



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:23 am GMT

PDB ID : 3W1K  
Title : Crystal structure of the selenocysteine synthase SelA and tRNA<sup>Sec</sup> complex  
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.  
Deposited on : 2012-11-15  
Resolution : 7.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

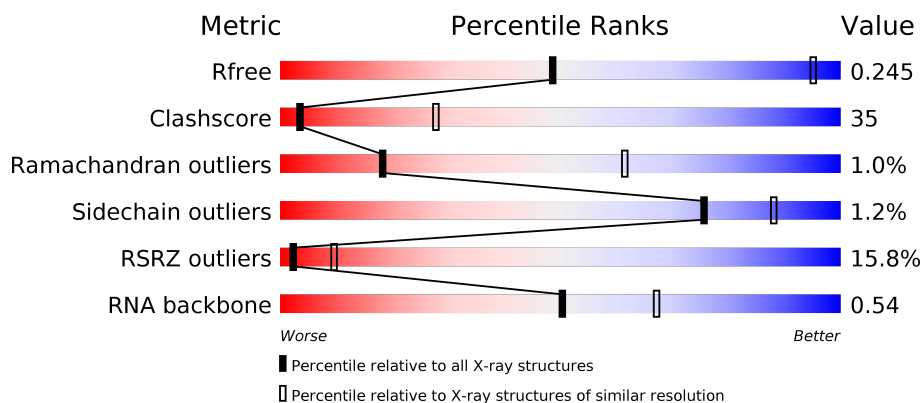
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 7.50 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))
$R_{free}$	100719	1100 (10.00-3.70)
Clashscore	112137	1035 (10.00-3.80)
Ramachandran outliers	110173	1003 (10.00-3.76)
Sidechain outliers	110143	1098 (10.00-3.70)
RSRZ outliers	101464	1003 (10.00-3.72)
RNA backbone	2435	1054 (11.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	452	<div> <div>16%</div> <div>44%</div> <div>54%</div> </div>
1	B	452	<div> <div>13%</div> <div>46%</div> <div>54%</div> </div>
1	C	452	<div> <div>13%</div> <div>48%</div> <div>51%</div> </div>
1	D	452	<div> <div>16%</div> <div>47%</div> <div>52%</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	452	<div> <div>20%</div> <div>46%</div> <div>53%</div> <div>•</div> </div>
2	F	95	<div> <div>5%</div> <div>16%</div> <div>78%</div> <div>• •</div> </div>
2	G	95	<div> <div>20%</div> <div>14%</div> <div>79%</div> <div>• •</div> </div>
2	H	95	<div> <div>33%</div> <div>17%</div> <div>77%</div> <div>• •</div> </div>
2	I	95	<div> <div>6%</div> <div>14%</div> <div>76%</div> <div>7%</div> <div>•</div> </div>
2	J	95	<div> <div>15%</div> <div>14%</div> <div>78%</div> <div>5%</div> <div>•</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27660 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 L-seryl-tRNA(Sec) selenium transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	B	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	C	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	D	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			
1	E	452	Total	C	N	O	P	S	0	0	0
			3575	2278	620	665	1	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
A	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
B	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
C	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140
D	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	19	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	21	ALA	LYS	ENGINEERED MUTATION	UNP O67140
E	46	ALA	LYS	ENGINEERED MUTATION	UNP O67140

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	48	ALA	LYS	ENGINEERED MUTATION	UNP O67140

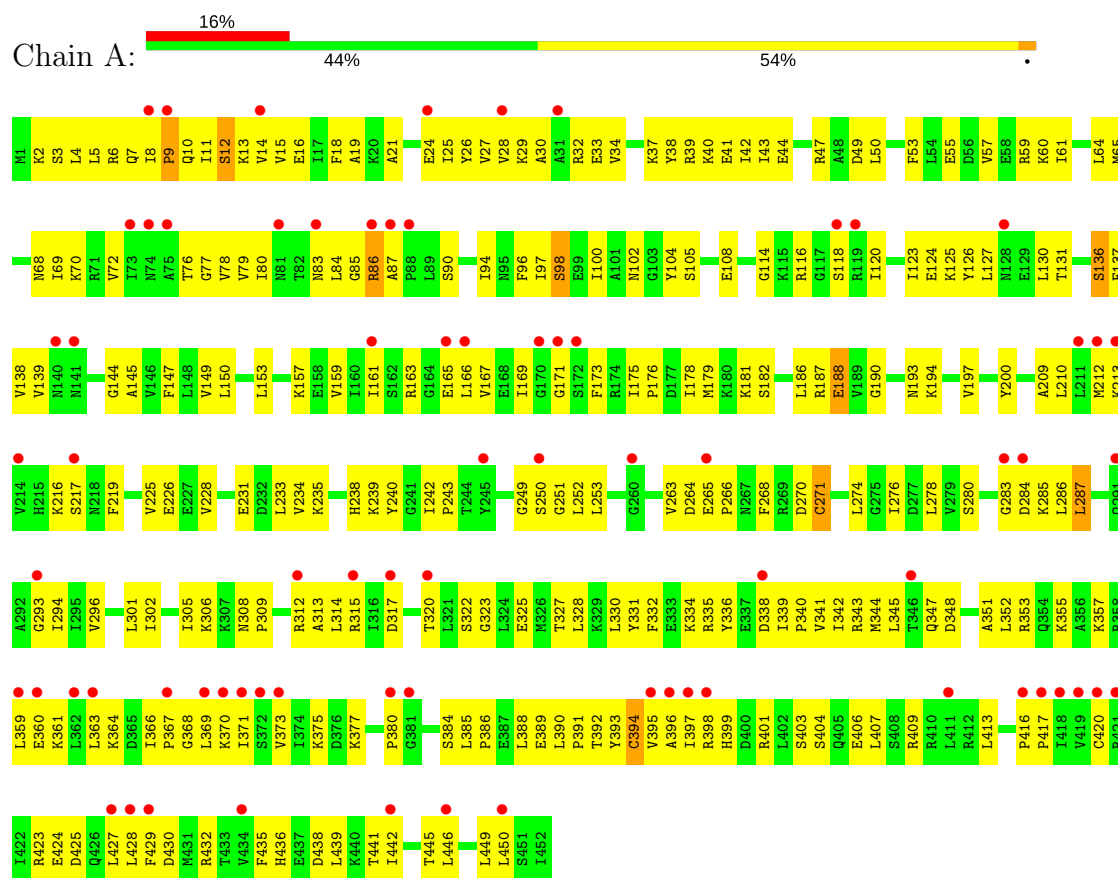
- Molecule 2 is a RNA chain called selenocysteine tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	G	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	H	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	I	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			
2	J	92	Total	C	N	O	P	0	0	0
			1957	873	342	650	92			

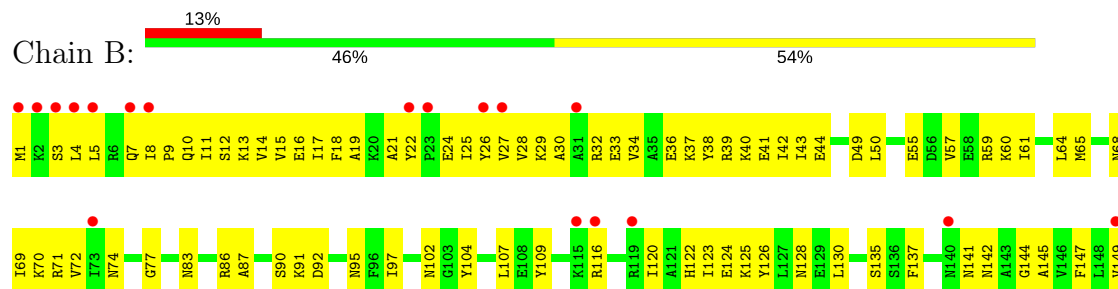
### 3 Residue-property plots

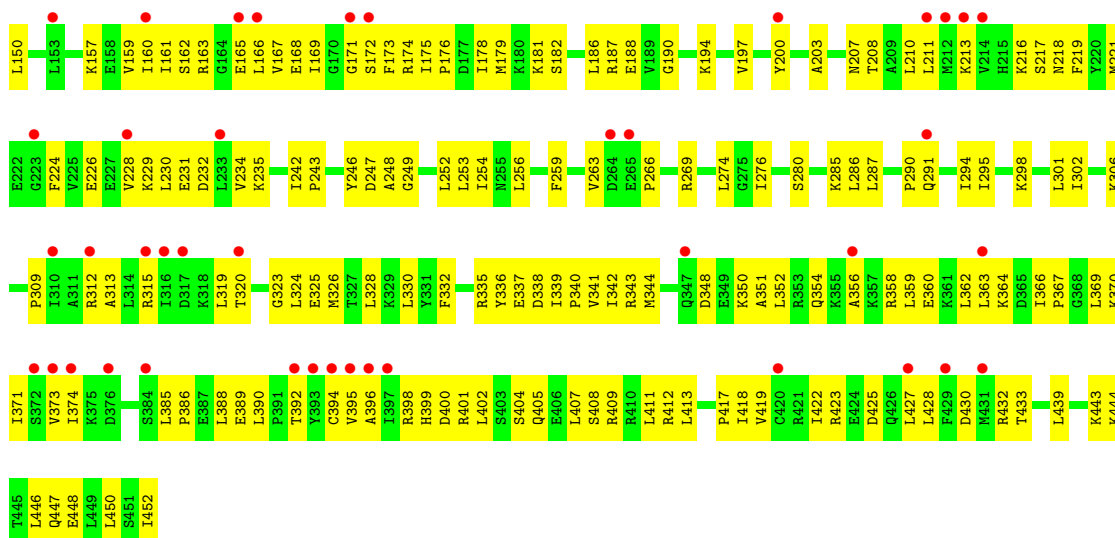
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: L-seryl-tRNA(Sec) selenium transferase

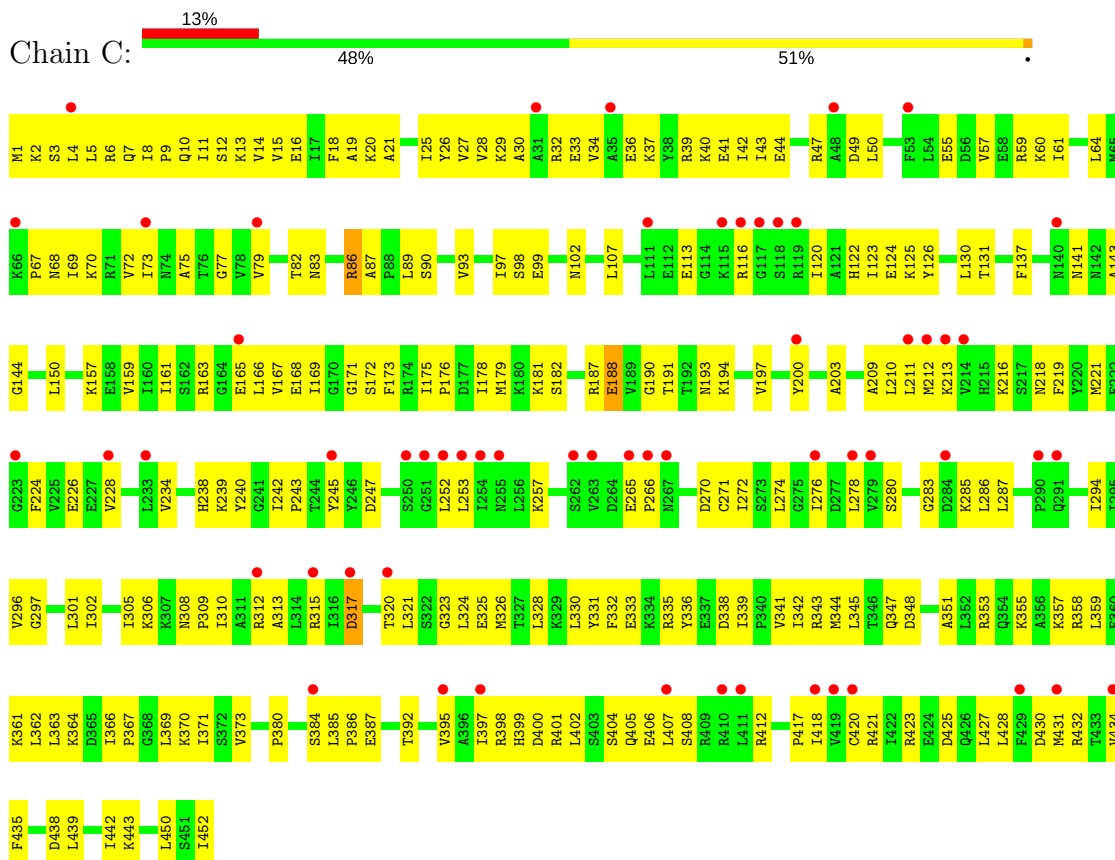


- Molecule 1: L-seryl-tRNA(Sec) selenium transferase

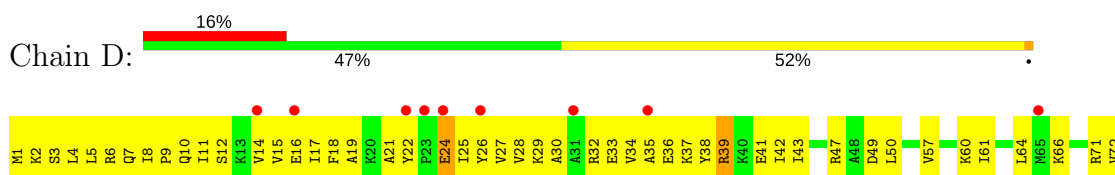


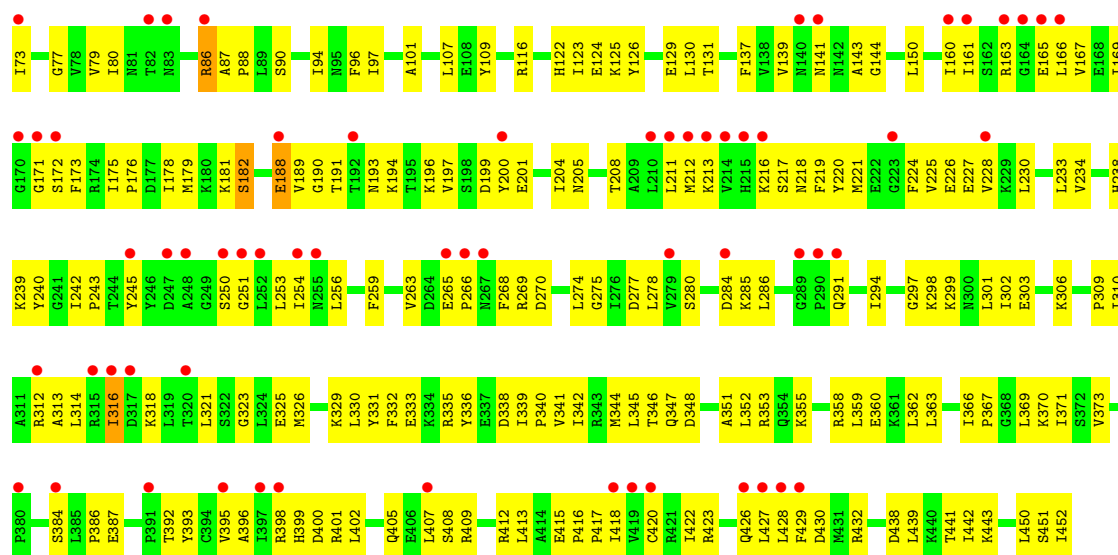


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

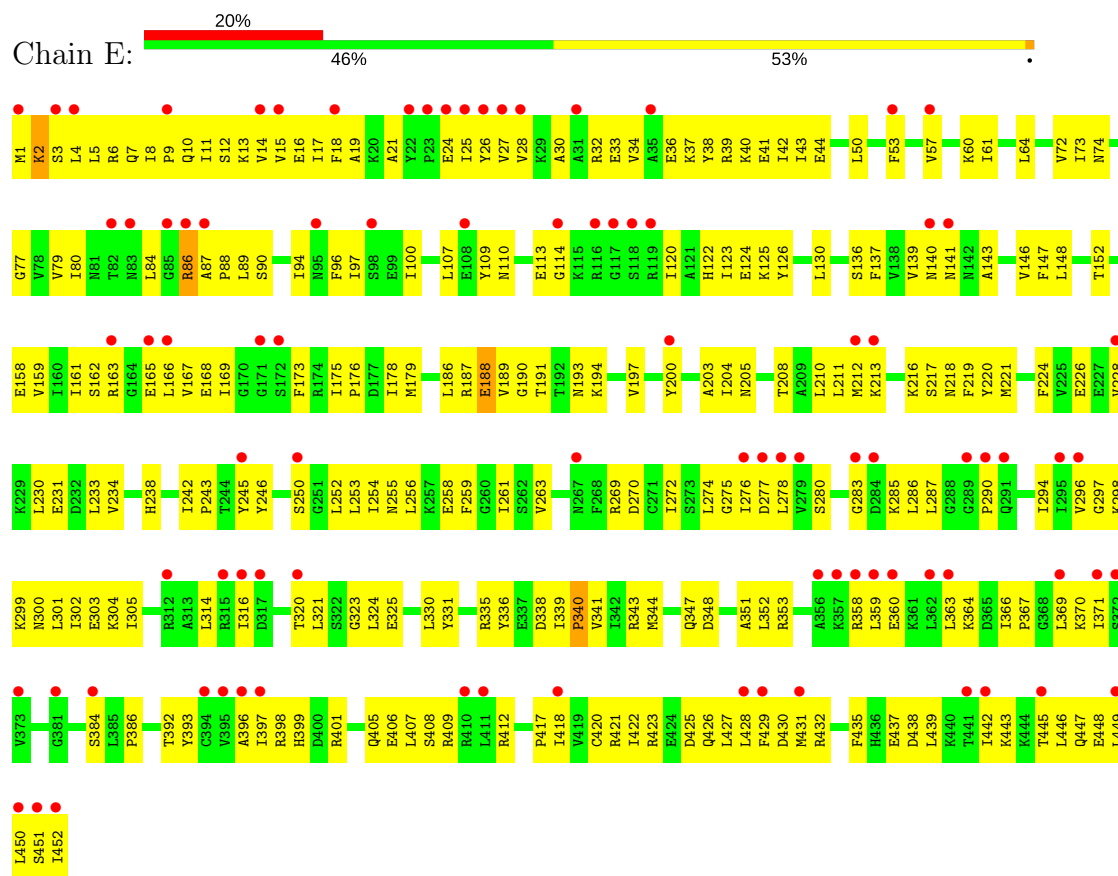


• Molecule 1: L-seryl-tRNA(Sec) selenium transferase

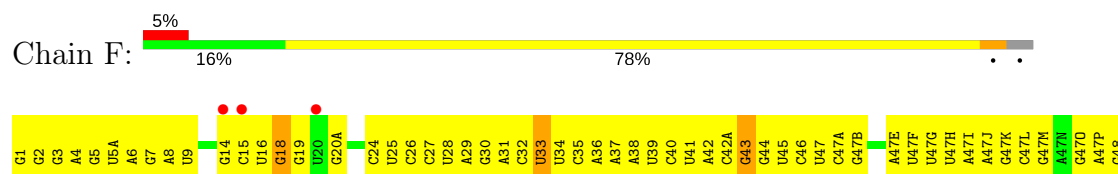




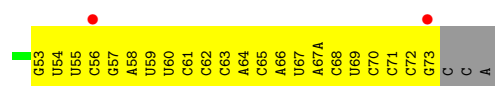
• Molecule 1: L-seryl-tRNA(Sec) selenium transferase



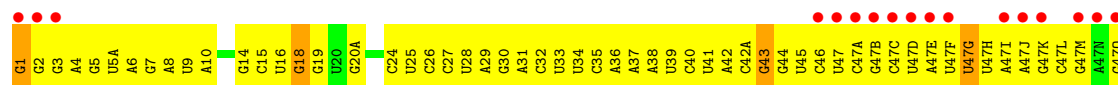
• Molecule 2: selenocysteine tRNA



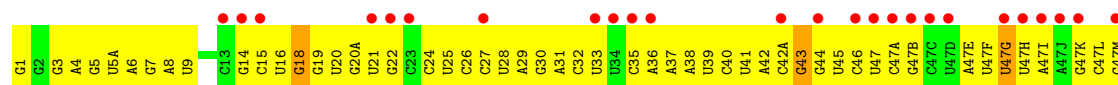




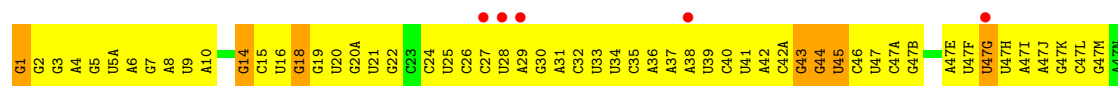
- Molecule 2: selenocysteine tRNA



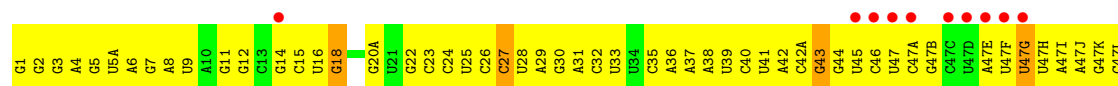
- Molecule 2: selenocysteine tRNA



- Molecule 2: selenocysteine tRNA



- Molecule 2: selenocysteine tRNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.55Å 355.97Å 165.50Å 90.00° 115.41° 90.00°	Depositor
Resolution (Å)	49.94 – 7.50 49.94 – 7.49	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.94-7.50) 98.0 (49.94-7.49)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 7.37Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.194 , 0.240 0.200 , 0.245	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	391.5	Xtriage
Anisotropy	0.388	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 562.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	27660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	525.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.56% 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: LLP

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	0.41	0/3597	0.65	0/4831
1	B	0.39	0/3597	0.65	0/4831
1	C	0.39	0/3597	0.64	0/4831
1	D	0.41	0/3597	0.65	0/4831
1	E	0.40	0/3597	0.64	0/4831
2	F	0.49	1/2185 (0.0%)	0.75	0/3401
2	G	0.44	1/2185 (0.0%)	0.73	0/3401
2	H	0.42	1/2185 (0.0%)	0.73	0/3401
2	I	0.43	1/2185 (0.0%)	0.72	0/3401
2	J	0.43	1/2185 (0.0%)	0.72	2/3401 (0.1%)
All	All	0.42	5/28910 (0.0%)	0.68	2/41160 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	G	OP3-P	-7.24	1.52	1.61
2	I	1	G	OP3-P	-7.05	1.52	1.61
2	J	1	G	OP3-P	-7.05	1.52	1.61
2	H	1	G	OP3-P	-6.86	1.52	1.61
2	G	1	G	OP3-P	-6.77	1.53	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	47(P)	A	OP2-P-O3'	6.24	118.93	105.20
2	J	27	C	OP2-P-O3'	5.73	117.81	105.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3575	0	3758	296	0
1	B	3575	0	3758	290	0
1	C	3575	0	3758	284	0
1	D	3575	0	3758	300	0
1	E	3575	0	3758	256	0
2	F	1957	0	989	102	0
2	G	1957	0	989	124	0
2	H	1957	0	989	105	0
2	I	1957	0	989	112	0
2	J	1957	0	989	91	0
All	All	27660	0	23735	1788	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 35.

All (1788) 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:C:157:LYS:HE2	1:C:209:ALA:HB2	1.27	1.14
1:B:1:MET:HG3	1:B:4:LEU:HD12	1.31	1.12
1:C:102:ASN:HB3	1:D:71:ARG:HH22	1.15	1.08
1:A:10:GLN:H	1:A:13:LYS:HD2	1.13	1.08
2:J:32:C:H2'	2:J:33:U:C6	1.93	1.02
1:B:10:GLN:H	1:B:13:LYS:HD2	1.20	1.02
1:C:353:ARG:HE	1:C:357:LYS:HD2	1.24	1.01
1:C:67:PRO:HD3	1:D:329:LYS:HE3	1.42	0.99
1:A:60:LYS:O	1:A:64:LEU:HG	1.63	0.98
1:B:374:ILE:HD11	1:B:428:LEU:HD21	1.42	0.97
1:D:221:MET:HG2	1:E:221:MET:HG2	1.47	0.97
2:G:47(H):U:H2'	2:G:47(I):A:O4'	1.65	0.97
1:D:4:LEU:O	1:D:42:ILE:HD13	1.65	0.95
1:B:423:ARG:HD2	1:B:428:LEU:HD12	1.49	0.95
1:B:373:VAL:HG22	1:B:395:VAL:HG22	1.49	0.94
1:A:157:LYS:HE2	1:A:209:ALA:HB2	1.50	0.94
1:A:442:ILE:O	1:A:446:LEU:HG	1.66	0.94

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:ILE:HD12	2:F:18:G:OP1	1.68	0.93
1:E:5:LEU:HD11	1:E:39:ARG:HA	1.47	0.93
1:A:181:LYS:HG3	1:B:309:PRO:HG2	1.49	0.93
1:C:163:ARG:HD2	1:C:190:GLY:O	1.67	0.93
2:F:36:A:H2'	2:F:37:A:O4'	1.67	0.93
1:C:10:GLN:H	1:C:13:LYS:HD2	1.31	0.92
1:C:399:HIS:HE1	1:C:401:ARG:HD3	1.35	0.91
1:C:83:ASN:HB3	1:D:109:TYR:HD2	1.36	0.91
1:B:10:GLN:HB3	1:B:13:LYS:HG3	1.51	0.91
1:E:187:ARG:HE	1:E:203:ALA:HB1	1.34	0.91
1:C:332:PHE:CZ	1:D:29:LYS:HD2	2.06	0.91
1:D:150:LEU:HD13	1:D:179:MET:HG3	1.52	0.91
2:J:7:G:H22	2:J:66:A:H2	1.18	0.90
1:A:97:ILE:HD11	1:A:323:GLY:HA3	1.52	0.90
1:E:254:ILE:HD11	1:E:259:PHE:CE2	2.08	0.89
2:I:33:U:H5'	2:I:34:U:OP2	1.70	0.89
1:B:366:ILE:HB	1:B:369:LEU:HD12	1.55	0.89
2:F:47(H):U:H2'	2:F:47(I):A:O4'	1.74	0.88
2:I:7:G:H22	2:I:66:A:H2	1.19	0.88
1:A:171:GLY:HA3	1:B:116:ARG:NH2	1.86	0.88
1:A:68:ASN:HD22	1:B:122:HIS:HA	1.37	0.88
2:G:29:A:H2'	2:G:30:G:O4'	1.74	0.87
2:F:7:G:H22	2:F:66:A:H2	1.23	0.87
2:G:7:G:H22	2:G:66:A:H2	1.20	0.87
1:B:221:MET:HG2	1:C:221:MET:HG2	1.56	0.86
1:D:29:LYS:HD3	1:D:64:LEU:HD13	1.55	0.86
1:B:358:ARG:HH21	1:B:439:LEU:HD12	1.39	0.86
1:E:254:ILE:HD11	1:E:259:PHE:HE2	1.39	0.86
1:B:231:GLU:HG3	1:B:274:LEU:HD11	1.58	0.85
1:E:330:LEU:HD23	1:E:335:ARG:HD3	1.58	0.85
2:G:65:C:H2'	2:G:66:A:C8	2.11	0.85
1:C:73:ILE:HB	1:C:418:ILE:HG12	1.57	0.85
1:B:10:GLN:HG2	1:B:12:SER:H	1.42	0.85
1:B:176:PRO:HG3	1:C:191:THR:HG22	1.59	0.84
1:A:136:SER:HB3	1:A:296:VAL:HG12	1.60	0.84
2:I:47(A):C:H2'	2:I:47(B):G:H8	1.40	0.84
1:E:1:MET:CG	1:E:4:LEU:HD12	2.07	0.84
1:C:29:LYS:HD2	1:D:332:PHE:CZ	2.11	0.84
1:E:252:LEU:HD21	1:E:256:LEU:HG	1.58	0.84
1:B:298:LYS:HB2	1:B:301:LEU:HD12	1.60	0.83
2:I:25:U:O2'	2:I:26:C:H5'	1.79	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:VAL:HG12	1:D:219:PHE:HE2	1.41	0.83
1:A:90:SER:HB3	1:A:338:ASP:O	1.77	0.83
2:F:47(G):U:H6	2:F:47(G):U:O5'	1.62	0.83
1:E:443:LYS:O	1:E:447:GLN:HG2	1.79	0.83
2:F:32:C:H2'	2:F:33:U:O4'	1.80	0.82
1:C:5:LEU:HD11	1:C:39:ARG:HA	1.60	0.82
2:I:47(H):U:H2'	2:I:47(I):A:O4'	1.80	0.82
1:B:263:VAL:HG11	1:B:388:LEU:HD13	1.62	0.82
2:H:7:G:H22	2:H:66:A:H2	1.24	0.81
1:A:10:GLN:HB2	1:A:13:LYS:HE3	1.61	0.81
1:A:29:LYS:HD2	1:B:332:PHE:CZ	2.16	0.81
1:B:97:ILE:HD11	1:B:323:GLY:HA3	1.61	0.81
1:D:362:LEU:HB3	1:D:443:LYS:HD2	1.62	0.81
2:G:25:U:H2'	2:G:26:C:H6	1.46	0.81
1:B:411:LEU:HD22	1:B:418:ILE:HD12	1.61	0.80
1:C:126:TYR:CB	1:C:328:LEU:HD13	2.12	0.80
1:A:171:GLY:HA3	1:B:116:ARG:HH22	1.44	0.80
2:G:25:U:H2'	2:G:26:C:C6	2.17	0.80
1:E:187:ARG:NE	1:E:203:ALA:HB1	1.97	0.80
2:J:47(L):C:H2'	2:J:47(M):G:C8	2.17	0.80
2:G:27:C:H2'	2:G:28:U:O4'	1.80	0.80
1:A:28:VAL:O	1:A:32:ARG:HG3	1.80	0.79
1:A:5:LEU:HD11	1:A:39:ARG:HG2	1.63	0.79
1:A:12:SER:O	1:A:16:GLU:HG3	1.82	0.79
1:B:60:LYS:O	1:B:64:LEU:HG	1.83	0.79
1:D:5:LEU:HD12	1:D:8:ILE:HD12	1.62	0.79
1:C:102:ASN:HB3	1:D:71:ARG:NH2	1.96	0.79
1:D:176:PRO:HG3	1:E:191:THR:HG22	1.64	0.79
2:J:47(L):C:H2'	2:J:47(M):G:H8	1.48	0.79
1:B:10:GLN:H	1:B:13:LYS:CD	1.95	0.79
1:A:366:ILE:HB	1:A:369:LEU:CD1	2.12	0.79
2:J:38:A:O2'	2:J:39:U:H5'	1.82	0.79
1:B:217:SER:O	1:B:386:PRO:HD3	1.83	0.79
2:H:67(A):A:H2'	2:H:68:C:C6	2.18	0.79
1:A:10:GLN:N	1:A:13:LYS:HD2	1.96	0.78
1:C:97:ILE:HD11	1:C:323:GLY:HA3	1.65	0.78
1:E:366:ILE:HB	1:E:369:LEU:HD12	1.66	0.78
1:C:234:VAL:CG2	1:C:276:ILE:HD13	2.14	0.78
1:D:344:MET:O	1:D:432:ARG:HD2	1.81	0.78
1:C:11:ILE:HB	2:I:16:U:H4'	1.65	0.78
1:B:197:VAL:HG22	1:B:228:VAL:HG13	1.64	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:55:U:H2'	2:I:57:G:OP2	1.84	0.78
2:J:47(H):U:H2'	2:J:47(I):A:O4'	1.84	0.78
1:B:405:GLN:HE22	1:B:422:ILE:HG21	1.49	0.78
1:C:126:TYR:HB2	1:C:328:LEU:HD13	1.64	0.78
1:C:253:LEU:HD23	1:C:331:TYR:CD1	2.19	0.78
1:D:10:GLN:HG2	1:D:12:SER:H	1.49	0.78
1:E:1:MET:C	1:E:3:SER:H	1.86	0.78
1:E:343:ARG:O	1:E:347:GLN:HG3	1.83	0.77
1:D:39:ARG:O	1:D:43:ILE:HG13	1.85	0.77
1:A:332:PHE:CZ	1:B:29:LYS:HD2	2.20	0.77
1:D:42:ILE:HD11	1:D:50:LEU:HD21	1.66	0.77
1:A:366:ILE:HB	1:A:369:LEU:HD12	1.64	0.77
1:C:126:TYR:CE2	1:C:325:GLU:HG3	2.20	0.77
1:B:37:LYS:O	1:B:41:GLU:HG3	1.85	0.76
2:I:47(A):C:H2'	2:I:47(B):G:C8	2.18	0.76
1:C:397:ILE:HD11	1:C:427:LEU:HD23	1.67	0.76
1:A:399:HIS:HE1	1:A:401:ARG:HD3	1.50	0.76
1:A:163:ARG:HD2	1:A:190:GLY:O	1.85	0.76
1:B:90:SER:HB3	1:B:338:ASP:O	1.84	0.76
1:E:5:LEU:CD1	1:E:39:ARG:HA	2.16	0.76
1:D:10:GLN:HB2	2:H:19:G:H3'	1.66	0.76
1:B:5:LEU:HD11	1:B:39:ARG:HA	1.68	0.76
1:A:217:SER:O	1:A:386:PRO:HD3	1.86	0.76
2:G:65:C:H2'	2:G:66:A:H8	1.52	0.75
1:C:130:LEU:HD13	1:C:253:LEU:HD21	1.69	0.75
2:F:65:C:H2'	2:F:66:A:C8	2.20	0.75
2:H:15:C:H2'	2:H:16:U:C6	2.20	0.75
1:D:1:MET:HG3	1:D:2:LYS:N	2.00	0.75
1:D:399:HIS:CE1	1:D:450:LEU:HD22	2.21	0.75
1:E:37:LYS:O	1:E:41:GLU:HG3	1.87	0.75
1:E:163:ARG:HD2	1:E:190:GLY:O	1.87	0.75
2:F:37:A:H2'	2:F:38:A:O4'	1.87	0.75
1:A:216:LYS:HG2	1:A:219:PHE:CZ	2.22	0.74
1:A:60:LYS:HD2	1:A:64:LEU:HD21	1.67	0.74
1:E:363:LEU:CD2	1:E:446:LEU:HD12	2.16	0.74
1:C:181:LYS:HG3	1:D:309:PRO:HG2	1.68	0.74
1:E:72:VAL:HG22	1:E:417:PRO:HG2	1.69	0.74
2:I:8:A:N6	2:I:21:U:O4	2.20	0.74
1:C:29:LYS:HD3	1:C:64:LEU:HD13	1.69	0.74
1:A:145:ALA:O	1:A:149:VAL:HG23	1.88	0.74
1:B:399:HIS:CE1	1:B:450:LEU:HD22	2.22	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:O	1:C:305:ILE:HG13	1.87	0.74
1:D:366:ILE:HB	1:D:369:LEU:HD12	1.69	0.74
2:F:47:U:H2'	2:F:47(A):C:C6	2.22	0.74
2:J:65:C:H2'	2:J:66:A:C8	2.23	0.74
1:A:28:VAL:HG12	1:A:32:ARG:NE	2.03	0.73
1:A:61:ILE:O	1:A:65:MET:HG3	1.88	0.73
1:B:169:ILE:O	1:B:173:PHE:HB3	1.88	0.73
1:E:73:ILE:HB	1:E:418:ILE:HG12	1.69	0.73
1:B:12:SER:O	1:B:16:GLU:HG3	1.88	0.73
1:E:363:LEU:HD21	1:E:446:LEU:HD12	1.69	0.73
2:H:46:C:C2'	2:H:47:U:H5'	2.18	0.73
2:G:58:A:H1'	2:G:60:U:OP2	1.88	0.73
1:A:147:PHE:HB2	1:A:178:ILE:HD11	1.69	0.73
2:G:28:U:O2'	2:G:29:A:H5'	1.88	0.73
1:C:39:ARG:HH22	2:I:18:G:H2'	1.54	0.73
1:A:68:ASN:ND2	1:B:122:HIS:HA	2.02	0.73
1:B:10:GLN:HB3	1:B:13:LYS:HE3	1.70	0.72
2:F:58:A:H1'	2:F:60:U:OP2	1.89	0.72
1:B:150:LEU:HD13	1:B:179:MET:HG3	1.70	0.72
1:D:5:LEU:HD11	1:D:39:ARG:HG3	1.70	0.72
1:B:39:ARG:O	1:B:43:ILE:HG13	1.88	0.72
2:J:55:U:H2'	2:J:57:G:OP2	1.89	0.72
1:C:359:LEU:HB2	1:C:439:LEU:HD22	1.70	0.72
2:F:47(A):C:H2'	2:F:47(B):G:H8	1.53	0.72
1:B:25:ILE:HG13	1:B:26:TYR:N	2.04	0.72
1:E:280:SER:HA	1:E:294:ILE:O	1.90	0.72
2:J:47(I):A:H2'	2:J:47(J):A:O4'	1.89	0.72
1:B:10:GLN:HB2	2:F:19:G:H3'	1.71	0.72
1:B:163:ARG:NH1	1:C:188:GLU:OE1	2.22	0.72
2:I:15:C:H2'	2:I:16:U:C6	2.24	0.72
1:B:224:PHE:CD1	1:C:218:ASN:HB2	2.25	0.72
2:F:47(A):C:H2'	2:F:47(B):G:C8	2.25	0.72
1:B:10:GLN:N	1:B:13:LYS:HD2	2.00	0.71
2:I:47:U:H2'	2:I:47(A):C:C6	2.26	0.71
1:B:336:TYR:O	1:B:339:ILE:HG12	1.90	0.71
1:E:30:ALA:O	1:E:34:VAL:HG23	1.91	0.71
2:H:37:A:H2'	2:H:38:A:O4'	1.91	0.71
2:G:47(J):A:O2'	2:G:47(K):G:H5'	1.91	0.71
1:D:169:ILE:HG22	1:D:218:ASN:OD1	1.91	0.71
2:G:63:C:H2'	2:G:64:A:C8	2.25	0.71
1:A:330:LEU:HD23	1:A:335:ARG:HD3	1.72	0.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:35:C:H2'	2:F:36:A:C8	2.26	0.71
2:F:63:C:H2'	2:F:64:A:C8	2.25	0.71
1:A:11:ILE:O	1:A:15:VAL:HG23	1.90	0.71
1:B:159:VAL:HG22	1:B:210:LEU:HB3	1.70	0.71
1:E:1:MET:SD	1:E:4:LEU:HD12	2.30	0.71
1:D:280:SER:HA	1:D:294:ILE:O	1.90	0.71
2:I:9:U:H4'	2:I:45:U:C2	2.26	0.71
1:A:407:LEU:CD2	1:A:427:LEU:HD22	2.21	0.70
1:B:28:VAL:HG12	1:B:32:ARG:NE	2.04	0.70
2:H:46:C:H2'	2:H:47:U:O4'	1.91	0.70
2:I:47(G):U:H2'	2:I:47(H):U:O4'	1.90	0.70
1:B:77:GLY:HA2	1:B:433:THR:HG23	1.73	0.70
1:E:90:SER:HB3	1:E:338:ASP:O	1.90	0.70
2:J:37:A:H2'	2:J:38:A:O4'	1.92	0.70
1:B:163:ARG:HD2	1:B:190:GLY:O	1.92	0.70
1:B:1:MET:HG3	1:B:4:LEU:CD1	2.18	0.70
1:C:12:SER:O	1:C:16:GLU:HG3	1.91	0.70
1:D:407:LEU:CD2	1:D:427:LEU:HD22	2.21	0.70
1:A:138:VAL:HG13	1:A:293:GLY:O	1.91	0.70
1:B:280:SER:HA	1:B:294:ILE:O	1.92	0.70
1:B:285:LLP:OP4	1:B:285:LLP:H4'1	1.91	0.70
1:E:330:LEU:CD2	1:E:335:ARG:HD3	2.22	0.70
2:F:47(O):G:H2'	2:F:47(P):A:C8	2.27	0.70
1:A:301:LEU:O	1:A:305:ILE:HG13	1.91	0.70
1:D:5:LEU:CD1	1:D:8:ILE:HD12	2.22	0.70
1:E:211:LEU:HG	1:E:242:ILE:CG2	2.21	0.70
1:E:77:GLY:HA3	1:E:430:ASP:CG	2.12	0.70
1:E:1:MET:HG3	1:E:4:LEU:HD12	1.72	0.70
1:D:408:SER:O	1:D:412:ARG:HG3	1.91	0.69
1:E:217:SER:O	1:E:386:PRO:HD3	1.93	0.69
2:G:47:U:H2'	2:G:47(A):C:C6	2.27	0.69
2:H:47:U:H2'	2:H:47(A):C:C6	2.27	0.69
1:B:290:PRO:HB2	1:B:320:THR:HG22	1.75	0.69
1:C:10:GLN:HG3	2:I:19:G:O5'	1.91	0.69
1:C:280:SER:HA	1:C:294:ILE:O	1.93	0.69
1:E:230:LEU:HD23	1:E:233:LEU:HD12	1.74	0.69
1:E:435:PHE:HB3	1:E:437:GLU:OE1	1.93	0.69
1:B:1:MET:CG	1:B:4:LEU:HD12	2.18	0.69
1:A:280:SER:HA	1:A:294:ILE:O	1.93	0.69
2:J:47(A):C:H2'	2:J:47(B):G:H8	1.57	0.69
2:I:37:A:H2'	2:I:38:A:O4'	1.91	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ILE:HD11	1:B:428:LEU:CD2	2.21	0.69
1:C:28:VAL:O	1:C:32:ARG:HG3	1.91	0.69
1:E:11:ILE:HG21	1:E:28:VAL:HG13	1.73	0.69
2:F:55:U:H2'	2:F:57:G:OP2	1.93	0.69
2:J:47:U:H2'	2:J:47(A):C:C6	2.28	0.69
1:A:253:LEU:HD23	1:A:331:TYR:CD1	2.28	0.69
1:D:200:TYR:CE2	1:D:228:VAL:HG21	2.28	0.69
2:G:37:A:H2'	2:G:38:A:O4'	1.93	0.69
1:E:10:GLN:HG2	1:E:12:SER:H	1.57	0.68
2:I:6:A:H2'	2:I:7:G:C8	2.29	0.68
1:B:187:ARG:HE	1:B:203:ALA:HB1	1.58	0.68
2:F:47(I):A:H2'	2:F:47(J):A:O4'	1.93	0.68
1:A:399:HIS:CE1	1:A:401:ARG:HD3	2.28	0.68
1:C:402:LEU:HD22	1:C:406:GLU:HG2	1.76	0.68
1:E:141:ASN:OD1	1:E:143:ALA:HB3	1.93	0.68
1:B:407:LEU:HD23	1:B:427:LEU:HD22	1.76	0.68
1:D:8:ILE:HD11	1:D:38:TYR:HB3	1.74	0.68
1:E:405:GLN:HE22	1:E:422:ILE:HG21	1.56	0.68
2:F:38:A:C2'	2:F:39:U:H5'	2.23	0.68
1:D:298:LYS:HB2	1:D:301:LEU:HD12	1.75	0.68
2:H:47(H):U:H2'	2:H:47(I):A:O4'	1.93	0.68
2:I:28:U:O2'	2:I:29:A:H5'	1.94	0.68
1:A:345:LEU:CD2	1:A:380:PRO:HB3	2.24	0.68
1:E:358:ARG:HH21	1:E:439:LEU:HD12	1.58	0.68
1:B:390:LEU:HB2	1:B:432:ARG:NH2	2.09	0.68
1:C:366:ILE:HG23	1:C:367:PRO:HD2	1.75	0.68
2:G:25:U:O2'	2:G:26:C:H5'	1.94	0.68
2:H:47(A):C:H2'	2:H:47(B):G:H8	1.59	0.68
1:A:320:THR:HG22	1:B:319:LEU:HD12	1.76	0.68
1:E:234:VAL:HG22	1:E:276:ILE:HD13	1.74	0.68
1:D:126:TYR:O	1:D:130:LEU:HG	1.94	0.67
2:F:65:C:H2'	2:F:66:A:H8	1.56	0.67
2:J:47(A):C:H2'	2:J:47(B):G:C8	2.29	0.67
1:E:162:SER:HB2	1:E:200:TYR:OH	1.94	0.67
1:E:197:VAL:HG22	1:E:228:VAL:HG13	1.77	0.67
2:I:47(L):C:H2'	2:I:47(M):G:C8	2.29	0.67
1:C:42:ILE:HD11	1:C:50:LEU:HD21	1.76	0.67
1:E:159:VAL:HG22	1:E:210:LEU:HB3	1.75	0.67
1:A:10:GLN:H	1:A:13:LYS:CD	2.00	0.67
1:A:2:LYS:O	1:A:6:ARG:HG3	1.94	0.67
2:J:47(O):G:H2'	2:J:47(P):A:C8	2.29	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HG2	1:B:226:GLU:HB2	1.76	0.67
1:B:390:LEU:CB	1:B:432:ARG:HH22	2.08	0.67
1:C:39:ARG:O	1:C:43:ILE:HG13	1.94	0.67
1:E:420:CYS:SG	1:E:427:LEU:HD11	2.35	0.67
1:E:8:ILE:HD11	1:E:38:TYR:HB3	1.75	0.67
1:A:123:ILE:CD1	1:A:325:GLU:HB2	2.23	0.67
1:A:85:GLY:HA2	1:B:107:LEU:HD23	1.76	0.67
1:B:256:LEU:HD23	1:B:263:VAL:CG2	2.24	0.67
1:C:302:ILE:HD13	1:C:305:ILE:HD12	1.76	0.67
1:D:2:LYS:HE2	1:D:6:ARG:NH2	2.10	0.67
1:E:8:ILE:CD1	1:E:38:TYR:HB3	2.24	0.67
1:B:28:VAL:HG12	1:B:32:ARG:HE	1.59	0.67
1:E:407:LEU:HD23	1:E:427:LEU:HD22	1.77	0.67
1:E:423:ARG:HD2	1:E:428:LEU:CD1	2.25	0.67
2:I:47(O):G:H2'	2:I:47(P):A:C8	2.30	0.67
1:A:392:THR:HG21	1:A:430:ASP:OD2	1.95	0.66
1:A:10:GLN:HB2	1:A:13:LYS:CE	2.25	0.66
1:C:187:ARG:HE	1:C:203:ALA:HB1	1.59	0.66
1:A:39:ARG:O	1:A:43:ILE:HG13	1.95	0.66
1:B:145:ALA:O	1:B:149:VAL:HG23	1.95	0.66
1:C:5:LEU:HD12	1:C:42:ILE:HD12	1.76	0.66
1:D:97:ILE:HD11	1:D:323:GLY:HA3	1.76	0.66
2:H:36:A:O2'	2:H:37:A:H5'	1.95	0.66
2:I:38:A:C2'	2:I:39:U:H5'	2.25	0.66
2:J:58:A:H1'	2:J:60:U:OP2	1.95	0.66
1:A:165:GLU:OE1	1:A:213:LYS:HG3	1.96	0.66
1:A:42:ILE:HD11	1:A:50:LEU:HD21	1.77	0.66
1:A:343:ARG:O	1:A:347:GLN:HG3	1.95	0.66
1:C:399:HIS:CD2	1:C:450:LEU:HD13	2.30	0.66
1:C:167:VAL:HG12	1:C:219:PHE:HE2	1.61	0.66
1:C:90:SER:HB3	1:C:338:ASP:O	1.95	0.66
1:D:340:PRO:O	1:D:344:MET:HG3	1.95	0.66
2:I:63:C:H2'	2:I:64:A:C8	2.31	0.66
1:A:30:ALA:O	1:A:34:VAL:HG23	1.95	0.66
1:B:390:LEU:HB2	1:B:432:ARG:HH22	1.58	0.66
2:G:30:G:O2'	2:G:31:A:H5'	1.95	0.66
2:H:58:A:H1'	2:H:60:U:OP2	1.95	0.66
1:A:361:LYS:HA	1:A:364:LYS:HE3	1.77	0.66
1:D:242:ILE:HG23	1:D:243:PRO:HD2	1.77	0.66
1:E:12:SER:O	1:E:16:GLU:HG3	1.96	0.66
2:J:27:C:H2'	2:J:28:U:O4'	1.95	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:VAL:HG12	1:A:265:GLU:H	1.59	0.65
1:B:412:ARG:HD2	1:B:419:VAL:HG22	1.78	0.65
2:G:63:C:H2'	2:G:64:A:H8	1.61	0.65
1:A:169:ILE:HG13	1:A:173:PHE:HD2	1.60	0.65
1:C:11:ILE:HG21	1:C:28:VAL:HG13	1.78	0.65
1:C:37:LYS:O	1:C:41:GLU:HG3	1.96	0.65
1:D:217:SER:O	1:D:386:PRO:HD3	1.96	0.65
2:G:47(O):G:H2'	2:G:47(P):A:C8	2.30	0.65
1:A:302:ILE:CG2	1:A:306:LYS:HE3	2.27	0.65
1:A:68:ASN:HD22	1:B:122:HIS:CA	2.07	0.65
1:D:302:ILE:CG2	1:D:306:LYS:HE3	2.26	0.65
1:E:130:LEU:HD13	1:E:253:LEU:HD21	1.79	0.65
1:E:211:LEU:HG	1:E:242:ILE:HG22	1.78	0.65
2:J:24:C:O2'	2:J:25:U:H5'	1.96	0.65
1:A:401:ARG:NH1	1:A:450:LEU:O	2.28	0.65
1:C:72:VAL:HG13	1:C:417:PRO:HG2	1.79	0.65
1:E:39:ARG:O	1:E:43:ILE:HG13	1.97	0.65
2:J:63:C:H2'	2:J:64:A:C8	2.32	0.65
1:D:39:ARG:HG2	2:H:56:C:N4	2.10	0.65
1:A:68:ASN:ND2	1:B:122:HIS:CD2	2.64	0.65
2:F:28:U:O2'	2:F:29:A:H5'	1.96	0.65
2:G:31:A:N7	2:G:32:C:C4	2.64	0.65
1:A:309:PRO:HG2	1:B:181:LYS:HG3	1.78	0.65
1:E:371:ILE:HG12	1:E:397:ILE:HG22	1.77	0.65
1:A:123:ILE:HG23	1:A:328:LEU:HD12	1.77	0.65
2:F:67(A):A:H2'	2:F:68:C:C6	2.32	0.65
2:F:69:U:H2'	2:F:70:C:C6	2.32	0.65
2:H:47(O):G:H2'	2:H:47(P):A:C8	2.32	0.65
1:A:83:ASN:HB3	1:B:109:TYR:HD2	1.62	0.65
1:B:32:ARG:HH22	2:F:18:G:P	2.19	0.65
1:A:13:LYS:HA	1:A:16:GLU:OE1	1.97	0.64
2:G:36:A:H2'	2:G:37:A:C8	2.31	0.64
1:D:250:SER:HB2	1:D:286:LEU:CD1	2.27	0.64
2:J:25:U:O2'	2:J:26:C:H5'	1.96	0.64
1:B:352:LEU:HD13	1:B:392:THR:HA	1.78	0.64
1:B:423:ARG:HD2	1:B:428:LEU:CD1	2.26	0.64
1:C:333:GLU:HA	1:D:25:ILE:HD12	1.80	0.64
1:D:218:ASN:ND2	1:E:224:PHE:HB2	2.13	0.64
2:I:47(L):C:H2'	2:I:47(M):G:H8	1.60	0.64
1:D:11:ILE:HG22	2:H:16:U:H4'	1.78	0.64
1:A:271:CYS:O	1:A:276:ILE:HG12	1.98	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:SER:OG	1:D:422:ILE:HD11	1.98	0.64
1:E:152:THR:HG21	1:E:305:ILE:HA	1.79	0.64
2:G:24:C:O2'	2:G:25:U:H5'	1.97	0.64
2:G:29:A:C2'	2:G:30:G:O4'	2.46	0.64
1:A:32:ARG:HH11	1:A:32:ARG:HG2	1.62	0.64
1:D:302:ILE:HG22	1:D:306:LYS:HE3	1.80	0.64
1:D:359:LEU:HB2	1:D:439:LEU:HD22	1.79	0.64
1:B:359:LEU:HB2	1:B:439:LEU:HD22	1.79	0.64
1:A:373:VAL:HG22	1:A:395:VAL:HG22	1.80	0.64
1:D:353:ARG:HB2	1:D:393:TYR:CE2	2.31	0.64
2:J:65:C:H2'	2:J:66:A:H8	1.62	0.64
2:F:6:A:H2'	2:F:7:G:C8	2.33	0.64
1:D:218:ASN:HD22	1:E:224:PHE:HB2	1.63	0.64
1:D:250:SER:HB2	1:D:286:LEU:HD12	1.79	0.64
1:E:86:ARG:NH1	1:E:285:LLP:HE2	2.12	0.64
1:B:10:GLN:NE2	2:F:19:G:OP1	2.31	0.63
1:C:11:ILE:O	1:C:15:VAL:HG23	1.97	0.63
1:D:161:ILE:HG21	1:D:166:LEU:HD21	1.79	0.63
1:A:309:PRO:CG	1:B:181:LYS:HG3	2.28	0.63
1:C:211:LEU:HG	1:C:242:ILE:HG21	1.80	0.63
1:D:3:SER:O	1:D:7:GLN:HG2	1.98	0.63
2:I:10:A:H4'	2:I:45:U:O4'	1.98	0.63
1:C:339:ILE:HD11	1:C:342:ILE:HG13	1.80	0.63
1:A:28:VAL:HG12	1:A:32:ARG:HE	1.63	0.63
1:C:5:LEU:CD1	1:C:42:ILE:HD12	2.28	0.63
1:D:259:PHE:HB3	1:D:346:THR:HG21	1.80	0.63
2:I:10:A:C5'	2:I:45:U:O4'	2.47	0.63
1:A:270:ASP:O	1:A:274:LEU:HG	1.98	0.63
1:C:317:ASP:HA	1:D:291:GLN:OE1	1.98	0.63
1:C:431:MET:CE	1:C:434:VAL:HG21	2.28	0.63
1:B:12:SER:OG	2:F:16:U:H1'	1.99	0.63
2:H:21:U:H2'	2:H:22:G:C8	2.34	0.63
2:H:63:C:H2'	2:H:64:A:C8	2.34	0.63
2:I:35:C:H2'	2:I:36:A:O4'	1.98	0.63
1:A:161:ILE:HG23	1:A:166:LEU:HD21	1.80	0.63
1:B:25:ILE:HG13	1:B:26:TYR:H	1.60	0.63
1:E:4:LEU:O	1:E:42:ILE:HD13	1.99	0.63
2:G:47(E):A:H2	2:G:47(I):A:N7	1.96	0.63
2:I:30:G:O2'	2:I:31:A:H5'	1.98	0.63
1:E:423:ARG:HD2	1:E:428:LEU:HD12	1.81	0.63
2:F:24:C:O2'	2:F:25:U:H5'	1.99	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASN:HD21	1:B:135:SER:HA	1.64	0.62
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.63	0.62
1:B:32:ARG:NH1	2:F:18:G:OP1	2.32	0.62
1:D:224:PHE:HD1	1:E:218:ASN:HB2	1.62	0.62
2:H:47(A):C:H2'	2:H:47(B):G:C8	2.34	0.62
1:B:178:ILE:HG23	1:B:179:MET:N	2.14	0.62
1:A:302:ILE:HG22	1:A:306:LYS:HE3	1.81	0.62
1:C:25:ILE:HG13	1:C:26:TYR:N	2.14	0.62
2:H:32:C:H2'	2:H:33:U:C6	2.34	0.62
1:E:396:ALA:HB2	1:E:428:LEU:HD23	1.82	0.62
2:F:63:C:H2'	2:F:64:A:H8	1.62	0.62
1:D:5:LEU:HD21	1:D:39:ARG:HG2	1.82	0.62
2:G:67(A):A:H2'	2:G:68:C:C6	2.34	0.62
1:A:37:LYS:O	1:A:41:GLU:HG3	1.99	0.62
1:B:33:GLU:OE1	1:B:60:LYS:HD2	2.00	0.62
2:G:47(H):U:O2'	2:G:47(I):A:H5'	1.99	0.62
2:G:32:C:H2'	2:G:33:U:C6	2.34	0.62
1:A:25:ILE:HG13	1:A:26:TYR:N	2.14	0.62
1:B:123:ILE:HD11	1:B:325:GLU:HB2	1.81	0.62
1:A:11:ILE:HD12	2:G:18:G:OP1	2.00	0.62
2:I:47(E):A:H2'	2:I:47(F):U:O4'	2.00	0.62
2:I:58:A:H1'	2:I:60:U:OP2	2.00	0.62
1:B:187:ARG:NE	1:B:203:ALA:HB1	2.14	0.62
1:C:57:VAL:O	1:C:61:ILE:HG13	2.00	0.62
1:C:312:ARG:HG2	1:D:173:PHE:HB2	1.82	0.62
1:D:1:MET:CG	1:D:2:LYS:N	2.62	0.62
1:A:425:ASP:CG	1:A:425:ASP:O	2.37	0.61
1:C:32:ARG:HH11	1:C:32:ARG:HG2	1.64	0.61
2:F:69:U:H2'	2:F:70:C:H6	1.64	0.61
1:A:69:ILE:HG12	1:B:122:HIS:ND1	2.14	0.61
1:C:187:ARG:NE	1:C:203:ALA:HB1	2.15	0.61
1:C:362:LEU:O	1:C:443:LYS:HG3	2.00	0.61
1:C:67:PRO:HB2	1:D:96:PHE:CZ	2.34	0.61
2:F:47(G):U:C6	2:F:47(G):U:O5'	2.51	0.61
1:C:348:ASP:HB2	1:C:351:ALA:HB2	1.82	0.61
1:B:61:ILE:O	1:B:65:MET:HG3	1.99	0.61
1:C:30:ALA:O	1:C:34:VAL:HG23	2.01	0.61
1:C:99:GLU:O	1:D:71:ARG:NH2	2.33	0.61
1:D:79:VAL:HG21	1:D:345:LEU:HG	1.81	0.61
1:E:33:GLU:OE1	1:E:60:LYS:HD2	2.01	0.61
1:C:150:LEU:HD13	1:C:179:MET:HG3	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:GLN:HG3	2:G:1:G:O4'	2.01	0.61
1:E:363:LEU:HB2	1:E:371:ILE:CD1	2.31	0.61
1:A:445:THR:O	1:A:449:LEU:HG	2.01	0.61
1:B:123:ILE:CD1	1:B:325:GLU:HB2	2.31	0.61
2:G:54:U:H2'	2:G:55:U:O4'	2.01	0.61
2:H:6:A:H2'	2:H:7:G:C8	2.36	0.61
2:I:67(A):A:H2'	2:I:68:C:C6	2.36	0.61
2:J:30:G:O2'	2:J:31:A:H5'	2.01	0.61
1:C:355:LYS:HG3	1:C:439:LEU:HD11	1.83	0.61
2:G:29:A:O2'	2:G:30:G:H5'	2.01	0.61
2:G:69:U:H2'	2:G:70:C:C6	2.35	0.61
1:B:405:GLN:NE2	1:B:422:ILE:HG21	2.15	0.61
1:D:125:LYS:O	1:D:129:GLU:HG3	2.00	0.60
1:D:347:GLN:NE2	1:D:352:LEU:HD21	2.16	0.60
1:C:102:ASN:CB	1:D:71:ARG:HH22	2.04	0.60
1:B:452:ILE:HG23	1:B:452:ILE:OXT	2.00	0.60
1:C:75:ALA:HB3	1:C:420:CYS:HB3	1.83	0.60
1:D:347:GLN:HE21	1:D:352:LEU:HD21	1.66	0.60
1:E:10:GLN:OE1	1:E:13:LYS:HE3	2.01	0.60
1:E:11:ILE:O	1:E:15:VAL:HG23	2.01	0.60
2:G:71:C:H2'	2:G:72:C:C6	2.36	0.60
1:A:251:GLY:HA2	1:A:268:PHE:HE2	1.66	0.60
1:E:158:GLU:OE2	1:E:187:ARG:HD2	2.00	0.60
2:H:69:U:H2'	2:H:70:C:C6	2.36	0.60
1:A:130:LEU:HD13	1:A:253:LEU:HD21	1.83	0.60
2:F:30:G:O2'	2:F:31:A:H5'	2.01	0.60
2:H:53:G:O2'	2:H:54:U:H5'	2.00	0.60
2:G:47(A):C:H2'	2:G:47(B):G:H8	1.66	0.60
2:I:71:C:H2'	2:I:72:C:C6	2.36	0.60
1:A:420:CYS:SG	1:A:427:LEU:HD21	2.41	0.60
1:E:88:PRO:HG2	1:E:340:PRO:CB	2.31	0.60
1:B:10:GLN:HG2	1:B:12:SER:N	2.15	0.60
1:B:57:VAL:O	1:B:61:ILE:HG13	2.01	0.60
1:C:344:MET:O	1:C:432:ARG:HD2	2.01	0.60
1:D:216:LYS:HG2	1:D:219:PHE:CZ	2.37	0.60
1:D:163:ARG:HH11	1:E:166:LEU:CD1	2.14	0.60
1:A:399:HIS:HE1	1:A:401:ARG:CD	2.14	0.60
1:B:28:VAL:O	1:B:32:ARG:HG3	2.02	0.60
1:D:123:ILE:CD1	1:D:325:GLU:HB2	2.32	0.60
1:E:57:VAL:O	1:E:61:ILE:HG13	2.01	0.60
2:I:69:U:H2'	2:I:70:C:C6	2.36	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:6:A:H2'	2:J:7:G:C8	2.37	0.60
1:A:32:ARG:NH1	1:A:32:ARG:HG2	2.16	0.60
1:B:11:ILE:O	1:B:15:VAL:HG23	2.02	0.60
1:B:178:ILE:CG2	1:B:179:MET:N	2.65	0.60
1:D:200:TYR:CD2	1:D:228:VAL:HG21	2.36	0.60
1:C:285:LLP:OP1	1:D:312:ARG:NH1	2.33	0.60
2:G:15:C:H2'	2:G:16:U:C6	2.37	0.60
1:A:363:LEU:O	1:A:371:ILE:HD11	2.02	0.60
1:C:14:VAL:HG13	1:C:18:PHE:HE2	1.66	0.60
1:C:423:ARG:HD2	1:C:428:LEU:CD1	2.32	0.60
2:G:6:A:H2'	2:G:7:G:C8	2.37	0.60
1:A:10:GLN:HB3	1:A:13:LYS:HG3	1.84	0.59
2:F:71:C:H2'	2:F:72:C:C6	2.36	0.59
1:C:11:ILE:CB	2:I:16:U:H4'	2.32	0.59
1:D:336:TYR:O	1:D:339:ILE:HG12	2.02	0.59
1:E:107:LEU:HD11	1:E:321:LEU:HD23	1.84	0.59
2:J:69:U:H2'	2:J:70:C:C6	2.36	0.59
1:B:10:GLN:CB	1:B:13:LYS:HE3	2.31	0.59
1:C:399:HIS:CE1	1:C:401:ARG:HD3	2.27	0.59
1:A:397:ILE:HD11	1:A:427:LEU:HD23	1.84	0.59
1:D:32:ARG:O	1:D:36:GLU:HG2	2.02	0.59
1:E:107:LEU:O	1:E:122:HIS:HE1	1.85	0.59
2:I:10:A:C2	2:I:26:C:O2	2.54	0.59
2:J:38:A:HO2'	2:J:39:U:H5'	1.67	0.59
1:B:32:ARG:NH1	1:B:32:ARG:HG2	2.18	0.59
1:C:187:ARG:HD3	1:C:203:ALA:HB1	1.84	0.59
1:C:93:VAL:HA	1:C:326:MET:HG2	1.84	0.59
1:A:10:GLN:HG3	2:G:19:G:P	2.43	0.59
2:I:38:A:O2'	2:I:39:U:H5'	2.02	0.59
2:J:71:C:H2'	2:J:72:C:C6	2.37	0.59
1:A:150:LEU:HD13	1:A:179:MET:HG3	1.84	0.59
1:D:2:LYS:O	1:D:2:LYS:HG2	2.03	0.59
1:D:208:THR:HG22	1:D:242:ILE:HD13	1.85	0.59
1:E:187:ARG:CD	1:E:203:ALA:HB1	2.32	0.59
1:C:366:ILE:HB	1:C:369:LEU:CD1	2.33	0.59
1:D:373:VAL:HG22	1:D:395:VAL:HG22	1.85	0.59
1:C:10:GLN:HG3	2:I:19:G:P	2.43	0.59
2:I:63:C:H2'	2:I:64:A:H8	1.67	0.59
1:A:193:ASN:O	1:A:225:VAL:HG13	2.03	0.59
1:C:285:LLP:P	1:D:312:ARG:HH22	2.26	0.59
1:E:2:LYS:O	1:E:6:ARG:HG3	2.02	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:SER:HG	2:F:16:U:H1'	1.68	0.59
1:B:30:ALA:O	1:B:34:VAL:HG23	2.02	0.58
2:G:4:A:H2'	2:G:5:G:C8	2.38	0.58
2:H:67(A):A:H2'	2:H:68:C:H6	1.68	0.58
1:A:153:LEU:HD11	1:A:301:LEU:HD22	1.85	0.58
1:B:242:ILE:HG23	1:B:243:PRO:HD2	1.85	0.58
1:C:13:LYS:HA	1:C:16:GLU:OE1	2.03	0.58
1:C:32:ARG:NH1	1:C:32:ARG:HG2	2.18	0.58
1:C:373:VAL:HG22	1:C:395:VAL:HG22	1.84	0.58
1:C:83:ASN:HB3	1:D:109:TYR:CD2	2.27	0.58
1:D:66:LYS:NZ	1:D:415:GLU:OE2	2.36	0.58
1:D:420:CYS:SG	1:D:427:LEU:HD11	2.43	0.58
2:G:39:U:H2'	2:G:40:C:O4'	2.04	0.58
1:B:1:MET:C	1:B:3:SER:H	2.06	0.58
2:F:67:U:H2'	2:F:67(A):A:H8	1.68	0.58
2:H:24:C:O2'	2:H:25:U:H5'	2.03	0.58
1:A:409:ARG:NH1	1:A:413:LEU:CD1	2.67	0.58
1:E:169:ILE:O	1:E:173:PHE:HB3	2.04	0.58
1:E:396:ALA:HB1	1:E:426:GLN:CD	2.24	0.58
2:I:10:A:C4'	2:I:45:U:O4'	2.51	0.58
1:A:181:LYS:HG3	1:B:309:PRO:CG	2.29	0.58
1:A:126:TYR:CB	1:A:328:LEU:HD13	2.34	0.58
1:B:256:LEU:HD23	1:B:263:VAL:HG21	1.83	0.58
1:D:10:GLN:HG2	1:D:12:SER:N	2.16	0.58
2:H:35:C:N4	2:H:36:A:N6	2.50	0.58
2:H:69:U:H2'	2:H:70:C:H6	1.68	0.58
2:J:53:G:H2'	2:J:54:U:H6	1.68	0.58
1:C:344:MET:O	1:C:432:ARG:CD	2.52	0.58
1:C:55:GLU:O	1:C:59:ARG:HG3	2.03	0.58
1:C:332:PHE:HZ	1:D:29:LYS:HD2	1.61	0.58
1:E:399:HIS:CE1	1:E:450:LEU:HD22	2.38	0.58
1:E:7:GLN:HB2	1:E:50:LEU:CD1	2.33	0.58
2:F:4:A:H2'	2:F:5:G:H8	1.69	0.58
2:H:71:C:H2'	2:H:72:C:C6	2.39	0.58
1:B:358:ARG:NH2	1:B:439:LEU:HD12	2.16	0.58
1:C:272:ILE:HD11	1:C:296:VAL:HG23	1.86	0.58
2:H:21:U:H2'	2:H:22:G:H8	1.67	0.58
2:I:59:U:O2'	2:I:60:U:H5'	2.03	0.58
2:J:69:U:H2'	2:J:70:C:H6	1.69	0.58
1:B:298:LYS:O	1:B:302:ILE:HG12	2.03	0.58
1:D:33:GLU:OE1	1:D:60:LYS:HD2	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:A:O2'	2:F:39:U:H5'	2.03	0.58
1:C:69:ILE:HD11	1:D:321:LEU:HG	1.85	0.58
1:D:344:MET:O	1:D:432:ARG:CD	2.52	0.58
2:J:54:U:H2'	2:J:55:U:O4'	2.04	0.58
1:B:32:ARG:O	1:B:36:GLU:HG2	2.04	0.58
1:C:363:LEU:HD22	1:C:366:ILE:HD12	1.86	0.58
1:D:37:LYS:O	1:D:41:GLU:HG3	2.04	0.58
2:J:18:G:O2'	2:J:57:G:N2	2.35	0.58
2:J:53:G:O2'	2:J:54:U:H5'	2.03	0.57
2:J:63:C:H2'	2:J:64:A:H8	1.69	0.57
1:A:409:ARG:HH12	1:A:413:LEU:CD1	2.17	0.57
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.70	0.57
1:C:10:GLN:HB3	1:C:13:LYS:HG3	1.85	0.57
1:D:224:PHE:CD1	1:E:218:ASN:HB2	2.38	0.57
1:E:353:ARG:HB2	1:E:393:TYR:CE2	2.39	0.57
2:G:4:A:H2'	2:G:5:G:H8	1.69	0.57
2:H:7:G:C2	2:H:49:G:C8	2.92	0.57
2:J:28:U:O2'	2:J:29:A:H5'	2.04	0.57
1:A:435:PHE:HB2	1:A:438:ASP:OD2	2.04	0.57
1:A:85:GLY:HA2	1:B:107:LEU:CD2	2.35	0.57
1:B:24:GLU:O	1:B:28:VAL:HG23	2.04	0.57
1:C:49:ASP:OD1	1:C:50:LEU:N	2.37	0.57
1:E:120:ILE:HG21	1:E:137:PHE:CD1	2.39	0.57
2:F:6:A:O2'	2:F:7:G:H5'	2.04	0.57
2:G:26:C:H2'	2:G:27:C:O4'	2.04	0.57
2:G:53:G:H2'	2:G:54:U:H6	1.68	0.57
2:J:53:G:H2'	2:J:54:U:C6	2.39	0.57
1:B:3:SER:O	1:B:7:GLN:HG2	2.04	0.57
1:B:10:GLN:HB2	2:F:19:G:C3'	2.34	0.57
2:F:54:U:H2'	2:F:55:U:O4'	2.04	0.57
2:H:30:G:O2'	2:H:31:A:H5'	2.05	0.57
2:H:53:G:H2'	2:H:54:U:H6	1.70	0.57
1:C:157:LYS:HE2	1:C:209:ALA:CB	2.19	0.57
1:C:423:ARG:HD2	1:C:428:LEU:HD12	1.86	0.57
1:D:399:HIS:CE1	1:D:401:ARG:HB2	2.40	0.57
2:F:71:C:H2'	2:F:72:C:H6	1.70	0.57
1:B:224:PHE:HD1	1:C:218:ASN:HB2	1.69	0.57
2:F:4:A:H2'	2:F:5:G:C8	2.39	0.57
2:G:25:U:C2	2:G:26:C:C5	2.93	0.57
2:H:48:G:H4'	2:H:49:G:H5''	1.86	0.57
1:A:251:GLY:HA2	1:A:268:PHE:CE2	2.40	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LEU:HB2	1:A:439:LEU:HD22	1.87	0.57
1:C:386:PRO:HG2	1:C:387:GLU:H	1.70	0.57
1:D:407:LEU:HD23	1:D:427:LEU:HD22	1.86	0.57
2:F:35:C:O2'	2:F:36:A:H5'	2.03	0.57
2:H:15:C:H2'	2:H:16:U:H6	1.70	0.57
1:B:175:ILE:N	1:B:176:PRO:HD2	2.19	0.57
1:C:339:ILE:CD1	1:C:342:ILE:HG13	2.34	0.57
1:C:421:ARG:HH11	1:C:421:ARG:HG2	1.68	0.57
1:E:169:ILE:HG22	1:E:218:ASN:OD1	2.05	0.57
1:E:408:SER:O	1:E:412:ARG:HG3	2.04	0.57
1:B:137:PHE:CE1	1:B:306:LYS:HG2	2.40	0.57
1:C:187:ARG:CD	1:C:203:ALA:HB1	2.33	0.57
1:D:234:VAL:HG11	1:D:275:GLY:HA3	1.87	0.57
1:E:25:ILE:HG13	1:E:26:TYR:N	2.19	0.57
2:F:53:G:H2'	2:F:54:U:H6	1.69	0.57
2:I:47(I):A:H2'	2:I:47(J):A:O4'	2.05	0.57
1:A:161:ILE:CG2	1:A:166:LEU:HD21	2.35	0.57
1:B:10:GLN:HB3	1:B:13:LYS:CG	2.30	0.57
2:G:26:C:O2'	2:G:27:C:H5'	2.04	0.57
2:H:4:A:H2'	2:H:5:G:H8	1.70	0.57
2:I:54:U:H2'	2:I:55:U:O4'	2.03	0.57
1:A:169:ILE:O	1:A:173:PHE:HB3	2.05	0.56
1:A:137:PHE:CD1	1:A:306:LYS:HG2	2.40	0.56
1:A:360:GLU:O	1:A:364:LYS:HG3	2.05	0.56
1:D:87:ALA:CB	1:D:341:VAL:HG21	2.35	0.56
1:E:299:LYS:O	1:E:303:GLU:HG2	2.05	0.56
2:F:53:G:O2'	2:F:54:U:H5'	2.05	0.56
2:G:43:G:H5'	2:G:43:G:H8	1.70	0.56
1:C:11:ILE:HD12	2:I:18:G:OP1	2.05	0.56
1:A:194:LYS:HG2	1:A:226:GLU:HB2	1.87	0.56
1:B:216:LYS:HG2	1:B:219:PHE:CZ	2.40	0.56
1:B:443:LYS:O	1:B:447:GLN:HG2	2.05	0.56
2:G:69:U:H2'	2:G:70:C:H6	1.69	0.56
2:I:38:A:H2'	2:I:39:U:O4'	2.04	0.56
2:J:14:G:O2'	2:J:15:C:H5'	2.05	0.56
1:E:200:TYR:CE2	1:E:228:VAL:HG21	2.41	0.56
1:E:1:MET:HG3	1:E:4:LEU:CD1	2.35	0.56
2:H:36:A:H2'	2:H:37:A:O4'	2.05	0.56
1:C:6:ARG:NH1	2:I:20:U:O4	2.38	0.56
1:C:141:ASN:OD1	1:C:143:ALA:HB3	2.05	0.56
1:C:14:VAL:HG13	1:C:18:PHE:CE2	2.40	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ILE:CD1	1:D:321:LEU:HG	2.36	0.56
1:D:360:GLU:HG3	1:D:371:ILE:HG21	1.87	0.56
1:E:336:TYR:O	1:E:339:ILE:HG12	2.04	0.56
2:G:53:G:H2'	2:G:54:U:C6	2.40	0.56
2:J:4:A:H2'	2:J:5:G:H8	1.70	0.56
1:C:169:ILE:O	1:C:173:PHE:HB3	2.05	0.56
2:H:41:U:O2'	2:H:42:A:H5'	2.05	0.56
2:H:47(E):A:H2'	2:H:47(F):U:H5'	1.88	0.56
1:B:15:VAL:HA	1:B:27:VAL:HG11	1.88	0.56
1:B:187:ARG:CD	1:B:203:ALA:HB1	2.36	0.56
1:C:194:LYS:NZ	1:C:224:PHE:HB3	2.21	0.56
1:C:211:LEU:HG	1:C:242:ILE:CG2	2.34	0.56
1:D:107:LEU:HD11	1:D:321:LEU:HD23	1.88	0.56
1:E:1:MET:C	1:E:3:SER:N	2.57	0.56
1:E:18:PHE:HB3	1:E:21:ALA:HB3	1.87	0.56
2:I:10:A:H5'	2:I:45:U:O4'	2.06	0.56
2:J:35:C:H2'	2:J:36:A:O4'	2.06	0.56
1:D:22:TYR:CG	1:D:61:ILE:HG21	2.41	0.56
1:E:401:ARG:NH1	1:E:450:LEU:O	2.39	0.56
2:G:47(K):G:O2'	2:G:47(L):C:H5'	2.06	0.56
2:H:32:C:C4	2:H:33:U:C4	2.93	0.56
2:H:47(E):A:C2'	2:H:47(F):U:H5'	2.35	0.56
2:I:15:C:H2'	2:I:16:U:H6	1.70	0.56
1:C:366:ILE:HB	1:C:369:LEU:HD12	1.88	0.56
1:D:194:LYS:HB2	1:E:168:GLU:OE1	2.06	0.56
2:H:4:A:H2'	2:H:5:G:C8	2.40	0.56
1:D:194:LYS:HG2	1:D:226:GLU:HB2	1.87	0.56
1:E:161:ILE:HG13	1:E:212:MET:O	2.05	0.56
1:E:269:ARG:HH11	1:E:269:ARG:HG3	1.71	0.56
1:E:88:PRO:HG2	1:E:340:PRO:HB2	1.88	0.56
2:G:53:G:O2'	2:G:54:U:H5'	2.05	0.56
1:D:5:LEU:HD21	2:H:56:C:N4	2.21	0.56
1:B:40:LYS:O	1:B:44:GLU:HG3	2.06	0.56
1:C:285:LLP:OP3	1:D:312:ARG:NH2	2.26	0.56
1:D:30:ALA:O	1:D:34:VAL:HG23	2.06	0.56
1:C:26:TYR:OH	1:D:333:GLU:CG	2.54	0.56
2:I:53:G:O2'	2:I:54:U:H5'	2.06	0.56
1:C:39:ARG:HH22	2:I:18:G:C2'	2.17	0.56
2:J:4:A:H2'	2:J:5:G:C8	2.41	0.56
1:A:57:VAL:O	1:A:61:ILE:HG13	2.05	0.55
1:B:402:LEU:HD12	1:B:450:LEU:CD2	2.36	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LEU:O	1:D:234:VAL:HG23	2.06	0.55
1:E:213:LYS:HE3	1:E:246:TYR:HE1	1.71	0.55
2:F:27:C:H2'	2:F:28:U:O4'	2.06	0.55
2:I:39:U:H2'	2:I:40:C:O4'	2.05	0.55
2:I:69:U:H2'	2:I:70:C:H6	1.69	0.55
1:A:366:ILE:HG23	1:A:367:PRO:HD2	1.89	0.55
1:B:72:VAL:HG22	1:B:417:PRO:HG2	1.88	0.55
1:D:201:GLU:OE2	1:D:239:LYS:NZ	2.37	0.55
1:E:399:HIS:CE1	1:E:401:ARG:HD3	2.41	0.55
2:F:67:U:H2'	2:F:67(A):A:C8	2.42	0.55
1:D:163:ARG:HG2	1:D:188:GLU:HB2	1.87	0.55
1:D:220:TYR:CD2	1:D:387:GLU:HG2	2.41	0.55
1:D:27:VAL:HG22	1:D:61:ILE:HD13	1.88	0.55
1:D:123:ILE:HD11	1:D:325:GLU:HB2	1.89	0.55
1:E:87:ALA:CB	1:E:341:VAL:HG21	2.37	0.55
1:A:39:ARG:NH2	2:G:18:G:O2'	2.40	0.55
1:C:107:LEU:O	1:C:122:HIS:HE1	1.90	0.55
1:C:420:CYS:SG	1:C:427:LEU:HD11	2.47	0.55
1:E:169:ILE:HD11	1:E:285:LLP:H5'1	1.87	0.55
2:I:4:A:H2'	2:I:5:G:C8	2.42	0.55
2:I:53:G:H2'	2:I:54:U:H6	1.72	0.55
1:A:234:VAL:HG12	1:A:238:HIS:CD2	2.41	0.55
1:A:123:ILE:HD11	1:A:325:GLU:HB2	1.87	0.55
1:C:216:LYS:HG2	1:C:219:PHE:CZ	2.42	0.55
1:C:242:ILE:HG23	1:C:243:PRO:HD2	1.88	0.55
2:F:59:U:O2'	2:F:60:U:H5'	2.07	0.55
2:G:47(A):C:H2'	2:G:47(B):G:C8	2.42	0.55
2:G:59:U:O2'	2:G:60:U:H5'	2.06	0.55
1:B:399:HIS:CD2	1:B:450:LEU:HD13	2.41	0.55
1:A:194:LYS:HG2	1:A:226:GLU:CB	2.36	0.55
1:D:326:MET:O	1:D:330:LEU:HG	2.06	0.55
1:A:169:ILE:HG13	1:A:173:PHE:CD2	2.41	0.55
1:A:157:LYS:CE	1:A:209:ALA:HB2	2.32	0.55
1:C:363:LEU:HD21	1:C:443:LYS:HA	1.88	0.55
1:C:39:ARG:NH2	2:I:18:G:O2'	2.39	0.55
1:D:150:LEU:HB3	1:D:182:SER:OG	2.07	0.55
2:H:47(L):C:H2'	2:H:47(M):G:C8	2.41	0.55
2:J:43:G:H8	2:J:43:G:H5'	1.72	0.55
1:A:348:ASP:O	1:A:351:ALA:HB3	2.06	0.55
1:C:26:TYR:OH	1:D:333:GLU:HG2	2.07	0.55
1:C:270:ASP:O	1:C:274:LEU:HG	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LLP:OP4	1:C:285:LLP:H4'1	2.05	0.55
1:D:10:GLN:HB2	2:H:19:G:C3'	2.37	0.55
2:G:41:U:O2'	2:G:42:A:H5'	2.07	0.55
2:H:28:U:O2'	2:H:29:A:H5'	2.06	0.55
2:H:63:C:H2'	2:H:64:A:H8	1.71	0.55
2:J:47(G):U:H2'	2:J:47(H):U:O4'	2.07	0.55
1:B:10:GLN:CB	1:B:13:LYS:HG3	2.33	0.55
1:D:163:ARG:HD2	1:D:190:GLY:O	2.07	0.55
1:E:80:ILE:HG22	1:E:80:ILE:O	2.07	0.55
1:B:208:THR:HG22	1:B:242:ILE:HD13	1.90	0.54
1:C:313:ALA:HB1	1:D:144:GLY:CA	2.37	0.54
1:E:278:LEU:HD23	1:E:297:GLY:HA3	1.89	0.54
1:E:430:ASP:OD1	1:E:432:ARG:HB3	2.06	0.54
1:E:74:ASN:HB2	1:E:84:LEU:HD13	1.89	0.54
2:F:47(K):G:O2'	2:F:47(L):C:H5'	2.07	0.54
2:J:3:G:H2'	2:J:4:A:O4'	2.08	0.54
1:A:436:HIS:CD2	1:A:439:LEU:HD12	2.42	0.54
1:C:435:PHE:HB2	1:C:438:ASP:OD2	2.07	0.54
2:F:38:A:H2'	2:F:39:U:H5'	1.90	0.54
1:A:239:LYS:HD3	1:A:240:TYR:CE2	2.42	0.54
1:C:171:GLY:HA3	1:D:116:ARG:NH2	2.22	0.54
1:D:402:LEU:HD12	1:D:450:LEU:CD2	2.38	0.54
2:H:47(F):U:O2'	2:H:47(G):U:H5''	2.08	0.54
2:J:26:C:O2'	2:J:27:C:H5'	2.08	0.54
2:J:39:U:H2'	2:J:40:C:O4'	2.07	0.54
1:A:265:GLU:HB2	1:A:385:LEU:HD21	1.90	0.54
1:B:169:ILE:HG22	1:B:218:ASN:OD1	2.08	0.54
1:C:317:ASP:HB3	1:D:291:GLN:HB3	1.90	0.54
1:D:392:THR:HG21	1:D:430:ASP:OD2	2.07	0.54
2:I:3:G:H2'	2:I:4:A:O4'	2.08	0.54
2:I:4:A:H2'	2:I:5:G:H8	1.72	0.54
1:A:396:ALA:HB2	1:A:428:LEU:CD2	2.37	0.54
1:D:57:VAL:O	1:D:61:ILE:HG13	2.07	0.54
1:C:278:LEU:HD23	1:C:297:GLY:HA3	1.89	0.54
1:C:302:ILE:CG2	1:C:306:LYS:HE3	2.38	0.54
1:D:405:GLN:HE22	1:D:422:ILE:HG21	1.72	0.54
1:D:438:ASP:O	1:D:442:ILE:HG13	2.08	0.54
2:I:47(K):G:O2'	2:I:47(L):C:H5'	2.07	0.54
1:A:388:LEU:HD21	1:A:390:LEU:HD11	1.90	0.54
1:A:40:LYS:O	1:A:44:GLU:HG3	2.08	0.54
1:C:10:GLN:N	1:C:13:LYS:HD2	2.13	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLY:O	1:C:287:LEU:HB3	2.08	0.54
1:C:420:CYS:HB2	1:C:428:LEU:O	2.06	0.54
2:I:71:C:H2'	2:I:72:C:H6	1.72	0.54
1:A:100:ILE:HD12	1:B:69:ILE:HG22	1.90	0.54
1:C:234:VAL:HG22	1:C:276:ILE:HD13	1.88	0.54
1:C:421:ARG:NH1	1:C:421:ARG:HG2	2.22	0.54
1:D:14:VAL:CG1	1:D:18:PHE:HE2	2.21	0.54
1:D:86:ARG:HD2	1:D:284:ASP:OD2	2.08	0.54
1:E:347:GLN:NE2	1:E:352:LEU:HD21	2.22	0.54
2:J:71:C:H2'	2:J:72:C:H6	1.73	0.54
1:A:25:ILE:HG13	1:A:26:TYR:H	1.71	0.54
1:A:96:PHE:O	1:A:100:ILE:HG12	2.08	0.54
1:C:407:LEU:CD2	1:C:427:LEU:HD22	2.38	0.54
1:D:139:VAL:HB	1:D:314:LEU:HB3	1.89	0.54
2:H:53:G:H2'	2:H:54:U:C6	2.43	0.54
1:A:263:VAL:HG12	1:A:264:ASP:N	2.22	0.54
1:C:28:VAL:HG11	2:I:16:U:OP1	2.08	0.54
1:D:176:PRO:HG3	1:E:191:THR:CG2	2.36	0.54
1:D:256:LEU:HD23	1:D:263:VAL:CG2	2.37	0.54
1:D:423:ARG:HD2	1:D:428:LEU:CD1	2.38	0.54
1:E:28:VAL:HG12	1:E:32:ARG:HE	1.71	0.54
1:E:220:TYR:HD2	1:E:386:PRO:HB2	1.74	0.53
2:G:55:U:H2'	2:G:57:G:OP2	2.08	0.53
2:G:64:A:H2'	2:G:65:C:C6	2.43	0.53
1:A:171:GLY:CA	1:B:116:ARG:NH2	2.67	0.53
1:D:191:THR:HG22	1:E:176:PRO:HG3	1.90	0.53
2:F:53:G:H2'	2:F:54:U:C6	2.42	0.53
2:G:5(A):U:C2'	2:G:6:A:H5'	2.38	0.53
2:H:59:U:O2'	2:H:60:U:H5'	2.08	0.53
2:I:39:U:H2'	2:I:40:C:C6	2.43	0.53
1:A:102:ASN:HB3	1:B:71:ARG:HH12	1.72	0.53
1:C:194:LYS:HG2	1:C:226:GLU:HB2	1.90	0.53
1:D:239:LYS:HD3	1:D:240:TYR:CE2	2.43	0.53
1:E:136:SER:HB3	1:E:296:VAL:HG12	1.89	0.53
2:G:71:C:H2'	2:G:72:C:H6	1.72	0.53
1:A:420:CYS:SG	1:A:427:LEU:HD11	2.49	0.53
1:D:348:ASP:HB2	1:D:351:ALA:HB2	1.90	0.53
1:E:32:ARG:O	1:E:36:GLU:HG2	2.08	0.53
2:G:10:A:C6	2:G:44:G:N1	2.76	0.53
1:A:340:PRO:HA	1:A:343:ARG:NH1	2.23	0.53
1:B:351:ALA:O	1:B:354:GLN:HB3	2.09	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:HIS:CE1	1:B:401:ARG:HB2	2.44	0.53
1:C:10:GLN:OE1	2:I:20:U:OP1	2.26	0.53
1:C:179:MET:O	1:C:182:SER:HB3	2.09	0.53
1:C:343:ARG:O	1:C:347:GLN:HG3	2.09	0.53
1:D:179:MET:HA	1:D:182:SER:HB3	1.90	0.53
1:D:47:ARG:HD3	1:D:49:ASP:O	2.08	0.53
1:E:178:ILE:HG23	1:E:179:MET:N	2.23	0.53
2:G:35:C:N4	2:G:36:A:N6	2.56	0.53
2:J:47(K):G:O2'	2:J:47(L):C:H5'	2.07	0.53
1:A:10:GLN:CB	1:A:13:LYS:HE3	2.35	0.53
1:C:159:VAL:HG13	1:C:210:LEU:HB3	1.90	0.53
1:D:107:LEU:O	1:D:122:HIS:HE1	1.92	0.53
1:D:197:VAL:HG22	1:D:228:VAL:HG13	1.91	0.53
1:D:7:GLN:HB2	1:D:50:LEU:CD1	2.39	0.53
1:E:79:VAL:HG12	1:E:341:VAL:HG13	1.91	0.53
1:D:39:ARG:NE	2:H:19:G:O6	2.42	0.53
1:C:29:LYS:CD	1:D:332:PHE:CZ	2.89	0.53
1:E:161:ILE:HG21	1:E:166:LEU:HD21	1.90	0.53
1:E:200:TYR:CD2	1:E:228:VAL:HG21	2.44	0.53
1:E:234:VAL:HG12	1:E:238:HIS:CD2	2.44	0.53
1:B:10:GLN:HG3	2:F:19:G:P	2.48	0.53
2:J:46:C:C4	2:J:47:U:C4	2.97	0.53
1:B:187:ARG:HD3	1:B:203:ALA:HB1	1.91	0.53
1:D:270:ASP:O	1:D:274:LEU:HG	2.08	0.53
1:E:79:VAL:HG13	1:E:344:MET:SD	2.48	0.53
2:F:39:U:H2'	2:F:40:C:O4'	2.08	0.53
2:J:15:C:H2'	2:J:16:U:C6	2.43	0.53
1:A:97:ILE:HD11	1:A:323:GLY:CA	2.34	0.53
1:B:194:LYS:HD3	1:C:168:GLU:OE2	2.09	0.53
2:H:3:G:H2'	2:H:4:A:O4'	2.09	0.53
1:A:231:GLU:O	1:A:235:LYS:HG3	2.09	0.52
1:A:347:GLN:NE2	1:A:352:LEU:HD21	2.24	0.52
1:B:179:MET:O	1:B:182:SER:HB3	2.09	0.52
1:A:11:ILE:HG21	1:A:28:VAL:HG13	1.90	0.52
1:A:334:LYS:HD2	1:A:336:TYR:OH	2.09	0.52
1:B:142:ASN:HB3	1:B:285:LLP:OP4	2.08	0.52
1:B:263:VAL:CG1	1:B:388:LEU:HD13	2.35	0.52
1:D:363:LEU:HB2	1:D:371:ILE:HD13	1.90	0.52
2:I:18:G:O2'	2:I:57:G:N2	2.38	0.52
1:A:161:ILE:HG13	1:A:212:MET:O	2.09	0.52
1:A:399:HIS:CE1	1:A:401:ARG:HB2	2.44	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:SER:HB2	1:B:200:TYR:OH	2.08	0.52
1:B:425:ASP:O	1:B:425:ASP:CG	2.48	0.52
1:C:11:ILE:CG2	2:I:16:U:H4'	2.39	0.52
1:C:86:ARG:NH1	1:C:285:LLP:HE2	2.24	0.52
1:D:396:ALA:HB1	1:D:426:GLN:CD	2.30	0.52
1:C:165:GLU:OE2	1:C:213:LYS:NZ	2.38	0.52
1:C:131:THR:HG21	1:C:296:VAL:HG11	1.92	0.52
1:D:77:GLY:HA3	1:D:430:ASP:CG	2.30	0.52
2:G:39:U:H2'	2:G:40:C:C6	2.45	0.52
2:G:10:A:C6	2:G:44:G:C6	2.97	0.52
2:I:31:A:H2'	2:I:32:C:O4'	2.09	0.52
2:I:41:U:O2'	2:I:42:A:H5'	2.08	0.52
1:B:200:TYR:CE2	1:B:228:VAL:HG21	2.44	0.52
1:B:210:LEU:HD12	1:B:243:PRO:HG2	1.92	0.52
1:C:25:ILE:HG13	1:C:26:TYR:H	1.72	0.52
1:C:407:LEU:HD23	1:C:427:LEU:HD22	1.90	0.52
1:E:211:LEU:HG	1:E:242:ILE:HG21	1.91	0.52
2:G:3:G:H2'	2:G:4:A:O4'	2.10	0.52
2:I:53:G:H2'	2:I:54:U:C6	2.44	0.52
1:D:165:GLU:OE1	1:D:213:LYS:HG3	2.10	0.52
2:H:71:C:H2'	2:H:72:C:H6	1.74	0.52
1:B:234:VAL:CG2	1:B:276:ILE:HD13	2.39	0.52
1:C:212:MET:HE3	1:C:245:TYR:HE1	1.75	0.52
1:D:169:ILE:O	1:D:169:ILE:HD12	2.09	0.52
1:E:194:LYS:HG2	1:E:226:GLU:HB2	1.91	0.52
2:J:5(A):U:C2'	2:J:6:A:H5'	2.39	0.52
1:A:370:LYS:HB2	1:A:398:ARG:O	2.10	0.52
1:B:252:LEU:HD12	1:B:253:LEU:N	2.25	0.52
1:C:28:VAL:HG12	1:C:32:ARG:NE	2.25	0.52
1:E:208:THR:HG22	1:E:242:ILE:HD13	1.92	0.52
1:B:169:ILE:O	1:B:169:ILE:HG13	2.08	0.52
1:C:47:ARG:HD3	1:C:49:ASP:O	2.09	0.52
1:D:254:ILE:HD13	1:D:336:TYR:HE1	1.74	0.52
1:D:35:ALA:HB1	1:D:39:ARG:NH2	2.25	0.52
1:E:25:ILE:HG13	1:E:26:TYR:H	1.73	0.52
2:G:47(E):A:C2	2:G:47(I):A:N7	2.77	0.52
2:H:6:A:O2'	2:H:7:G:H5'	2.10	0.52
1:A:427:LEU:HD23	1:A:429:PHE:HE1	1.75	0.51
1:B:230:LEU:HB3	1:B:274:LEU:CD2	2.39	0.51
1:E:147:PHE:HB2	1:E:178:ILE:HD11	1.92	0.51
1:B:142:ASN:HD22	1:B:285:LLP:C5	2.23	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASN:ND2	1:C:224:PHE:HB2	2.25	0.51
1:B:224:PHE:HB2	1:C:218:ASN:ND2	2.25	0.51
1:B:360:GLU:HG3	1:B:371:ILE:CG2	2.41	0.51
1:B:38:TYR:O	1:B:42:ILE:HG13	2.10	0.51
1:B:91:LYS:HE2	1:B:95:ASN:HD21	1.75	0.51
1:C:29:LYS:HD2	1:D:332:PHE:CE2	2.45	0.51
1:A:15:VAL:HA	1:A:27:VAL:HG11	1.91	0.51
1:B:5:LEU:HD12	1:B:8:ILE:CD1	2.41	0.51
1:E:123:ILE:HD13	1:E:324:LEU:HD23	1.92	0.51
1:E:234:VAL:HG11	1:E:275:GLY:HA3	1.92	0.51
2:F:39:U:H2'	2:F:40:C:C6	2.45	0.51
2:F:47(E):A:O2'	2:F:47(I):A:N6	2.41	0.51
2:G:27:C:O2'	2:G:28:U:H5'	2.10	0.51
2:G:6:A:O2'	2:G:7:G:H5'	2.11	0.51
1:A:278:LEU:HD11	1:A:305:ILE:HD11	1.93	0.51
1:C:2:LYS:O	1:C:6:ARG:HG3	2.09	0.51
1:D:227:GLU:HG2	1:D:228:VAL:N	2.26	0.51
2:F:43:G:H8	2:F:43:G:H5'	1.75	0.51
2:F:47:U:H2'	2:F:47(A):C:H6	1.72	0.51
2:F:67(A):A:H2'	2:F:68:C:H6	1.76	0.51
2:G:47(G):U:H2'	2:G:47(H):U:O4'	2.11	0.51
2:H:39:U:H2'	2:H:40:C:O4'	2.10	0.51
2:I:6:A:O2'	2:I:7:G:H5'	2.09	0.51
1:A:33:GLU:CD	1:A:60:LYS:HE3	2.30	0.51
1:D:208:THR:CG2	1:D:242:ILE:HD13	2.39	0.51
1:E:363:LEU:HD22	1:E:446:LEU:HD12	1.91	0.51
2:J:6:A:O2'	2:J:7:G:H5'	2.10	0.51
1:B:147:PHE:CD2	1:B:147:PHE:C	2.83	0.51
1:B:396:ALA:HB2	1:B:428:LEU:HD23	1.93	0.51
2:F:64:A:H2'	2:F:65:C:C6	2.46	0.51
2:J:59:U:O2'	2:J:60:U:H5'	2.10	0.51
1:C:361:LYS:HA	1:C:364:LYS:HE3	1.93	0.51
2:F:3:G:H2'	2:F:4:A:O4'	2.10	0.51
2:F:47(G):U:H2'	2:F:47(H):U:O4'	2.11	0.51
2:H:54:U:H2'	2:H:55:U:O4'	2.09	0.51
2:H:7:G:O2'	2:H:8:A:H5'	2.11	0.51
2:I:14:G:O2'	2:I:15:C:H5'	2.10	0.51
2:I:43:G:H5'	2:I:43:G:H8	1.75	0.51
2:J:41:U:O2'	2:J:42:A:H5'	2.11	0.51
2:J:64:A:H2'	2:J:65:C:C6	2.45	0.51
1:B:14:VAL:O	1:B:18:PHE:HD2	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:14:G:O2'	2:H:15:C:H5'	2.11	0.51
2:J:52:G:O2'	2:J:53:G:H5'	2.11	0.51
2:I:64:A:H2'	2:I:65:C:C6	2.46	0.51
2:I:67:U:H2'	2:I:67(A):A:H8	1.76	0.51
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.76	0.51
1:B:10:GLN:NE2	1:B:12:SER:OG	2.44	0.51
1:B:404:SER:OG	1:B:425:ASP:HA	2.11	0.51
1:B:5:LEU:CD1	1:B:42:ILE:HD12	2.41	0.51
1:C:392:THR:HG21	1:C:430:ASP:OD2	2.10	0.51
1:E:1:MET:O	1:E:3:SER:N	2.44	0.51
1:E:242:ILE:HG23	1:E:243:PRO:HD2	1.93	0.51
1:E:261:ILE:HG22	1:E:263:VAL:HG13	1.92	0.51
1:E:285:LLP:O3	1:E:285:LLP:NZ	2.44	0.51
1:B:11:ILE:HG22	2:F:16:U:H4'	1.93	0.51
2:F:36:A:O2'	2:F:37:A:H5'	2.11	0.51
1:A:179:MET:O	1:A:182:SER:HB3	2.11	0.50
1:A:3:SER:O	1:A:7:GLN:HG2	2.10	0.50
1:A:87:ALA:CB	1:A:341:VAL:HG21	2.41	0.50
2:G:31:A:N7	2:G:32:C:C5	2.80	0.50
1:B:337:GLU:N	1:B:337:GLU:OE1	2.43	0.50
1:B:5:LEU:HD12	1:B:8:ILE:HD12	1.93	0.50
1:C:252:LEU:HD13	1:C:286:LEU:HB3	1.94	0.50
2:G:25:U:N3	2:G:26:C:C4	2.80	0.50
2:H:47(K):G:O2'	2:H:47(L):C:H5'	2.11	0.50
2:H:47(L):C:H2'	2:H:47(M):G:H8	1.75	0.50
2:H:64:A:H2'	2:H:65:C:C6	2.45	0.50
1:A:126:TYR:HB2	1:A:328:LEU:HD13	1.92	0.50
1:A:153:LEU:CD1	1:A:301:LEU:HD22	2.42	0.50
1:C:173:PHE:HB2	1:D:312:ARG:HG2	1.93	0.50
1:D:25:ILE:HG13	1:D:26:TYR:N	2.27	0.50
2:J:32:C:H2'	2:J:33:U:C5	2.41	0.50
1:C:12:SER:OG	2:I:16:U:H1'	2.11	0.50
1:C:4:LEU:O	1:C:42:ILE:HD13	2.12	0.50
1:C:79:VAL:HG21	1:C:345:LEU:CD2	2.42	0.50
1:D:452:ILE:OXT	1:D:452:ILE:HG23	2.12	0.50
1:E:363:LEU:CB	1:E:371:ILE:CD1	2.89	0.50
2:H:45:U:H2'	2:H:46:C:O4'	2.12	0.50
1:A:357:LYS:O	1:A:361:LYS:HG3	2.11	0.50
1:A:34:VAL:HG12	1:A:53:PHE:CE1	2.46	0.50
1:B:230:LEU:HB3	1:B:274:LEU:HD21	1.94	0.50
1:C:157:LYS:CE	1:C:209:ALA:HB2	2.20	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ARG:NH2	1:C:439:LEU:HD12	2.27	0.50
1:C:68:ASN:ND2	1:D:122:HIS:CD2	2.79	0.50
1:D:278:LEU:HD23	1:D:297:GLY:HA3	1.94	0.50
1:D:369:LEU:HD21	1:D:450:LEU:CD1	2.42	0.50
2:G:5(A):U:H2'	2:G:6:A:H5'	1.93	0.50
1:A:396:ALA:HB2	1:A:428:LEU:HD21	1.94	0.50
1:C:168:GLU:O	1:C:168:GLU:HG2	2.12	0.50
1:D:299:LYS:O	1:D:303:GLU:HG2	2.11	0.50
1:A:72:VAL:HG22	1:A:417:PRO:HG2	1.94	0.50
1:B:123:ILE:O	1:B:125:LYS:N	2.44	0.50
1:D:18:PHE:HB3	1:D:21:ALA:HB3	1.92	0.50
1:E:34:VAL:HG21	1:E:57:VAL:HA	1.94	0.50
1:D:6:ARG:NH1	2:H:20:U:O4	2.45	0.50
2:H:46:C:H2'	2:H:47:U:H5'	1.93	0.50
1:A:161:ILE:HG22	1:A:186:LEU:HD11	1.93	0.50
1:B:55:GLU:O	1:B:59:ARG:HG3	2.11	0.50
1:C:161:ILE:CG2	1:C:166:LEU:HD21	2.41	0.50
1:D:90:SER:HB3	1:D:338:ASP:O	2.12	0.50
1:E:34:VAL:O	1:E:38:TYR:HD1	1.95	0.50
2:H:25:U:O2'	2:H:26:C:H5'	2.11	0.50
2:H:46:C:O2'	2:H:47:U:H5'	2.12	0.50
2:I:24:C:O2'	2:I:25:U:H5'	2.11	0.50
2:I:26:C:H2'	2:I:27:C:O4'	2.11	0.50
1:B:186:LEU:HD12	1:B:187:ARG:N	2.27	0.50
1:B:22:TYR:CG	1:B:61:ILE:HG21	2.46	0.50
1:C:161:ILE:HD13	1:C:166:LEU:CD2	2.42	0.50
1:E:7:GLN:HB2	1:E:50:LEU:HD11	1.92	0.50
1:E:97:ILE:HD11	1:E:323:GLY:HA3	1.94	0.50
1:B:396:ALA:HB2	1:B:428:LEU:CD2	2.41	0.49
1:D:396:ALA:HB1	1:D:426:GLN:HG2	1.94	0.49
1:E:396:ALA:HB2	1:E:428:LEU:CD2	2.41	0.49
1:E:435:PHE:HB2	1:E:438:ASP:OD2	2.12	0.49
1:E:79:VAL:CG1	1:E:341:VAL:HG13	2.41	0.49
2:G:9:U:C4	2:G:48:G:C8	2.99	0.49
2:J:47(N):A:C6	2:J:47(O):G:C6	3.00	0.49
1:A:340:PRO:O	1:A:344:MET:HG3	2.12	0.49
1:B:174:ARG:C	1:B:176:PRO:HD2	2.33	0.49
1:D:363:LEU:HB2	1:D:371:ILE:CD1	2.42	0.49
1:D:72:VAL:HG22	1:D:417:PRO:HG2	1.94	0.49
2:I:47:U:H2'	2:I:47(A):C:H6	1.76	0.49
1:D:163:ARG:HG3	1:D:189:VAL:O	2.13	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:TYR:HE2	1:D:228:VAL:HG21	1.75	0.49
1:E:28:VAL:HG12	1:E:32:ARG:NE	2.28	0.49
2:H:43:G:H8	2:H:43:G:H5'	1.77	0.49
1:A:409:ARG:NH1	1:A:413:LEU:HD11	2.27	0.49
1:B:18:PHE:HB3	1:B:21:ALA:HB3	1.93	0.49
2:F:5(A):U:C2'	2:F:6:A:H5'	2.42	0.49
2:I:25:U:C2'	2:I:26:C:H5'	2.42	0.49
2:I:47(I):A:C2'	2:I:47(J):A:H5'	2.43	0.49
1:C:194:LYS:HG2	1:C:226:GLU:N	2.27	0.49
2:H:39:U:H2'	2:H:40:C:C6	2.47	0.49
2:H:47(F):U:C2'	2:H:47(G):U:H5''	2.42	0.49
2:H:67:U:H2'	2:H:67(A):A:H8	1.77	0.49
2:J:31:A:H2'	2:J:32:C:O4'	2.13	0.49
1:A:8:ILE:CD1	1:A:38:TYR:HB3	2.42	0.49
1:C:312:ARG:HD2	1:C:315:ARG:NH1	2.28	0.49
1:E:347:GLN:NE2	1:E:352:LEU:CD2	2.75	0.49
1:E:77:GLY:HA3	1:E:430:ASP:CB	2.42	0.49
2:F:47(L):C:H2'	2:F:47(M):G:C8	2.48	0.49
1:A:313:ALA:HB1	1:B:144:GLY:CA	2.43	0.49
1:C:123:ILE:HG23	1:C:328:LEU:HD12	1.95	0.49
1:C:257:LYS:HD2	2:H:5:G:H4'	1.94	0.49
1:C:1:MET:HG3	1:C:4:LEU:HD12	1.94	0.49
1:D:360:GLU:HG3	1:D:371:ILE:CG2	2.42	0.49
1:D:358:ARG:HH21	1:D:439:LEU:HD12	1.76	0.49
1:E:399:HIS:HE1	1:E:401:ARG:HD3	1.77	0.49
2:J:47(E):A:H2	2:J:47(I):A:N7	2.11	0.49
2:J:5(A):U:H2'	2:J:6:A:H5'	1.95	0.49
1:A:200:TYR:CD2	1:A:233:LEU:HD21	2.48	0.49
1:A:250:SER:HB2	1:A:286:LEU:HD12	1.94	0.49
1:C:330:LEU:HD22	1:C:335:ARG:HD3	1.95	0.49
1:D:178:ILE:CG2	1:D:179:MET:N	2.76	0.49
1:C:172:SER:OG	1:D:312:ARG:HB2	2.13	0.49
1:D:163:ARG:NH1	1:E:188:GLU:OE1	2.46	0.49
1:E:366:ILE:HG23	1:E:367:PRO:HD2	1.95	0.49
2:G:47(G):U:O5'	2:G:47(G):U:H6	1.95	0.49
1:A:5:LEU:HD12	1:A:8:ILE:HD12	1.94	0.49
1:B:408:SER:O	1:B:412:ARG:HG3	2.12	0.49
1:D:161:ILE:HD13	1:D:166:LEU:HD23	1.94	0.49
2:G:67:U:H2'	2:G:67(A):A:H8	1.78	0.49
2:I:26:C:O2'	2:I:27:C:H5'	2.13	0.49
2:I:46:C:C4	2:I:47:U:C4	3.00	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ALA:HB1	1:B:295:ILE:HD11	1.95	0.49
1:D:196:LYS:N	1:D:199:ASP:OD2	2.46	0.49
1:B:324:LEU:O	1:B:324:LEU:HD12	2.12	0.48
1:C:266:PRO:HB2	1:C:271:CYS:SG	2.53	0.48
1:D:123:ILE:O	1:D:125:LYS:N	2.46	0.48
1:E:363:LEU:HD22	1:E:366:ILE:HD12	1.95	0.48
1:E:370:LYS:HG3	1:E:398:ARG:O	2.13	0.48
1:E:421:ARG:HG2	1:E:421:ARG:NH1	2.27	0.48
2:F:28:U:H2'	2:F:29:A:C8	2.48	0.48
2:G:14:G:O2'	2:G:15:C:H5'	2.13	0.48
2:G:49:G:O5'	2:G:49:G:C8	2.66	0.48
1:A:197:VAL:HG22	1:A:228:VAL:HG13	1.95	0.48
1:A:377:LYS:HE2	1:A:389:GLU:OE2	2.14	0.48
1:A:344:MET:O	1:A:432:ARG:CD	2.60	0.48
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.78	0.48
1:B:229:LYS:HB2	1:B:232:ASP:OD2	2.13	0.48
1:B:231:GLU:O	1:B:235:LYS:HG3	2.12	0.48
1:B:335:ARG:NH1	1:B:338:ASP:OD2	2.45	0.48
1:B:339:ILE:HG13	1:B:342:ILE:HB	1.95	0.48
1:C:89:LEU:HD12	1:D:101:ALA:HB1	1.95	0.48
1:D:11:ILE:O	1:D:15:VAL:HG23	2.13	0.48
1:D:439:LEU:HD23	1:D:442:ILE:HD12	1.96	0.48
1:E:406:GLU:HA	1:E:406:GLU:OE1	2.11	0.48
2:G:46:C:O2'	2:G:47:U:H5'	2.13	0.48
1:A:163:ARG:HG2	1:A:188:GLU:HB2	1.94	0.48
1:C:194:LYS:HZ1	1:C:224:PHE:HB3	1.78	0.48
1:C:408:SER:O	1:C:412:ARG:HG3	2.13	0.48
1:E:353:ARG:HB2	1:E:393:TYR:CD2	2.47	0.48
1:E:72:VAL:HG22	1:E:417:PRO:CG	2.42	0.48
2:I:35:C:O2'	2:I:36:A:H5'	2.14	0.48
1:A:286:LEU:HG	1:A:384:SER:HB2	1.95	0.48
1:A:442:ILE:O	1:A:446:LEU:CG	2.53	0.48
1:B:211:LEU:HG	1:B:242:ILE:HG21	1.94	0.48
1:B:219:PHE:CD2	1:C:193:ASN:HB3	2.48	0.48
1:C:370:LYS:HB2	1:C:398:ARG:O	2.14	0.48
1:D:254:ILE:HD12	1:D:259:PHE:CE2	2.49	0.48
1:E:96:PHE:O	1:E:100:ILE:HG12	2.13	0.48
2:G:34:U:H6	2:G:34:U:O5'	1.96	0.48
2:H:47(E):A:H2'	2:H:47(F):U:O4'	2.13	0.48
2:H:5(A):U:C2'	2:H:6:A:H5'	2.42	0.48
2:I:47(E):A:C2'	2:I:47(F):U:H5'	2.43	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:67:U:H2'	2:I:67(A):A:C8	2.49	0.48
1:A:250:SER:O	1:A:286:LEU:HB2	2.13	0.48
1:A:268:PHE:HD2	1:A:268:PHE:H	1.62	0.48
1:D:11:ILE:HG21	1:D:28:VAL:HG13	1.95	0.48
1:E:163:ARG:CD	1:E:190:GLY:O	2.61	0.48
1:E:204:ILE:HG22	1:E:205:ASN:N	2.28	0.48
1:A:126:TYR:HB3	1:A:328:LEU:HD13	1.95	0.48
1:A:442:ILE:CG2	1:A:446:LEU:HD11	2.43	0.48
1:B:400:ASP:OD1	1:B:401:ARG:N	2.47	0.48
1:B:411:LEU:CD2	1:B:418:ILE:HD12	2.37	0.48
1:C:169:ILE:HG13	1:C:173:PHE:HD2	1.77	0.48
1:C:212:MET:CE	1:C:245:TYR:HE1	2.26	0.48
1:D:163:ARG:NH1	1:E:166:LEU:HD13	2.28	0.48
1:D:5:LEU:CD1	1:D:39:ARG:HA	2.44	0.48
1:E:421:ARG:HG2	1:E:421:ARG:HH11	1.77	0.48
2:F:14:G:O2'	2:F:15:C:H5'	2.14	0.48
2:I:45:U:H2'	2:I:46:C:O4'	2.13	0.48
2:I:48:G:H4'	2:I:49:G:H5''	1.96	0.48
2:J:3:G:O2'	2:J:4:A:H5'	2.13	0.48
1:B:254:ILE:CD1	1:B:259:PHE:HE2	2.27	0.48
1:C:197:VAL:CG2	1:C:228:VAL:HG13	2.43	0.48
1:C:123:ILE:HD13	1:C:325:GLU:HB2	1.96	0.48
1:C:5:LEU:HD13	1:C:42:ILE:HB	1.95	0.48
1:D:39:ARG:HG2	2:H:56:C:H42	1.78	0.48
2:G:10:A:H4'	2:G:45:U:O4'	2.14	0.48
2:I:10:A:C2	2:I:26:C:C2	3.00	0.48
1:A:210:LEU:HD12	1:A:243:PRO:HG2	1.96	0.48
1:A:231:GLU:H	1:A:231:GLU:CD	2.16	0.48
1:A:366:ILE:HB	1:A:369:LEU:HD11	1.92	0.48
1:A:432:ARG:O	1:A:432:ARG:HG3	2.12	0.48
1:B:165:GLU:OE1	1:B:213:LYS:HG3	2.13	0.48
1:C:200:TYR:CE2	1:C:228:VAL:HG21	2.48	0.48
1:C:40:LYS:O	1:C:44:GLU:HG3	2.14	0.48
2:F:9:U:H5	2:F:48:G:H5'	1.78	0.48
1:A:108:GLU:HB2	1:B:83:ASN:HA	1.96	0.48
1:A:165:GLU:OE2	1:A:213:LYS:NZ	2.47	0.48
1:C:363:LEU:O	1:C:371:ILE:HD11	2.13	0.48
1:C:68:ASN:HD22	1:D:122:HIS:CB	2.26	0.48
1:D:10:GLN:CG	1:D:12:SER:H	2.22	0.48
1:D:131:THR:O	1:D:269:ARG:HA	2.13	0.48
1:D:176:PRO:CG	1:E:191:THR:HG22	2.39	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:VAL:HG22	1:E:245:TYR:OH	2.13	0.48
1:E:425:ASP:O	1:E:425:ASP:CG	2.51	0.48
2:F:26:C:H2'	2:F:27:C:O4'	2.13	0.48
2:F:37:A:O2'	2:F:38:A:H5'	2.14	0.48
2:G:36:A:O2'	2:G:37:A:H5'	2.14	0.48
2:J:35:C:H2'	2:J:36:A:C8	2.49	0.48
1:A:242:ILE:HG23	1:A:243:PRO:HD2	1.95	0.47
1:A:87:ALA:HB2	1:A:341:VAL:HG21	1.96	0.47
1:A:34:VAL:O	1:A:38:TYR:HD1	1.97	0.47
1:B:150:LEU:HB3	1:B:182:SER:OG	2.14	0.47
1:C:313:ALA:HB1	1:D:144:GLY:HA2	1.95	0.47
1:D:335:ARG:NH1	1:D:338:ASP:OD2	2.47	0.47
1:E:452:ILE:OXT	1:E:452:ILE:HG23	2.14	0.47
2:I:3:G:O2'	2:I:4:A:H5'	2.14	0.47
1:B:128:ASN:ND2	1:B:135:SER:HA	2.29	0.47
1:B:285:LLP:O3	1:B:285:LLP:NZ	2.43	0.47
1:B:5:LEU:CD1	1:B:39:ARG:HA	2.42	0.47
1:B:409:ARG:HH12	1:B:413:LEU:HD11	1.79	0.47
1:D:191:THR:HB	1:E:166:LEU:O	2.14	0.47
2:F:41:U:O2'	2:F:42:A:H5'	2.14	0.47
2:G:31:A:C8	2:G:32:C:C5	3.02	0.47
2:H:5(A):U:H2'	2:H:6:A:H5'	1.96	0.47
2:I:37:A:O2'	2:I:38:A:H5'	2.14	0.47
2:I:5(A):U:C2'	2:I:6:A:H5'	2.44	0.47
1:E:344:MET:O	1:E:432:ARG:CD	2.63	0.47
2:G:27:C:C2'	2:G:28:U:O4'	2.58	0.47
1:B:42:ILE:HD11	1:B:50:LEU:HD21	1.96	0.47
1:A:116:ARG:HD3	1:B:83:ASN:OD1	2.15	0.47
1:C:302:ILE:HA	1:C:305:ILE:HD12	1.94	0.47
1:C:358:ARG:HH21	1:C:439:LEU:HD12	1.79	0.47
1:E:187:ARG:HD3	1:E:203:ALA:HB1	1.95	0.47
1:E:298:LYS:O	1:E:302:ILE:HG12	2.14	0.47
2:F:61:C:H2'	2:F:62:C:C6	2.49	0.47
2:G:10:A:C4	2:G:44:G:C2	3.02	0.47
2:J:67:U:H2'	2:J:67(A):A:H8	1.78	0.47
1:A:138:VAL:HG22	1:A:294:ILE:HA	1.96	0.47
1:A:33:GLU:OE1	1:A:60:LYS:HD2	2.14	0.47
1:C:363:LEU:HB2	1:C:371:ILE:HD13	1.97	0.47
1:D:228:VAL:CG1	1:D:233:LEU:HG	2.45	0.47
1:D:24:GLU:O	1:D:24:GLU:HG3	2.14	0.47
1:D:339:ILE:HG13	1:D:339:ILE:O	2.15	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:GLN:HG2	1:E:12:SER:N	2.25	0.47
2:I:47(E):A:H2'	2:I:47(F):U:H5'	1.95	0.47
1:B:166:LEU:O	1:C:191:THR:HB	2.15	0.47
1:C:68:ASN:HD22	1:D:122:HIS:HB3	1.80	0.47
1:D:87:ALA:HB2	1:D:341:VAL:HG21	1.97	0.47
1:E:216:LYS:HG2	1:E:219:PHE:CE2	2.49	0.47
2:I:47(I):A:H2'	2:I:47(J):A:H5'	1.96	0.47
2:J:39:U:H2'	2:J:40:C:C6	2.48	0.47
1:A:178:ILE:HG23	1:A:179:MET:N	2.29	0.47
1:A:406:GLU:OE1	1:A:406:GLU:HA	2.13	0.47
1:A:407:LEU:HD21	1:A:427:LEU:HD22	1.94	0.47
1:A:55:GLU:O	1:A:59:ARG:HG3	2.14	0.47
1:B:10:GLN:HB3	1:B:13:LYS:CE	2.43	0.47
1:C:366:ILE:CG2	1:C:367:PRO:HD2	2.43	0.47
1:E:123:ILE:O	1:E:126:TYR:N	2.41	0.47
1:D:163:ARG:NH1	1:E:166:LEU:CD1	2.78	0.47
1:E:188:GLU:H	1:E:188:GLU:HG2	1.47	0.47
1:E:194:LYS:HE3	1:E:224:PHE:HB3	1.95	0.47
1:E:283:GLY:O	1:E:287:LEU:HB3	2.14	0.47
2:H:26:C:H2'	2:H:27:C:O4'	2.14	0.47
1:B:423:ARG:NH1	1:B:423:ARG:HG2	2.30	0.47
1:C:18:PHE:HB3	1:C:21:ALA:HB3	1.96	0.47
1:C:60:LYS:HA	1:C:60:LYS:HD3	1.70	0.47
1:C:33:GLU:OE1	1:C:60:LYS:HD2	2.14	0.47
1:D:131:THR:HG22	1:D:268:PHE:HB3	1.97	0.47
1:E:161:ILE:CG2	1:E:166:LEU:HD21	2.45	0.47
1:E:37:LYS:O	1:E:41:GLU:CG	2.59	0.47
2:G:31:A:C5	2:G:32:C:C4	3.01	0.47
2:I:47(P):A:H2'	2:I:48:G:H5'	1.96	0.47
2:J:36:A:H2'	2:J:37:A:O4'	2.14	0.47
2:J:8:A:HO2'	2:J:9:U:P	2.37	0.47
1:B:402:LEU:HD12	1:B:450:LEU:HD21	1.97	0.47
1:C:181:LYS:HB3	1:D:310:ILE:HD11	1.96	0.47
1:E:139:VAL:HB	1:E:314:LEU:HB3	1.97	0.47
1:E:348:ASP:O	1:E:351:ALA:HB3	2.14	0.47
1:E:8:ILE:HD13	1:E:38:TYR:HB3	1.96	0.47
2:F:47(E):A:H2'	2:F:47(F):U:H5'	1.97	0.47
2:H:65:C:H2'	2:H:66:A:H8	1.79	0.47
1:A:72:VAL:HG22	1:A:417:PRO:CG	2.45	0.47
1:C:309:PRO:HG2	1:D:181:LYS:HG3	1.96	0.47
1:D:161:ILE:CG2	1:D:166:LEU:HD21	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ILE:N	1:D:176:PRO:HD2	2.29	0.47
1:D:251:GLY:HA2	1:D:268:PHE:HE2	1.79	0.47
1:D:318:LYS:HB3	1:D:318:LYS:HE2	1.73	0.47
1:E:107:LEU:O	1:E:122:HIS:CE1	2.66	0.47
2:G:37:A:O2'	2:G:38:A:H5'	2.15	0.47
1:B:123:ILE:O	1:B:126:TYR:N	2.43	0.47
1:D:335:ARG:O	1:D:338:ASP:HB2	2.15	0.47
1:D:7:GLN:CB	1:D:50:LEU:CD1	2.93	0.47
2:F:42:A:O2'	2:F:43:G:C8	2.68	0.47
2:G:10:A:N6	2:G:44:G:C6	2.83	0.47
2:G:40:C:H2'	2:G:41:U:C6	2.51	0.47
2:H:43:G:O2'	2:H:44:G:H5'	2.15	0.47
2:I:59:U:C2'	2:I:60:U:H5'	2.45	0.47
1:A:18:PHE:HB3	1:A:21:ALA:HB3	1.97	0.46
1:A:366:ILE:CG2	1:A:367:PRO:HD2	2.45	0.46
1:B:444:LYS:O	1:B:448:GLU:HG3	2.15	0.46
1:C:285:LLP:O3	1:C:285:LLP:NZ	2.46	0.46
1:C:348:ASP:HB2	1:C:351:ALA:CB	2.44	0.46
1:E:255:ASN:HB3	1:E:258:GLU:OE2	2.15	0.46
1:E:429:PHE:HB3	1:E:431:MET:CE	2.46	0.46
2:G:47(F):U:O2'	2:G:47(H):U:OP2	2.21	0.46
1:A:175:ILE:N	1:A:176:PRO:HD2	2.30	0.46
1:A:399:HIS:ND1	1:A:401:ARG:HB2	2.30	0.46
1:A:72:VAL:HG13	1:A:417:PRO:HG2	1.97	0.46
1:B:161:ILE:HG22	1:B:186:LEU:HD11	1.97	0.46
1:D:107:LEU:CD1	1:D:321:LEU:HD23	2.45	0.46
1:E:123:ILE:O	1:E:125:LYS:N	2.48	0.46
1:E:230:LEU:O	1:E:234:VAL:HG23	2.15	0.46
2:G:25:U:C2	2:G:26:C:C6	3.04	0.46
1:A:345:LEU:CD2	1:A:380:PRO:CB	2.91	0.46
1:A:68:ASN:HD22	1:B:122:HIS:CB	2.27	0.46
1:A:80:ILE:HD12	1:A:285:LLP:HA	1.97	0.46
2:I:47(H):U:O2'	2:I:47(I):A:H5'	2.16	0.46
2:J:47:U:H2'	2:J:47(A):C:H6	1.76	0.46
1:A:2:LYS:O	1:A:6:ARG:NE	2.48	0.46
1:B:344:MET:O	1:B:432:ARG:HD2	2.15	0.46
1:C:302:ILE:HG22	1:C:306:LYS:HE3	1.97	0.46
1:D:234:VAL:HG12	1:D:238:HIS:CD2	2.50	0.46
1:D:7:GLN:HB2	1:D:50:LEU:HD13	1.95	0.46
2:I:65:C:H2'	2:I:66:A:C8	2.50	0.46
1:A:369:LEU:HD21	1:A:450:LEU:CD1	2.45	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:O	1:B:269:ARG:NH2	2.49	0.46
1:B:11:ILE:HG21	1:B:28:VAL:HG13	1.98	0.46
1:C:123:ILE:O	1:C:125:LYS:N	2.48	0.46
1:C:169:ILE:HD11	1:C:285:LLP:H5'1	1.98	0.46
1:C:317:ASP:HA	1:D:291:GLN:CD	2.36	0.46
1:C:68:ASN:HD21	1:D:122:HIS:HD2	1.63	0.46
1:D:34:VAL:HG21	1:D:57:VAL:HA	1.97	0.46
1:E:254:ILE:HD11	1:E:259:PHE:CZ	2.50	0.46
1:E:270:ASP:O	1:E:274:LEU:HG	2.15	0.46
2:H:9:U:H4'	2:H:45:U:C2	2.50	0.46
2:J:46:C:C4	2:J:47:U:O4	2.69	0.46
1:C:123:ILE:HG23	1:C:328:LEU:CD1	2.45	0.46
1:D:228:VAL:HG11	1:D:233:LEU:HG	1.98	0.46
1:D:2:LYS:CE	2:H:56:C:O2'	2.63	0.46
1:D:316:ILE:H	1:D:316:ILE:HG12	1.48	0.46
1:D:339:ILE:HG13	1:D:342:ILE:HB	1.97	0.46
1:A:334:LYS:CD	1:A:336:TYR:OH	2.64	0.46
1:B:160:ILE:HD12	1:B:211:LEU:CD2	2.45	0.46
1:C:308:ASN:OD1	1:C:310:ILE:HG13	2.16	0.46
1:C:320:THR:O	1:C:324:LEU:HB2	2.15	0.46
1:C:87:ALA:HB2	1:C:341:VAL:HG21	1.97	0.46
1:D:2:LYS:HE2	1:D:6:ARG:CZ	2.45	0.46
1:E:442:ILE:O	1:E:446:LEU:HG	2.15	0.46
2:F:36:A:C2'	2:F:37:A:H5'	2.46	0.46
2:F:47(J):A:N6	2:F:47(K):G:O6	2.48	0.46
2:G:25:U:O2'	2:G:26:C:C5'	2.64	0.46
2:G:9:U:O4	2:G:48:G:C8	2.68	0.46
1:A:348:ASP:HB2	1:A:351:ALA:HB2	1.97	0.46
1:A:427:LEU:HD23	1:A:429:PHE:CE1	2.50	0.46
1:A:436:HIS:HD2	1:A:439:LEU:HD12	1.81	0.46
1:A:68:ASN:O	1:A:70:LYS:HE3	2.15	0.46
1:B:246:TYR:OH	1:B:266:PRO:HG3	2.16	0.46
1:B:326:MET:O	1:B:330:LEU:HG	2.15	0.46
1:D:60:LYS:HD3	1:D:60:LYS:HA	1.77	0.46
1:C:67:PRO:HB2	1:D:96:PHE:CE1	2.51	0.46
2:G:10:A:C5	2:G:44:G:C2	3.04	0.46
1:B:126:TYR:O	1:B:130:LEU:HG	2.15	0.46
1:C:60:LYS:O	1:C:64:LEU:HG	2.16	0.46
1:D:169:ILE:O	1:D:173:PHE:HB3	2.15	0.46
2:F:26:C:O2'	2:F:27:C:H5'	2.15	0.46
2:H:67:U:H2'	2:H:67(A):A:C8	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:8:A:O2'	2:H:9:U:P	2.74	0.46
2:I:47(E):A:C2	2:I:47(J):A:C6	3.04	0.46
2:J:59:U:C2'	2:J:60:U:H5'	2.46	0.46
1:A:24:GLU:O	1:A:28:VAL:HG23	2.16	0.46
1:A:120:ILE:HD11	1:A:315:ARG:HG3	1.97	0.46
1:A:60:LYS:HA	1:A:60:LYS:HD3	1.73	0.46
1:A:116:ARG:HH22	1:B:171:GLY:HA3	1.81	0.46
1:A:309:PRO:HG3	1:B:181:LYS:HG3	1.97	0.46
1:A:320:THR:CG2	1:B:319:LEU:HD12	2.45	0.46
1:B:370:LYS:HB2	1:B:398:ARG:O	2.16	0.46
1:E:109:TYR:OH	1:E:114:GLY:O	2.32	0.46
1:E:40:LYS:O	1:E:44:GLU:HG3	2.16	0.46
1:B:14:VAL:CG1	1:B:18:PHE:HE2	2.29	0.45
1:C:234:VAL:HG12	1:C:238:HIS:CD2	2.51	0.45
1:D:167:VAL:HG12	1:D:219:PHE:CE2	2.34	0.45
1:E:73:ILE:HD13	1:E:438:ASP:HB3	1.97	0.45
1:A:68:ASN:ND2	1:B:122:HIS:HD2	2.11	0.45
1:A:181:LYS:HE3	1:B:309:PRO:HD2	1.99	0.45
1:D:347:GLN:NE2	1:D:352:LEU:CD2	2.80	0.45
2:G:40:C:H2'	2:G:41:U:O4'	2.16	0.45
2:G:67:U:H2'	2:G:67(A):A:C8	2.51	0.45
2:I:36:A:H2'	2:I:37:A:O4'	2.16	0.45
1:A:123:ILE:O	1:A:126:TYR:N	2.45	0.45
1:A:375:LYS:NZ	1:A:391:PRO:HB2	2.32	0.45
1:C:14:VAL:O	1:C:18:PHE:HD2	1.98	0.45
1:C:431:MET:HE2	1:C:434:VAL:HG21	1.98	0.45
1:C:67:PRO:CG	1:D:96:PHE:CE1	2.99	0.45
1:D:212:MET:HG2	1:D:213:LYS:N	2.29	0.45
1:E:432:ARG:HG3	1:E:432:ARG:O	2.16	0.45
2:G:31:A:C6	2:G:32:C:N3	2.84	0.45
2:J:65:C:H2'	2:J:66:A:O4'	2.17	0.45
1:A:420:CYS:HB2	1:A:428:LEU:O	2.16	0.45
1:D:123:ILE:HG12	1:D:321:LEU:HD11	1.99	0.45
1:D:285:LLP:H4'1	1:D:285:LLP:OP4	2.16	0.45
1:D:409:ARG:NH1	1:D:413:LEU:HD11	2.30	0.45
2:F:38:A:H2'	2:F:39:U:C5'	2.46	0.45
1:B:92:ASP:CG	1:B:335:ARG:HH12	2.19	0.45
1:C:181:LYS:HG3	1:D:309:PRO:CG	2.44	0.45
1:E:14:VAL:CG1	1:E:18:PHE:HE2	2.29	0.45
1:E:234:VAL:HG12	1:E:238:HIS:HD2	1.80	0.45
2:G:18:G:O2'	2:G:57:G:N2	2.50	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:28:U:H2'	2:G:29:A:C8	2.52	0.45
2:H:55:U:H2'	2:H:57:G:OP2	2.17	0.45
1:C:107:LEU:O	1:C:122:HIS:CE1	2.68	0.45
1:C:73:ILE:CB	1:C:418:ILE:HG12	2.40	0.45
1:D:169:ILE:HG13	1:D:173:PHE:HD2	1.82	0.45
1:D:1:MET:CG	1:D:2:LYS:H	2.28	0.45
1:E:15:VAL:HA	1:E:27:VAL:HG11	1.98	0.45
1:E:187:ARG:HE	1:E:203:ALA:CB	2.15	0.45
1:E:360:GLU:O	1:E:364:LYS:HG3	2.16	0.45
1:E:445:THR:O	1:E:449:LEU:HG	2.16	0.45
2:F:25:U:O2'	2:F:26:C:H5'	2.16	0.45
2:F:8:A:HO2'	2:F:9:U:P	2.39	0.45
2:G:47(C):C:O2'	2:G:47(D):U:H5'	2.16	0.45
2:I:25:U:HO2'	2:I:26:C:H5'	1.78	0.45
1:D:33:GLU:CD	1:D:60:LYS:HE3	2.37	0.45
2:G:25:U:C4	2:G:26:C:N4	2.85	0.45
2:H:47(E):A:H2'	2:H:47(F):U:C5'	2.45	0.45
2:I:21:U:H2'	2:I:22:G:H8	1.81	0.45
2:I:28:U:H2'	2:I:29:A:C8	2.52	0.45
2:I:47(I):A:H2'	2:I:47(J):A:C5'	2.47	0.45
2:I:5(A):U:H2'	2:I:6:A:H5'	1.99	0.45
2:J:67:U:H2'	2:J:67(A):A:C8	2.50	0.45
1:A:283:GLY:O	1:A:287:LEU:HB3	2.17	0.45
1:B:34:VAL:HG21	1:B:57:VAL:HA	1.99	0.45
1:B:360:GLU:O	1:B:364:LYS:HG3	2.17	0.45
1:C:70:LYS:O	1:C:72:VAL:HG23	2.17	0.45
1:D:188:GLU:OE1	1:E:163:ARG:NH1	2.38	0.45
1:E:88:PRO:HD2	1:E:341:VAL:HG22	1.98	0.45
2:F:43:G:O2'	2:F:44:G:H5'	2.17	0.45
2:H:42:A:O2'	2:H:43:G:C8	2.64	0.45
1:B:363:LEU:O	1:B:371:ILE:HD11	2.17	0.45
1:E:193:ASN:HB2	1:E:224:PHE:O	2.17	0.45
1:E:344:MET:O	1:E:432:ARG:HD2	2.17	0.45
1:E:89:LEU:HB2	1:E:94:ILE:HD11	1.99	0.45
1:A:34:VAL:HG21	1:A:57:VAL:HA	1.98	0.45
1:A:353:ARG:HB2	1:A:393:TYR:CE2	2.52	0.45
1:B:60:LYS:HD3	1:B:60:LYS:HA	1.58	0.45
1:D:10:GLN:HA	2:H:19:G:H2'	1.98	0.45
1:D:219:PHE:CD2	1:E:193:ASN:HB3	2.52	0.45
2:H:46:C:H2'	2:H:47:U:C5'	2.46	0.45
2:J:28:U:H2'	2:J:29:A:C8	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:SER:OG	1:A:323:GLY:N	2.50	0.44
1:A:123:ILE:HD13	1:A:325:GLU:HB2	1.99	0.44
1:C:335:ARG:O	1:C:338:ASP:HB2	2.17	0.44
1:C:358:ARG:O	1:C:362:LEU:HG	2.17	0.44
1:D:396:ALA:HB1	1:D:426:GLN:CG	2.47	0.44
1:D:5:LEU:HD13	1:D:39:ARG:HA	1.98	0.44
1:C:120:ILE:HG21	1:C:137:PHE:CD1	2.52	0.44
1:C:5:LEU:CD1	1:C:39:ARG:HA	2.40	0.44
1:C:77:GLY:CA	1:C:430:ASP:HB3	2.46	0.44
1:E:165:GLU:OE1	1:E:213:LYS:HG3	2.17	0.44
1:E:438:ASP:O	1:E:442:ILE:HG13	2.18	0.44
2:H:28:U:H2'	2:H:29:A:C8	2.53	0.44
2:H:47:U:H2'	2:H:47(A):C:H6	1.78	0.44
1:A:263:VAL:CG2	1:A:388:LEU:HD13	2.48	0.44
1:A:359:LEU:HD11	1:A:363:LEU:HD11	2.00	0.44
1:C:423:ARG:HD2	1:C:428:LEU:HD11	2.00	0.44
1:E:7:GLN:CB	1:E:50:LEU:CD1	2.95	0.44
2:H:26:C:O2'	2:H:27:C:H5'	2.17	0.44
2:H:37:A:O2'	2:H:38:A:H5'	2.17	0.44
2:H:49:G:O5'	2:H:49:G:C8	2.70	0.44
1:B:348:ASP:O	1:B:351:ALA:HB3	2.17	0.44
1:C:5:LEU:HD12	1:C:8:ILE:CD1	2.48	0.44
1:D:11:ILE:HD13	2:H:18:G:OP1	2.16	0.44
1:E:316:ILE:HD11	1:E:321:LEU:HD13	1.99	0.44
1:E:347:GLN:HE21	1:E:352:LEU:CD2	2.31	0.44
2:F:43:G:H2'	2:F:44:G:C8	2.53	0.44
1:A:14:VAL:HG13	1:A:18:PHE:HE2	1.82	0.44
1:A:423:ARG:O	1:A:424:GLU:HB3	2.18	0.44
1:A:94:ILE:HD11	1:B:102:ASN:HA	1.99	0.44
1:B:87:ALA:HB2	1:B:341:VAL:HG21	2.00	0.44
1:C:123:ILE:O	1:C:126:TYR:N	2.43	0.44
1:C:197:VAL:HG22	1:C:228:VAL:HG13	1.98	0.44
1:E:367:PRO:HG3	1:E:451:SER:OG	2.17	0.44
2:J:26:C:H2'	2:J:27:C:O4'	2.17	0.44
1:A:77:GLY:CA	1:A:430:ASP:HB3	2.47	0.44
1:B:141:ASN:HB2	1:B:285:LLP:OP1	2.18	0.44
1:A:317:ASP:HB2	1:B:291:GLN:HB3	2.00	0.44
1:C:161:ILE:HG21	1:C:166:LEU:HD21	1.98	0.44
1:C:423:ARG:HH11	1:C:423:ARG:HG2	1.82	0.44
1:C:77:GLY:HA3	1:C:430:ASP:HB3	1.99	0.44
1:D:286:LEU:HD21	1:D:384:SER:OG	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:ASP:OD1	1:D:401:ARG:N	2.51	0.44
1:E:359:LEU:HB2	1:E:439:LEU:HD22	1.98	0.44
2:F:5(A):U:H2'	2:F:6:A:H5'	1.99	0.44
1:A:131:THR:HG21	1:A:296:VAL:HG11	1.99	0.44
1:A:159:VAL:HG13	1:A:210:LEU:HB3	2.00	0.44
1:A:200:TYR:CE2	1:A:233:LEU:HD21	2.53	0.44
1:C:404:SER:OG	1:C:425:ASP:HA	2.18	0.44
1:D:254:ILE:HD12	1:D:259:PHE:HE2	1.82	0.44
1:D:254:ILE:HD13	1:D:336:TYR:CE1	2.53	0.44
1:E:110:ASN:ND2	1:E:113:GLU:OE1	2.51	0.44
1:E:42:ILE:HD11	1:E:50:LEU:HD21	2.00	0.44
2:G:47:U:H2'	2:G:47(A):C:H6	1.77	0.44
1:C:169:ILE:HG13	1:C:169:ILE:O	2.17	0.44
1:C:178:ILE:CG2	1:C:179:MET:N	2.81	0.44
1:D:14:VAL:HG12	1:D:18:PHE:CE2	2.52	0.44
1:E:17:ILE:HG22	1:E:17:ILE:O	2.18	0.44
1:E:213:LYS:HD3	1:E:230:LEU:HD21	2.00	0.44
1:E:148:LEU:HG	1:E:305:ILE:HG23	1.99	0.44
1:E:123:ILE:CD1	1:E:321:LEU:HD12	2.48	0.44
2:G:29:A:C2'	2:G:30:G:H5'	2.47	0.44
1:D:2:LYS:NZ	2:H:56:C:O2'	2.49	0.44
1:A:347:GLN:HE21	1:A:352:LEU:HD21	1.80	0.44
1:A:375:LYS:HB2	1:A:393:TYR:CE1	2.52	0.44
1:B:366:ILE:HG23	1:B:367:PRO:HD2	2.00	0.44
1:B:409:ARG:NH1	1:B:413:LEU:HD11	2.32	0.44
1:E:77:GLY:CA	1:E:430:ASP:HB3	2.48	0.44
1:E:448:GLU:O	1:E:452:ILE:CG2	2.65	0.44
2:I:47(E):A:H2'	2:I:47(F):U:C5'	2.48	0.44
2:I:65:C:H2'	2:I:66:A:H8	1.83	0.44
2:J:47(E):A:C2	2:J:47(I):A:N7	2.85	0.44
2:J:47(N):A:H2'	2:J:47(O):G:C8	2.52	0.44
1:A:363:LEU:HB2	1:A:371:ILE:HD13	2.00	0.43
1:B:157:LYS:HB3	1:B:207:ASN:O	2.17	0.43
1:B:37:LYS:O	1:B:41:GLU:CG	2.59	0.43
1:C:167:VAL:HG12	1:C:219:PHE:CE2	2.48	0.43
1:C:175:ILE:N	1:C:176:PRO:HD2	2.33	0.43
1:C:431:MET:HE1	1:C:434:VAL:HG21	2.00	0.43
1:D:123:ILE:O	1:D:126:TYR:N	2.44	0.43
1:D:17:ILE:HG22	1:D:17:ILE:O	2.18	0.43
1:D:194:LYS:CB	1:E:168:GLU:OE1	2.66	0.43
1:E:443:LYS:HE2	1:E:447:GLN:OE1	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:15:C:H2'	2:F:16:U:C6	2.53	0.43
2:F:2:G:O2'	2:F:3:G:H5'	2.18	0.43
2:F:56:C:H2'	2:F:57:G:C8	2.53	0.43
2:G:47(J):A:H2'	2:G:47(K):G:O4'	2.18	0.43
1:C:11:ILE:HD12	2:I:18:G:P	2.58	0.43
1:A:127:LEU:O	1:A:131:THR:HG23	2.18	0.43
1:A:360:GLU:HG3	1:A:371:ILE:HG21	1.99	0.43
1:B:392:THR:HG21	1:B:430:ASP:OD2	2.19	0.43
1:C:98:SER:HA	1:D:94:ILE:CG2	2.48	0.43
1:E:159:VAL:HG13	1:E:210:LEU:HB3	2.00	0.43
1:E:269:ARG:HG3	1:E:269:ARG:NH1	2.32	0.43
2:F:59:U:C2'	2:F:60:U:H5'	2.48	0.43
2:J:46:C:H2'	2:J:47:U:C6	2.53	0.43
1:A:252:LEU:HD12	1:A:253:LEU:N	2.33	0.43
1:A:271:CYS:HA	1:A:274:LEU:HD12	2.00	0.43
1:A:8:ILE:HD11	1:A:38:TYR:HB3	2.00	0.43
1:D:285:LLP:NZ	1:D:285:LLP:O3	2.50	0.43
1:D:367:PRO:HG3	1:D:451:SER:OG	2.18	0.43
2:F:28:U:H2'	2:F:29:A:H8	1.83	0.43
2:G:10:A:C2	2:G:26:C:O2	2.71	0.43
2:G:31:A:H2'	2:G:32:C:O4'	2.18	0.43
2:I:27:C:C4	2:I:28:U:C4	3.06	0.43
1:A:339:ILE:HG13	1:A:342:ILE:HB	2.01	0.43
1:A:344:MET:O	1:A:432:ARG:HD2	2.17	0.43
1:B:312:ARG:HD2	1:B:315:ARG:NH1	2.33	0.43
1:C:107:LEU:HD11	1:C:321:LEU:HD23	2.00	0.43
1:C:265:GLU:OE1	1:C:385:LEU:CD2	2.66	0.43
1:D:259:PHE:HB3	1:D:346:THR:CG2	2.48	0.43
1:D:259:PHE:CB	1:D:346:THR:HG21	2.48	0.43
1:E:348:ASP:HB2	1:E:351:ALA:HB2	2.00	0.43
2:F:45:U:H2'	2:F:46:C:O4'	2.19	0.43
2:G:29:A:H2'	2:G:30:G:C8	2.53	0.43
1:A:104:TYR:CD1	1:A:104:TYR:N	2.86	0.43
1:A:123:ILE:CG2	1:A:328:LEU:HD12	2.48	0.43
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.80	0.43
1:B:120:ILE:HG21	1:B:137:PHE:CD1	2.54	0.43
1:B:200:TYR:HE2	1:B:228:VAL:HG21	1.83	0.43
1:B:254:ILE:HD12	1:B:259:PHE:HE2	1.82	0.43
1:B:287:LEU:HD23	1:B:287:LEU:C	2.39	0.43
1:C:312:ARG:CD	1:C:315:ARG:NH1	2.82	0.43
1:D:86:ARG:CD	1:D:284:ASP:OD2	2.66	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:ILE:HB	1:D:369:LEU:CD1	2.44	0.43
1:E:253:LEU:HD23	1:E:331:TYR:CG	2.54	0.43
2:G:28:U:C2'	2:G:29:A:H5'	2.48	0.43
2:G:47(L):C:H2'	2:G:47(M):G:C8	2.53	0.43
2:J:11:G:C2	2:J:12:G:N7	2.86	0.43
2:J:45:U:H2'	2:J:46:C:O4'	2.18	0.43
2:J:47(P):A:H2'	2:J:48:G:H5'	1.99	0.43
1:A:76:THR:OG1	1:A:78:VAL:HG23	2.17	0.43
1:B:25:ILE:CG1	1:B:26:TYR:N	2.80	0.43
1:B:343:ARG:HH21	1:B:343:ARG:HG2	1.84	0.43
1:D:1:MET:HG3	1:D:2:LYS:H	1.81	0.43
1:E:5:LEU:HD13	1:E:42:ILE:HB	2.00	0.43
2:F:8:A:C5	2:F:48:G:N2	2.86	0.43
1:A:271:CYS:O	1:A:274:LEU:HB2	2.19	0.43
1:A:442:ILE:HG23	1:A:446:LEU:HD11	1.99	0.43
1:B:360:GLU:HG3	1:B:371:ILE:HG22	1.99	0.43
1:D:399:HIS:CD2	1:D:450:LEU:HD13	2.54	0.43
1:E:28:VAL:O	1:E:32:ARG:HG3	2.17	0.43
1:E:8:ILE:HD13	1:E:38:TYR:CB	2.49	0.43
1:E:405:GLN:HE22	1:E:422:ILE:CG2	2.29	0.43
2:G:26:C:C4	2:G:27:C:C4	3.06	0.43
1:D:11:ILE:HB	2:H:16:U:O2'	2.19	0.43
2:J:47(E):A:H2'	2:J:47(F):U:H5'	2.00	0.43
1:A:312:ARG:HB2	1:B:172:SER:OG	2.19	0.43
1:B:286:LEU:HA	1:B:286:LEU:HD23	1.76	0.43
1:B:77:GLY:CA	1:B:433:THR:HG23	2.47	0.43
1:D:370:LYS:HB2	1:D:398:ARG:O	2.18	0.43
1:A:313:ALA:HB1	1:B:144:GLY:HA2	2.00	0.43
1:C:336:TYR:O	1:C:339:ILE:HG12	2.18	0.43
1:D:14:VAL:O	1:D:18:PHE:HD2	2.01	0.43
1:D:169:ILE:HG13	1:D:173:PHE:CD2	2.54	0.43
1:E:88:PRO:HD2	1:E:341:VAL:CG2	2.49	0.43
2:G:47(E):A:H2'	2:G:47(F):U:O4'	2.19	0.43
2:J:38:A:C2'	2:J:39:U:H5'	2.49	0.43
1:A:169:ILE:CG1	1:A:173:PHE:HD2	2.30	0.43
1:B:179:MET:HA	1:B:182:SER:HB3	2.01	0.43
1:B:348:ASP:HB2	1:B:351:ALA:HB2	2.00	0.43
1:C:179:MET:HA	1:C:182:SER:HB3	2.00	0.43
1:C:345:LEU:CD2	1:C:380:PRO:HB3	2.49	0.43
1:E:14:VAL:HG21	1:E:53:PHE:HE2	1.84	0.43
1:A:345:LEU:HD21	1:A:380:PRO:HB3	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:O	1:A:98:SER:HB2	2.19	0.42
1:B:87:ALA:CB	1:B:341:VAL:HG21	2.48	0.42
1:A:325:GLU:OE2	1:B:68:ASN:HB2	2.19	0.42
1:C:126:TYR:HB3	1:C:328:LEU:HD13	1.96	0.42
1:D:73:ILE:HB	1:D:418:ILE:HG12	2.00	0.42
2:G:15:C:H2'	2:G:16:U:H6	1.81	0.42
2:H:3:G:O2'	2:H:4:A:H5'	2.19	0.42
2:J:2:G:O2'	2:J:3:G:H5'	2.18	0.42
1:A:79:VAL:HG12	1:A:341:VAL:HG13	2.00	0.42
1:B:230:LEU:HD22	1:B:276:ILE:HD11	2.00	0.42
1:D:212:MET:HG3	1:D:245:TYR:CD1	2.54	0.42
1:D:80:ILE:HD12	1:D:285:LLP:HA	2.01	0.42
1:B:10:GLN:HB2	2:F:19:G:C2'	2.49	0.42
2:G:59:U:C2'	2:G:60:U:H5'	2.49	0.42
2:G:8:A:O2'	2:G:9:U:P	2.77	0.42
1:D:11:ILE:CD1	2:H:18:G:OP1	2.67	0.42
1:A:169:ILE:CG1	1:A:173:PHE:CD2	3.03	0.42
1:A:8:ILE:HA	1:A:9:PRO:HD2	1.82	0.42
1:C:386:PRO:HG2	1:C:387:GLU:N	2.32	0.42
1:D:193:ASN:O	1:D:225:VAL:HG13	2.19	0.42
1:D:88:PRO:HG2	1:D:340:PRO:CB	2.49	0.42
1:E:277:ASP:O	1:E:297:GLY:HA3	2.19	0.42
2:H:47(G):U:H2'	2:H:47(H):U:O4'	2.18	0.42
2:I:21:U:H2'	2:I:22:G:C8	2.55	0.42
1:A:123:ILE:O	1:A:125:LYS:N	2.52	0.42
1:A:161:ILE:CG2	1:A:186:LEU:HD11	2.49	0.42
1:B:168:GLU:OE2	1:C:194:LYS:HD2	2.20	0.42
1:B:350:LYS:HG3	1:B:350:LYS:H	1.51	0.42
1:A:114:GLY:HA3	1:B:412:ARG:NH2	2.35	0.42
1:B:70:LYS:O	1:B:72:VAL:HG23	2.18	0.42
1:C:5:LEU:HD21	1:C:39:ARG:HG2	2.00	0.42
1:D:14:VAL:HG12	1:D:18:PHE:HE2	1.84	0.42
1:D:218:ASN:HD22	1:E:224:PHE:CB	2.29	0.42
1:D:427:LEU:HD23	1:D:429:PHE:HE1	1.84	0.42
1:D:5:LEU:HD21	1:D:39:ARG:CG	2.48	0.42
1:E:216:LYS:HG2	1:E:219:PHE:CZ	2.55	0.42
1:E:347:GLN:HE21	1:E:352:LEU:HD21	1.82	0.42
2:G:36:A:H2'	2:G:37:A:H8	1.81	0.42
2:G:45:U:H2'	2:G:46:C:O4'	2.18	0.42
2:J:22:G:H2'	2:J:23:C:H6	1.83	0.42
1:A:114:GLY:CA	1:B:412:ARG:HH21	2.33	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:HG3	1:A:439:LEU:HD11	2.01	0.42
1:A:5:LEU:HD11	1:A:39:ARG:CG	2.44	0.42
1:C:239:LYS:HD3	1:C:240:TYR:CE2	2.54	0.42
1:C:343:ARG:HH21	1:C:343:ARG:HG2	1.85	0.42
1:C:425:ASP:O	1:C:425:ASP:CG	2.57	0.42
1:D:25:ILE:HG13	1:D:26:TYR:H	1.84	0.42
1:D:137:PHE:CD1	1:D:306:LYS:HG2	2.54	0.42
1:E:250:SER:O	1:E:286:LEU:HB2	2.20	0.42
1:E:358:ARG:NH2	1:E:439:LEU:HD12	2.28	0.42
2:G:27:C:C4	2:G:28:U:C4	3.08	0.42
2:I:38:A:H2'	2:I:39:U:H5'	2.00	0.42
1:A:169:ILE:HD11	1:A:285:LLP:H5'1	2.02	0.42
1:B:49:ASP:OD1	1:B:50:LEU:N	2.53	0.42
1:C:116:ARG:HH22	1:D:171:GLY:HA3	1.84	0.42
1:D:7:GLN:O	1:D:8:ILE:C	2.58	0.42
1:E:167:VAL:HG12	1:E:219:PHE:HE2	1.85	0.42
1:B:287:LEU:HD23	1:B:287:LEU:O	2.20	0.42
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.85	0.42
1:B:394:CYS:HB3	1:B:428:LEU:HD22	2.00	0.42
1:D:160:ILE:HB	1:D:211:LEU:HD23	2.01	0.42
1:E:300:ASN:O	1:E:304:LYS:HG3	2.20	0.42
2:F:3:G:O2'	2:F:4:A:H5'	2.20	0.42
1:D:16:GLU:OE2	2:H:22:G:H5'	2.20	0.42
1:B:13:LYS:O	1:B:17:ILE:HG13	2.20	0.42
1:B:167:VAL:HG12	1:B:219:PHE:HE2	1.85	0.42
1:C:82:THR:HG22	1:C:86:ARG:HE	1.85	0.42
1:C:68:ASN:HD22	1:D:122:HIS:HA	1.85	0.42
1:D:141:ASN:OD1	1:D:143:ALA:HB3	2.19	0.42
1:C:144:GLY:CA	1:D:313:ALA:HB1	2.50	0.42
1:E:126:TYR:CE2	1:E:325:GLU:HG3	2.54	0.42
1:A:97:ILE:HG12	1:A:322:SER:OG	2.20	0.42
1:B:363:LEU:HD21	1:B:446:LEU:HD12	2.02	0.42
1:B:5:LEU:HD12	1:B:42:ILE:HD12	2.01	0.42
1:B:77:GLY:HA3	1:B:430:ASP:CG	2.40	0.42
1:C:423:ARG:NH1	1:C:423:ARG:HG2	2.35	0.42
1:C:452:ILE:OXT	1:C:452:ILE:HG23	2.20	0.42
1:D:194:LYS:HD2	1:E:168:GLU:CD	2.39	0.42
2:F:34:U:O2'	2:F:35:C:H5'	2.20	0.42
2:H:46:C:C2'	2:H:47:U:C5'	2.96	0.42
1:A:4:LEU:O	1:A:42:ILE:HD13	2.19	0.42
1:B:33:GLU:CD	1:B:60:LYS:HE3	2.40	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:CD2	1:B:446:LEU:HD12	2.50	0.42
1:C:6:ARG:HG2	1:C:6:ARG:HH11	1.85	0.42
1:D:77:GLY:CA	1:D:430:ASP:HB3	2.49	0.42
2:G:3:G:O2'	2:G:4:A:H5'	2.19	0.42
2:G:47(E):A:H2'	2:G:47(F):U:H5'	2.01	0.42
2:J:15:C:H2'	2:J:16:U:H6	1.84	0.42
2:J:47(E):A:O2'	2:J:47(I):A:N6	2.53	0.42
1:A:394:CYS:HB2	1:A:428:LEU:HD22	2.01	0.41
1:C:20:LYS:HG2	1:C:20:LYS:O	2.20	0.41
1:E:392:THR:HG21	1:E:430:ASP:OD2	2.20	0.41
1:D:2:LYS:HE3	2:H:56:C:O2'	2.19	0.41
2:H:59:U:C2'	2:H:60:U:H5'	2.50	0.41
1:A:249:GLY:O	1:A:285:LLP:HD3	2.20	0.41
1:A:363:LEU:C	1:A:371:ILE:HD11	2.40	0.41
1:A:368:GLY:O	1:A:399:HIS:HA	2.20	0.41
1:B:444:LYS:HA	1:B:447:GLN:HG2	2.03	0.41
1:C:344:MET:O	1:C:432:ARG:HD3	2.19	0.41
1:C:7:GLN:O	1:C:8:ILE:C	2.58	0.41
1:D:42:ILE:HD11	1:D:50:LEU:CD2	2.44	0.41
1:D:49:ASP:OD1	1:D:50:LEU:N	2.53	0.41
1:E:7:GLN:O	1:E:8:ILE:C	2.56	0.41
2:F:26:C:C4	2:F:27:C:C4	3.07	0.41
2:F:47(E):A:C2'	2:F:47(F):U:H5'	2.49	0.41
1:A:11:ILE:HB	2:G:16:U:H4'	2.02	0.41
2:J:38:A:H2'	2:J:39:U:O4'	2.20	0.41
1:A:268:PHE:N	1:A:268:PHE:CD2	2.88	0.41
1:A:285:LLP:NZ	1:A:285:LLP:O3	2.50	0.41
1:B:249:GLY:O	1:B:285:LLP:HD3	2.19	0.41
1:C:328:LEU:HA	1:C:328:LEU:HD23	1.89	0.41
1:C:362:LEU:HB3	1:C:443:LYS:HD2	2.03	0.41
1:D:432:ARG:HG3	1:D:432:ARG:O	2.20	0.41
1:C:67:PRO:CG	1:D:96:PHE:HE1	2.33	0.41
1:E:189:VAL:HG21	1:E:200:TYR:CD1	2.55	0.41
2:F:9:U:C4	2:F:48:G:C8	3.07	0.41
2:G:56:C:H2'	2:G:57:G:C8	2.55	0.41
2:G:7:G:O2'	2:G:8:A:H5'	2.20	0.41
2:H:32:C:C4	2:H:33:U:O4	2.74	0.41
1:A:250:SER:HB2	1:A:286:LEU:CD1	2.50	0.41
1:A:308:ASN:OD1	1:A:308:ASN:C	2.58	0.41
1:A:114:GLY:CA	1:B:412:ARG:NH2	2.84	0.41
1:B:97:ILE:HD11	1:B:323:GLY:CA	2.41	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:GLU:H	1:C:113:GLU:HG3	1.71	0.41
1:D:227:GLU:CG	1:D:228:VAL:N	2.83	0.41
1:D:38:TYR:CE2	1:D:47:ARG:NE	2.88	0.41
1:E:140:ASN:ND2	1:E:141:ASN:ND2	2.69	0.41
1:E:14:VAL:O	1:E:18:PHE:HD2	2.03	0.41
1:E:88:PRO:HG2	1:E:340:PRO:HB3	2.00	0.41
2:F:7:G:O2'	2:F:8:A:H5'	2.19	0.41
1:A:144:GLY:HA2	1:B:313:ALA:HB1	2.03	0.41
1:A:339:ILE:HA	1:A:340:PRO:HD3	1.88	0.41
1:A:388:LEU:HD21	1:A:390:LEU:CD1	2.50	0.41
1:B:175:ILE:N	1:B:176:PRO:CD	2.83	0.41
1:B:247:ASP:C	1:B:247:ASP:OD1	2.59	0.41
1:B:452:ILE:CG2	1:B:452:ILE:OXT	2.68	0.41
1:C:15:VAL:HA	1:C:27:VAL:HG11	2.01	0.41
1:C:355:LYS:CG	1:C:439:LEU:HD11	2.48	0.41
1:D:191:THR:HG22	1:E:176:PRO:CG	2.51	0.41
1:D:298:LYS:O	1:D:302:ILE:HG12	2.19	0.41
1:E:286:LEU:HG	1:E:384:SER:HB2	2.03	0.41
1:E:290:PRO:HB2	1:E:320:THR:HG22	2.03	0.41
1:E:409:ARG:HG3	1:E:412:ARG:NH2	2.34	0.41
2:F:66:A:H2'	2:F:67:U:C6	2.56	0.41
1:A:60:LYS:C	1:A:64:LEU:HG	2.37	0.41
1:A:144:GLY:CA	1:B:313:ALA:HB1	2.50	0.41
1:B:366:ILE:CG2	1:B:367:PRO:HD2	2.51	0.41
1:A:102:ASN:HB3	1:B:71:ARG:HH22	1.85	0.41
1:D:253:LEU:HD23	1:D:331:TYR:CD2	2.55	0.41
1:D:333:GLU:OE1	1:D:335:ARG:HD2	2.21	0.41
2:F:35:C:H2'	2:F:36:A:O4'	2.21	0.41
2:G:43:G:N1	2:G:44:G:C6	2.88	0.41
2:H:46:C:C3'	2:H:47:U:H5'	2.49	0.41
1:A:216:LYS:HG2	1:A:219:PHE:CE2	2.55	0.41
1:A:359:LEU:CD1	1:A:363:LEU:HD11	2.50	0.41
1:A:404:SER:O	1:A:407:LEU:HB3	2.20	0.41
1:A:407:LEU:HD23	1:A:427:LEU:HD22	2.00	0.41
1:B:167:VAL:HG12	1:B:219:PHE:CE2	2.55	0.41
1:B:7:GLN:O	1:B:8:ILE:C	2.58	0.41
1:C:178:ILE:HG23	1:C:179:MET:N	2.36	0.41
1:D:277:ASP:O	1:D:278:LEU:HD23	2.20	0.41
1:D:369:LEU:HD21	1:D:450:LEU:HD11	2.03	0.41
1:C:67:PRO:CB	1:D:96:PHE:CE1	3.04	0.41
1:E:178:ILE:CG2	1:E:179:MET:N	2.83	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:60:LYS:O	1:E:64:LEU:HG	2.20	0.41
2:G:10:A:N6	2:G:44:G:O6	2.54	0.41
2:I:67(A):A:H2'	2:I:68:C:H6	1.83	0.41
2:J:43:G:H2'	2:J:44:G:C8	2.56	0.41
1:A:77:GLY:HA3	1:A:430:ASP:HB3	2.03	0.41
1:B:160:ILE:HB	1:B:211:LEU:HD23	2.03	0.41
1:B:246:TYR:CE2	1:B:248:ALA:HA	2.56	0.41
1:B:356:ALA:O	1:B:395:VAL:HG21	2.20	0.41
1:B:362:LEU:HD22	1:B:443:LYS:HD2	2.01	0.41
1:C:32:ARG:O	1:C:36:GLU:HG2	2.21	0.41
1:C:79:VAL:HG21	1:C:345:LEU:HG	2.03	0.41
1:D:355:LYS:HG3	1:D:439:LEU:HD11	2.03	0.41
1:E:179:MET:SD	1:E:186:LEU:HB2	2.61	0.41
2:J:32:C:C4	2:J:33:U:O4	2.74	0.41
1:B:74:ASN:OD1	1:B:74:ASN:C	2.59	0.41
1:C:72:VAL:HG22	1:C:417:PRO:CG	2.51	0.41
1:D:256:LEU:HD23	1:D:263:VAL:HG21	2.03	0.41
1:D:265:GLU:HG3	1:D:266:PRO:HD2	2.03	0.41
1:D:399:HIS:ND1	1:D:450:LEU:HD22	2.35	0.41
1:A:12:SER:HG	2:G:16:U:H1'	1.86	0.41
2:I:10:A:C5'	2:I:45:U:C1'	2.99	0.41
2:J:7:G:O2'	2:J:49:G:OP2	2.37	0.41
1:A:139:VAL:HB	1:A:314:LEU:HB3	2.02	0.41
1:A:79:VAL:HG21	1:A:345:LEU:CD2	2.51	0.41
1:B:137:PHE:CD1	1:B:306:LYS:HG2	2.55	0.41
1:B:339:ILE:HG13	1:B:342:ILE:CG1	2.51	0.41
1:B:389:GLU:O	1:B:390:LEU:HD23	2.21	0.41
1:D:204:ILE:HG22	1:D:205:ASN:N	2.35	0.41
1:E:211:LEU:CD2	1:E:242:ILE:HG21	2.51	0.41
1:E:90:SER:CB	1:E:338:ASP:O	2.66	0.41
2:H:26:C:C4	2:H:27:C:C4	3.09	0.41
2:J:47(J):A:H2'	2:J:47(K):G:C8	2.56	0.41
1:A:126:TYR:O	1:A:130:LEU:HG	2.21	0.41
1:A:265:GLU:CD	1:A:266:PRO:HD2	2.40	0.41
1:B:1:MET:C	1:B:3:SER:N	2.74	0.41
1:B:385:LEU:HD13	1:B:388:LEU:HD22	2.03	0.41
1:C:432:ARG:HG3	1:C:432:ARG:O	2.20	0.41
1:C:33:GLU:CD	1:C:60:LYS:HE3	2.42	0.41
1:D:254:ILE:CD1	1:D:336:TYR:CE1	3.04	0.41
1:E:88:PRO:HG3	1:E:344:MET:CE	2.51	0.41
2:I:43:G:H2'	2:I:44:G:C8	2.56	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LYS:HD2	1:B:332:PHE:CE1	2.56	0.40
1:A:84:LEU:HB3	1:B:104:TYR:HB3	2.02	0.40
1:C:438:ASP:O	1:C:442:ILE:HG13	2.20	0.40
1:E:272:ILE:HD11	1:E:296:VAL:HG23	2.03	0.40
1:E:301:LEU:HA	1:E:301:LEU:HD23	1.75	0.40
1:E:30:ALA:O	1:E:34:VAL:CG2	2.66	0.40
1:E:409:ARG:HA	1:E:412:ARG:CZ	2.52	0.40
2:G:47(H):U:H2'	2:G:47(I):A:C4'	2.51	0.40
2:G:66:A:H2'	2:G:67:U:C6	2.56	0.40
2:I:30:G:N2	2:I:40:C:O2	2.44	0.40
1:A:327:THR:O	1:A:331:TYR:HD2	2.05	0.40
1:A:79:VAL:CG1	1:A:341:VAL:HG13	2.51	0.40
1:A:396:ALA:HB2	1:A:428:LEU:HD23	2.03	0.40
1:C:99:GLU:O	1:D:71:ARG:CZ	2.69	0.40
1:D:86:ARG:HB3	1:D:284:ASP:O	2.21	0.40
1:E:15:VAL:HG11	1:E:24:GLU:OE2	2.21	0.40
1:D:163:ARG:HH11	1:E:166:LEU:HD13	1.83	0.40
1:E:231:GLU:H	1:E:231:GLU:CD	2.23	0.40
2:H:65:C:H2'	2:H:66:A:C8	2.56	0.40
2:J:23:C:N4	2:J:24:C:N4	2.69	0.40
1:A:169:ILE:HG13	1:A:169:ILE:O	2.21	0.40
1:A:263:VAL:CG1	1:A:264:ASP:N	2.85	0.40
1:A:47:ARG:HD3	1:A:49:ASP:O	2.22	0.40
1:A:86:ARG:HD2	1:A:284:ASP:OD2	2.22	0.40
1:B:137:PHE:HD1	1:B:306:LYS:HE2	1.86	0.40
1:B:7:GLN:HB2	1:B:50:LEU:CD1	2.51	0.40
1:C:193:ASN:HB2	1:C:224:PHE:O	2.21	0.40
1:B:10:GLN:HB2	2:F:19:G:H2'	2.02	0.40
2:F:38:A:H2'	2:F:39:U:O4'	2.20	0.40
2:I:1:G:H2'	2:I:2:G:C8	2.56	0.40
2:J:47(E):A:C2'	2:J:47(F):U:H5'	2.51	0.40
2:J:56:C:H2'	2:J:57:G:C8	2.56	0.40
1:C:247:ASP:OD1	1:C:247:ASP:C	2.60	0.40
1:C:87:ALA:CB	1:C:341:VAL:HG21	2.52	0.40
1:C:70:LYS:HE2	1:C:70:LYS:HB3	1.88	0.40
1:D:220:TYR:CD1	1:D:220:TYR:C	2.95	0.40
1:D:348:ASP:O	1:D:351:ALA:HB3	2.21	0.40
1:D:363:LEU:O	1:D:371:ILE:HD11	2.22	0.40
1:E:175:ILE:N	1:E:176:PRO:HD2	2.36	0.40
2:G:29:A:O2'	2:G:30:G:O4'	2.39	0.40
2:G:2:G:H2'	2:G:3:G:C8	2.56	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:28:U:H2'	2:I:29:A:H8	1.86	0.40
2:J:35:C:C2'	2:J:36:A:O4'	2.69	0.40
1:A:167:VAL:HG12	1:A:219:PHE:CE2	2.56	0.40
1:A:335:ARG:NE	1:A:338:ASP:OD2	2.54	0.40
1:A:416:PRO:HG3	1:A:441:THR:HG21	2.04	0.40
1:D:416:PRO:CG	1:D:441:THR:HG21	2.51	0.40
1:E:136:SER:CB	1:E:296:VAL:HG12	2.49	0.40
2:H:8:A:HO2'	2:H:9:U:P	2.44	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	449/452 (99%)	423 (94%)	22 (5%)	4 (1%)	20	63
1	B	449/452 (99%)	419 (93%)	25 (6%)	5 (1%)	17	60
1	C	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	20	63
1	D	449/452 (99%)	421 (94%)	24 (5%)	4 (1%)	20	63
1	E	449/452 (99%)	420 (94%)	23 (5%)	6 (1%)	14	56
All	All	2245/2260 (99%)	2104 (94%)	118 (5%)	23 (1%)	18	61

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	9	PRO
1	E	9	PRO
1	B	124	GLU
1	C	124	GLU
1	D	124	GLU
1	E	2	LYS

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type
1	E	124	GLU
1	A	86	ARG
1	A	124	GLU
1	B	19	ALA
1	C	86	ARG
1	D	19	ALA
1	A	19	ALA
1	B	86	ARG
1	C	19	ALA
1	D	86	ARG
1	E	19	ALA
1	E	86	ARG
1	A	9	PRO
1	C	9	PRO
1	E	340	PRO
1	B	9	PRO
1	B	340	PRO

### 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	390/390 (100%)	380 (97%)	10 (3%)	51	75
1	B	390/390 (100%)	389 (100%)	1 (0%)	94	96
1	C	390/390 (100%)	385 (99%)	5 (1%)	73	87
1	D	390/390 (100%)	384 (98%)	6 (2%)	70	85
1	E	390/390 (100%)	389 (100%)	1 (0%)	94	96
All	All	1950/1950 (100%)	1927 (99%)	23 (1%)	75	88

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	98	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	105	SER
1	A	118	SER
1	A	136	SER
1	A	188	GLU
1	A	271	CYS
1	A	287	LEU
1	A	394	CYS
1	A	403	SER
1	B	188	GLU
1	C	3	SER
1	C	188	GLU
1	C	317	ASP
1	C	384	SER
1	C	400	ASP
1	D	24	GLU
1	D	39	ARG
1	D	172	SER
1	D	182	SER
1	D	188	GLU
1	D	316	ILE
1	E	188	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	140	ASN
1	A	347	GLN
1	A	399	HIS
1	A	436	HIS
1	B	10	GLN
1	B	95	ASN
1	B	122	HIS
1	B	142	ASN
1	B	399	HIS
1	B	405	GLN
1	C	10	GLN
1	C	68	ASN
1	C	95	ASN
1	C	122	HIS
1	C	291	GLN
1	C	347	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	405	GLN
1	D	122	HIS
1	D	347	GLN
1	D	399	HIS
1	D	436	HIS
1	E	122	HIS
1	E	140	ASN
1	E	238	HIS
1	E	347	GLN
1	E	399	HIS
1	E	405	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	F	91/95 (95%)	6 (6%)	0
2	G	91/95 (95%)	6 (6%)	0
2	H	91/95 (95%)	6 (6%)	0
2	I	91/95 (95%)	9 (9%)	0
2	J	91/95 (95%)	6 (6%)	0
All	All	455/475 (95%)	33 (7%)	0

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	F	18	G
2	F	20(A)	G
2	F	33	U
2	F	42(A)	C
2	F	43	G
2	F	73	G
2	G	18	G
2	G	20(A)	G
2	G	42(A)	C
2	G	43	G
2	G	47(G)	U
2	G	73	G
2	H	18	G
2	H	20(A)	G
2	H	42(A)	C
2	H	43	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	47(G)	U
2	H	73	G
2	I	14	G
2	I	18	G
2	I	20(A)	G
2	I	42(A)	C
2	I	43	G
2	I	44	G
2	I	45	U
2	I	47(G)	U
2	I	73	G
2	J	18	G
2	J	20(A)	G
2	J	42(A)	C
2	J	43	G
2	J	47(G)	U
2	J	73	G

There are no RNA pucker outliers to report.

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

5 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	LLP	A	285	1	24,24,25	1.18	1 (4%)	28,32,34	0.95	1 (3%)
1	LLP	B	285	1	24,24,25	1.23	2 (8%)	28,32,34	1.03	1 (3%)
1	LLP	C	285	1	24,24,25	1.15	2 (8%)	28,32,34	0.95	1 (3%)
1	LLP	D	285	1	24,24,25	1.12	1 (4%)	28,32,34	0.92	1 (3%)
1	LLP	E	285	1	24,24,25	1.16	1 (4%)	28,32,34	1.07	1 (3%)

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	LLP	A	285	1	-	0/15/17/19	0/1/1/1
1	LLP	B	285	1	-	0/15/17/19	0/1/1/1
1	LLP	C	285	1	-	0/15/17/19	0/1/1/1
1	LLP	D	285	1	-	0/15/17/19	0/1/1/1
1	LLP	E	285	1	-	0/15/17/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	LLP	C4-C4'	-3.21	1.40	1.46
1	E	285	LLP	C4-C4'	-2.95	1.41	1.46
1	A	285	LLP	C4-C4'	-2.82	1.41	1.46
1	C	285	LLP	C4-C4'	-2.56	1.41	1.46
1	D	285	LLP	C4-C4'	-2.47	1.42	1.46
1	B	285	LLP	C3-C2	-2.17	1.39	1.40
1	C	285	LLP	C4'-NZ	2.11	1.33	1.27

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	LLP	OP4-P-OP1	2.22	112.69	106.47
1	D	285	LLP	OP4-P-OP1	2.23	112.73	106.47
1	A	285	LLP	OP4-P-OP1	2.33	113.00	106.47
1	B	285	LLP	OP4-P-OP1	2.54	113.59	106.47
1	E	285	LLP	OP4-P-OP1	2.68	114.00	106.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	285	LLP	4	0
1	B	285	LLP	6	0
1	C	285	LLP	7	0
1	D	285	LLP	3	0
1	E	285	LLP	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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	451/452 (99%)	0.98	74 (16%) 2 9	363, 478, 546, 629	0
1	B	451/452 (99%)	0.87	59 (13%) 4 11	371, 474, 554, 648	0
1	C	451/452 (99%)	0.70	58 (12%) 4 12	364, 474, 549, 625	0
1	D	451/452 (99%)	0.90	71 (15%) 2 10	356, 463, 536, 601	0
1	E	451/452 (99%)	1.08	91 (20%) 1 8	330, 466, 539, 617	0
2	F	92/95 (96%)	0.21	5 (5%) 26 30	505, 594, 716, 786	0
2	G	92/95 (96%)	0.75	19 (20%) 1 8	505, 594, 744, 870	0
2	H	92/95 (96%)	1.43	31 (33%) 0 6	506, 596, 753, 853	0
2	I	92/95 (96%)	0.48	6 (6%) 20 24	506, 596, 746, 774	0
2	J	92/95 (96%)	0.73	14 (15%) 2 10	506, 595, 744, 791	0
All	All	2715/2735 (99%)	0.87	428 (15%) 2 9	330, 482, 656, 870	0

All (428) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	GLN	6.7
1	A	420	CYS	6.0
2	H	47(O)	G	6.0
1	E	228	VAL	5.5
1	D	165	GLU	5.4
1	D	291	GLN	5.3
2	G	47(O)	G	5.2
1	C	116	ARG	5.2
1	E	395	VAL	5.1
2	G	47(N)	A	5.1
1	D	23	PRO	5.1
2	J	47(O)	G	5.0
1	A	317	ASP	5.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	317	ASP	5.0
1	E	397	ILE	4.9
1	E	373	VAL	4.9
1	E	396	ALA	4.8
1	B	317	ASP	4.8
1	B	373	VAL	4.8
1	B	397	ILE	4.8
1	D	212	MET	4.7
1	E	315	ARG	4.7
1	D	211	LEU	4.7
1	D	213	LYS	4.6
1	C	317	ASP	4.6
2	H	22	G	4.6
1	D	397	ILE	4.5
1	D	429	PHE	4.5
1	E	371	ILE	4.5
1	A	291	GLN	4.4
1	E	171	GLY	4.4
1	B	395	VAL	4.4
1	D	171	GLY	4.3
1	B	394	CYS	4.2
1	D	284	ASP	4.2
1	E	360	GLU	4.2
1	D	251	GLY	4.1
1	A	165	GLU	4.1
2	J	47(N)	A	4.1
1	E	140	ASN	4.0
1	A	73	ILE	4.0
1	C	73	ILE	4.0
1	D	317	ASP	4.0
1	E	372	SER	4.0
2	G	73	G	4.0
1	A	140	ASN	3.9
1	A	284	ASP	3.9
2	J	47(F)	U	3.9
2	G	47	U	3.9
1	D	170	GLY	3.9
2	H	14	G	3.9
1	A	8	ILE	3.8
1	A	427	LEU	3.8
1	B	372	SER	3.8
2	H	47(A)	C	3.8

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	315	ARG	3.8
1	D	214	VAL	3.8
2	H	34	U	3.8
1	C	418	ILE	3.7
1	E	23	PRO	3.7
1	E	172	SER	3.7
2	H	47(I)	A	3.7
1	D	250	SER	3.7
1	E	31	ALA	3.7
1	C	291	GLN	3.6
1	C	212	MET	3.6
2	J	73	G	3.6
1	A	87	ALA	3.6
1	D	267	ASN	3.6
1	A	418	ILE	3.6
2	J	47(E)	A	3.5
2	H	42(A)	C	3.5
1	E	27	VAL	3.5
1	B	396	ALA	3.5
1	B	2	LYS	3.5
1	E	3	SER	3.5
2	F	73	G	3.5
1	E	284	ASP	3.5
1	A	397	ILE	3.5
1	B	140	ASN	3.4
1	B	165	GLU	3.4
1	D	172	SER	3.4
1	E	1	MET	3.4
1	E	14	VAL	3.4
1	B	429	PHE	3.4
2	H	47	U	3.4
1	E	24	GLU	3.4
1	B	291	GLN	3.4
1	A	395	VAL	3.4
1	C	165	GLU	3.4
1	E	312	ARG	3.3
1	C	119	ARG	3.3
1	D	266	PRO	3.3
1	D	420	CYS	3.3
2	H	47(N)	A	3.3
1	A	212	MET	3.3
2	H	21	U	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	211	LEU	3.3
1	A	428	LEU	3.3
1	C	31	ALA	3.2
1	D	320	THR	3.2
2	J	47(D)	U	3.2
2	J	46	C	3.2
1	E	429	PHE	3.2
1	E	119	ARG	3.2
1	C	265	GLU	3.2
1	A	369	LEU	3.2
1	B	214	VAL	3.2
2	G	72	C	3.2
1	E	26	TYR	3.1
1	D	255	ASN	3.1
1	E	277	ASP	3.1
1	D	14	VAL	3.1
1	B	212	MET	3.1
1	C	266	PRO	3.1
1	A	429	PHE	3.1
1	E	250	SER	3.1
1	E	212	MET	3.1
1	D	247	ASP	3.1
1	C	429	PHE	3.1
2	H	35	C	3.1
1	D	82	THR	3.1
1	B	265	GLU	3.0
1	D	86	ARG	3.0
2	G	47(E)	A	3.0
1	C	228	VAL	3.0
2	J	47	U	3.0
1	B	393	TYR	3.0
1	D	140	ASN	3.0
1	A	213	LYS	3.0
1	E	28	VAL	3.0
1	E	116	ARG	3.0
2	H	46	C	3.0
1	B	376	ASP	3.0
1	A	315	ARG	3.0
1	E	394	CYS	3.0
1	B	431	MET	3.0
1	E	316	ILE	2.9
1	E	83	ASN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	320	THR	2.9
2	H	47(P)	A	2.9
1	D	192	THR	2.9
1	D	200	TYR	2.9
1	D	215	HIS	2.9
1	A	421	ARG	2.9
2	H	47(H)	U	2.9
1	A	166	LEU	2.9
2	G	46	C	2.9
2	G	47(A)	C	2.9
1	E	445	THR	2.9
2	F	14	G	2.9
2	H	47(B)	G	2.9
1	B	3	SER	2.8
1	C	410	ARG	2.8
1	E	290	PRO	2.8
1	A	442	ILE	2.8
1	B	172	SER	2.8
1	A	419	VAL	2.8
2	H	47(C)	C	2.8
1	C	200	TYR	2.8
2	J	47(M)	G	2.8
1	C	118	SER	2.8
1	B	316	ILE	2.8
1	A	31	ALA	2.8
1	B	315	ARG	2.8
1	C	214	VAL	2.8
1	A	371	ILE	2.8
1	D	24	GLU	2.8
1	B	211	LEU	2.8
1	A	312	ARG	2.8
1	E	442	ILE	2.8
2	J	47(C)	C	2.8
1	A	320	THR	2.7
1	E	357	LYS	2.8
1	C	213	LYS	2.7
1	C	279	VAL	2.7
1	E	118	SER	2.7
1	B	374	ILE	2.7
1	D	419	VAL	2.7
1	D	22	TYR	2.7
1	D	427	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	22	TYR	2.7
1	A	172	SER	2.7
1	E	95	ASN	2.7
1	E	200	TYR	2.7
2	G	47(M)	G	2.7
1	D	265	GLU	2.7
1	E	15	VAL	2.7
1	E	441	THR	2.7
2	G	2	G	2.7
2	J	14	G	2.7
1	A	373	VAL	2.7
1	C	420	CYS	2.7
2	F	15	C	2.7
1	D	248	ALA	2.7
1	C	245	TYR	2.7
1	C	312	ARG	2.7
1	C	384	SER	2.7
1	E	359	LEU	2.7
1	C	434	VAL	2.7
1	E	418	ILE	2.7
1	B	228	VAL	2.7
1	E	141	ASN	2.6
1	D	418	ILE	2.6
1	E	278	LEU	2.6
1	E	9	PRO	2.6
1	B	8	ILE	2.6
1	A	74	ASN	2.6
1	E	279	VAL	2.6
1	A	370	LYS	2.6
1	C	48	ALA	2.6
1	A	88	PRO	2.6
1	B	115	LYS	2.6
1	C	411	LEU	2.6
1	E	82	THR	2.6
1	C	53	PHE	2.6
1	C	211	LEU	2.6
1	C	419	VAL	2.6
2	G	47(F)	U	2.6
1	E	289	GLY	2.6
1	D	407	LEU	2.6
1	D	161	ILE	2.6
1	D	228	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	320	THR	2.6
1	E	114	GLY	2.6
1	C	263	VAL	2.6
1	D	384	SER	2.6
2	G	3	G	2.6
2	H	47(J)	A	2.6
1	B	356	ALA	2.6
1	D	245	TYR	2.6
1	E	449	LEU	2.6
1	A	338	ASP	2.6
1	C	4	LEU	2.5
1	E	369	LEU	2.5
1	D	31	ALA	2.5
1	C	284	ASP	2.5
1	E	431	MET	2.5
2	G	47(K)	G	2.5
2	I	29	A	2.5
1	B	153	LEU	2.5
1	E	25	ILE	2.5
1	A	372	SER	2.5
1	C	252	LEU	2.5
2	G	47(B)	G	2.5
1	D	163	ARG	2.5
1	A	83	ASN	2.5
1	C	320	THR	2.5
1	A	141	ASN	2.5
1	E	87	ALA	2.5
1	D	188	GLU	2.5
2	J	47(A)	C	2.5
2	H	55	U	2.5
1	B	1	MET	2.5
1	B	31	ALA	2.5
1	B	160	ILE	2.5
1	C	253	LEU	2.5
1	A	381	GLY	2.5
1	B	213	LYS	2.5
1	A	118	SER	2.5
1	B	7	GLN	2.5
1	D	428	LEU	2.5
2	G	47(D)	U	2.5
1	A	417	PRO	2.5
1	B	23	PRO	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	86	ARG	2.5
1	E	267	ASN	2.5
1	A	363	LEU	2.4
1	E	245	TYR	2.4
1	A	250	SER	2.4
1	A	28	VAL	2.4
1	A	14	VAL	2.4
1	D	210	LEU	2.4
1	E	86	ARG	2.4
1	A	214	VAL	2.4
1	C	254	ILE	2.4
1	B	420	CYS	2.4
1	B	347	GLN	2.4
1	C	251	GLY	2.4
1	E	276	ILE	2.4
2	G	47(C)	C	2.4
1	B	171	GLY	2.4
1	C	117	GLY	2.4
1	C	223	GLY	2.4
1	C	276	ILE	2.4
1	A	170	GLY	2.4
1	C	395	VAL	2.4
1	A	360	GLU	2.4
1	E	4	LEU	2.4
1	D	279	VAL	2.4
1	E	213	LYS	2.4
2	I	38	A	2.4
1	B	223	GLY	2.4
1	D	380	PRO	2.4
1	E	410	ARG	2.4
1	E	165	GLU	2.4
2	H	47(G)	U	2.4
1	B	427	LEU	2.4
1	C	290	PRO	2.4
1	E	166	LEU	2.3
2	H	27	C	2.3
2	J	45	U	2.3
1	B	384	SER	2.3
2	G	1	G	2.3
1	A	446	LEU	2.3
1	D	160	ILE	2.3
1	D	26	TYR	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	141	ASN	2.3
2	H	15	C	2.3
1	A	411	LEU	2.3
1	D	316	ILE	2.3
1	D	166	LEU	2.3
1	A	398	ARG	2.3
1	D	216	LYS	2.3
1	B	310	ILE	2.3
1	C	267	ASN	2.3
1	A	362	LEU	2.3
1	A	171	GLY	2.3
2	H	44	G	2.3
1	D	315	ARG	2.3
1	C	262	SER	2.3
1	A	434	VAL	2.3
2	I	72	C	2.3
1	E	428	LEU	2.3
1	E	296	VAL	2.3
1	B	166	LEU	2.3
1	B	233	LEU	2.3
2	I	28	U	2.3
1	D	426	GLN	2.3
1	E	85	GLY	2.3
1	B	312	ARG	2.3
1	D	391	PRO	2.3
1	C	35	ALA	2.2
1	A	128	ASN	2.2
1	D	83	ASN	2.2
1	E	108	GLU	2.2
1	E	356	ALA	2.2
1	A	9	PRO	2.2
1	E	57	VAL	2.2
1	A	416	PRO	2.2
1	C	115	LYS	2.2
2	H	47(M)	G	2.2
1	D	289	GLY	2.2
2	H	36	A	2.2
2	H	56	C	2.2
1	A	161	ILE	2.2
1	B	26	TYR	2.2
1	D	73	ILE	2.2
1	D	35	ALA	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	431	MET	2.2
1	D	164	GLY	2.2
1	C	140	ASN	2.2
1	A	359	LEU	2.2
1	C	407	LEU	2.2
1	C	233	LEU	2.2
1	A	346	THR	2.2
1	B	149	VAL	2.2
1	B	116	ARG	2.2
2	H	33	U	2.2
1	E	117	GLY	2.2
1	A	75	ALA	2.2
2	G	47(J)	A	2.2
1	E	450	LEU	2.2
1	C	79	VAL	2.2
1	E	452	ILE	2.2
1	A	450	LEU	2.2
1	A	24	GLU	2.2
1	A	119	ARG	2.2
1	D	65	MET	2.2
1	D	223	GLY	2.2
1	E	18	PHE	2.2
1	D	254	ILE	2.2
2	F	56	C	2.1
1	A	396	ALA	2.1
1	A	367	PRO	2.1
1	A	380	PRO	2.1
1	A	245	TYR	2.1
1	A	265	GLU	2.1
1	D	395	VAL	2.1
1	E	381	GLY	2.1
1	D	290	PRO	2.1
1	D	312	ARG	2.1
2	F	20	U	2.1
1	B	4	LEU	2.1
1	B	264	ASP	2.1
1	C	397	ILE	2.1
1	E	363	LEU	2.1
1	D	398	ARG	2.1
1	E	35	ALA	2.1
1	B	392	THR	2.1
2	H	13	C	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	217	SER	2.1
1	D	252	LEU	2.1
1	C	66	LYS	2.1
1	C	278	LEU	2.1
2	H	47(K)	G	2.1
1	A	260	GLY	2.1
1	E	163	ARG	2.1
2	H	73	G	2.1
1	E	384	SER	2.1
2	H	47(D)	U	2.1
1	A	293	GLY	2.1
2	I	47(G)	U	2.1
1	E	98	SER	2.1
1	E	283	GLY	2.1
1	B	119	ARG	2.1
1	B	200	TYR	2.1
1	C	111	LEU	2.1
2	J	47(G)	U	2.1
1	A	81	ASN	2.1
1	E	411	LEU	2.0
1	E	22	TYR	2.0
2	I	27	C	2.0
1	E	53	PHE	2.0
1	E	295	ILE	2.0
1	B	363	LEU	2.0
1	E	362	LEU	2.0
1	E	358	ARG	2.0
1	A	283	GLY	2.0
2	H	23	C	2.0
1	B	73	ILE	2.0
1	D	16	GLU	2.0
1	C	250	SER	2.0
1	C	255	ASN	2.0
1	E	451	SER	2.0
2	G	47(I)	A	2.0
1	B	5	LEU	2.0
1	B	27	VAL	2.0

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

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	B	285	24/25	0.75	0.61	-	429,446,491,495	0
1	LLP	E	285	24/25	0.70	0.67	-	290,384,467,493	0
1	LLP	D	285	24/25	0.57	0.71	-	310,432,455,471	0
1	LLP	A	285	24/25	0.64	0.69	-	384,433,449,452	0
1	LLP	C	285	24/25	0.63	0.65	-	416,449,487,497	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.