
2	E	26	GLU
2	E	79	THR
2	E	81	GLN
2	E	99	ASP
2	E	106	LEU
2	E	113	GLU
2	E	121	PHE
2	E	140	ARG
2	E	151	PHE
2	E	154	TYR
2	E	171	LEU
2	E	177	THR
2	E	178	THR
2	E	181	THR
2	E	183	GLU
2	E	185	ILE
2	E	186	GLU
2	E	203	ASN
2	E	209	ASN
2	E	212	GLU
2	E	216	ARG
2	E	223	LEU
2	E	228	THR
2	E	256	GLN
2	E	270	LEU
2	E	300	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	E	320	SER
2	E	321	ARG
2	E	325	LEU
2	E	333	MET
2	E	342	ASN
2	E	360	LEU
2	E	371	LYS
2	E	375	ILE
2	E	417	ASP
2	E	451	ARG
2	E	453	ILE
2	E	458	MET
2	E	464	ASP
2	E	471	MET
2	E	474	ASP
2	E	501	GLU
2	E	505	LEU
1	F	26	GLU
1	F	33	HIS
1	F	45	SER
1	F	77	GLU
1	F	79	THR
1	F	99	ASP
1	F	106	LEU
1	F	116	GLU
1	F	121	PHE
1	F	123	LEU
1	F	140	ARG
1	F	151	PHE
1	F	154	TYR
1	F	181	THR
1	F	183	GLU
1	F	184	ARG
1	F	185	ILE
1	F	186	GLU
1	F	198	GLU
1	F	203	ASN
1	F	212	GLU
1	F	223	LEU
1	F	256	GLN
1	F	287	THR
1	F	300	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	302	VAL
1	F	314	LEU
1	F	321	ARG
1	F	325	LEU
1	F	333	MET
1	F	342	ASN
1	F	360	LEU
1	F	369	ASP
1	F	371	LYS
1	F	375	ILE
1	F	381	SER
1	F	417	ASP
1	F	451	ARG
1	F	458	MET
1	F	462	TRP
1	F	469	GLU
1	F	471	MET
1	F	496	ARG
1	F	501	GLU
1	F	504	GLU
1	F	507	ARG
1	F	514	GLU
1	F	515	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	33	HIS
1	A	62	ASN
1	A	81	GLN
1	A	209	ASN
1	A	304	ASN
1	A	368	ASN
1	A	414	ASN
1	A	441	GLN
1	A	463	HIS
2	B	58	GLN
2	B	62	ASN
2	B	81	GLN
2	B	209	ASN
2	B	256	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	260	ASN
2	B	323	GLN
2	B	361	GLN
2	B	368	ASN
2	B	414	ASN
2	B	441	GLN
2	B	454	ASN
2	C	33	HIS
2	C	58	GLN
2	C	81	GLN
2	C	209	ASN
2	C	256	GLN
2	C	260	ASN
2	C	304	ASN
2	C	368	ASN
2	C	389	ASN
2	C	414	ASN
2	C	429	HIS
2	C	441	GLN
2	D	33	HIS
2	D	81	GLN
2	D	209	ASN
2	D	327	ASN
2	D	414	ASN
2	E	81	GLN
2	E	203	ASN
2	E	209	ASN
2	E	256	GLN
2	E	304	ASN
2	E	361	GLN
2	E	368	ASN
2	E	414	ASN
2	E	441	GLN
2	E	454	ASN
1	F	16	GLN
1	F	33	HIS
1	F	81	GLN
1	F	209	ASN
1	F	260	ASN
1	F	323	GLN
1	F	361	GLN
1	F	368	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	F	414	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	SEP	F	320	1	8,9,10	2.12	3 (37%)	8,12,14	3.15	3 (37%)
1	SEP	A	320	1	8,9,10	1.89	1 (12%)	8,12,14	2.97	2 (25%)

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
1	SEP	F	320	1	-	1/5/8/10	-
1	SEP	A	320	1	-	2/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	SEP	P-O1P	4.83	1.66	1.50
1	F	320	SEP	P-O1P	4.48	1.65	1.50
1	F	320	SEP	P-O2P	2.63	1.65	1.54
1	F	320	SEP	CB-CA	2.61	1.59	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	SEP	OG-CB-CA	6.04	114.02	108.14
1	F	320	SEP	OG-CB-CA	-5.44	102.85	108.14
1	F	320	SEP	P-OG-CB	-5.23	103.89	118.30
1	A	320	SEP	P-OG-CB	-4.99	104.56	118.30
1	F	320	SEP	O3P-P-OG	3.99	117.36	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	320	SEP	N-CA-CB-OG
1	F	320	SEP	CA-CB-OG-P
1	A	320	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	320	SEP	11	0
1	A	320	SEP	16	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 21 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	F	903	4	26,33,33	1.44	3 (11%)	31,52,52	1.74	5 (16%)
3	ATP	F	901	4	26,33,33	1.31	4 (15%)	31,52,52	1.73	6 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	ATP	E	901	4	26,33,33	1.37	4 (15%)	31,52,52	1.84	6 (19%)
3	ATP	B	901	4	26,33,33	1.32	4 (15%)	31,52,52	1.71	4 (12%)
3	ATP	A	901	4	26,33,33	1.31	3 (11%)	31,52,52	1.78	6 (19%)
3	ATP	C	901	4	26,33,33	1.42	4 (15%)	31,52,52	1.72	5 (16%)
3	ATP	D	901	4	26,33,33	1.33	3 (11%)	31,52,52	1.67	4 (12%)
3	ATP	D	903	4	26,33,33	1.17	2 (7%)	31,52,52	1.79	4 (12%)
3	ATP	B	903	4	26,33,33	1.37	4 (15%)	31,52,52	1.83	8 (25%)
3	ATP	E	903	-	26,33,33	1.32	3 (11%)	31,52,52	1.66	6 (19%)
3	ATP	C	903	4	26,33,33	1.16	2 (7%)	31,52,52	1.82	4 (12%)
3	ATP	A	903	4	26,33,33	1.36	4 (15%)	31,52,52	1.70	6 (19%)

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
3	ATP	F	903	4	-	7/18/38/38	0/3/3/3
3	ATP	F	901	4	-	6/18/38/38	0/3/3/3
3	ATP	E	901	4	-	6/18/38/38	0/3/3/3
3	ATP	B	901	4	-	7/18/38/38	0/3/3/3
3	ATP	A	901	4	-	7/18/38/38	0/3/3/3
3	ATP	C	901	4	-	6/18/38/38	0/3/3/3
3	ATP	D	901	4	-	10/18/38/38	0/3/3/3
3	ATP	D	903	4	-	8/18/38/38	0/3/3/3
3	ATP	B	903	4	-	8/18/38/38	0/3/3/3
3	ATP	E	903	-	-	9/18/38/38	0/3/3/3
3	ATP	C	903	4	-	9/18/38/38	0/3/3/3
3	ATP	A	903	4	-	9/18/38/38	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	903	ATP	C2-N3	4.79	1.39	1.32
3	C	901	ATP	C2-N3	4.44	1.39	1.32
3	E	901	ATP	C2-N3	4.27	1.39	1.32
3	A	901	ATP	C2-N3	4.22	1.38	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	901	ATP	C2-N3	4.16	1.38	1.32
3	E	903	ATP	C2-N3	4.11	1.38	1.32
3	B	903	ATP	C2-N3	4.01	1.38	1.32
3	B	901	ATP	C2-N3	3.80	1.38	1.32
3	D	901	ATP	C2-N3	3.78	1.38	1.32
3	A	903	ATP	C2-N3	3.77	1.38	1.32
3	D	903	ATP	C2-N3	3.41	1.37	1.32
3	C	903	ATP	C2-N3	3.37	1.37	1.32
3	B	903	ATP	O4'-C1'	3.12	1.45	1.41
3	A	903	ATP	C2'-C1'	-2.93	1.49	1.53
3	A	901	ATP	O4'-C1'	2.80	1.45	1.41
3	F	901	ATP	O4'-C1'	2.72	1.44	1.41
3	B	901	ATP	O4'-C1'	2.56	1.44	1.41
3	F	903	ATP	C2-N1	2.55	1.38	1.33
3	B	901	ATP	C2-N1	2.52	1.38	1.33
3	A	903	ATP	O4'-C1'	2.51	1.44	1.41
3	D	901	ATP	O4'-C1'	2.48	1.44	1.41
3	D	903	ATP	C2'-C1'	-2.46	1.50	1.53
3	F	901	ATP	C2-N1	2.36	1.38	1.33
3	C	901	ATP	C2'-C1'	-2.33	1.50	1.53
3	B	903	ATP	C4-N3	2.28	1.38	1.35
3	E	901	ATP	C2-N1	2.27	1.38	1.33
3	E	901	ATP	C4-N3	2.27	1.38	1.35
3	C	901	ATP	O4'-C1'	2.24	1.44	1.41
3	A	903	ATP	C2-N1	2.22	1.38	1.33
3	B	903	ATP	C2-N1	2.20	1.38	1.33
3	B	901	ATP	C4-N3	2.19	1.38	1.35
3	C	903	ATP	O4'-C4'	-2.16	1.40	1.45
3	E	903	ATP	C2'-C3'	-2.15	1.47	1.53
3	F	903	ATP	C2'-C1'	-2.14	1.50	1.53
3	A	901	ATP	C2-N1	2.14	1.37	1.33
3	F	901	ATP	C4-N3	2.12	1.38	1.35
3	D	901	ATP	C2'-C1'	-2.09	1.50	1.53
3	C	901	ATP	C4-N3	2.09	1.38	1.35
3	E	901	ATP	O4'-C1'	2.01	1.43	1.41
3	E	903	ATP	C2-N1	2.01	1.37	1.33

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	901	ATP	N3-C2-N1	-5.75	119.69	128.68
3	C	903	ATP	N3-C2-N1	-5.74	119.71	128.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	ATP	N3-C2-N1	-5.57	119.97	128.68
3	B	903	ATP	N3-C2-N1	-5.51	120.06	128.68
3	B	901	ATP	N3-C2-N1	-5.50	120.08	128.68
3	A	903	ATP	N3-C2-N1	-5.43	120.19	128.68
3	D	903	ATP	N3-C2-N1	-5.39	120.25	128.68
3	E	901	ATP	N3-C2-N1	-5.33	120.35	128.68
3	F	903	ATP	N3-C2-N1	-5.32	120.37	128.68
3	F	901	ATP	N3-C2-N1	-5.27	120.44	128.68
3	A	901	ATP	N3-C2-N1	-5.22	120.51	128.68
3	E	903	ATP	N3-C2-N1	-5.17	120.59	128.68
3	D	903	ATP	C4-C5-N7	-4.65	104.55	109.40
3	E	901	ATP	C4-C5-N7	-4.40	104.81	109.40
3	D	903	ATP	C5-C6-N6	4.39	127.02	120.35
3	A	901	ATP	C4-C5-N7	-4.25	104.97	109.40
3	A	901	ATP	C5-C6-N6	4.20	126.73	120.35
3	E	901	ATP	C5-C6-N6	4.19	126.72	120.35
3	E	903	ATP	C4-C5-N7	-4.17	105.06	109.40
3	F	901	ATP	C4-C5-N7	-4.14	105.09	109.40
3	B	903	ATP	C4-C5-N7	-4.05	105.17	109.40
3	C	903	ATP	C5-C6-N6	3.99	126.42	120.35
3	F	901	ATP	C5-C6-N6	3.98	126.39	120.35
3	C	903	ATP	C4-C5-N7	-3.93	105.30	109.40
3	F	903	ATP	C4-C5-N7	-3.92	105.31	109.40
3	B	903	ATP	C5-C6-N6	3.91	126.29	120.35
3	C	901	ATP	C4-C5-N7	-3.87	105.37	109.40
3	B	901	ATP	C4-C5-N7	-3.86	105.38	109.40
3	B	901	ATP	C5-C6-N6	3.83	126.17	120.35
3	A	903	ATP	C5-C6-N6	3.81	126.14	120.35
3	A	903	ATP	C4-C5-N7	-3.80	105.43	109.40
3	D	901	ATP	C4-C5-N7	-3.61	105.64	109.40
3	E	903	ATP	C5-C6-N6	3.48	125.65	120.35
3	F	903	ATP	C5-C6-N6	3.46	125.60	120.35
3	D	901	ATP	C5-C6-N6	3.36	125.46	120.35
3	C	901	ATP	C5-C6-N6	3.35	125.44	120.35
3	B	903	ATP	PB-O3B-PG	-2.69	123.60	132.83
3	E	901	ATP	C3'-C2'-C1'	2.65	104.96	100.98
3	C	901	ATP	O2'-C2'-C3'	2.60	120.23	111.82
3	D	901	ATP	C3'-C2'-C1'	2.47	104.70	100.98
3	F	903	ATP	C3'-C2'-C1'	2.45	104.67	100.98
3	E	901	ATP	N6-C6-N1	-2.33	113.74	118.57
3	D	903	ATP	N6-C6-N1	-2.32	113.76	118.57
3	B	903	ATP	O2'-C2'-C3'	2.31	119.30	111.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	ATP	O2G-PG-O3B	2.30	112.34	104.64
3	A	903	ATP	PB-O3B-PG	-2.28	125.00	132.83
3	A	901	ATP	N6-C6-N1	-2.25	113.89	118.57
3	C	901	ATP	C3'-C2'-C1'	2.23	104.34	100.98
3	A	901	ATP	C3'-C2'-C1'	2.23	104.34	100.98
3	E	901	ATP	O2'-C2'-C3'	2.21	118.96	111.82
3	B	903	ATP	N6-C6-N1	-2.20	114.01	118.57
3	F	901	ATP	PB-O3B-PG	-2.20	125.28	132.83
3	F	901	ATP	N6-C6-N1	-2.18	114.06	118.57
3	B	901	ATP	O2G-PG-O3B	2.17	111.91	104.64
3	B	903	ATP	O2G-PG-O3B	2.11	111.70	104.64
3	E	903	ATP	O2G-PG-O3B	2.09	111.64	104.64
3	C	903	ATP	N6-C6-N1	-2.08	114.25	118.57
3	F	901	ATP	O2'-C2'-C3'	2.08	118.55	111.82
3	A	901	ATP	PB-O3B-PG	-2.08	125.70	132.83
3	A	903	ATP	N6-C6-N1	-2.05	114.31	118.57
3	E	903	ATP	PA-O3A-PB	2.05	139.86	132.83
3	E	903	ATP	PB-O3B-PG	-2.03	125.86	132.83
3	B	903	ATP	C3'-C2'-C1'	2.02	104.02	100.98
3	F	903	ATP	O2G-PG-O3B	2.02	111.40	104.64

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	ATP	C5'-O5'-PA-O1A
3	A	901	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	C3'-C4'-C5'-O5'
3	C	901	ATP	C5'-O5'-PA-O3A
3	C	901	ATP	C3'-C4'-C5'-O5'
3	B	903	ATP	PB-O3B-PG-O3G
3	B	903	ATP	O4'-C4'-C5'-O5'
3	B	903	ATP	C3'-C4'-C5'-O5'
3	E	901	ATP	C5'-O5'-PA-O1A
3	E	901	ATP	C5'-O5'-PA-O3A
3	E	901	ATP	C3'-C4'-C5'-O5'
3	B	901	ATP	C5'-O5'-PA-O1A
3	B	901	ATP	C3'-C4'-C5'-O5'
3	D	901	ATP	PB-O3B-PG-O2G
3	D	901	ATP	PB-O3B-PG-O3G
3	D	901	ATP	C5'-O5'-PA-O3A
3	D	901	ATP	C3'-C4'-C5'-O5'

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	D	903	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	PB-O3B-PG-O3G
3	E	903	ATP	C5'-O5'-PA-O1A
3	E	903	ATP	C3'-C4'-C5'-O5'
3	C	903	ATP	PB-O3B-PG-O3G
3	C	903	ATP	C5'-O5'-PA-O1A
3	C	903	ATP	C3'-C4'-C5'-O5'
3	F	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	C3'-C4'-C5'-O5'
3	F	901	ATP	C5'-O5'-PA-O1A
3	F	901	ATP	C3'-C4'-C5'-O5'
3	A	903	ATP	PB-O3B-PG-O3G
3	A	903	ATP	C3'-C4'-C5'-O5'
3	D	903	ATP	C3'-C4'-C5'-O5'
3	A	901	ATP	O4'-C4'-C5'-O5'
3	C	901	ATP	O4'-C4'-C5'-O5'
3	E	901	ATP	O4'-C4'-C5'-O5'
3	B	901	ATP	O4'-C4'-C5'-O5'
3	D	901	ATP	O4'-C4'-C5'-O5'
3	E	903	ATP	O4'-C4'-C5'-O5'
3	C	903	ATP	O4'-C4'-C5'-O5'
3	F	901	ATP	O4'-C4'-C5'-O5'
3	A	903	ATP	O4'-C4'-C5'-O5'
3	F	903	ATP	PB-O3B-PG-O1G
3	B	903	ATP	PB-O3A-PA-O1A
3	E	903	ATP	PB-O3A-PA-O1A
3	F	903	ATP	PB-O3A-PA-O1A
3	A	901	ATP	PB-O3A-PA-O5'
3	C	901	ATP	PB-O3A-PA-O5'
3	E	901	ATP	PB-O3A-PA-O5'
3	B	901	ATP	PB-O3A-PA-O5'
3	D	901	ATP	PB-O3A-PA-O5'
3	D	903	ATP	PB-O3A-PA-O5'
3	C	903	ATP	PB-O3A-PA-O5'
3	F	901	ATP	PB-O3A-PA-O5'
3	A	903	ATP	PB-O3A-PA-O5'
3	D	903	ATP	PB-O3B-PG-O3G
3	B	901	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	PA-O3A-PB-O2B
3	C	901	ATP	PA-O3A-PB-O2B
3	B	903	ATP	PA-O3A-PB-O2B
3	E	901	ATP	PA-O3A-PB-O2B

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	B	901	ATP	PA-O3A-PB-O2B
3	D	901	ATP	PA-O3A-PB-O2B
3	D	903	ATP	PA-O3A-PB-O2B
3	D	903	ATP	PB-O3A-PA-O1A
3	E	903	ATP	PA-O3A-PB-O2B
3	C	903	ATP	PA-O3A-PB-O2B
3	F	903	ATP	PA-O3A-PB-O2B
3	F	901	ATP	PA-O3A-PB-O2B
3	A	903	ATP	PA-O3A-PB-O2B
3	C	901	ATP	C5'-O5'-PA-O1A
3	D	901	ATP	C5'-O5'-PA-O1A
3	D	903	ATP	PB-O3B-PG-O1G
3	B	903	ATP	PB-O3A-PA-O5'
3	E	903	ATP	PB-O3A-PA-O5'
3	F	903	ATP	PB-O3A-PA-O5'
3	E	903	ATP	PB-O3B-PG-O1G
3	C	903	ATP	PB-O3B-PG-O1G
3	B	903	ATP	PB-O3B-PG-O2G
3	E	903	ATP	PB-O3B-PG-O2G
3	C	903	ATP	C5'-O5'-PA-O3A
3	F	901	ATP	C5'-O5'-PA-O3A
3	A	901	ATP	PA-O3A-PB-O1B
3	B	903	ATP	PA-O3A-PB-O1B
3	B	901	ATP	PB-O3A-PA-O2A
3	D	901	ATP	PA-O3A-PB-O1B
3	D	901	ATP	PB-O3A-PA-O2A
3	C	903	ATP	PB-O3A-PA-O1A
3	A	903	ATP	PA-O3A-PB-O1B
3	A	903	ATP	PB-O3A-PA-O1A
3	D	903	ATP	C5'-O5'-PA-O1A
3	F	903	ATP	C5'-O5'-PA-O1A
3	A	903	ATP	C5'-O5'-PA-O1A
3	A	903	ATP	PB-O3B-PG-O1G

There are no ring outliers.

12 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	903	ATP	2	0
3	F	901	ATP	4	0
3	E	901	ATP	6	0
3	B	901	ATP	3	0

*Continued on next page...*

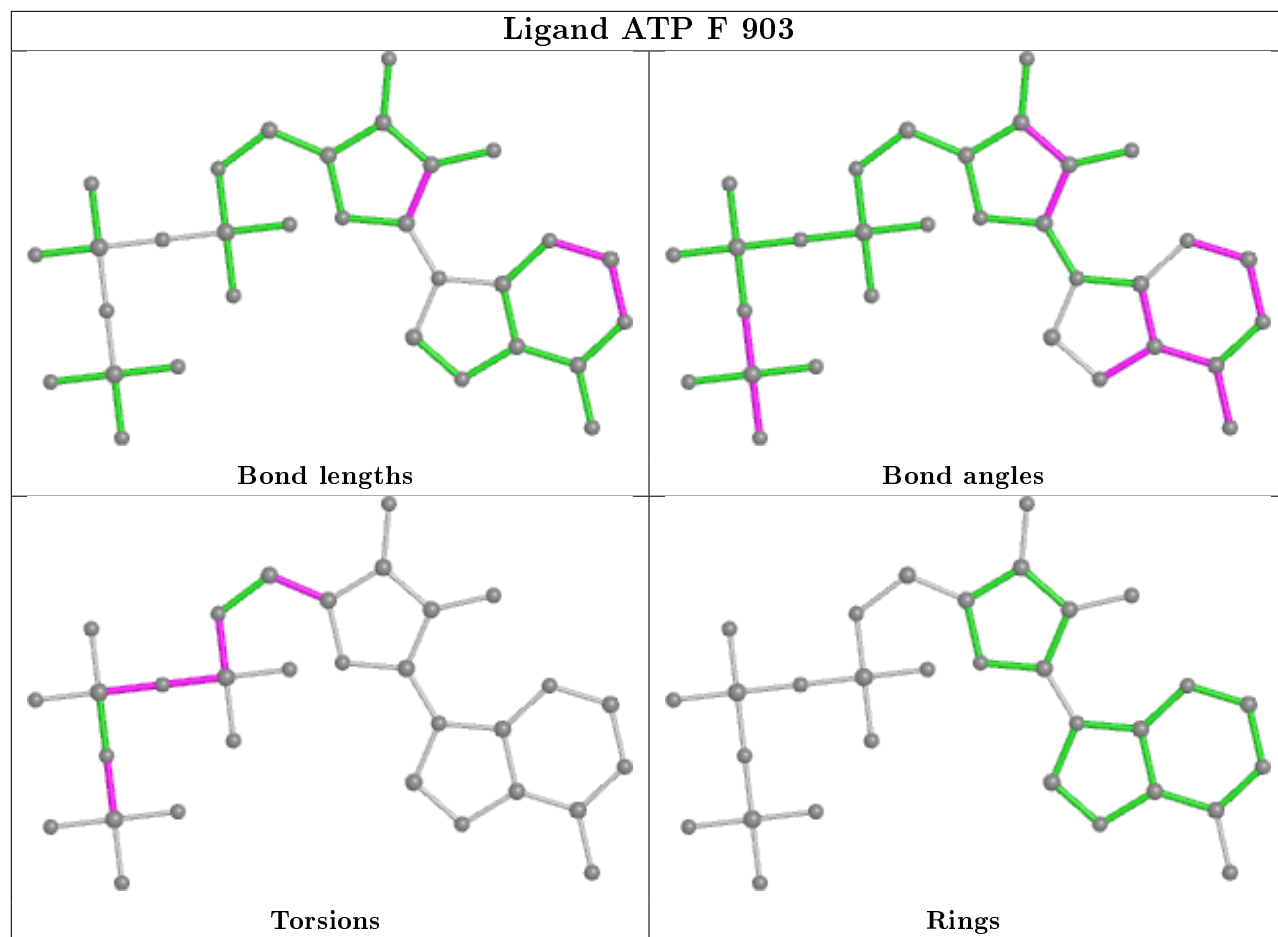


*Continued from previous page...*

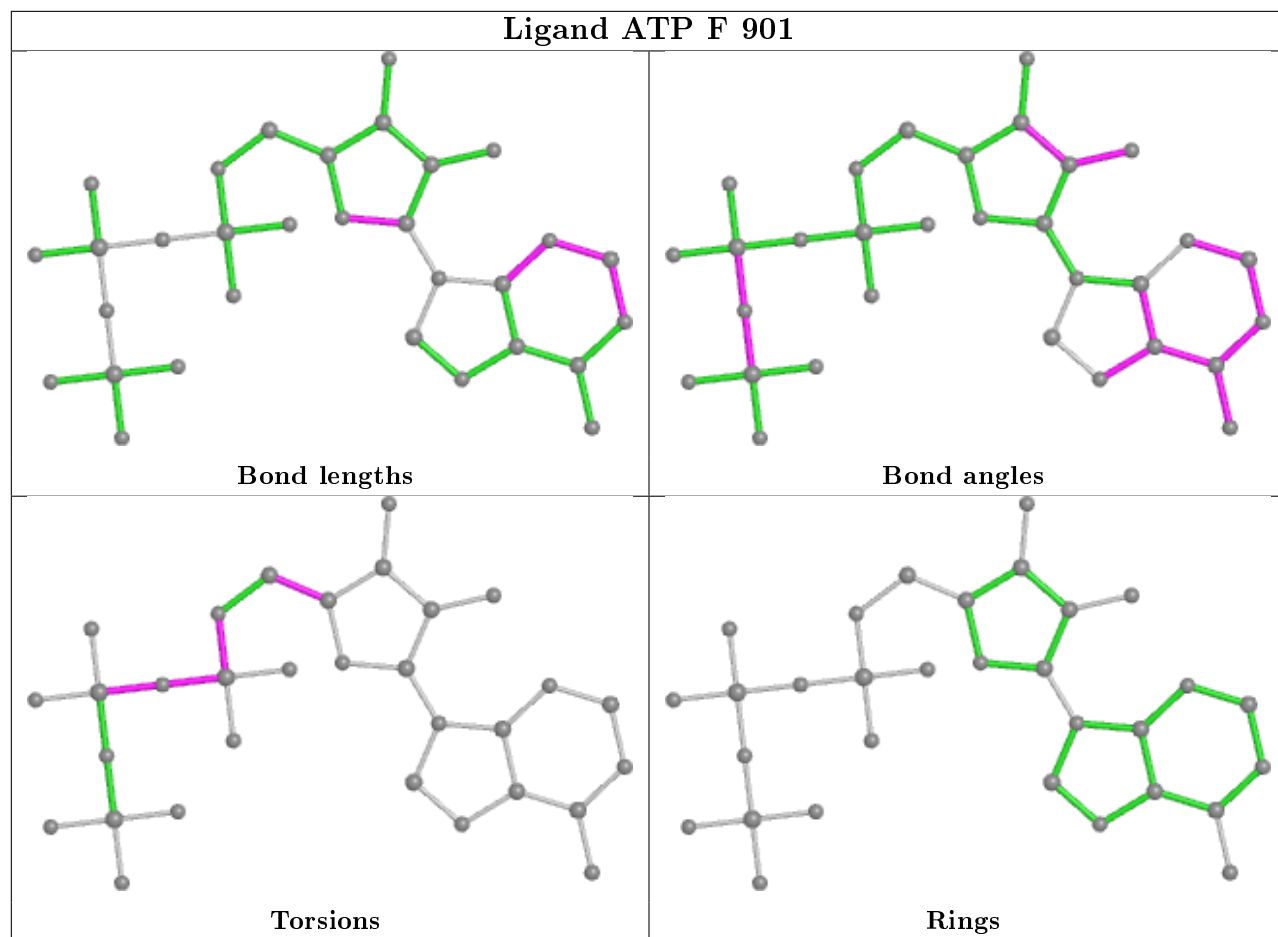
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	ATP	6	0
3	C	901	ATP	3	0
3	D	901	ATP	2	0
3	D	903	ATP	4	0
3	B	903	ATP	5	0
3	E	903	ATP	5	0
3	C	903	ATP	2	0
3	A	903	ATP	1	0

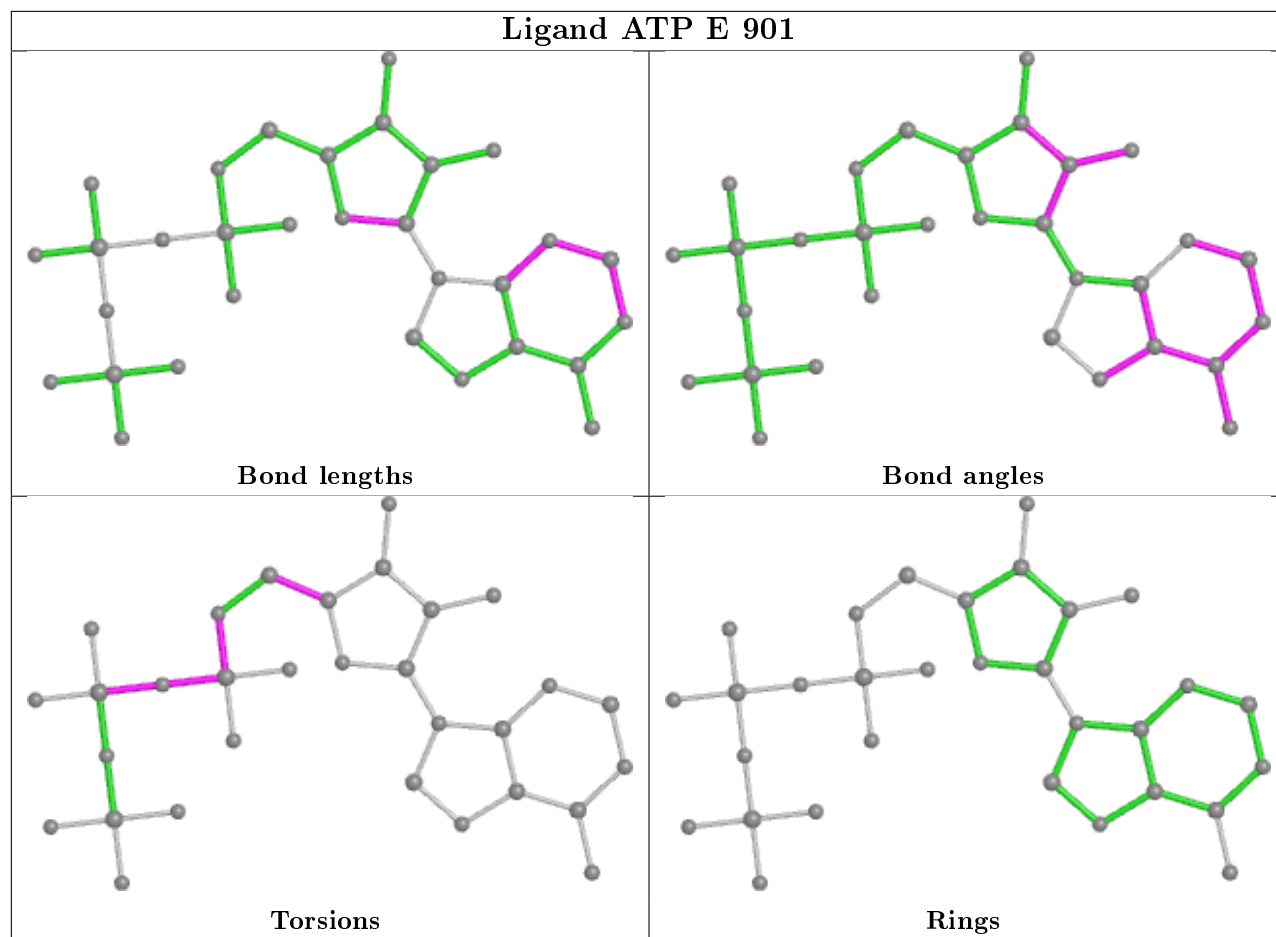
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

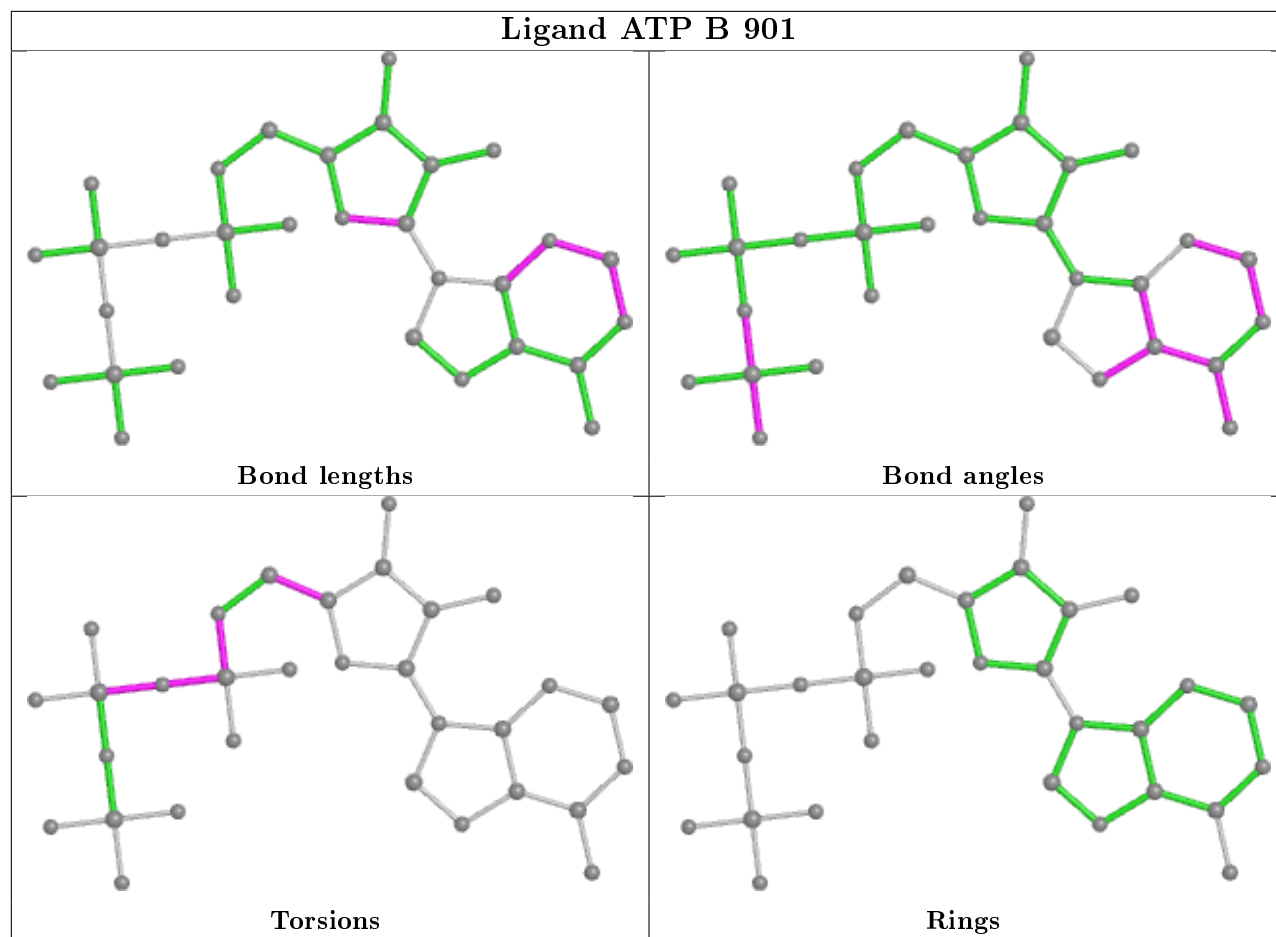
## Ligand ATP F 903

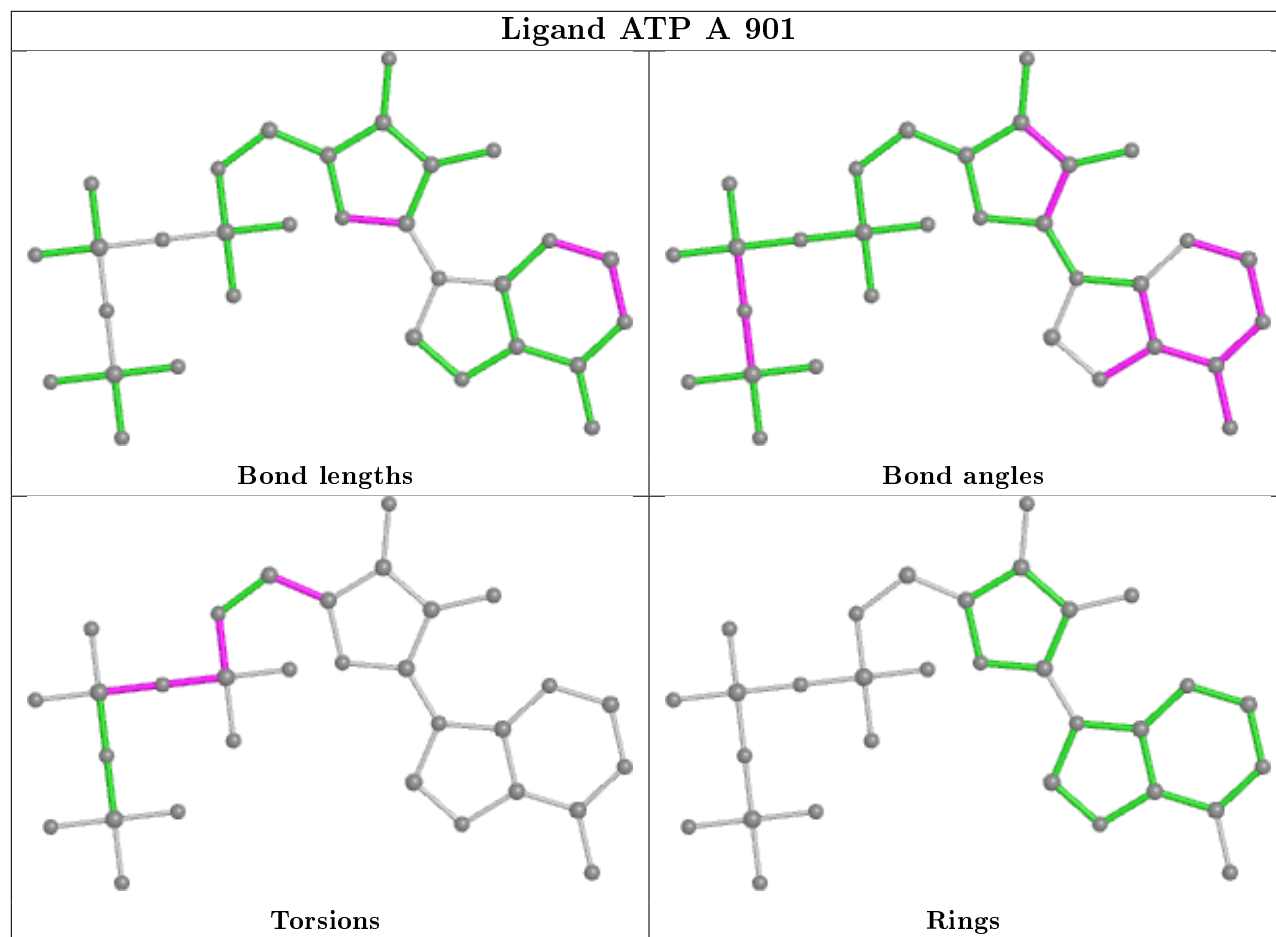


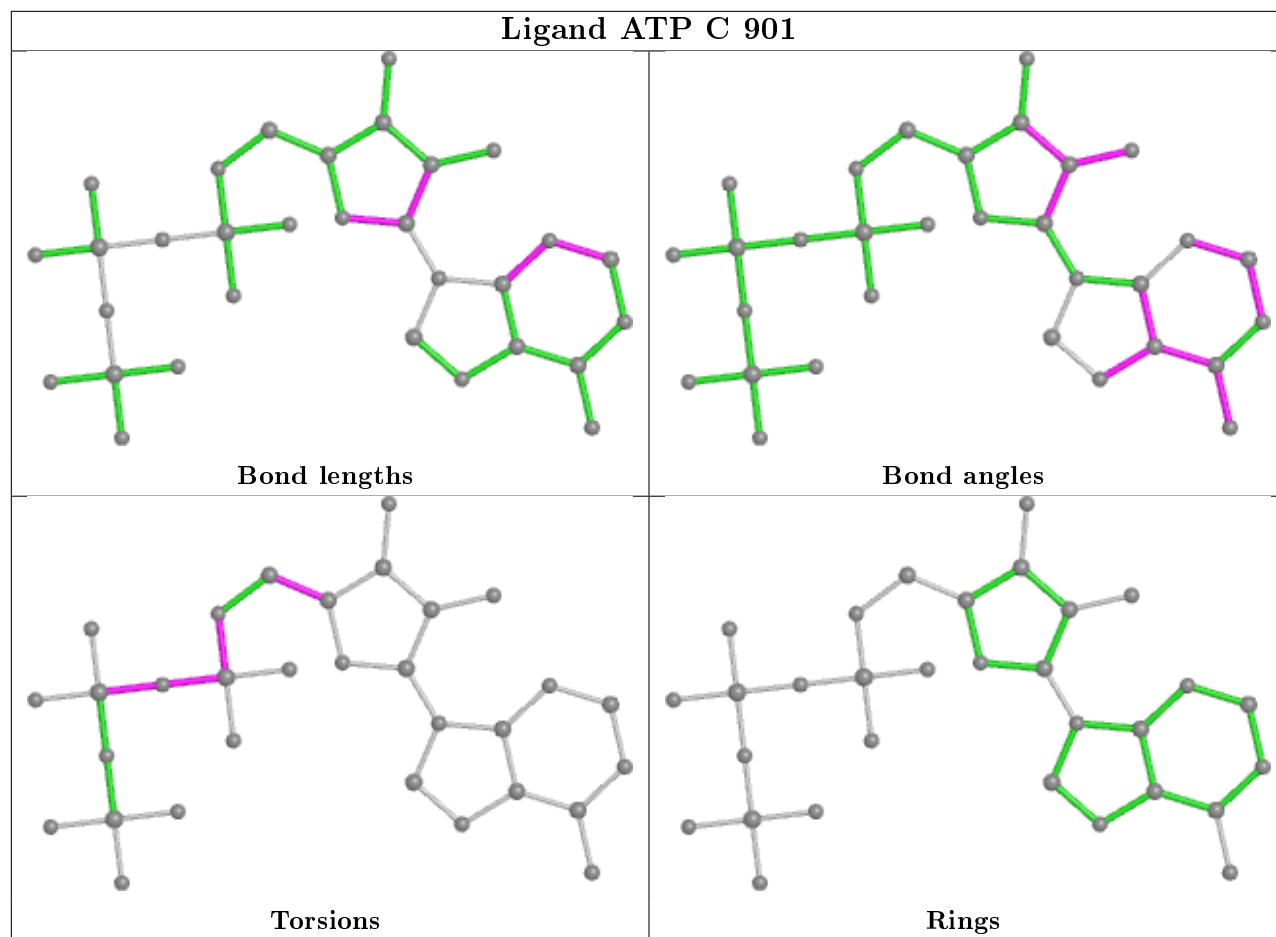
## Ligand ATP F 901

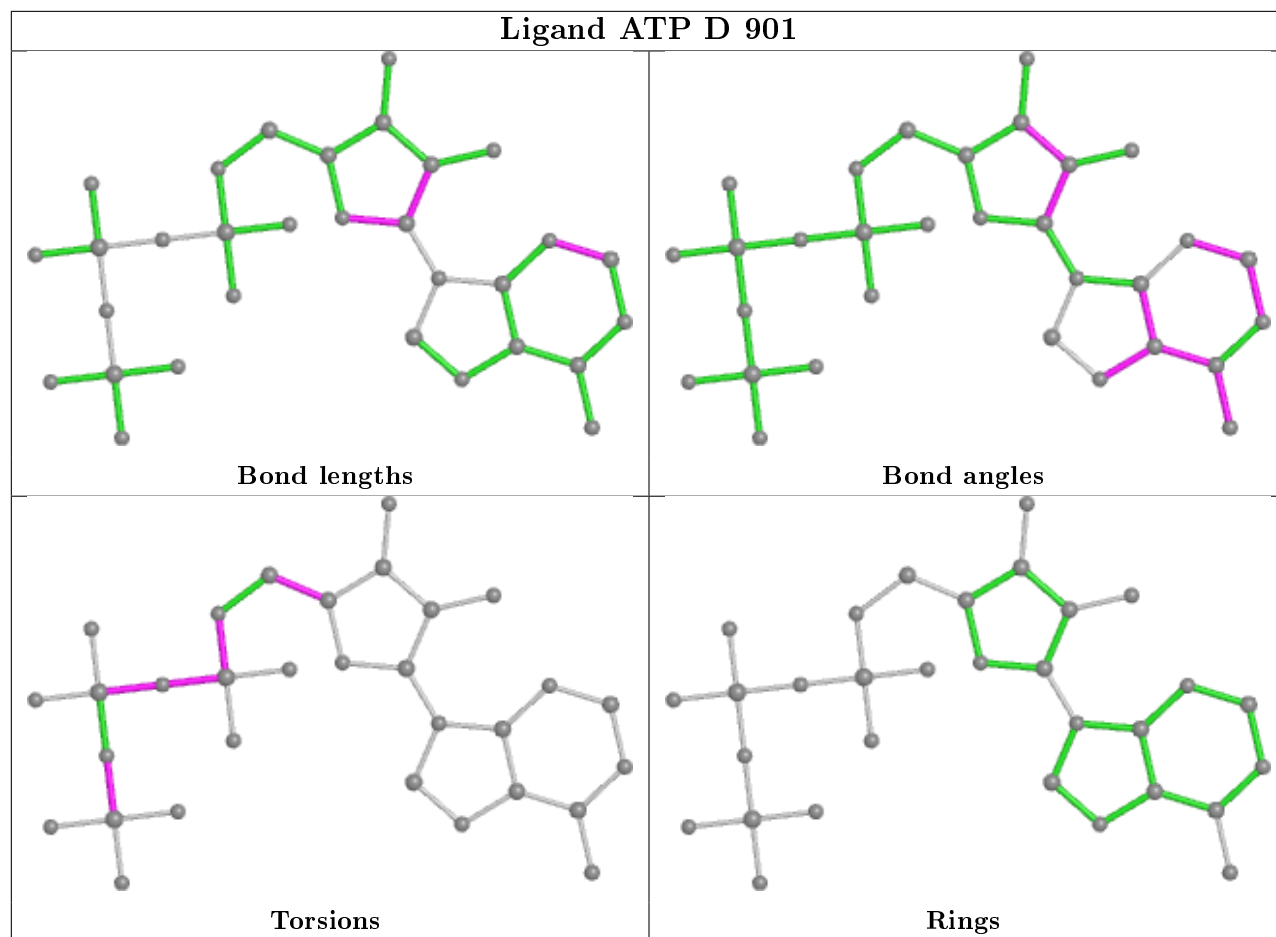




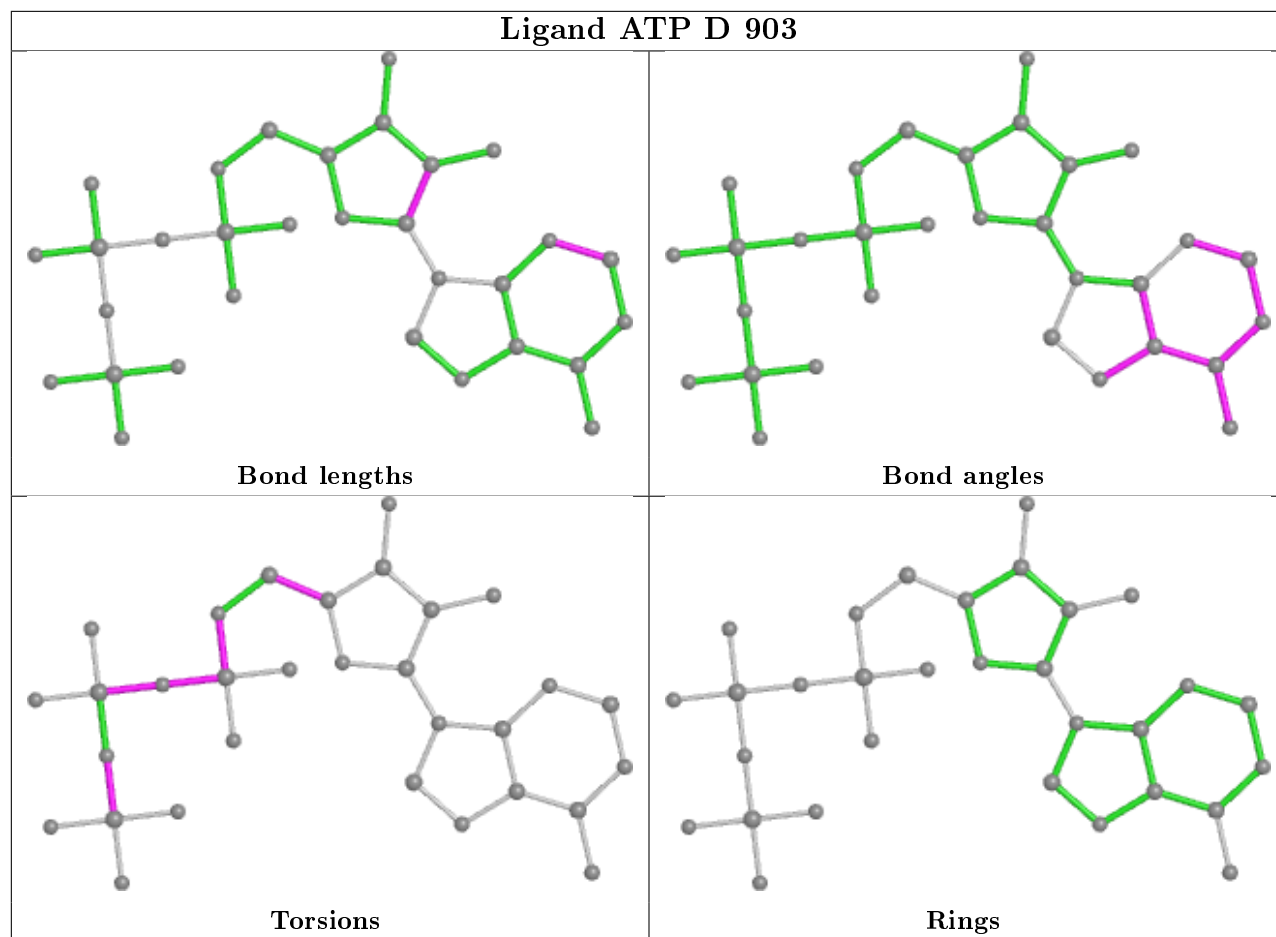




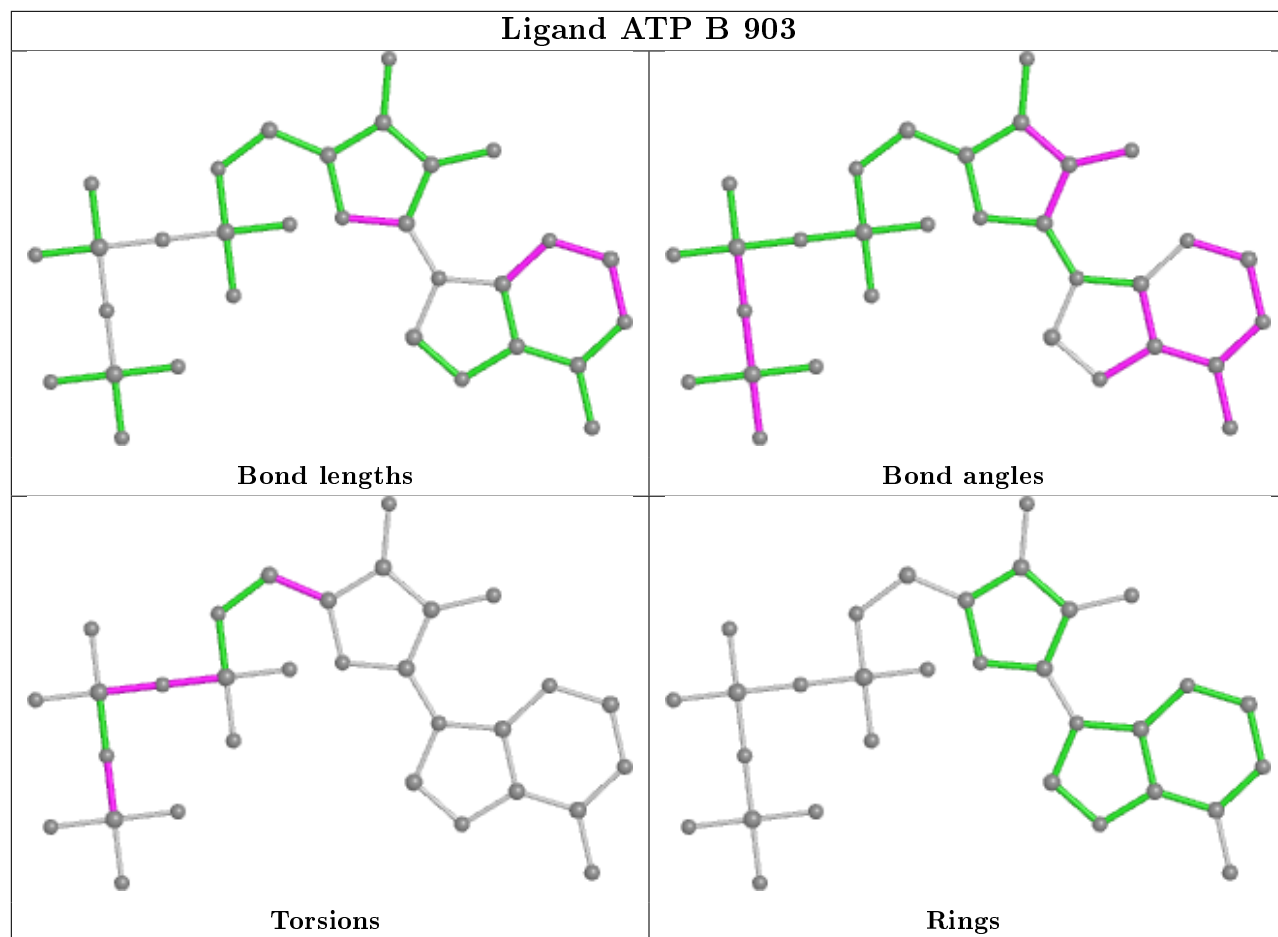




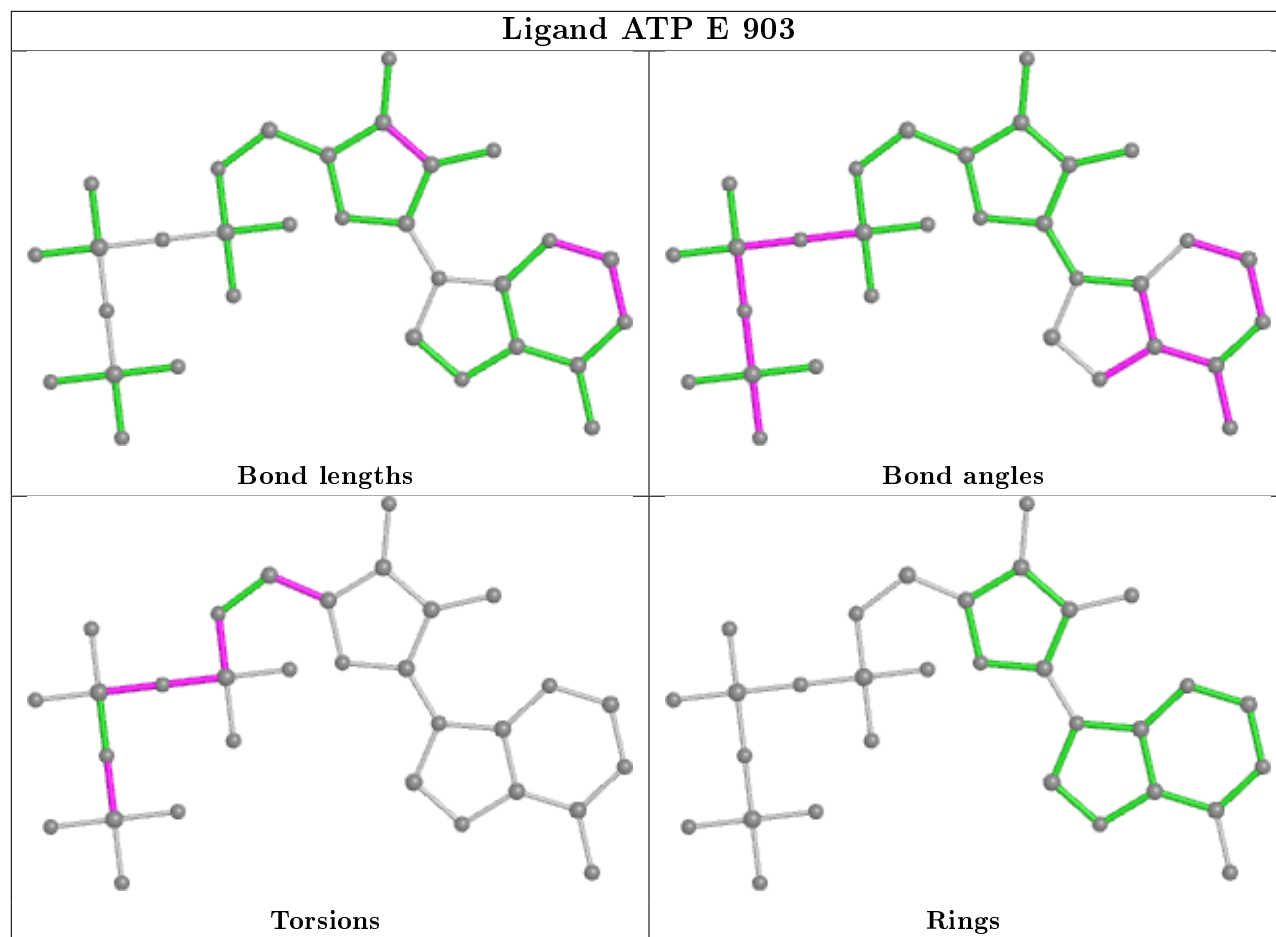


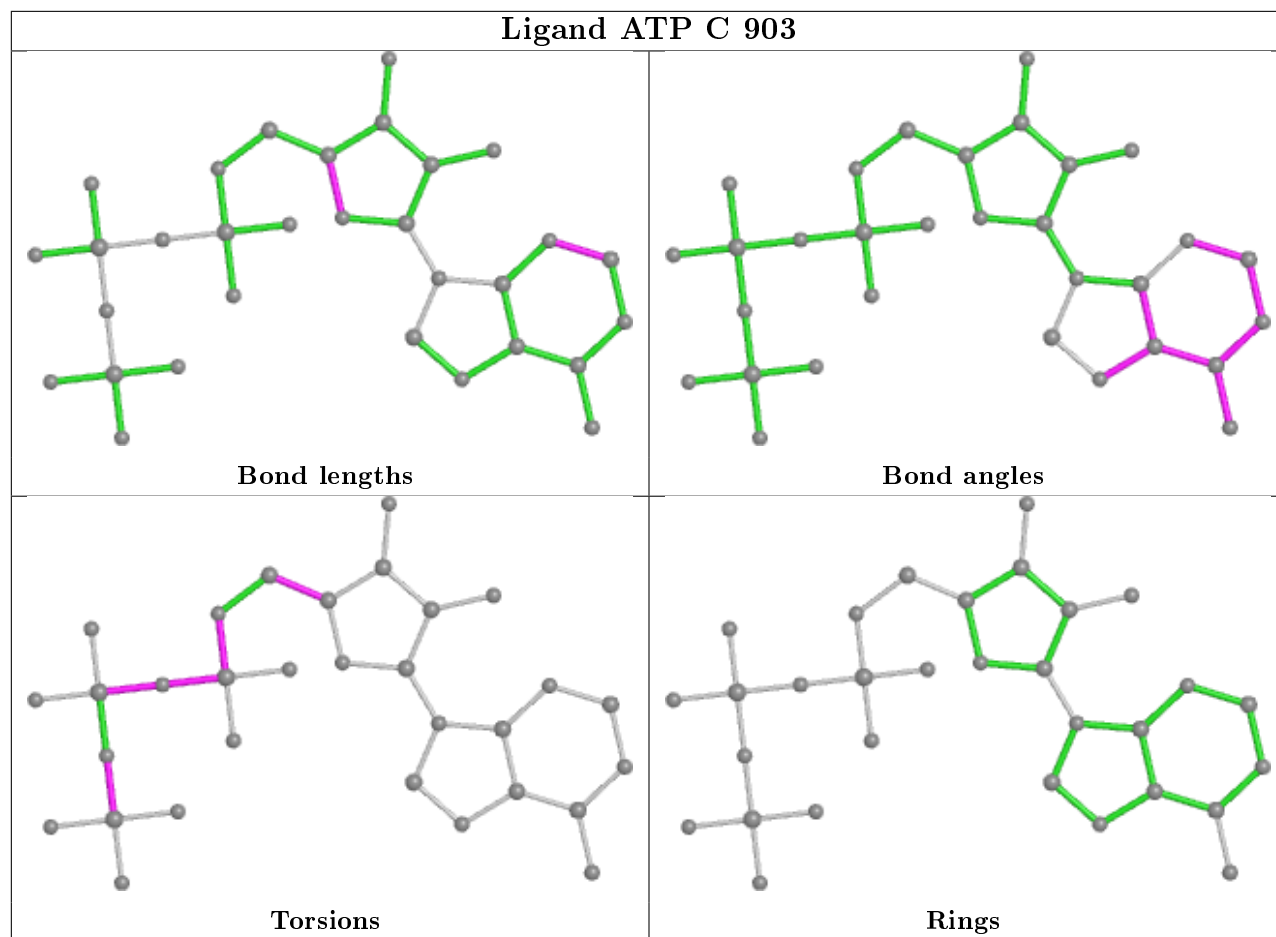


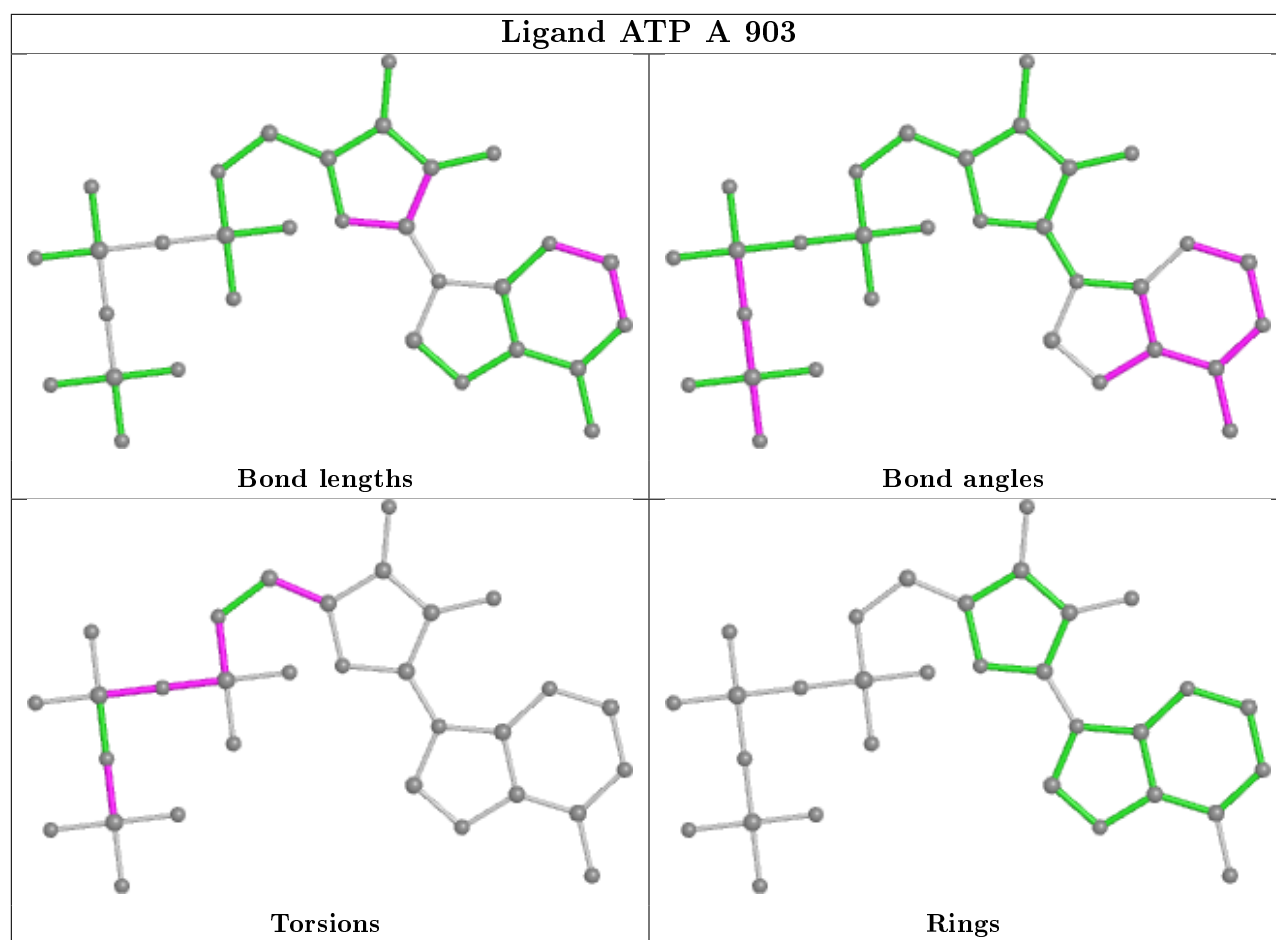
## Ligand ATP B 903



## Ligand ATP E 903







## 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	505/525 (96%)	0.17	49 (9%) 7 2	31, 77, 121, 154	0
1	F	505/525 (96%)	-0.10	31 (6%) 21 7	18, 66, 113, 145	0
2	B	491/525 (93%)	0.13	32 (6%) 18 5	43, 82, 126, 158	0
2	C	488/525 (92%)	-0.17	21 (4%) 35 13	30, 69, 122, 160	0
2	D	485/525 (92%)	-0.37	13 (2%) 54 26	20, 53, 106, 152	0
2	E	492/525 (93%)	-0.26	15 (3%) 50 22	15, 59, 104, 148	0
All	All	2966/3150 (94%)	-0.10	161 (5%) 25 9	15, 69, 117, 160	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	118	VAL	7.7
1	F	516	GLY	6.9
2	D	119	GLY	6.4
1	A	509	VAL	5.8
2	D	117	VAL	5.6
2	D	121	PHE	5.4
1	F	517	PRO	5.4
2	B	500	ASP	5.3
1	F	500	ASP	5.1
2	C	117	VAL	5.1
1	F	506	SER	5.1
2	E	500	ASP	5.1
2	C	119	GLY	4.9
1	A	519	SER	4.9
1	A	513	GLN	4.8
1	A	500	ASP	4.7
1	A	258	SER	4.7
2	B	503	SER	4.7
1	F	509	VAL	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	504	GLU	4.7
1	F	515	LYS	4.7
1	F	507	ARG	4.6
1	A	120	GLY	4.6
2	B	255	THR	4.5
1	A	16	GLN	4.5
1	A	506	SER	4.5
2	D	120	GLY	4.4
2	C	118	VAL	4.4
2	B	501	GLU	4.4
2	B	117	VAL	4.4
1	F	154	TYR	4.3
1	A	503	SER	4.2
1	A	257	ARG	4.2
1	A	507	ARG	4.1
2	B	15	HIS	4.1
1	F	508	ILE	4.0
1	A	518	GLU	4.0
2	C	120	GLY	4.0
1	A	508	ILE	4.0
2	C	499	VAL	3.9
2	E	154	TYR	3.9
2	E	504	GLU	3.9
1	F	121	PHE	3.8
2	B	251	ALA	3.8
1	F	519	SER	3.8
1	A	511	GLY	3.8
2	B	254	LEU	3.8
1	A	517	PRO	3.7
2	E	121	PHE	3.7
2	E	501	GLU	3.6
1	A	254	LEU	3.6
1	A	117	VAL	3.5
2	B	158	SER	3.5
2	B	307	ALA	3.4
1	A	516	GLY	3.4
1	F	511	GLY	3.4
2	B	498	THR	3.4
1	F	501	GLU	3.4
2	E	499	VAL	3.3
2	C	154	TYR	3.3
2	C	251	ALA	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	E	503	SER	3.3
1	A	121	PHE	3.3
2	B	175	GLY	3.3
1	A	115	GLN	3.3
2	B	499	VAL	3.3
2	B	157	SER	3.2
2	D	154	TYR	3.2
1	F	518	GLU	3.2
2	C	500	ASP	3.1
2	B	153	GLN	3.1
1	F	512	VAL	3.0
1	A	510	ARG	3.0
1	A	251	ALA	3.0
1	F	498	THR	3.0
1	A	498	THR	3.0
1	F	257	ARG	2.9
2	D	113	GLU	2.9
2	B	119	GLY	2.9
2	E	505	LEU	2.9
1	A	334	ASP	2.9
1	F	255	THR	2.9
2	B	257	ARG	2.9
2	B	407	GLU	2.9
2	C	252	MET	2.9
1	F	513	GLN	2.8
2	D	498	THR	2.8
1	F	514	GLU	2.8
2	B	116	GLU	2.8
1	A	502	LYS	2.8
2	B	135	GLN	2.8
1	A	241	ASP	2.8
2	B	118	VAL	2.8
1	F	504	GLU	2.8
2	E	113	GLU	2.8
2	D	16	GLN	2.8
2	B	502	LYS	2.8
2	E	116	GLU	2.7
1	A	505	LEU	2.7
1	F	503	SER	2.7
2	C	77	GLU	2.7
2	C	257	ARG	2.6
2	E	118	VAL	2.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	117	VAL	2.6
2	C	116	GLU	2.6
1	A	152	GLN	2.6
2	C	115	GLN	2.6
1	A	253	ARG	2.6
1	A	256	GLN	2.6
2	B	253	ARG	2.6
2	B	16	GLN	2.5
2	D	15	HIS	2.5
2	D	155	ASP	2.5
2	C	15	HIS	2.5
2	B	132	TYR	2.5
1	A	499	VAL	2.5
2	B	154	TYR	2.5
2	B	504	GLU	2.5
2	C	423	HIS	2.5
1	F	510	ARG	2.5
1	A	255	THR	2.5
1	A	337	GLU	2.5
2	C	501	GLU	2.5
1	A	116	GLU	2.5
1	F	155	ASP	2.5
1	F	499	VAL	2.4
1	A	17	ALA	2.4
1	A	112	PRO	2.4
2	E	332	GLY	2.4
1	A	153	GLN	2.4
1	A	71	GLY	2.4
1	F	311	ARG	2.4
2	B	121	PHE	2.4
1	F	251	ALA	2.3
1	A	310	GLU	2.3
1	A	311	ARG	2.3
1	A	154	TYR	2.3
1	A	114	GLY	2.3
2	E	310	GLU	2.3
1	A	475	LYS	2.2
1	F	502	LYS	2.2
2	B	14	GLU	2.2
1	A	342	ASN	2.2
2	B	342	ASN	2.2
2	B	250	GLY	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	256	GLN	2.2
2	C	121	PHE	2.2
2	C	153	GLN	2.2
1	F	120	GLY	2.2
2	C	102	LYS	2.1
2	D	257	ARG	2.1
1	A	113	GLU	2.1
2	B	115	GLN	2.1
2	C	176	ALA	2.1
2	E	115	GLN	2.1
1	A	368	ASN	2.1
1	A	515	LYS	2.1
2	D	115	GLN	2.0
2	E	155	ASP	2.0
2	C	250	GLY	2.0
1	A	340	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	A	320	10/11	0.58	0.54	49,59,66,68	0
1	SEP	F	320	10/11	0.60	0.39	45,57,63,66	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

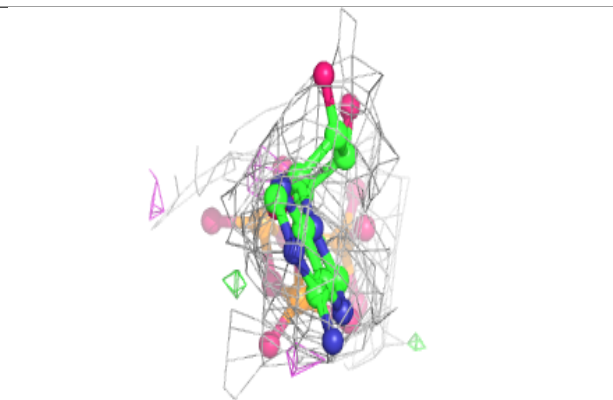
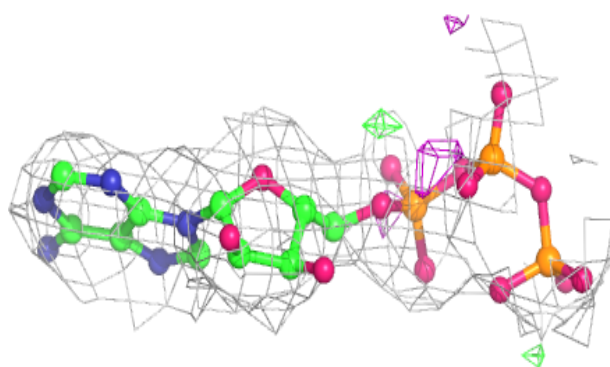
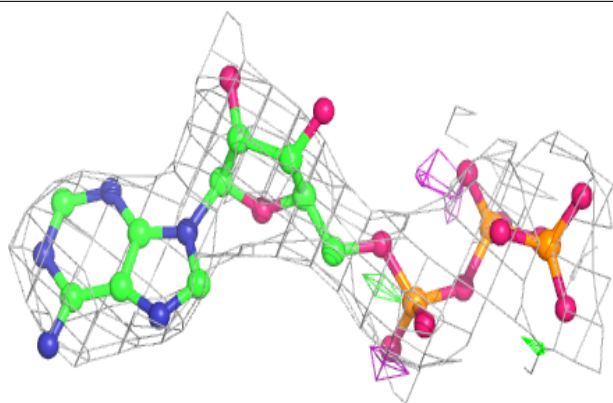
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	B	801	1/1	0.68	0.12	45,45,45,45	0
4	MG	A	526	1/1	0.74	0.48	58,58,58,58	0
4	MG	C	701	1/1	0.82	0.26	70,70,70,70	0
4	MG	B	701	1/1	0.83	0.23	58,58,58,58	0
4	MG	D	701	1/1	0.85	0.35	59,59,59,59	0
4	MG	C	702	1/1	0.85	0.49	65,65,65,65	0
4	MG	B	702	1/1	0.88	0.24	79,79,79,79	0
4	MG	F	701	1/1	0.89	0.19	45,45,45,45	0
3	ATP	B	903	31/31	0.91	0.17	77,81,94,95	0
3	ATP	B	901	31/31	0.92	0.20	67,70,85,87	0
3	ATP	C	903	31/31	0.92	0.19	42,52,85,85	0
3	ATP	A	903	31/31	0.92	0.19	61,66,76,77	0
3	ATP	A	901	31/31	0.93	0.19	84,86,89,90	0
4	MG	F	802	1/1	0.93	0.26	53,53,53,53	0
4	MG	D	801	1/1	0.94	0.34	44,44,44,44	0
4	MG	A	802	1/1	0.94	0.31	82,82,82,82	0
3	ATP	F	903	31/31	0.94	0.15	44,48,62,62	0
3	ATP	F	901	31/31	0.94	0.18	74,83,88,89	0
4	MG	D	702	1/1	0.94	0.24	49,49,49,49	0
4	MG	A	701	1/1	0.94	0.33	63,63,63,63	0
4	MG	A	801	1/1	0.94	0.14	46,46,46,46	0
3	ATP	E	901	31/31	0.95	0.16	65,72,81,81	0
3	ATP	D	901	31/31	0.95	0.17	50,54,60,62	0
4	MG	E	801	1/1	0.95	0.18	38,38,38,38	0
3	ATP	D	903	31/31	0.95	0.15	26,35,60,62	0
4	MG	E	802	1/1	0.95	0.18	46,46,46,46	0
3	ATP	E	903	31/31	0.96	0.14	22,28,60,62	0
4	MG	D	802	1/1	0.96	0.12	17,17,17,17	0
3	ATP	C	901	31/31	0.96	0.17	36,47,56,56	0
4	MG	F	702	1/1	0.96	0.24	68,68,68,68	0
4	MG	C	802	1/1	0.96	0.18	41,41,41,41	0
4	MG	C	801	1/1	0.97	0.08	25,25,25,25	0
4	MG	B	802	1/1	0.98	0.18	64,64,64,64	0

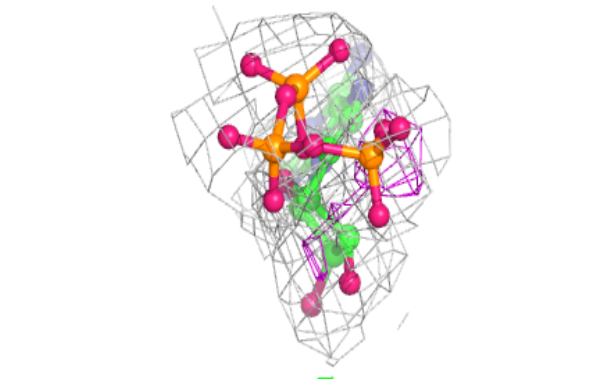
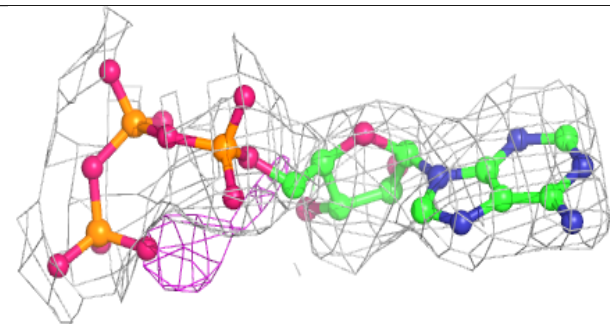
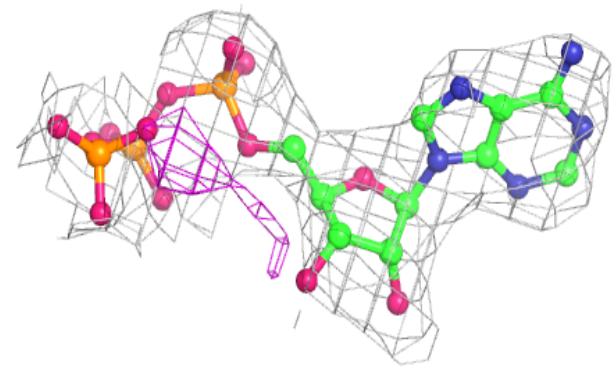
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ATP B 903:**

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

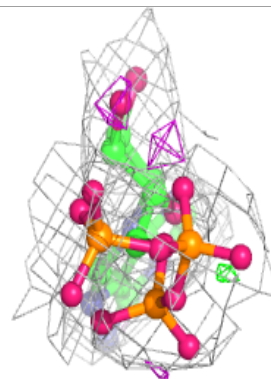
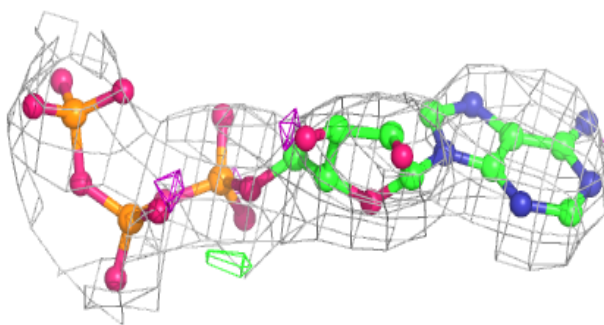
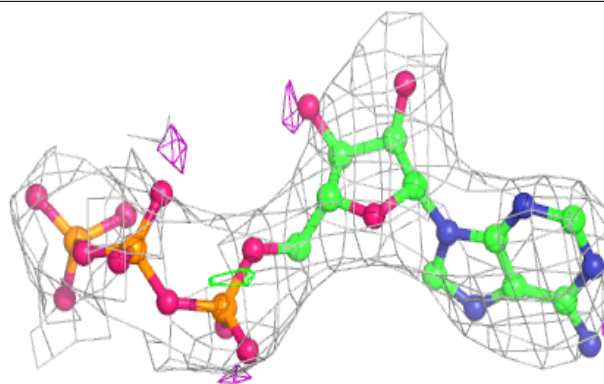
**Electron density around ATP B 901:**

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

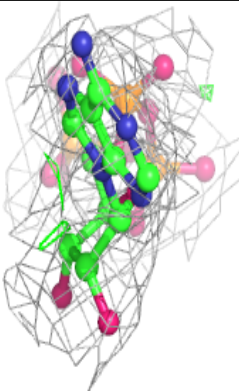
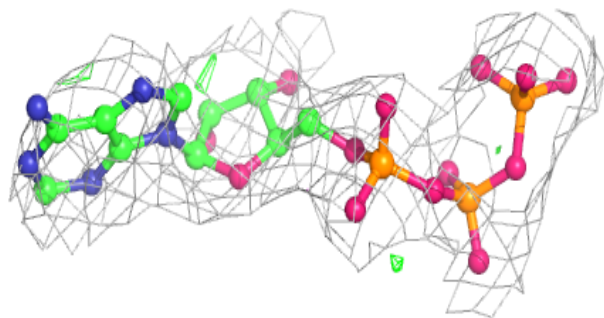
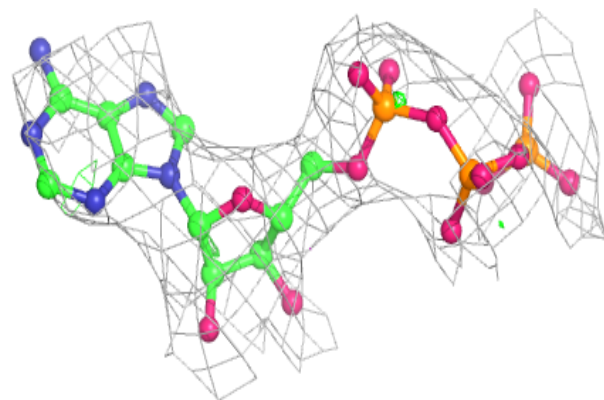


**Electron density around ATP C 903:**

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

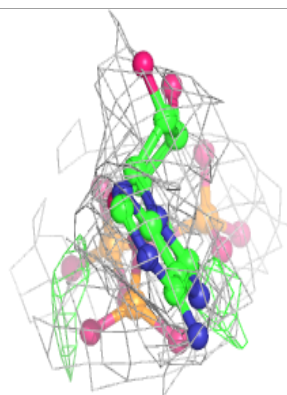
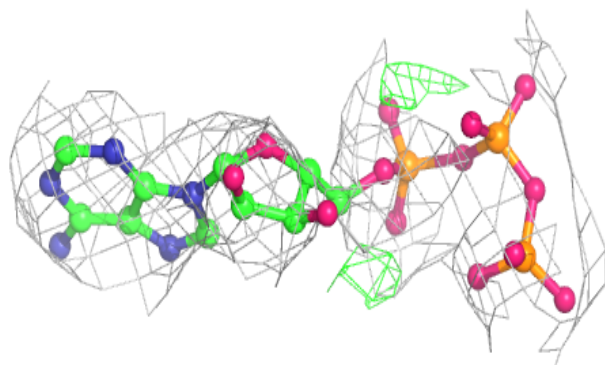
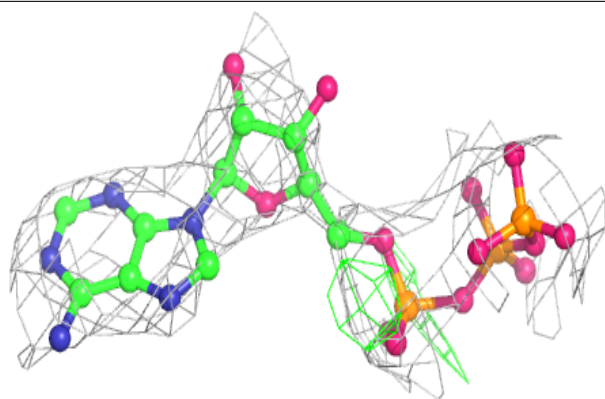
**Electron density around ATP A 903:**

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

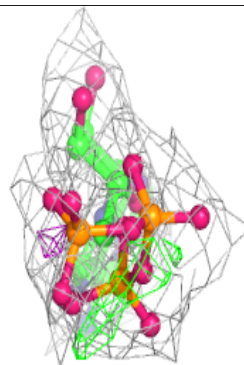
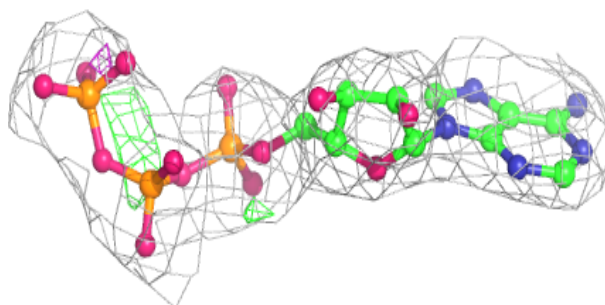
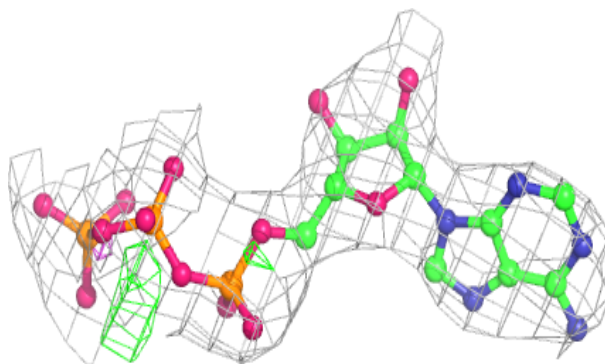


**Electron density around ATP A 901:**

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

**Electron density around ATP F 903:**

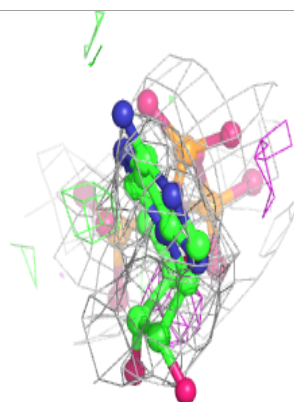
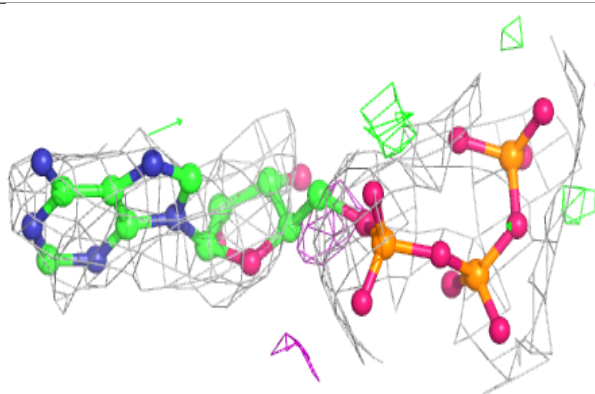
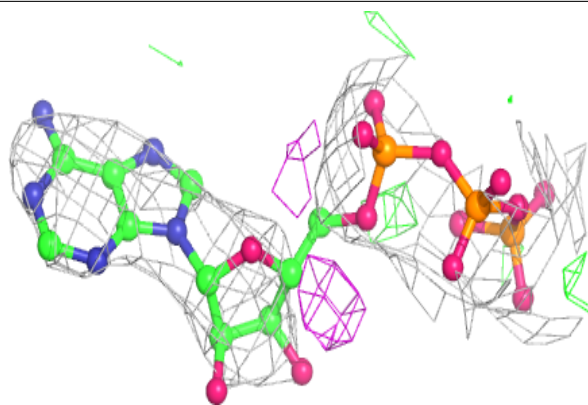
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



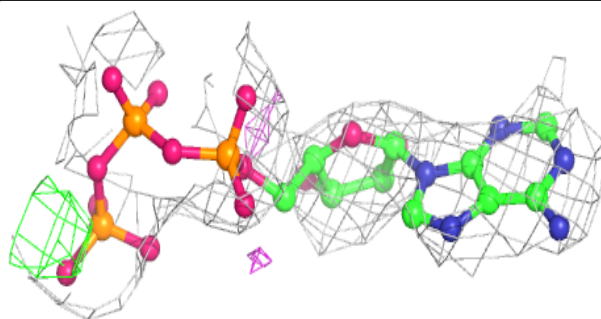
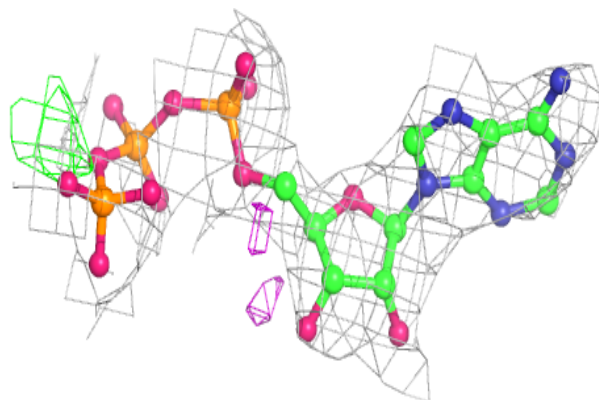


**Electron density around ATP F 901:**

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

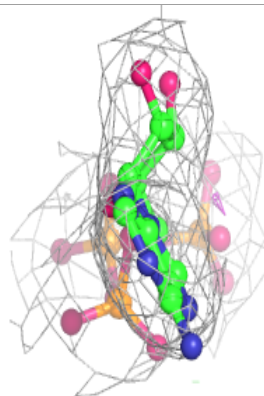
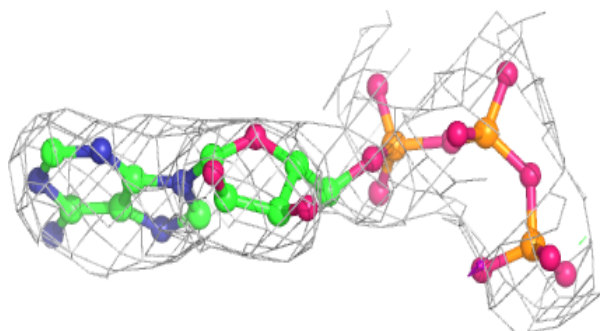
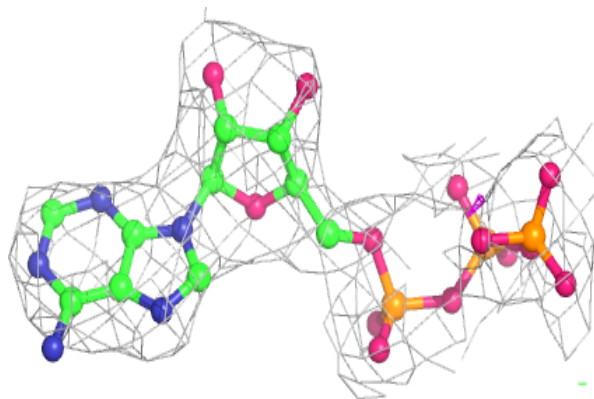
**Electron density around ATP E 901:**

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

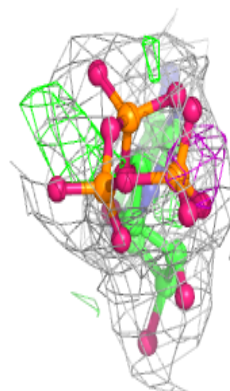
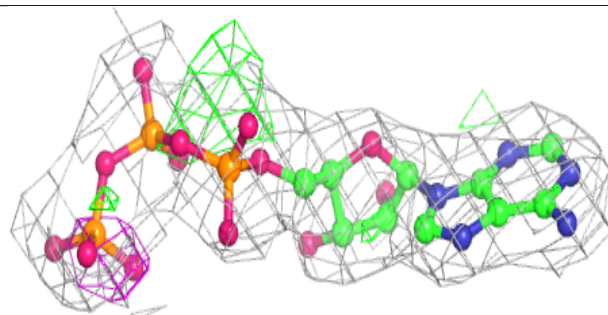
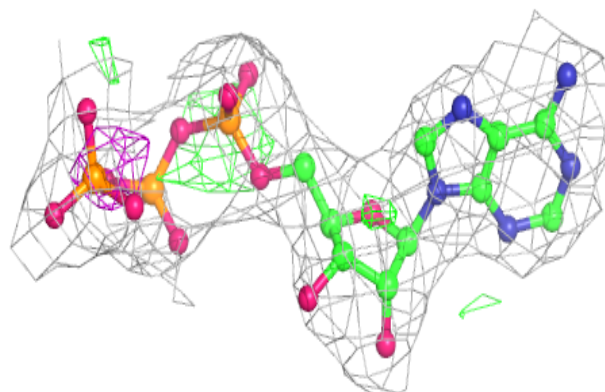


**Electron density around ATP D 901:**

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

**Electron density around ATP D 903:**

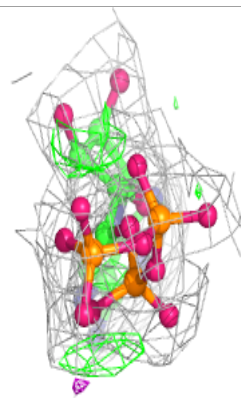
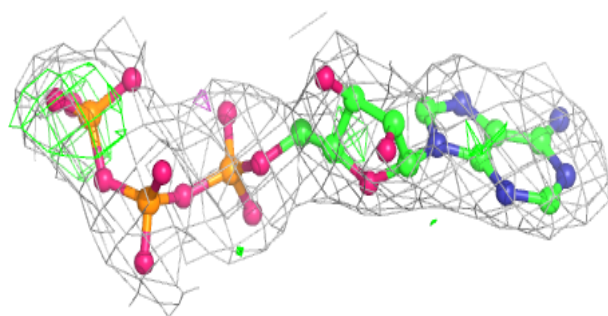
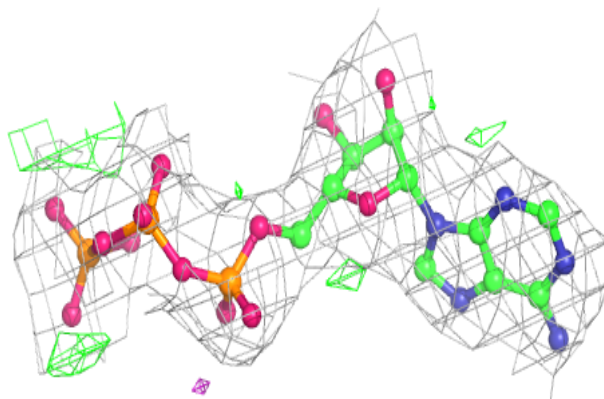
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



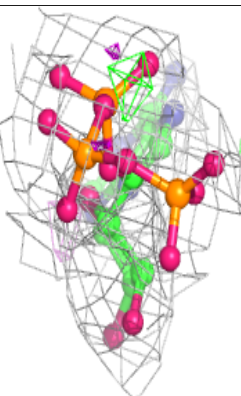
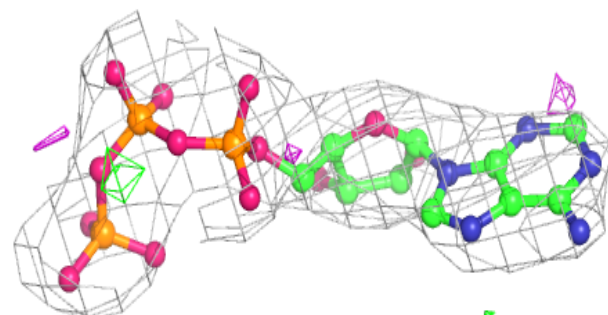
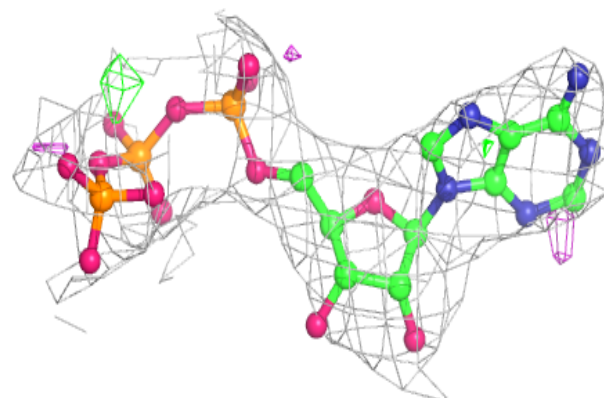


**Electron density around ATP E 903:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around ATP C 901:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.