Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2021 – 03:33 PM EDT

PDB ID	:	3K5N
Title	:	Crystal structure of E.coli Pol II-abasic DNA binary complex
Authors	:	Yang, W.; Wang, F.
Deposited on	:	2009-10-07
Resolution	:	3.15 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

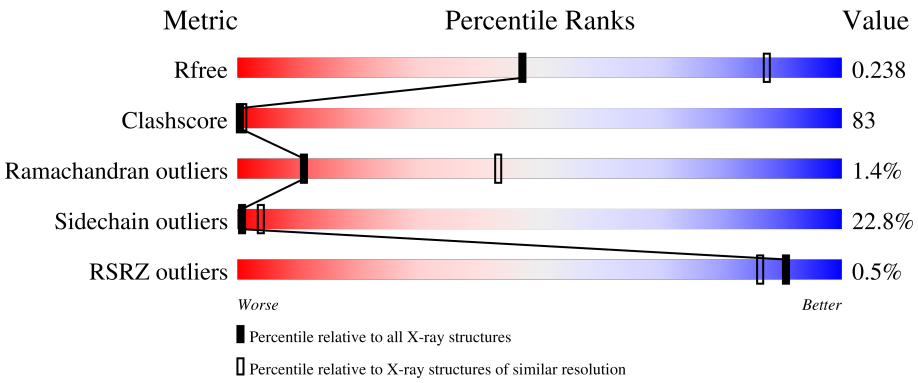
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	786	.% 28% 50% 17% • •
1	B	786	27% 49% 17% • 6%
2	T	20	5% 30% 35% 35%
3	P	13	69% 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12722 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 DNA polymerase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	759	6169	3934	1093	1117	25	0	0	0
1	B	738	6007	3832	1066	1086	23	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P21189
A	-1	PRO	-	expression tag	UNP P21189
A	0	HIS	-	expression tag	UNP P21189
A	335	ASN	ASP	engineered mutation	UNP P21189
B	-2	GLY	-	expression tag	UNP P21189
B	-1	PRO	-	expression tag	UNP P21189
B	0	HIS	-	expression tag	UNP P21189
B	335	ASN	ASP	engineered mutation	UNP P21189

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*CP*CP*TP*GP*(3DR)*TP*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	13	263	126	51	74	12	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	13	255	122	45	76	12	0	0	0

- Molecule 4 is water.

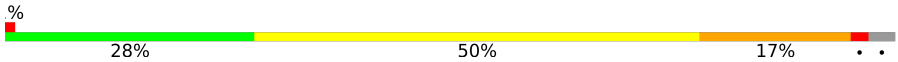
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	18	18	18	0	0
			Total	O		
4	B	10	10	10	0	0

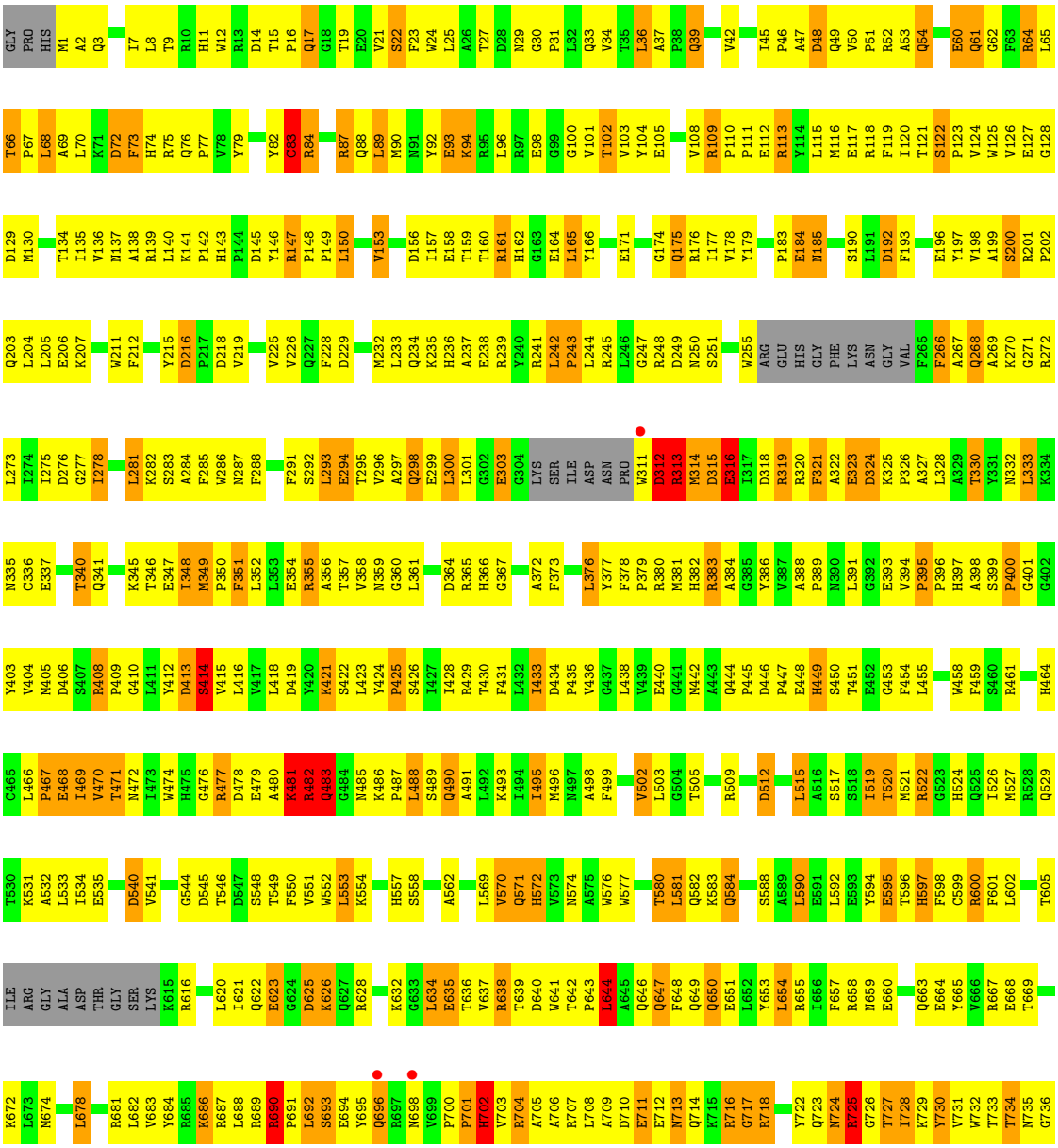
3 Residue-property plots (i)

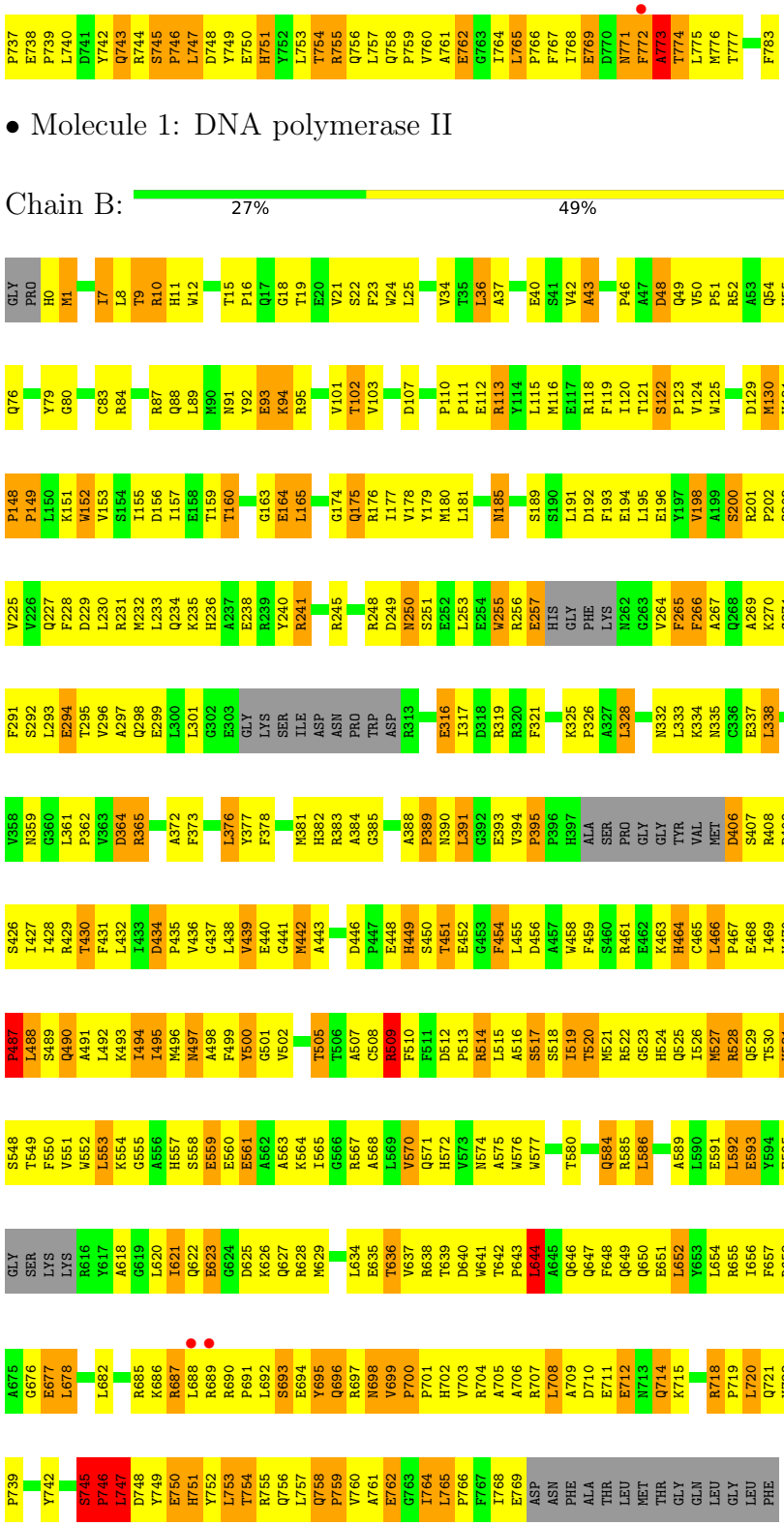
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA polymerase II

Chain A:







• Molecule 1: DNA polymerase II

Chain B: 27% 49% 17% • 6%

• Molecule 2: DNA (5'-D(*GP*TP*CP*CP*TP*GP*(3DR)*TP*AP*CP*GP*CP*TP*AP*GP*GP*CP*AP*CP*A)-3')

Chain T: 5% 30% 35% 35%

• Molecule 3: DNA (5'-D(*GP*TP*GP*CP*CP*TP*AP*GP*CP*GP*TP*AP*G)-3')

Chain P:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.41Å 147.55Å 96.28Å 90.00° 99.98° 90.00°	Depositor
Resolution (Å)	31.31 – 3.15 46.18 – 3.15	Depositor EDS
% Data completeness (in resolution range)	95.2 (31.31-3.15) 95.2 (46.18-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.236 0.232 , 0.238	Depositor DCC
R_{free} test set	1696 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12722	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.98	3/6331 (0.0%)	1.13	32/8587 (0.4%)
1	B	0.94	2/6163 (0.0%)	1.05	18/8359 (0.2%)
2	T	1.27	2/295 (0.7%)	1.67	11/453 (2.4%)
3	P	1.50	4/285 (1.4%)	1.66	9/438 (2.1%)
All	All	0.98	11/13074 (0.1%)	1.13	70/17837 (0.4%)

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

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	725	ARG	CG-CD	-17.75	1.07	1.51
1	B	255	TRP	CB-CG	-8.48	1.34	1.50
3	P	902	DT	C5-C6	-6.43	1.29	1.34
1	B	152	TRP	CB-CG	-6.00	1.39	1.50
2	T	808	DT	C5-C6	-5.86	1.30	1.34
1	A	725	ARG	CB-CG	-5.75	1.37	1.52
2	T	819	DC	C5-C6	-5.45	1.29	1.34
1	A	83	CYS	CB-SG	-5.27	1.73	1.81
3	P	905	DC	C2'-C1'	5.14	1.57	1.52
3	P	905	DC	N1-C2	5.08	1.45	1.40
3	P	908	DG	N9-C4	-5.01	1.33	1.38

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	725	ARG	NE-CZ-NH1	-24.14	108.23	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	725	ARG	NE-CZ-NH2	15.19	127.90	120.30
1	A	725	ARG	CA-CB-CG	13.00	142.00	113.40
1	A	725	ARG	CB-CA-C	-9.47	91.46	110.40
1	B	746	PRO	CA-N-CD	-7.91	100.42	111.50
2	T	820	DA	O5'-P-OP1	7.64	119.86	110.70
3	P	902	DT	C6-N1-C1'	-7.58	109.03	120.40
1	A	773	ALA	N-CA-C	-7.38	91.08	111.00
1	B	413	ASP	N-CA-C	-7.38	91.08	111.00
1	B	623	GLU	N-CA-C	-7.29	91.31	111.00
2	T	819	DC	O4'-C1'-N1	-7.21	102.95	108.00
3	P	905	DC	OP1-P-O3'	7.20	121.03	105.20
3	P	902	DT	C2-N1-C1'	7.18	129.68	118.20
1	A	774	THR	N-CA-C	-6.88	92.43	111.00
3	P	902	DT	O4'-C1'-N1	-6.64	103.35	108.00
2	T	817	DC	O4'-C1'-N1	-6.63	103.36	108.00
2	T	808	DT	C6-N1-C1'	-6.57	110.54	120.40
1	B	745	SER	N-CA-C	6.49	128.53	111.00
1	A	266	PHE	N-CA-C	-6.46	93.57	111.00
1	B	195	LEU	N-CA-C	-6.46	93.57	111.00
1	B	700	PRO	N-CA-C	-6.41	95.43	112.10
1	A	584	GLN	N-CA-C	-6.37	93.80	111.00
3	P	905	DC	N1-C1'-C2'	6.36	124.68	112.60
1	A	150	LEU	CA-CB-CG	6.26	129.71	115.30
1	A	60	GLU	N-CA-C	-6.26	94.10	111.00
1	B	149	PRO	N-CA-C	-6.17	96.05	112.10
1	A	269	ALA	N-CA-C	-6.17	94.34	111.00
1	B	555	GLY	N-CA-C	6.13	128.44	113.10
1	A	644	LEU	CA-CB-CG	6.05	129.21	115.30
3	P	902	DT	O4'-C4'-C3'	-6.01	102.09	104.50
1	B	747	LEU	N-CA-C	-5.99	94.83	111.00
1	A	701	PRO	N-CA-C	5.88	127.40	112.10
1	A	572	HIS	N-CA-C	-5.79	95.37	111.00
1	A	725	ARG	CD-NE-CZ	5.79	131.71	123.60
1	B	746	PRO	N-CA-C	5.79	127.14	112.10
3	P	906	DT	C1'-O4'-C4'	-5.74	104.36	110.10
1	B	728	ILE	CB-CA-C	-5.73	100.14	111.60
1	A	678	LEU	CA-CB-CG	5.66	128.32	115.30
3	P	908	DG	O4'-C1'-N9	-5.65	104.04	108.00
1	B	644	LEU	CA-CB-CG	5.63	128.26	115.30
1	A	702	HIS	N-CA-C	-5.60	95.88	111.00
1	B	487	PRO	CA-N-CD	-5.55	103.73	111.50
1	A	125	TRP	N-CA-C	-5.51	96.14	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	482	ARG	N-CA-C	-5.47	96.23	111.00
2	T	808	DT	C2-N1-C1'	5.45	126.92	118.20
1	A	718	ARG	N-CA-C	-5.45	96.28	111.00
1	A	312	ASP	N-CA-C	5.44	125.69	111.00
1	A	453	GLY	N-CA-C	-5.43	99.51	113.10
1	A	570	VAL	C-N-CA	-5.41	108.18	121.70
2	T	816	DG	N9-C1'-C2'	5.32	122.71	112.60
1	A	519	ILE	CB-CA-C	-5.30	101.00	111.60
2	T	819	DC	C6-N1-C1'	-5.27	114.47	120.80
1	B	125	TRP	N-CA-C	-5.21	96.92	111.00
1	B	509	ARG	N-CA-C	-5.20	96.95	111.00
1	B	486	LYS	C-N-CD	-5.19	109.18	120.60
2	T	818	DA	O4'-C4'-C3'	-5.15	102.44	104.50
1	B	165	LEU	CA-CB-CG	5.14	127.12	115.30
2	T	817	DC	C2-N1-C1'	5.12	124.43	118.80
1	A	512	ASP	N-CA-C	-5.11	97.20	111.00
1	A	147	ARG	N-CA-C	-5.11	97.21	111.00
2	T	809	DA	C3'-C2'-C1'	-5.09	96.39	102.50
1	A	316	GLU	N-CA-C	-5.09	97.25	111.00
3	P	905	DC	O3'-P-O5'	-5.09	94.34	104.00
1	A	68	LEU	CA-CB-CG	5.08	126.99	115.30
1	A	413	ASP	N-CA-C	-5.07	97.32	111.00
1	A	190	SER	N-CA-C	5.06	124.66	111.00
2	T	819	DC	C2-N1-C1'	5.05	124.36	118.80
1	B	43	ALA	N-CA-C	-5.03	97.42	111.00
1	A	281	LEU	CA-CB-CG	-5.01	103.77	115.30
1	A	481	LYS	N-CA-C	-5.01	97.46	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	745	SER	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6169	0	6040	865	2
1	B	6007	0	5881	1075	4
2	T	263	0	147	67	0
3	P	255	0	143	59	0
4	A	18	0	0	1	0
4	B	10	0	0	0	0
All	All	12722	0	12211	2057	4

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 83.

All (2057) 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:B:688:LEU:CD1	1:B:728:ILE:HD11	1.34	1.51
1:B:231:ARG:HD2	1:B:265:PHE:CE1	1.42	1.51
1:B:688:LEU:HD11	1:B:728:ILE:CD1	1.45	1.44
1:B:642:THR:CB	1:B:756:GLN:NE2	1.85	1.37
1:A:14:ASP:OD2	1:A:87:ARG:HG2	1.20	1.35
1:B:732:TRP:CB	1:B:751:HIS:HD2	1.38	1.34
1:B:673:LEU:HD23	1:B:674:MET:N	1.43	1.33
1:A:413:ASP:O	1:A:552:TRP:HZ3	1.09	1.32
1:B:733:THR:HG23	1:B:746:PRO:O	1.24	1.32
1:A:688:LEU:HB2	1:A:726:GLY:N	1.44	1.32
1:B:231:ARG:CD	1:B:265:PHE:HE1	1.42	1.32
1:A:772:PHE:N	1:A:773:ALA:HB2	1.44	1.31
1:B:733:THR:CG2	1:B:735:ASN:OD1	1.80	1.30
1:B:689:ARG:O	1:B:725:ARG:CD	1.80	1.29
1:A:16:PRO:CG	1:A:17:GLN:OE1	1.81	1.27
1:A:688:LEU:N	1:A:726:GLY:O	1.67	1.26
1:B:428:ILE:CD1	1:B:519:ILE:HD11	1.65	1.25
1:B:9:THR:HG21	1:B:11:HIS:CE1	1.71	1.25
1:B:732:TRP:CB	1:B:751:HIS:CD2	2.19	1.24
1:B:691:PRO:HD3	1:B:725:ARG:NH1	1.51	1.24
1:B:421:LYS:HG2	1:B:593:GLU:OE1	1.37	1.23
1:A:751:HIS:CE1	1:A:755:ARG:HG2	1.72	1.22
1:B:231:ARG:CD	1:B:265:PHE:CE1	2.19	1.22
1:A:700:PRO:O	1:A:703:VAL:CB	1.87	1.22
1:B:642:THR:HB	1:B:756:GLN:NE2	0.89	1.21
1:A:740:LEU:C	1:A:740:LEU:HD23	1.60	1.20
1:A:292:SER:O	1:A:296:VAL:HG23	1.41	1.19
1:B:428:ILE:HD11	1:B:519:ILE:CD1	1.73	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:740:LEU:HD23	1:A:740:LEU:O	1.42	1.17
1:B:692:LEU:HD11	1:B:722:TYR:O	1.43	1.17
1:B:733:THR:HG21	1:B:735:ASN:OD1	1.39	1.17
1:B:337:GLU:O	1:B:341:GLN:HG3	1.42	1.16
1:B:9:THR:CG2	1:B:11:HIS:CE1	2.29	1.16
1:B:554:LYS:N	1:B:554:LYS:HD3	1.53	1.16
1:B:668:GLU:O	1:B:672:LYS:HG2	1.43	1.16
1:B:418:LEU:HD12	1:B:418:LEU:H	1.05	1.16
1:A:21:VAL:O	1:A:36:LEU:CD1	1.93	1.15
1:A:722:TYR:CZ	1:A:728:ILE:HG13	1.80	1.15
1:B:495:ILE:O	1:B:495:ILE:HD12	1.47	1.15
1:A:413:ASP:O	1:A:552:TRP:CZ3	1.99	1.15
1:A:160:THR:HG22	1:A:162:HIS:H	0.98	1.14
1:A:700:PRO:O	1:A:703:VAL:HB	0.98	1.14
1:B:334:LYS:O	1:B:338:LEU:HD23	1.47	1.14
1:B:218:ASP:OD2	1:B:248:ARG:NH2	1.78	1.14
1:B:689:ARG:O	1:B:725:ARG:HD2	1.41	1.14
1:B:753:LEU:HD12	1:B:753:LEU:O	1.44	1.14
1:B:699:VAL:HG21	1:B:704:ARG:HD3	1.28	1.13
1:A:94:LYS:O	1:A:98:GLU:HG3	1.46	1.13
1:B:200:SER:HB2	1:B:202:PRO:HD2	1.16	1.13
1:B:495:ILE:HD12	1:B:495:ILE:C	1.69	1.13
1:A:48:ASP:O	1:A:51:PRO:HD2	1.46	1.12
1:B:732:TRP:HB3	1:B:751:HIS:HD2	0.98	1.12
1:A:600:ARG:HG2	1:A:600:ARG:HH11	1.10	1.12
1:B:255:TRP:CE3	1:B:267:ALA:HB2	1.84	1.12
1:B:229:ASP:O	1:B:233:LEU:CD1	1.97	1.12
1:B:553:LEU:HD23	1:B:553:LEU:H	1.01	1.12
1:B:644:LEU:HD13	1:B:757:LEU:HD11	1.26	1.11
1:B:592:LEU:HD23	1:B:593:GLU:N	1.66	1.11
1:B:644:LEU:HD13	1:B:757:LEU:CD1	1.79	1.11
1:B:351:PHE:CE2	1:B:352:LEU:HD23	1.87	1.10
1:A:638:ARG:HH11	1:A:638:ARG:CG	1.65	1.10
1:B:723:GLN:C	1:B:724:ASN:HD22	1.53	1.10
1:A:408:ARG:HH11	1:A:408:ARG:CG	1.63	1.10
1:A:751:HIS:O	1:A:755:ARG:HB2	1.52	1.09
1:A:692:LEU:H	1:A:692:LEU:CD1	1.60	1.09
1:B:732:TRP:CG	1:B:751:HIS:CD2	2.39	1.09
1:B:747:LEU:O	1:B:747:LEU:HD23	1.51	1.09
3:P:901:DG:H2'	3:P:902:DT:H73	1.35	1.09
1:B:48:ASP:HB3	1:B:76:GLN:NE2	1.67	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:CYS:HB3	1:B:88:GLN:HE21	1.16	1.08
1:B:733:THR:HA	1:B:747:LEU:HA	1.26	1.08
1:B:747:LEU:H	1:B:747:LEU:CD2	1.66	1.08
1:A:692:LEU:N	1:A:692:LEU:HD12	1.63	1.08
3:P:901:DG:H2'	3:P:902:DT:C7	1.83	1.08
1:A:408:ARG:HG2	1:A:408:ARG:NH1	1.47	1.07
1:A:688:LEU:CB	1:A:726:GLY:H	1.66	1.07
1:B:696:GLN:OE1	1:B:696:GLN:HA	1.47	1.07
1:B:292:SER:O	1:B:296:VAL:HG23	1.55	1.07
1:B:733:THR:CG2	1:B:746:PRO:O	2.01	1.07
3:P:902:DT:H6	3:P:902:DT:H5"	1.04	1.07
1:A:36:LEU:CD1	1:A:36:LEU:H	1.61	1.07
1:B:407:SER:O	1:B:409:PRO:HD3	1.52	1.07
1:B:638:ARG:HG3	1:B:640:ASP:OD1	1.54	1.07
1:B:485:ASN:C	1:B:487:PRO:HD3	1.73	1.07
1:A:638:ARG:HH11	1:A:638:ARG:HG2	0.96	1.06
1:B:576:TRP:O	1:B:580:THR:HG22	1.53	1.06
1:B:672:LYS:O	1:B:677:GLU:HB2	1.54	1.06
1:B:378:PHE:O	1:B:382:HIS:HD2	1.36	1.06
1:B:755:ARG:HA	1:B:755:ARG:HE	1.19	1.06
1:A:64:ARG:HH11	1:A:64:ARG:HG3	1.15	1.05
1:A:642:THR:HG22	1:A:644:LEU:H	1.22	1.05
1:B:121:THR:HG23	1:B:122:SER:H	0.91	1.05
1:B:257:GLU:HG2	1:B:265:PHE:HA	1.35	1.05
1:B:381:MET:HE3	1:B:388:ALA:N	1.69	1.05
1:B:200:SER:CB	1:B:202:PRO:HD2	1.87	1.05
1:B:216:ASP:OD2	1:B:248:ARG:NH1	1.89	1.05
1:B:692:LEU:CD1	1:B:722:TYR:O	2.03	1.05
2:T:809:DA:H2"	2:T:810:DC:OP2	1.53	1.05
1:A:654:LEU:HD12	1:A:655:ARG:N	1.71	1.05
3:P:913:DG:OP2	3:P:913:DG:H2'	1.55	1.05
1:A:692:LEU:HD11	1:A:722:TYR:O	1.57	1.05
3:P:901:DG:C2'	3:P:902:DT:H71	1.87	1.04
3:P:901:DG:C2'	3:P:902:DT:C7	2.35	1.04
1:B:528:ARG:O	1:B:531:LYS:HG2	1.56	1.04
1:B:464:HIS:HB2	1:B:468:GLU:OE1	1.57	1.04
3:P:902:DT:H5"	3:P:902:DT:C6	1.93	1.04
1:B:257:GLU:HG2	1:B:265:PHE:CB	1.87	1.04
1:B:586:LEU:HD12	1:B:586:LEU:N	1.72	1.04
1:B:691:PRO:HD3	1:B:725:ARG:HH11	0.92	1.04
3:P:901:DG:H2"	3:P:902:DT:H71	1.40	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:SER:HB3	1:B:458:TRP:HE3	1.23	1.03
1:B:500:TYR:HD2	1:B:500:TYR:C	1.62	1.03
1:A:724:ASN:O	1:A:725:ARG:HB2	1.24	1.03
1:A:64:ARG:HH11	1:A:64:ARG:CG	1.68	1.03
1:A:771:ASN:C	1:A:773:ALA:HB2	1.76	1.03
1:B:440:GLU:OE2	1:B:463:LYS:HE3	1.57	1.03
1:B:450:SER:HB3	1:B:458:TRP:CE3	1.94	1.03
1:B:655:ARG:NH1	1:B:661:PRO:O	1.90	1.03
1:B:636:THR:HB	1:B:649:GLN:OE1	1.57	1.03
1:B:747:LEU:HD23	1:B:747:LEU:H	1.20	1.03
1:B:528:ARG:HH11	1:B:528:ARG:CG	1.69	1.02
1:B:377:TYR:OH	1:B:434:ASP:OD1	1.78	1.02
1:B:553:LEU:HD23	1:B:553:LEU:N	1.71	1.02
1:A:16:PRO:HG2	1:A:17:GLN:OE1	0.85	1.02
1:A:485:ASN:C	1:A:487:PRO:HD2	1.79	1.02
1:A:113:ARG:HH11	1:A:113:ARG:HG3	1.15	1.02
1:B:688:LEU:CD1	1:B:728:ILE:CD1	2.15	1.01
1:A:337:GLU:O	1:A:341:GLN:HG3	1.60	1.01
2:T:812:DC:H2'	2:T:813:DT:C7	1.90	1.01
1:B:416:LEU:HB2	1:B:551:VAL:CG1	1.91	1.01
1:A:36:LEU:H	1:A:36:LEU:HD12	0.85	1.00
1:B:121:THR:HG23	1:B:122:SER:N	1.69	1.00
1:B:429:ARG:HE	1:B:471:THR:HG22	1.23	1.00
1:A:485:ASN:OD1	1:A:487:PRO:HD2	1.59	1.00
1:B:349:MET:HB3	1:B:350:PRO:HD3	1.42	1.00
1:A:36:LEU:HD12	1:A:36:LEU:N	1.67	1.00
1:A:358:VAL:CG1	1:A:495:ILE:HD13	1.90	1.00
1:B:500:TYR:C	1:B:500:TYR:CD2	2.34	1.00
1:A:160:THR:HG22	1:A:162:HIS:N	1.77	1.00
1:B:466:LEU:HD12	1:B:470:VAL:HG23	1.38	1.00
1:B:733:THR:HG22	1:B:735:ASN:OD1	1.60	0.99
1:B:121:THR:CG2	1:B:122:SER:H	1.74	0.99
1:B:528:ARG:HH11	1:B:528:ARG:HG2	0.85	0.99
1:B:528:ARG:HG2	1:B:528:ARG:NH1	1.61	0.99
1:B:699:VAL:HG21	1:B:704:ARG:CD	1.91	0.99
1:B:431:PHE:CE2	1:B:522:ARG:HD3	1.97	0.99
1:B:225:VAL:O	1:B:230:LEU:HB2	1.63	0.99
1:B:688:LEU:CG	1:B:728:ILE:HD11	1.93	0.99
1:A:768:ILE:O	1:A:769:GLU:HB2	1.62	0.99
1:B:351:PHE:HE2	1:B:352:LEU:HD23	1.21	0.99
2:T:819:DC:H2"	2:T:820:DA:C4'	1.93	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:LEU:C	1:B:411:LEU:HD12	1.81	0.99
1:B:592:LEU:HD23	1:B:592:LEU:C	1.83	0.98
1:A:383:ARG:HH11	1:A:383:ARG:HG3	1.25	0.98
2:T:813:DT:H2'	2:T:814:DA:C8	1.98	0.98
3:P:912:DA:H2"	3:P:913:DG:O5'	1.60	0.98
1:B:278:ILE:O	1:B:282:LYS:HG3	1.64	0.98
1:B:584:GLN:HB3	1:B:586:LEU:HD13	1.46	0.98
1:B:543:TYR:HD2	1:B:550:PHE:CD2	1.81	0.98
1:A:732:TRP:CG	1:A:751:HIS:HD2	1.82	0.97
1:B:551:VAL:HG13	1:B:551:VAL:O	1.61	0.97
1:A:692:LEU:H	1:A:692:LEU:HD12	0.82	0.97
1:A:724:ASN:O	1:A:725:ARG:CB	2.13	0.97
1:B:454:PHE:H	1:B:454:PHE:HD2	0.99	0.97
1:B:466:LEU:HD12	1:B:470:VAL:CG2	1.95	0.97
1:B:543:TYR:HD2	1:B:550:PHE:CE2	1.81	0.97
1:B:750:GLU:O	1:B:754:THR:CG2	2.12	0.96
1:A:377:TYR:OH	1:A:434:ASP:OD2	1.80	0.96
1:A:454:PHE:C	1:A:455:LEU:HD12	1.84	0.96
1:B:257:GLU:HG2	1:B:265:PHE:CA	1.94	0.96
1:A:688:LEU:HB2	1:A:726:GLY:H	0.94	0.96
1:B:694:GLU:HG3	1:B:694:GLU:O	1.62	0.96
1:A:351:PHE:CD2	1:A:352:LEU:HD12	2.00	0.96
1:B:584:GLN:HB3	1:B:586:LEU:CD1	1.95	0.96
1:A:540:ASP:OD1	1:A:554:LYS:HE3	1.64	0.95
1:B:454:PHE:CD2	1:B:454:PHE:N	2.31	0.95
1:B:231:ARG:HG2	1:B:265:PHE:CZ	2.01	0.95
1:B:231:ARG:CG	1:B:265:PHE:CE1	2.50	0.95
1:B:495:ILE:O	1:B:498:ALA:HB3	1.66	0.95
1:A:467:PRO:O	1:A:471:THR:HG22	1.65	0.95
1:A:600:ARG:HH11	1:A:600:ARG:CG	1.80	0.95
1:A:700:PRO:HG2	1:A:703:VAL:HG21	1.49	0.95
1:B:160:THR:HG23	1:B:164:GLU:O	1.65	0.94
1:A:419:ASP:HB2	1:A:595:GLU:OE1	1.67	0.94
1:B:745:SER:HB2	1:B:746:PRO:HD3	1.46	0.94
1:A:72:ASP:HB3	1:A:74:HIS:H	1.32	0.94
1:A:446:ASP:OD2	1:A:449:HIS:HD2	1.51	0.94
1:B:732:TRP:HB3	1:B:751:HIS:CD2	1.88	0.94
1:A:113:ARG:HH11	1:A:113:ARG:CG	1.80	0.94
1:B:554:LYS:HD3	1:B:554:LYS:H	1.18	0.94
1:B:673:LEU:HD23	1:B:674:MET:H	1.20	0.94
1:B:689:ARG:O	1:B:725:ARG:HD3	1.66	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:817:DC:H2'	2:T:818:DA:H1'	1.50	0.94
1:A:113:ARG:HG3	1:A:113:ARG:NH1	1.74	0.94
1:B:418:LEU:HD12	1:B:418:LEU:N	1.80	0.94
2:T:817:DC:H2'	2:T:818:DA:C1'	1.98	0.94
1:B:255:TRP:O	1:B:256:ARG:HG2	1.68	0.93
1:B:420:TYR:CE1	1:B:592:LEU:HB2	2.03	0.93
1:B:0:HIS:O	1:B:1:MET:HG2	1.67	0.93
1:A:638:ARG:HG2	1:A:638:ARG:NH1	1.72	0.93
1:B:686:LYS:HG2	1:B:702:HIS:CD2	2.04	0.93
1:A:83:CYS:SG	1:A:89:LEU:HD23	2.09	0.93
3:P:902:DT:H6	3:P:902:DT:C5'	1.82	0.93
1:A:740:LEU:C	1:A:740:LEU:CD2	2.36	0.92
1:A:14:ASP:OD2	1:A:87:ARG:CG	2.15	0.92
1:A:49:GLN:HE21	1:A:101:VAL:HG13	1.31	0.92
1:B:413:ASP:HA	1:B:599:CYS:O	1.70	0.92
1:A:161:ARG:HB3	1:A:314:MET:HE1	1.50	0.92
1:A:481:LYS:NZ	1:A:481:LYS:CB	2.33	0.92
1:B:481:LYS:O	1:B:481:LYS:HD3	1.70	0.92
1:B:266:PHE:C	1:B:266:PHE:CD2	2.40	0.92
1:A:255:TRP:CE3	1:A:266:PHE:O	2.23	0.91
1:B:485:ASN:HD21	1:B:488:LEU:CD2	1.83	0.91
1:B:416:LEU:O	1:B:551:VAL:HG12	1.71	0.91
1:A:668:GLU:O	1:A:672:LYS:HG3	1.71	0.91
1:B:485:ASN:O	1:B:487:PRO:HD2	1.69	0.91
1:B:553:LEU:N	1:B:553:LEU:CD2	2.32	0.91
1:B:233:LEU:H	1:B:233:LEU:HD12	1.35	0.91
1:B:755:ARG:HA	1:B:755:ARG:NE	1.78	0.91
1:B:753:LEU:HD12	1:B:753:LEU:C	1.80	0.91
2:T:819:DC:H2"	2:T:820:DA:C5'	2.01	0.91
1:B:554:LYS:N	1:B:554:LYS:CD	2.33	0.91
1:B:485:ASN:C	1:B:487:PRO:CD	2.39	0.91
1:B:711:GLU:O	1:B:714:GLN:HB3	1.70	0.91
1:B:411:LEU:C	1:B:411:LEU:CD1	2.38	0.91
1:B:440:GLU:O	1:B:443:ALA:HB3	1.70	0.91
1:B:333:LEU:O	1:B:337:GLU:HG3	1.72	0.90
1:B:411:LEU:HD12	1:B:412:TYR:N	1.86	0.90
1:A:376:LEU:N	1:A:376:LEU:CD1	2.35	0.90
1:A:724:ASN:HD22	1:A:724:ASN:H	1.05	0.90
1:B:255:TRP:CZ3	1:B:267:ALA:HB2	2.06	0.90
1:B:751:HIS:O	1:B:755:ARG:CB	2.20	0.90
1:A:433:ILE:HG22	1:A:433:ILE:O	1.68	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ILE:HD11	1:B:519:ILE:HD11	0.91	0.90
1:B:627:GLN:OE1	1:B:658:ARG:NH1	2.05	0.90
1:A:438:LEU:O	1:A:442:MET:HB2	1.72	0.90
1:A:549:THR:C	1:A:550:PHE:HD2	1.74	0.90
1:B:431:PHE:CE1	1:B:522:ARG:NH1	2.40	0.90
1:B:768:ILE:O	1:B:769:GLU:HG3	1.72	0.90
2:T:813:DT:H2"	2:T:814:DA:O5'	1.70	0.90
1:B:181:LEU:O	1:B:325:LYS:NZ	2.05	0.90
1:A:397:HIS:HD2	1:A:398:ALA:N	1.70	0.90
1:A:710:ASP:OD2	1:A:722:TYR:HB2	1.71	0.90
3:P:905:DC:H2'	3:P:906:DT:C7	2.02	0.90
1:A:278:ILE:O	1:A:282:LYS:HG3	1.70	0.89
1:B:524:HIS:O	1:B:528:ARG:HD2	1.72	0.89
2:T:811:DG:O6	3:P:909:DC:N4	2.04	0.89
1:A:351:PHE:HD2	1:A:352:LEU:HD12	1.38	0.89
1:B:277:GLY:O	1:B:281:LEU:HB2	1.70	0.89
1:B:231:ARG:CG	1:B:265:PHE:CZ	2.55	0.89
1:B:688:LEU:HD11	1:B:728:ILE:HD11	0.95	0.89
1:A:549:THR:O	1:A:550:PHE:HD2	1.54	0.89
2:T:819:DC:C2'	2:T:820:DA:H5'	2.01	0.89
1:A:397:HIS:CD2	1:A:399:SER:H	1.91	0.89
2:T:811:DG:H2'	2:T:812:DC:C6	2.08	0.89
1:B:351:PHE:C	1:B:351:PHE:CD2	2.42	0.89
1:B:673:LEU:CD2	1:B:674:MET:N	2.33	0.89
1:B:699:VAL:O	1:B:699:VAL:HG22	1.68	0.89
1:A:600:ARG:CD	1:A:657:PHE:O	2.21	0.88
1:A:311:TRP:HB3	1:A:312:ASP:OD1	1.74	0.88
1:A:695:TYR:O	1:A:707:ARG:NH2	2.05	0.88
1:B:454:PHE:CB	1:B:521:MET:HE2	2.03	0.88
1:A:200:SER:OG	1:A:202:PRO:HD2	1.72	0.88
1:B:411:LEU:CD1	1:B:412:TYR:N	2.36	0.88
1:A:50:VAL:O	1:A:54:GLN:HG2	1.74	0.88
1:B:198:VAL:HG21	1:B:204:LEU:CD2	2.03	0.88
1:A:712:GLU:O	1:A:716:ARG:HD2	1.74	0.88
1:B:710:ASP:OD2	1:B:723:GLN:NE2	2.05	0.88
2:T:816:DG:N1	3:P:904:DC:N3	2.22	0.88
1:A:724:ASN:H	1:A:724:ASN:ND2	1.72	0.88
1:A:234:GLN:OE1	1:A:255:TRP:NE1	2.06	0.87
1:B:669:THR:O	1:B:672:LYS:HB2	1.73	0.87
1:B:442:MET:HE1	1:B:458:TRP:H	1.37	0.87
1:A:713:ASN:HD21	1:A:742:TYR:HE2	1.22	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:TYR:O	1:B:601:PHE:N	2.06	0.87
1:B:733:THR:HB	1:B:736:GLY:O	1.75	0.87
1:B:454:PHE:CD1	1:B:521:MET:HE2	2.08	0.87
1:B:378:PHE:O	1:B:382:HIS:CD2	2.27	0.87
2:T:819:DC:H2'	2:T:820:DA:C8	2.08	0.87
1:B:415:VAL:CG1	1:B:601:PHE:HB3	2.04	0.87
1:B:60:GLU:HG2	1:B:92:TYR:OH	1.74	0.87
1:B:553:LEU:H	1:B:553:LEU:CD2	1.85	0.87
1:B:421:LYS:CG	1:B:593:GLU:OE1	2.23	0.87
1:B:697:ARG:O	1:B:698:ASN:HB3	1.72	0.87
1:A:692:LEU:HD13	1:A:723:GLN:HA	1.56	0.86
1:B:691:PRO:CD	1:B:725:ARG:HH11	1.85	0.86
1:B:732:TRP:CG	1:B:751:HIS:HD2	1.86	0.86
2:T:813:DT:H2'	2:T:814:DA:N7	1.89	0.86
1:B:416:LEU:HB2	1:B:551:VAL:HG11	1.56	0.86
1:B:691:PRO:CD	1:B:725:ARG:NH1	2.38	0.86
1:A:481:LYS:HB2	1:A:481:LYS:HZ2	1.39	0.86
1:B:376:LEU:N	1:B:376:LEU:CD1	2.36	0.86
1:B:454:PHE:CD1	1:B:521:MET:CE	2.58	0.86
1:B:692:LEU:O	1:B:695:TYR:HB2	1.73	0.86
1:B:733:THR:CG2	1:B:734:THR:N	2.38	0.86
1:A:400:PRO:HG2	1:A:401:GLY:H	1.39	0.86
1:A:196:GLU:OE2	1:A:207:LYS:HE2	1.74	0.86
1:B:688:LEU:HD12	1:B:728:ILE:HD11	1.55	0.86
1:A:21:VAL:O	1:A:36:LEU:HD12	1.73	0.86
1:A:700:PRO:C	1:A:703:VAL:HB	1.95	0.86
1:B:9:THR:HG21	1:B:11:HIS:HE1	1.40	0.86
1:B:201:ARG:N	1:B:202:PRO:CD	2.38	0.86
1:A:775:LEU:HD23	1:A:777:THR:CG2	2.05	0.85
1:B:682:LEU:O	1:B:752:TYR:OH	1.95	0.85
1:B:732:TRP:HB2	1:B:751:HIS:CD2	2.11	0.85
2:T:812:DC:H2'	2:T:813:DT:C5	2.10	0.85
1:A:732:TRP:CG	1:A:751:HIS:CD2	2.64	0.85
1:B:212:PHE:HD1	1:B:272:ARG:HH12	1.22	0.85
1:B:654:LEU:O	1:B:658:ARG:HG3	1.76	0.85
1:B:316:GLU:CD	1:B:319:ARG:HH21	1.79	0.85
1:B:543:TYR:CD2	1:B:550:PHE:CE2	2.63	0.85
1:B:600:ARG:HD3	1:B:657:PHE:O	1.76	0.85
1:B:266:PHE:C	1:B:266:PHE:HD2	1.78	0.85
2:T:819:DC:H2"	2:T:820:DA:H5'	1.57	0.85
1:B:417:VAL:HG12	1:B:595:GLU:HB2	1.56	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:THR:HG22	1:B:735:ASN:H	1.41	0.85
1:B:233:LEU:HD12	1:B:233:LEU:N	1.92	0.85
1:B:467:PRO:O	1:B:471:THR:HG23	1.75	0.85
1:B:642:THR:CB	1:B:756:GLN:HE22	1.63	0.85
1:A:658:ARG:HH12	1:A:660:GLU:CD	1.80	0.84
1:B:180:MET:O	1:B:198:VAL:HG23	1.77	0.84
1:B:755:ARG:HE	1:B:755:ARG:CA	1.89	0.84
3:P:902:DT:H2"	3:P:903:DG:O4'	1.78	0.84
1:A:751:HIS:ND1	1:A:755:ARG:HG2	1.92	0.84
1:B:231:ARG:HD2	1:B:265:PHE:CZ	2.12	0.84
1:B:584:GLN:O	1:B:585:ARG:HB2	1.77	0.84
1:B:600:ARG:HB3	1:B:600:ARG:CZ	2.04	0.84
1:A:636:THR:OG1	1:A:649:GLN:OE1	1.93	0.84
1:B:464:HIS:CB	1:B:468:GLU:OE1	2.26	0.84
1:A:160:THR:CG2	1:A:162:HIS:H	1.87	0.84
1:B:485:ASN:O	1:B:487:PRO:CD	2.24	0.84
1:B:509:ARG:O	1:B:510:PHE:HB2	1.77	0.84
1:A:312:ASP:O	1:A:313:ARG:HB2	1.74	0.84
1:A:348:ILE:CG2	1:A:349:MET:N	2.40	0.84
1:B:751:HIS:O	1:B:755:ARG:HB3	1.77	0.84
1:A:482:ARG:O	1:A:483:GLN:HB2	1.76	0.84
1:A:600:ARG:HG2	1:A:600:ARG:NH1	1.89	0.84
1:B:83:CYS:CB	1:B:88:GLN:HE21	1.90	0.84
1:A:419:ASP:OD2	1:A:595:GLU:OE1	1.95	0.84
1:B:466:LEU:CD1	1:B:470:VAL:CG2	2.55	0.84
2:T:818:DA:N6	3:P:902:DT:O4	2.11	0.84
1:B:436:VAL:HG13	1:B:437:GLY:N	1.93	0.83
1:B:636:THR:HG22	1:B:637:VAL:HG23	1.59	0.83
1:A:405:MET:HE3	1:A:544:GLY:HA3	1.60	0.83
1:B:531:LYS:HG3	1:B:532:ALA:N	1.92	0.83
3:P:901:DG:H2"	3:P:902:DT:C7	2.05	0.83
1:B:563:ALA:O	1:B:567:ARG:HG3	1.79	0.83
1:A:348:ILE:HG22	1:A:349:MET:N	1.92	0.83
1:A:485:ASN:O	1:A:487:PRO:HD2	1.78	0.83
1:B:484:GLY:HA2	1:B:485:ASN:HB3	1.60	0.83
1:B:83:CYS:HB3	1:B:88:GLN:NE2	1.93	0.82
1:A:722:TYR:CE1	1:A:728:ILE:HG13	2.14	0.82
1:B:212:PHE:HD1	1:B:272:ARG:NH1	1.77	0.82
1:B:750:GLU:O	1:B:754:THR:HG22	1.78	0.82
1:B:748:ASP:O	1:B:751:HIS:HB3	1.78	0.82
1:A:722:TYR:OH	1:A:728:ILE:HG13	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:816:DG:O6	3:P:904:DC:N4	2.09	0.82
3:P:901:DG:C2'	3:P:902:DT:H73	2.04	0.82
1:B:55:HIS:O	1:B:58:GLN:HG2	1.79	0.82
1:A:772:PHE:N	1:A:773:ALA:CB	2.37	0.82
1:B:256:ARG:O	1:B:266:PHE:O	1.96	0.82
1:B:642:THR:HB	1:B:756:GLN:HE22	0.99	0.81
1:B:734:THR:HB	1:B:746:PRO:HG2	1.61	0.81
1:B:755:ARG:O	1:B:755:ARG:HD3	1.80	0.81
1:A:446:ASP:OD2	1:A:449:HIS:CD2	2.33	0.81
1:A:562:ALA:CB	1:A:597:HIS:CD2	2.63	0.81
1:B:454:PHE:CG	1:B:521:MET:HE2	2.14	0.81
1:A:419:ASP:CB	1:A:595:GLU:OE1	2.29	0.81
1:A:713:ASN:ND2	1:A:742:TYR:CE2	2.48	0.81
1:A:499:PHE:O	1:A:502:VAL:CG2	2.28	0.81
1:B:349:MET:HB3	1:B:350:PRO:CD	2.10	0.81
1:A:321:PHE:CD2	1:A:321:PHE:O	2.34	0.81
1:A:383:ARG:HH11	1:A:383:ARG:CG	1.92	0.81
1:B:539:TYR:OH	1:B:565:ILE:HG21	1.79	0.81
2:T:820:DA:H3'	2:T:820:DA:OP2	1.80	0.81
1:A:499:PHE:O	1:A:502:VAL:HG23	1.80	0.81
2:T:813:DT:C2'	2:T:814:DA:C8	2.62	0.81
1:A:485:ASN:OD1	1:A:487:PRO:CD	2.28	0.81
1:A:712:GLU:C	1:A:714:GLN:H	1.80	0.81
1:B:430:THR:OG1	1:B:589:ALA:CB	2.28	0.81
1:A:468:GLU:HA	1:A:471:THR:HG23	1.63	0.81
2:T:812:DC:C2'	2:T:813:DT:C5	2.64	0.81
1:A:64:ARG:CB	1:A:64:ARG:NH1	2.45	0.80
1:A:139:ARG:C	1:A:140:LEU:HD12	2.02	0.80
1:B:7:ILE:HG12	1:B:7:ILE:O	1.81	0.80
1:B:0:HIS:CD2	1:B:1:MET:H	1.97	0.80
1:A:49:GLN:NE2	1:A:101:VAL:HA	1.96	0.80
1:A:376:LEU:N	1:A:376:LEU:HD12	1.95	0.80
1:A:713:ASN:ND2	1:A:742:TYR:HE2	1.79	0.80
1:A:654:LEU:HD12	1:A:654:LEU:C	2.01	0.80
1:B:407:SER:C	1:B:409:PRO:HD3	2.00	0.80
1:A:481:LYS:HB3	1:A:481:LYS:HZ3	1.46	0.80
1:B:644:LEU:CD1	1:B:757:LEU:HD11	2.10	0.80
1:B:586:LEU:N	1:B:586:LEU:CD1	2.45	0.80
1:B:699:VAL:HG23	1:B:700:PRO:O	1.82	0.80
1:B:753:LEU:HG	1:B:754:THR:N	1.96	0.80
1:B:758:GLN:N	1:B:759:PRO:CD	2.44	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:913:DG:H2'	3:P:913:DG:P	2.21	0.80
1:A:64:ARG:HH11	1:A:64:ARG:CB	1.94	0.80
1:A:1:MET:O	1:A:1:MET:HG3	1.80	0.79
1:A:166:TYR:OH	1:A:318:ASP:OD1	1.99	0.79
1:A:688:LEU:CB	1:A:726:GLY:N	2.33	0.79
1:B:466:LEU:HD12	1:B:466:LEU:O	1.82	0.79
1:B:642:THR:CA	1:B:756:GLN:HE22	1.94	0.79
1:A:692:LEU:CD1	1:A:723:GLN:HA	2.11	0.79
1:B:413:ASP:CA	1:B:599:CYS:O	2.31	0.79
1:A:751:HIS:CE1	1:A:755:ARG:CG	2.61	0.79
1:B:454:PHE:HB3	1:B:521:MET:CE	2.12	0.79
1:A:112:GLU:O	1:A:116:MET:HB2	1.81	0.79
1:B:266:PHE:CD2	1:B:266:PHE:O	2.36	0.79
1:B:688:LEU:O	1:B:725:ARG:HG3	1.83	0.79
1:A:159:THR:HG22	1:A:165:LEU:HA	1.63	0.79
1:A:775:LEU:HD23	1:A:777:THR:HG21	1.65	0.79
1:B:454:PHE:HD1	1:B:521:MET:CE	1.94	0.79
2:T:819:DC:H2"	2:T:820:DA:O4'	1.82	0.79
1:A:358:VAL:HG11	1:A:495:ILE:HD13	1.65	0.79
1:A:408:ARG:NH2	1:A:540:ASP:OD2	2.16	0.79
1:B:416:LEU:CB	1:B:551:VAL:CG1	2.60	0.79
1:B:753:LEU:HD11	1:B:758:GLN:HG3	1.62	0.79
1:B:130:MET:CE	1:B:133:GLY:HA2	2.13	0.78
1:A:744:ARG:HG2	1:A:744:ARG:HH11	1.47	0.78
1:B:413:ASP:CB	1:B:599:CYS:O	2.31	0.78
1:B:567:ARG:O	1:B:570:VAL:HG22	1.83	0.78
1:A:738:GLU:OE2	1:A:745:SER:OG	2.01	0.78
1:B:63:PHE:HD1	1:B:64:ARG:N	1.81	0.78
1:B:232:MET:O	1:B:236:HIS:HD2	1.66	0.78
1:B:485:ASN:OD1	1:B:487:PRO:CD	2.31	0.78
1:A:658:ARG:NH1	1:A:660:GLU:CD	2.37	0.78
1:B:48:ASP:HB3	1:B:76:GLN:HE21	1.47	0.78
1:B:710:ASP:OD2	1:B:720:LEU:HB3	1.83	0.78
1:A:89:LEU:O	1:A:93:GLU:HG2	1.83	0.78
1:A:772:PHE:N	1:A:772:PHE:HD2	1.78	0.78
1:B:354:GLU:HG2	1:B:488:LEU:HB3	1.65	0.78
1:A:444:GLN:N	1:A:445:PRO:CD	2.46	0.78
1:A:690:ARG:O	1:A:725:ARG:N	2.16	0.78
1:A:692:LEU:HD21	1:A:722:TYR:O	1.84	0.78
1:B:429:ARG:NE	1:B:471:THR:HG22	1.98	0.78
1:A:21:VAL:O	1:A:36:LEU:HD11	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:OE1	1:A:139:ARG:NH2	2.14	0.78
1:A:127:GLU:CD	1:A:139:ARG:HH21	1.87	0.78
1:A:690:ARG:HG3	1:A:691:PRO:N	1.99	0.78
1:B:747:LEU:CD2	1:B:747:LEU:N	2.34	0.78
1:A:481:LYS:NZ	1:A:481:LYS:HB3	1.96	0.77
2:T:818:DA:H4'	2:T:818:DA:OP1	1.81	0.77
1:A:540:ASP:OD1	1:A:554:LYS:CE	2.32	0.77
1:A:734:THR:CG2	1:A:735:ASN:OD1	2.32	0.77
1:B:451:THR:HG21	1:B:586:LEU:HD21	1.64	0.77
1:A:161:ARG:HB3	1:A:314:MET:CE	2.13	0.77
1:A:768:ILE:O	1:A:769:GLU:CB	2.32	0.77
1:B:234:GLN:OE1	1:B:255:TRP:NE1	2.17	0.77
1:B:733:THR:CB	1:B:746:PRO:O	2.32	0.77
2:T:812:DC:H2'	2:T:813:DT:H73	1.65	0.77
1:A:467:PRO:O	1:A:471:THR:CG2	2.32	0.77
1:A:502:VAL:HG23	1:A:503:LEU:H	1.50	0.77
1:A:687:ARG:HA	1:A:727:THR:HA	1.65	0.77
1:A:772:PHE:N	1:A:772:PHE:CD2	2.49	0.77
1:B:164:GLU:HG2	1:B:201:ARG:NH1	1.99	0.77
1:B:257:GLU:CG	1:B:265:PHE:HA	2.12	0.77
1:B:431:PHE:CZ	1:B:522:ARG:HD3	2.19	0.77
1:B:696:GLN:OE1	1:B:696:GLN:CA	2.32	0.77
1:B:703:VAL:CG1	1:B:704:ARG:N	2.47	0.77
1:A:127:GLU:CD	1:A:139:ARG:NH2	2.38	0.77
1:A:620:LEU:HD22	1:A:657:PHE:HB3	1.67	0.77
1:B:430:THR:OG1	1:B:589:ALA:N	2.17	0.77
1:A:654:LEU:O	1:A:658:ARG:HG3	1.84	0.77
1:A:689:ARG:O	1:A:690:ARG:HB2	1.84	0.77
1:B:130:MET:CE	1:B:133:GLY:CA	2.63	0.77
1:B:175:GLN:OE1	1:B:215:TYR:HE1	1.68	0.77
1:B:541:VAL:O	1:B:541:VAL:HG12	1.82	0.77
1:A:485:ASN:C	1:A:487:PRO:CD	2.53	0.76
1:A:577:TRP:O	1:A:581:LEU:HD12	1.85	0.76
1:B:200:SER:HB2	1:B:202:PRO:CD	2.07	0.76
1:B:231:ARG:CD	1:B:265:PHE:CZ	2.66	0.76
1:B:376:LEU:N	1:B:376:LEU:HD12	1.99	0.76
1:B:750:GLU:O	1:B:754:THR:HG23	1.82	0.76
1:A:284:ALA:O	1:A:285:PHE:HB2	1.86	0.76
1:B:229:ASP:O	1:B:233:LEU:HD12	1.85	0.76
1:B:543:TYR:CD2	1:B:550:PHE:CD2	2.71	0.76
1:B:351:PHE:HE2	1:B:352:LEU:CD2	1.98	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:MET:HE2	1:B:458:TRP:HB2	1.67	0.76
1:B:485:ASN:HD21	1:B:488:LEU:HD23	1.47	0.76
1:B:500:TYR:HD2	1:B:501:GLY:N	1.83	0.76
1:A:408:ARG:HH11	1:A:408:ARG:HG2	0.70	0.76
1:B:656:ILE:HD12	1:B:764:ILE:HD13	1.67	0.76
1:B:434:ASP:OD2	1:B:436:VAL:CG1	2.33	0.76
1:B:466:LEU:O	1:B:470:VAL:HG23	1.85	0.76
1:A:481:LYS:CB	1:A:481:LYS:HZ2	1.96	0.76
1:B:416:LEU:HB2	1:B:551:VAL:HG13	1.67	0.76
1:B:0:HIS:O	1:B:1:MET:CG	2.34	0.76
1:B:418:LEU:H	1:B:418:LEU:CD1	1.88	0.76
1:B:495:ILE:O	1:B:498:ALA:CB	2.34	0.76
3:P:903:DG:OP1	3:P:903:DG:H4'	1.85	0.76
1:B:682:LEU:HD22	1:B:752:TYR:CD1	2.20	0.76
1:B:201:ARG:N	1:B:202:PRO:HD3	2.01	0.76
2:T:819:DC:H1'	2:T:820:DA:H5'	1.68	0.76
3:P:905:DC:H2'	3:P:906:DT:H72	1.66	0.75
1:A:94:LYS:O	1:A:98:GLU:CG	2.31	0.75
1:A:600:ARG:NE	1:A:657:PHE:O	2.19	0.75
1:A:140:LEU:HD12	1:A:140:LEU:N	2.02	0.75
1:B:642:THR:HB	1:B:756:GLN:HE21	0.93	0.75
2:T:819:DC:C2'	2:T:820:DA:H2'	2.16	0.75
1:A:9:THR:OG1	1:A:11:HIS:CE1	2.40	0.75
1:B:551:VAL:CG1	1:B:551:VAL:O	2.35	0.75
1:B:692:LEU:HD13	1:B:723:GLN:HA	1.68	0.75
1:B:733:THR:HG22	1:B:734:THR:N	2.01	0.75
2:T:819:DC:C1'	2:T:820:DA:H5'	2.16	0.75
1:B:669:THR:HA	1:B:672:LYS:HG3	1.68	0.75
1:A:397:HIS:CD2	1:A:399:SER:N	2.54	0.75
1:B:224:ASN:N	1:B:276:ASP:OD2	2.18	0.75
1:B:440:GLU:OE2	1:B:463:LYS:CE	2.35	0.75
1:B:688:LEU:HD11	1:B:728:ILE:HD13	1.65	0.75
1:A:234:GLN:OE1	1:A:255:TRP:CD1	2.40	0.75
1:B:229:ASP:O	1:B:233:LEU:HD13	1.87	0.75
1:B:415:VAL:CG1	1:B:601:PHE:CB	2.64	0.75
1:A:298:GLN:HB2	1:A:303:GLU:O	1.85	0.75
1:A:386:TYR:OH	1:A:440:GLU:OE2	2.02	0.75
1:A:455:LEU:HD12	1:A:455:LEU:N	2.01	0.75
1:A:482:ARG:O	1:A:482:ARG:CD	2.35	0.75
1:A:686:LYS:O	1:A:727:THR:HG22	1.86	0.75
1:B:694:GLU:O	1:B:694:GLU:CG	2.34	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:HIS:CD2	1:A:398:ALA:N	2.53	0.74
1:A:400:PRO:HG2	1:A:401:GLY:N	2.03	0.74
1:B:231:ARG:HD2	1:B:265:PHE:HE1	0.71	0.74
1:B:63:PHE:CD1	1:B:64:ARG:N	2.55	0.74
3:P:911:DT:H2"	3:P:912:DA:C8	2.22	0.74
1:A:232:MET:CE	1:A:235:LYS:NZ	2.50	0.74
1:A:355:ARG:HG2	1:A:356:ALA:N	2.02	0.74
1:A:365:ARG:HH11	1:A:365:ARG:HG3	1.51	0.74
1:B:450:SER:CB	1:B:458:TRP:CE3	2.69	0.74
1:A:634:LEU:O	1:A:637:VAL:HB	1.88	0.74
1:B:177:ILE:HG13	1:B:194:GLU:HB2	1.68	0.74
1:A:744:ARG:HG2	1:A:744:ARG:NH1	2.00	0.74
1:A:642:THR:CG2	1:A:681:ARG:O	2.35	0.74
1:B:524:HIS:O	1:B:528:ARG:CD	2.36	0.74
1:A:647:GLN:O	1:A:651:GLU:HG3	1.87	0.74
1:B:60:GLU:CG	1:B:92:TYR:OH	2.35	0.74
1:B:48:ASP:HB3	1:B:76:GLN:HE22	1.52	0.74
1:B:113:ARG:NH1	1:B:113:ARG:HG3	2.01	0.74
1:A:64:ARG:HG3	1:A:64:ARG:NH1	1.94	0.73
2:T:819:DC:H2"	2:T:820:DA:C2'	2.17	0.73
1:B:415:VAL:HG23	1:B:551:VAL:O	1.88	0.73
1:B:699:VAL:O	1:B:699:VAL:CG2	2.33	0.73
1:B:703:VAL:O	1:B:706:ALA:HB3	1.88	0.73
2:T:812:DC:C2'	2:T:813:DT:C7	2.65	0.73
1:B:755:ARG:NE	1:B:755:ARG:CA	2.43	0.73
1:A:529:GLN:HG3	1:A:533:LEU:HD13	1.70	0.73
1:B:342:ILE:O	1:B:346:THR:HG23	1.88	0.73
1:B:660:GLU:HB3	1:B:661:PRO:HD2	1.71	0.73
1:B:690:ARG:HB3	1:B:694:GLU:OE2	1.89	0.73
1:A:146:TYR:O	1:A:147:ARG:NH1	2.20	0.73
1:A:193:PHE:CG	1:A:333:LEU:HD12	2.24	0.73
1:B:487:PRO:CD	1:B:488:LEU:H	2.02	0.73
1:B:733:THR:HA	1:B:747:LEU:CA	2.14	0.73
1:A:105:GLU:OE2	1:A:382:HIS:HE1	1.71	0.73
1:A:255:TRP:HE3	1:A:266:PHE:O	1.70	0.73
1:B:159:THR:OG1	1:B:163:GLY:HA2	1.89	0.73
1:B:55:HIS:O	1:B:58:GLN:CG	2.37	0.72
1:B:642:THR:HG22	1:B:644:LEU:H	1.54	0.72
1:A:49:GLN:NE2	1:A:101:VAL:HG13	2.04	0.72
1:A:688:LEU:HB2	1:A:726:GLY:CA	2.18	0.72
1:B:248:ARG:O	1:B:249:ASP:HB3	1.89	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HG12	1:B:601:PHE:HB3	1.69	0.72
1:A:732:TRP:CB	1:A:751:HIS:HD2	2.02	0.72
1:B:1:MET:HA	1:B:1:MET:CE	2.17	0.72
1:B:733:THR:N	1:B:736:GLY:O	2.22	0.72
1:A:159:THR:HB	1:A:164:GLU:O	1.88	0.72
1:A:689:ARG:O	1:A:690:ARG:CB	2.35	0.72
1:B:732:TRP:O	1:B:747:LEU:HA	1.88	0.72
1:A:326:PRO:O	1:A:330:THR:HG22	1.89	0.72
1:A:664:GLU:O	1:A:668:GLU:HG3	1.89	0.72
1:A:712:GLU:C	1:A:714:GLN:N	2.39	0.72
1:A:734:THR:HG22	1:A:735:ASN:N	2.03	0.72
1:B:430:THR:OG1	1:B:589:ALA:HB3	1.89	0.72
1:B:591:GLU:HG2	1:B:591:GLU:O	1.87	0.72
1:B:747:LEU:O	1:B:747:LEU:CD2	2.34	0.72
1:A:380:ARG:HD2	1:A:469:ILE:HG12	1.72	0.72
1:B:120:ILE:HG22	1:B:121:THR:N	2.04	0.72
1:A:577:TRP:O	1:A:581:LEU:CD1	2.37	0.72
1:B:113:ARG:CG	1:B:113:ARG:HH11	2.02	0.72
1:B:175:GLN:CD	1:B:215:TYR:CE1	2.63	0.72
1:B:351:PHE:CD2	1:B:352:LEU:HD23	2.22	0.72
1:B:629:MET:HE1	1:B:657:PHE:HE2	1.54	0.72
1:A:482:ARG:O	1:A:482:ARG:CG	2.33	0.72
1:A:316:GLU:OE1	1:A:316:GLU:CA	2.38	0.72
1:B:481:LYS:HD3	1:B:481:LYS:C	2.05	0.72
1:A:324:ASP:OD2	1:A:327:ALA:CB	2.38	0.72
1:B:248:ARG:O	1:B:249:ASP:CB	2.35	0.72
1:B:476:GLY:O	1:B:480:ALA:CB	2.38	0.72
1:B:334:LYS:O	1:B:338:LEU:CD2	2.32	0.71
1:B:454:PHE:HB3	1:B:521:MET:HE2	1.71	0.71
1:A:37:ALA:O	1:A:39:GLN:NE2	2.23	0.71
1:A:311:TRP:C	1:A:312:ASP:OD1	2.29	0.71
1:B:121:THR:CG2	1:B:123:PRO:HD2	2.20	0.71
1:B:421:LYS:O	1:B:422:SER:C	2.26	0.71
1:B:416:LEU:CB	1:B:551:VAL:HG11	2.18	0.71
1:B:454:PHE:HD1	1:B:521:MET:HE3	1.54	0.71
1:A:298:GLN:NE2	1:A:303:GLU:O	2.23	0.71
1:A:454:PHE:C	1:A:455:LEU:CD1	2.59	0.71
1:B:625:ASP:O	1:B:626:LYS:CG	2.39	0.71
1:B:703:VAL:HG13	1:B:704:ARG:N	2.04	0.71
1:A:292:SER:O	1:A:296:VAL:CG2	2.31	0.71
1:B:417:VAL:O	1:B:595:GLU:HB2	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:LEU:CD2	1:B:593:GLU:N	2.52	0.71
1:A:171:GLU:OE1	1:A:340:THR:HG21	1.89	0.71
1:A:277:GLY:O	1:A:281:LEU:HB2	1.91	0.71
1:A:479:GLU:HA	1:A:479:GLU:OE2	1.90	0.71
1:A:571:GLN:OE1	1:A:572:HIS:N	2.24	0.71
1:A:654:LEU:C	1:A:654:LEU:CD1	2.58	0.71
1:B:113:ARG:HG3	1:B:113:ARG:HH11	1.56	0.71
1:B:485:ASN:ND2	1:B:488:LEU:HD23	2.05	0.71
1:B:9:THR:HG22	1:B:11:HIS:CE1	2.26	0.71
1:B:359:ASN:ND2	1:B:361:LEU:HB2	2.05	0.71
1:B:750:GLU:OE1	1:B:754:THR:CG2	2.39	0.71
1:A:21:VAL:HB	1:A:36:LEU:HD13	1.72	0.71
1:B:584:GLN:CB	1:B:586:LEU:HD13	2.21	0.71
1:B:669:THR:HA	1:B:672:LYS:CG	2.20	0.71
3:P:907:DA:H2"	3:P:908:DG:O5'	1.90	0.71
1:B:415:VAL:HG11	1:B:601:PHE:CG	2.26	0.71
1:A:358:VAL:CG1	1:A:495:ILE:CD1	2.67	0.70
1:A:600:ARG:HD3	1:A:657:PHE:O	1.91	0.70
1:B:600:ARG:CD	1:B:657:PHE:O	2.38	0.70
1:B:753:LEU:HD11	1:B:758:GLN:CG	2.21	0.70
2:T:817:DC:H2'	2:T:818:DA:O4'	1.89	0.70
1:A:549:THR:O	1:A:550:PHE:CD2	2.42	0.70
1:B:381:MET:HE3	1:B:388:ALA:CA	2.20	0.70
1:B:381:MET:CE	1:B:388:ALA:HB2	2.21	0.70
1:B:487:PRO:HD2	1:B:488:LEU:H	1.57	0.70
1:A:477:ARG:HD2	1:A:477:ARG:C	2.10	0.70
1:B:764:ILE:O	1:B:764:ILE:HG12	1.90	0.70
1:A:351:PHE:CE2	1:A:352:LEU:HD12	2.26	0.70
1:A:688:LEU:O	1:A:726:GLY:N	2.25	0.70
1:B:495:ILE:C	1:B:495:ILE:CD1	2.42	0.70
1:B:592:LEU:C	1:B:592:LEU:CD2	2.58	0.70
2:T:815:DG:H2"	2:T:816:DG:O5'	1.92	0.70
1:A:636:THR:CG2	1:A:650:GLN:OE1	2.40	0.70
1:B:528:ARG:O	1:B:531:LYS:CG	2.36	0.70
1:A:128:GLY:HA3	1:A:135:ILE:HG23	1.72	0.70
1:A:117:GLU:OE2	1:A:382:HIS:HD2	1.74	0.70
1:A:394:VAL:HG13	1:A:395:PRO:HD2	1.72	0.70
1:A:549:THR:C	1:A:550:PHE:CD2	2.63	0.70
1:B:60:GLU:HG2	1:B:92:TYR:CZ	2.25	0.70
1:B:469:ILE:O	1:B:473:ILE:HG13	1.92	0.70
1:B:586:LEU:HD12	1:B:586:LEU:H	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ASN:OD1	1:A:487:PRO:HG2	1.92	0.70
1:A:197:TYR:HE1	1:A:325:LYS:HD3	1.56	0.69
1:B:264:VAL:CG2	1:B:264:VAL:O	2.39	0.69
1:B:376:LEU:H	1:B:376:LEU:HD13	1.56	0.69
1:A:692:LEU:CD1	1:A:723:GLN:O	2.40	0.69
1:A:724:ASN:ND2	1:A:724:ASN:N	2.33	0.69
1:B:200:SER:CB	1:B:202:PRO:CD	2.69	0.69
1:B:753:LEU:C	1:B:753:LEU:CD1	2.43	0.69
1:B:214:ASN:HB3	1:B:215:TYR:CD2	2.27	0.69
1:B:706:ALA:HB2	1:B:728:ILE:HD12	1.74	0.69
1:A:405:MET:CE	1:A:544:GLY:HA3	2.22	0.69
1:A:481:LYS:O	1:A:482:ARG:C	2.31	0.69
1:A:517:SER:O	1:A:521:MET:HB2	1.93	0.69
1:A:771:ASN:C	1:A:773:ALA:CB	2.59	0.69
1:B:1:MET:HA	1:B:1:MET:HE3	1.73	0.69
1:A:160:THR:CG2	1:A:161:ARG:N	2.55	0.69
1:A:218:ASP:OD1	1:A:248:ARG:NH2	2.16	0.69
1:A:421:LYS:O	1:A:422:SER:C	2.29	0.69
1:B:584:GLN:O	1:B:586:LEU:CD1	2.40	0.69
1:B:731:VAL:HG12	1:B:732:TRP:N	2.06	0.69
1:A:398:ALA:O	1:A:399:SER:C	2.29	0.69
1:B:733:THR:HG22	1:B:735:ASN:N	2.07	0.69
1:A:110:PRO:HB2	1:A:111:PRO:HD3	1.75	0.69
1:A:751:HIS:HE1	1:A:755:ARG:HG2	1.48	0.69
1:B:249:ASP:C	1:B:250:ASN:HD22	1.95	0.69
1:B:745:SER:HB2	1:B:746:PRO:CD	2.22	0.69
1:B:751:HIS:O	1:B:755:ARG:HB2	1.91	0.69
1:A:686:LYS:O	1:A:727:THR:CG2	2.41	0.69
1:B:229:ASP:O	1:B:233:LEU:HD11	1.93	0.69
1:B:522:ARG:O	1:B:526:ILE:HG13	1.93	0.69
1:B:570:VAL:CG2	1:B:571:GLN:N	2.55	0.69
1:B:672:LYS:O	1:B:677:GLU:CB	2.37	0.69
1:A:50:VAL:HG21	1:A:79:TYR:CD1	2.27	0.69
1:A:724:ASN:HD22	1:A:724:ASN:N	1.73	0.68
1:B:376:LEU:N	1:B:376:LEU:HD13	2.09	0.68
1:A:140:LEU:N	1:A:140:LEU:CD1	2.56	0.68
1:B:747:LEU:HD23	1:B:747:LEU:N	1.93	0.68
1:A:351:PHE:CD2	1:A:351:PHE:C	2.67	0.68
1:B:233:LEU:CD1	1:B:233:LEU:H	2.05	0.68
1:B:234:GLN:OE1	1:B:255:TRP:CD1	2.46	0.68
1:B:768:ILE:O	1:B:769:GLU:CG	2.42	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:GLU:OE1	1:B:84:ARG:NH1	2.26	0.68
1:B:434:ASP:OD2	1:B:436:VAL:HG13	1.93	0.68
1:A:351:PHE:HD2	1:A:352:LEU:CD1	2.05	0.68
1:B:9:THR:HG21	1:B:11:HIS:NE2	2.08	0.68
1:B:720:LEU:HD13	1:B:720:LEU:N	2.08	0.68
1:B:485:ASN:ND2	1:B:488:LEU:CD2	2.56	0.68
1:B:601:PHE:HE2	1:B:603:MET:HB3	1.57	0.68
1:B:750:GLU:OE1	1:B:754:THR:HG21	1.93	0.68
3:P:902:DT:H2"	3:P:903:DG:OP1	1.94	0.68
1:A:748:ASP:C	1:A:748:ASP:OD1	2.32	0.68
1:A:312:ASP:OD1	1:A:312:ASP:N	2.26	0.68
1:A:333:LEU:O	1:A:337:GLU:HG3	1.94	0.68
1:B:647:GLN:O	1:B:651:GLU:HG3	1.93	0.68
1:A:64:ARG:NH1	1:A:64:ARG:HB2	2.09	0.68
1:A:321:PHE:CD2	1:A:321:PHE:C	2.68	0.68
1:A:376:LEU:HD13	1:A:376:LEU:H	1.59	0.68
1:B:407:SER:O	1:B:409:PRO:CD	2.38	0.68
1:B:592:LEU:HD23	1:B:593:GLU:CA	2.24	0.68
1:A:449:HIS:O	1:A:450:SER:OG	2.11	0.67
1:A:716:ARG:O	1:A:717:GLY:C	2.30	0.67
1:B:0:HIS:O	1:B:1:MET:CB	2.42	0.67
1:B:198:VAL:CG2	1:B:204:LEU:CD2	2.71	0.67
1:A:479:GLU:OE2	1:A:479:GLU:CA	2.42	0.67
1:A:549:THR:HG22	1:A:550:PHE:N	2.08	0.67
1:B:160:THR:HG21	1:B:164:GLU:HB3	1.76	0.67
1:B:234:GLN:O	1:B:238:GLU:HG3	1.95	0.67
1:B:381:MET:HE1	1:B:388:ALA:HB2	1.75	0.67
1:A:118:ARG:NH1	1:A:140:LEU:O	2.27	0.67
1:B:316:GLU:CD	1:B:319:ARG:NH2	2.48	0.67
2:T:811:DG:H2"	2:T:812:DC:O5'	1.93	0.67
1:B:143:HIS:CD2	1:B:144:PRO:HD2	2.29	0.67
1:B:466:LEU:HD11	1:B:470:VAL:HG22	1.76	0.67
1:B:636:THR:CG2	1:B:637:VAL:HG23	2.25	0.67
1:B:714:GLN:HG3	1:B:715:LYS:N	2.06	0.67
3:P:908:DG:H2"	3:P:909:DC:O5'	1.94	0.67
1:A:15:THR:HB	1:A:16:PRO:HD2	1.77	0.67
1:A:42:VAL:HG23	1:A:82:TYR:CD1	2.29	0.67
1:B:196:GLU:OE2	1:B:207:LYS:HE2	1.93	0.67
1:B:428:ILE:CD1	1:B:519:ILE:CD1	2.50	0.67
1:B:584:GLN:HB3	1:B:586:LEU:HD11	1.76	0.67
1:A:692:LEU:CD1	1:A:723:GLN:C	2.63	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:PRO:O	1:A:746:PRO:HG2	1.94	0.67
1:A:482:ARG:C	1:A:482:ARG:HD2	2.15	0.67
1:B:638:ARG:HG2	1:B:641:TRP:CD1	2.29	0.67
1:A:49:GLN:HE22	1:A:101:VAL:HA	1.57	0.67
1:A:203:GLN:HA	1:A:206:GLU:HG2	1.77	0.67
1:B:198:VAL:HG21	1:B:204:LEU:HD23	1.75	0.67
1:B:584:GLN:C	1:B:586:LEU:CD1	2.62	0.67
1:A:294:GLU:N	1:A:294:GLU:OE1	2.28	0.67
1:A:692:LEU:CD1	1:A:722:TYR:O	2.40	0.67
1:B:91:ASN:C	1:B:91:ASN:OD1	2.34	0.67
1:B:411:LEU:HD13	1:B:412:TYR:N	2.09	0.67
1:B:485:ASN:O	1:B:485:ASN:CG	2.30	0.67
1:A:294:GLU:H	1:A:294:GLU:CD	1.98	0.66
1:B:625:ASP:O	1:B:626:LYS:HG2	1.95	0.66
1:B:543:TYR:O	1:B:550:PHE:N	2.26	0.66
3:P:910:DG:H2'	3:P:911:DT:C6	2.29	0.66
1:A:200:SER:OG	1:A:202:PRO:CD	2.42	0.66
1:B:257:GLU:HG2	1:B:265:PHE:HB3	1.76	0.66
1:A:316:GLU:OE1	1:A:319:ARG:NH1	2.29	0.66
1:A:758:GLN:HB3	1:A:759:PRO:CD	2.25	0.66
1:B:411:LEU:HD22	1:B:602:LEU:HB2	1.77	0.66
1:B:485:ASN:OD1	1:B:487:PRO:CG	2.43	0.66
1:B:442:MET:CE	1:B:458:TRP:HB2	2.25	0.66
1:A:772:PHE:H	1:A:773:ALA:HB2	1.56	0.66
1:B:629:MET:HE1	1:B:657:PHE:CE2	2.29	0.66
1:B:638:ARG:HG2	1:B:641:TRP:HD1	1.61	0.66
1:A:355:ARG:CG	1:A:356:ALA:N	2.58	0.66
1:B:623:GLU:OE1	1:B:628:ARG:NH1	2.29	0.66
1:A:179:TYR:CE1	1:A:207:LYS:HD2	2.31	0.66
1:A:376:LEU:N	1:A:376:LEU:HD13	2.09	0.66
1:B:121:THR:HG23	1:B:123:PRO:HD2	1.76	0.66
1:B:698:ASN:C	1:B:698:ASN:OD1	2.34	0.66
1:A:454:PHE:O	1:A:455:LEU:HB2	1.95	0.66
1:B:644:LEU:CD1	1:B:757:LEU:CD1	2.66	0.66
1:B:733:THR:HG23	1:B:734:THR:H	1.60	0.66
1:A:83:CYS:SG	1:A:89:LEU:CD2	2.84	0.66
1:B:94:LYS:HG3	1:B:95:ARG:N	2.10	0.66
1:B:539:TYR:OH	1:B:565:ILE:CG2	2.44	0.66
1:B:642:THR:CB	1:B:756:GLN:HE21	1.77	0.66
1:B:688:LEU:O	1:B:725:ARG:CG	2.43	0.66
1:A:284:ALA:HB2	1:A:348:ILE:HD11	1.76	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:GLU:OE1	1:A:628:ARG:NH2	2.30	0.65
1:B:466:LEU:HD12	1:B:466:LEU:C	2.15	0.65
1:B:516:ALA:O	1:B:519:ILE:HB	1.96	0.65
1:B:699:VAL:CG2	1:B:704:ARG:CD	2.72	0.65
1:B:753:LEU:O	1:B:753:LEU:CD1	2.34	0.65
1:A:232:MET:HE1	1:A:235:LYS:NZ	2.11	0.65
1:A:648:PHE:HD2	1:A:760:VAL:HG21	1.61	0.65
1:B:673:LEU:O	1:B:676:GLY:N	2.29	0.65
1:B:724:ASN:HD22	1:B:724:ASN:N	1.89	0.65
2:T:812:DC:H2"	2:T:813:DT:C5	2.32	0.65
1:B:215:TYR:CD2	1:B:215:TYR:N	2.64	0.65
1:A:482:ARG:O	1:A:482:ARG:NE	2.29	0.65
1:B:487:PRO:CG	1:B:488:LEU:H	2.09	0.65
1:A:400:PRO:CG	1:A:401:GLY:H	2.09	0.65
2:T:820:DA:OP2	2:T:820:DA:C3'	2.45	0.65
1:A:450:SER:HA	1:A:459:PHE:O	1.95	0.65
1:B:231:ARG:HG2	1:B:265:PHE:HZ	1.56	0.65
1:B:454:PHE:HB3	1:B:521:MET:HE1	1.79	0.65
1:B:534:ILE:HG22	1:B:535:GLU:N	2.12	0.65
1:A:105:GLU:OE2	1:A:382:HIS:CE1	2.50	0.65
1:B:430:THR:HG1	1:B:589:ALA:H	1.45	0.65
1:B:634:LEU:CD2	1:B:635:GLU:OE1	2.45	0.65
2:T:818:DA:C2	3:P:903:DG:C2	2.84	0.65
1:A:424:TYR:O	1:A:428:ILE:HG13	1.97	0.65
1:A:479:GLU:O	1:A:481:LYS:O	2.15	0.65
1:A:731:VAL:HG12	1:A:732:TRP:N	2.12	0.65
1:B:689:ARG:O	1:B:725:ARG:CG	2.45	0.65
1:A:419:ASP:CG	1:A:595:GLU:OE1	2.35	0.65
1:A:636:THR:HG21	1:A:650:GLN:OE1	1.96	0.65
1:A:761:ALA:HB1	1:A:776:MET:HE1	1.77	0.65
1:A:68:LEU:HD21	1:A:82:TYR:OH	1.96	0.64
1:A:468:GLU:HA	1:A:471:THR:CG2	2.27	0.64
1:B:505:THR:HB	1:B:507:ALA:H	1.62	0.64
1:B:758:GLN:N	1:B:759:PRO:HD3	2.10	0.64
1:A:351:PHE:CD2	1:A:352:LEU:CD1	2.77	0.64
1:A:540:ASP:HB2	1:A:552:TRP:HB3	1.79	0.64
1:B:509:ARG:O	1:B:510:PHE:CB	2.43	0.64
1:B:747:LEU:H	1:B:747:LEU:HD22	1.56	0.64
1:A:185:ASN:C	1:A:185:ASN:OD1	2.34	0.64
1:A:426:SER:HB3	1:A:590:LEU:HD12	1.78	0.64
1:B:440:GLU:O	1:B:443:ALA:CB	2.43	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ASP:HB3	1:A:548:SER:OG	1.96	0.64
1:B:0:HIS:HD2	1:B:1:MET:H	1.44	0.64
1:B:598:PHE:CD2	1:B:601:PHE:HD1	2.14	0.64
1:B:621:ILE:O	1:B:621:ILE:HG12	1.98	0.64
1:A:135:ILE:HG22	1:A:138:ALA:HB2	1.79	0.64
1:A:136:VAL:HG12	1:A:137:ASN:N	2.11	0.64
1:A:176:ARG:NH1	1:A:192:ASP:O	2.30	0.64
1:A:638:ARG:CG	1:A:638:ARG:NH1	2.36	0.64
1:B:7:ILE:HG23	1:B:122:SER:O	1.97	0.64
1:B:561:GLU:CA	1:B:561:GLU:OE1	2.45	0.64
1:A:23:PHE:HE2	1:A:36:LEU:HD21	1.62	0.64
1:A:69:ALA:O	1:A:70:LEU:HD12	1.98	0.64
1:A:281:LEU:O	1:A:284:ALA:HB3	1.97	0.64
1:A:336:CYS:O	1:A:340:THR:CG2	2.45	0.64
1:A:745:SER:HB2	1:A:746:PRO:HD2	1.79	0.64
1:B:0:HIS:CD2	1:B:1:MET:N	2.65	0.64
1:A:626:LYS:HD3	1:A:626:LYS:N	2.13	0.64
1:B:544:GLY:HA2	1:B:549:THR:HA	1.80	0.64
1:B:723:GLN:O	1:B:724:ASN:ND2	2.31	0.64
2:T:812:DC:H2"	2:T:813:DT:C6	2.32	0.64
1:A:485:ASN:OD1	1:A:487:PRO:CG	2.44	0.64
1:B:461:ARG:O	1:B:464:HIS:CE1	2.50	0.64
1:B:464:HIS:C	1:B:468:GLU:OE1	2.36	0.64
1:B:642:THR:N	1:B:756:GLN:HE22	1.95	0.64
1:B:695:TYR:O	1:B:696:GLN:OE1	2.16	0.64
1:A:380:ARG:HD2	1:A:469:ILE:CG1	2.28	0.64
1:A:520:THR:HG22	1:A:521:MET:N	2.11	0.64
1:A:623:GLU:CD	1:A:628:ARG:HH21	2.01	0.64
1:A:734:THR:CG2	1:A:735:ASN:N	2.58	0.64
1:B:63:PHE:CD1	1:B:63:PHE:C	2.71	0.64
1:B:212:PHE:CD1	1:B:272:ARG:NH1	2.64	0.64
1:B:673:LEU:HD23	1:B:674:MET:CA	2.27	0.64
1:B:442:MET:HE1	1:B:458:TRP:N	2.10	0.63
1:B:570:VAL:HG23	1:B:571:GLN:N	2.14	0.63
1:A:247:GLY:HA3	1:A:251:SER:HB3	1.80	0.63
1:A:315:ASP:OD2	1:A:315:ASP:N	2.30	0.63
1:A:436:VAL:O	1:A:436:VAL:CG1	2.46	0.63
1:B:177:ILE:HG12	1:B:178:VAL:N	2.14	0.63
1:B:316:GLU:OE2	1:B:319:ARG:NH2	2.31	0.63
1:B:481:LYS:C	1:B:481:LYS:CD	2.67	0.63
1:B:500:TYR:CD2	1:B:500:TYR:O	2.50	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ASP:OD2	1:B:514:ARG:HG3	1.98	0.63
1:A:529:GLN:HG3	1:A:533:LEU:CD1	2.29	0.63
1:B:416:LEU:CD1	1:B:597:HIS:HD2	2.12	0.63
1:B:586:LEU:CD1	1:B:586:LEU:H	2.12	0.63
1:A:486:LYS:N	1:A:487:PRO:CD	2.61	0.63
1:A:734:THR:HG23	1:A:735:ASN:OD1	1.99	0.63
1:B:68:LEU:CD2	1:B:80:GLY:N	2.61	0.63
1:B:301:LEU:HD11	1:B:342:ILE:HG13	1.79	0.63
1:A:17:GLN:OE1	1:A:17:GLN:N	2.31	0.63
1:A:160:THR:HG22	1:A:161:ARG:N	2.13	0.63
1:A:502:VAL:HG23	1:A:503:LEU:N	2.13	0.63
1:A:775:LEU:CD2	1:A:777:THR:CG2	2.75	0.63
1:B:256:ARG:C	1:B:257:GLU:HG3	2.18	0.63
3:P:906:DT:C2'	3:P:907:DA:OP2	2.41	0.63
1:A:105:GLU:OE1	1:A:113:ARG:NH2	2.26	0.63
1:A:639:THR:HG22	1:A:639:THR:O	1.98	0.63
1:B:545:ASP:N	1:B:548:SER:O	2.30	0.63
1:A:751:HIS:O	1:A:755:ARG:CB	2.39	0.63
1:B:332:ASN:O	1:B:335:ASN:N	2.28	0.63
1:A:482:ARG:O	1:A:482:ARG:HG3	1.99	0.63
1:B:641:TRP:CE3	1:B:756:GLN:OE1	2.51	0.63
1:A:700:PRO:HG2	1:A:703:VAL:CG2	2.27	0.63
1:B:316:GLU:OE1	1:B:319:ARG:NH2	2.32	0.63
1:B:351:PHE:CD2	1:B:351:PHE:O	2.52	0.63
1:B:466:LEU:CD1	1:B:470:VAL:HG22	2.28	0.63
1:B:487:PRO:CD	1:B:488:LEU:N	2.61	0.63
1:A:482:ARG:O	1:A:483:GLN:CB	2.47	0.62
1:A:303:GLU:OE1	1:A:303:GLU:CA	2.46	0.62
1:A:418:LEU:HD11	1:A:551:VAL:HG21	1.81	0.62
1:A:17:GLN:H	1:A:17:GLN:CD	2.02	0.62
1:A:700:PRO:O	1:A:703:VAL:CA	2.46	0.62
1:B:88:GLN:O	1:B:91:ASN:HB3	1.99	0.62
1:B:278:ILE:O	1:B:282:LYS:CG	2.45	0.62
1:B:520:THR:O	1:B:523:GLY:N	2.31	0.62
1:A:49:GLN:HB3	1:A:101:VAL:HG13	1.81	0.62
1:A:74:HIS:O	1:A:75:ARG:HB2	2.00	0.62
1:B:131:HIS:O	1:B:132:ASN:HB2	1.98	0.62
1:B:436:VAL:CG1	1:B:437:GLY:N	2.61	0.62
1:B:93:GLU:C	1:B:93:GLU:OE1	2.38	0.62
1:B:584:GLN:O	1:B:585:ARG:CB	2.47	0.62
1:B:688:LEU:O	1:B:725:ARG:HA	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASP:OD2	1:A:327:ALA:HB3	1.99	0.62
1:A:480:ALA:HB3	1:A:489:SER:OG	1.99	0.62
1:B:160:THR:HG21	1:B:164:GLU:CB	2.28	0.62
1:B:257:GLU:HG2	1:B:265:PHE:HB2	1.78	0.62
1:A:725:ARG:NH2	1:A:725:ARG:HG2	2.08	0.62
1:A:436:VAL:O	1:A:436:VAL:HG12	1.97	0.62
1:B:135:ILE:HG22	1:B:135:ILE:O	1.99	0.62
1:B:224:ASN:CA	1:B:276:ASP:OD2	2.48	0.62
1:B:232:MET:HE1	1:B:235:LYS:HD2	1.82	0.62
1:B:406:ASP:OD1	1:B:406:ASP:N	2.31	0.62
1:B:601:PHE:CE2	1:B:603:MET:HE2	2.35	0.62
1:B:648:PHE:O	1:B:652:LEU:HB2	2.00	0.62
1:B:745:SER:CB	1:B:746:PRO:HD3	2.27	0.62
1:A:365:ARG:NH1	1:A:367:GLY:O	2.33	0.62
1:B:359:ASN:HD22	1:B:361:LEU:HB2	1.65	0.62
1:B:547:ASP:C	1:B:547:ASP:OD1	2.38	0.62
1:B:598:PHE:HD1	1:B:620:LEU:O	1.82	0.62
1:A:179:TYR:HE1	1:A:207:LYS:HD2	1.62	0.61
1:A:746:PRO:O	1:A:746:PRO:CG	2.48	0.61
2:T:820:DA:H3'	2:T:820:DA:P	2.38	0.61
1:A:478:ASP:O	1:A:481:LYS:HG2	1.99	0.61
1:A:692:LEU:HA	1:A:695:TYR:CD2	2.35	0.61
1:A:705:ALA:HA	1:A:708:LEU:HB2	1.81	0.61
1:B:153:VAL:O	1:B:153:VAL:CG1	2.48	0.61
1:B:497:ASN:N	1:B:497:ASN:OD1	2.33	0.61
1:A:297:ALA:O	1:A:301:LEU:HB2	2.00	0.61
1:A:751:HIS:ND1	1:A:755:ARG:CG	2.63	0.61
1:B:600:ARG:NE	1:B:657:PHE:O	2.33	0.61
1:A:682:LEU:HD23	1:A:747:LEU:HD22	1.83	0.61
1:B:454:PHE:CD1	1:B:521:MET:HE3	2.33	0.61
1:B:751:HIS:C	1:B:751:HIS:ND1	2.53	0.61
2:T:813:DT:O5'	2:T:813:DT:H6	1.82	0.61
3:P:903:DG:OP1	3:P:903:DG:C4'	2.48	0.61
1:A:201:ARG:O	1:A:204:LEU:HB2	1.99	0.61
1:A:270:LYS:HG3	1:A:270:LYS:O	1.99	0.61
1:A:276:ASP:OD2	1:A:278:ILE:N	2.31	0.61
1:A:316:GLU:OE1	1:A:316:GLU:HA	1.99	0.61
1:B:436:VAL:HG13	1:B:437:GLY:H	1.66	0.61
1:B:643:PRO:HA	1:B:646:GLN:HG3	1.82	0.61
1:B:720:LEU:N	1:B:720:LEU:CD1	2.62	0.61
1:A:702:HIS:O	1:A:706:ALA:HB2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:LYS:N	1:B:487:PRO:HD3	2.14	0.61
1:B:646:GLN:O	1:B:650:GLN:HG3	2.01	0.61
1:A:48:ASP:OD2	1:A:48:ASP:N	2.30	0.61
1:A:702:HIS:O	1:A:706:ALA:N	2.32	0.61
1:B:481:LYS:O	1:B:481:LYS:CD	2.47	0.61
1:B:553:LEU:O	1:B:557:HIS:NE2	2.32	0.61
1:A:700:PRO:O	1:A:704:ARG:N	2.34	0.61
1:A:651:GLU:O	1:A:655:ARG:HG3	2.00	0.61
1:A:758:GLN:HB3	1:A:759:PRO:HD3	1.83	0.61
1:B:113:ARG:NH1	1:B:113:ARG:CG	2.63	0.61
1:B:527:MET:CE	1:B:549:THR:HG22	2.31	0.61
1:A:425:PRO:HB3	1:A:496:MET:HE3	1.83	0.60
1:A:732:TRP:CB	1:A:751:HIS:CD2	2.84	0.60
1:B:467:PRO:O	1:B:471:THR:CG2	2.46	0.60
2:T:819:DC:H2'	2:T:820:DA:H8	1.65	0.60
1:A:600:ARG:CG	1:A:600:ARG:NH1	2.51	0.60
1:A:759:PRO:HA	1:A:762:GLU:HB2	1.83	0.60
1:B:156:ASP:OD2	1:B:157:ILE:N	2.34	0.60
1:B:295:THR:O	1:B:299:GLU:HG3	2.01	0.60
1:B:477:ARG:O	1:B:481:LYS:N	2.34	0.60
1:B:638:ARG:CG	1:B:641:TRP:HD1	2.15	0.60
1:A:1:MET:O	1:A:1:MET:CG	2.49	0.60
1:A:688:LEU:CA	1:A:726:GLY:O	2.47	0.60
1:B:231:ARG:HG3	1:B:265:PHE:CE1	2.36	0.60
1:B:232:MET:O	1:B:236:HIS:CD2	2.53	0.60
1:B:264:VAL:O	1:B:264:VAL:HG23	2.01	0.60
1:B:294:GLU:O	1:B:298:GLN:HG3	2.02	0.60
1:B:687:ARG:O	1:B:687:ARG:CD	2.50	0.60
1:B:688:LEU:HG	1:B:728:ILE:HD11	1.83	0.60
1:B:751:HIS:O	1:B:751:HIS:ND1	2.33	0.60
1:A:562:ALA:CB	1:A:597:HIS:HD2	2.12	0.60
1:B:732:TRP:O	1:B:747:LEU:HB2	2.01	0.60
1:A:354:GLU:OE1	1:A:488:LEU:HD23	2.02	0.60
1:A:450:SER:HB2	1:A:458:TRP:HE3	1.66	0.60
1:A:761:ALA:CB	1:A:776:MET:HE1	2.32	0.60
2:T:819:DC:C2'	2:T:820:DA:C2'	2.77	0.60
1:B:499:PHE:O	1:B:502:VAL:HB	2.02	0.60
1:A:215:TYR:CD2	1:A:215:TYR:N	2.70	0.60
1:A:658:ARG:NH1	1:A:660:GLU:OE1	2.34	0.60
1:B:348:ILE:O	1:B:349:MET:C	2.36	0.60
1:B:486:LYS:O	1:B:487:PRO:C	2.38	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:PHE:CE2	1:B:603:MET:CE	2.85	0.60
3:P:903:DG:H2'	3:P:904:DC:C5	2.37	0.60
1:A:761:ALA:HB3	1:A:776:MET:HE3	1.84	0.60
1:B:466:LEU:CD1	1:B:470:VAL:HG23	2.20	0.60
1:B:687:ARG:N	1:B:687:ARG:HD2	2.16	0.60
1:A:545:ASP:CB	1:A:548:SER:OG	2.50	0.59
1:B:10:ARG:HB3	1:B:23:PHE:CD1	2.37	0.59
1:B:253:LEU:HD12	1:B:269:ALA:HB2	1.84	0.59
1:B:478:ASP:OD1	1:B:478:ASP:N	2.34	0.59
1:B:561:GLU:OE1	1:B:561:GLU:N	2.35	0.59
1:B:434:ASP:OD1	1:B:436:VAL:HG12	2.01	0.59
1:B:732:TRP:O	1:B:747:LEU:CA	2.49	0.59
1:B:733:THR:HG23	1:B:734:THR:N	2.15	0.59
1:A:324:ASP:OD2	1:A:327:ALA:HB2	2.01	0.59
1:B:48:ASP:C	1:B:48:ASP:OD1	2.41	0.59
1:B:351:PHE:HD2	1:B:352:LEU:N	2.00	0.59
1:B:688:LEU:HD12	1:B:728:ILE:CD1	2.21	0.59
1:A:761:ALA:CB	1:A:776:MET:CE	2.80	0.59
1:B:180:MET:HG3	1:B:181:LEU:H	1.67	0.59
1:B:733:THR:CB	1:B:736:GLY:O	2.49	0.59
1:B:94:LYS:CG	1:B:95:ARG:N	2.65	0.59
1:B:500:TYR:CD2	1:B:501:GLY:N	2.67	0.59
1:A:354:GLU:OE1	1:A:488:LEU:CD2	2.50	0.59
1:A:400:PRO:CG	1:A:401:GLY:N	2.64	0.59
1:B:577:TRP:HA	1:B:580:THR:CG2	2.32	0.59
1:A:212:PHE:HD1	1:A:272:ARG:NH1	2.00	0.59
1:A:278:ILE:O	1:A:282:LYS:CG	2.46	0.59
1:A:640:ASP:C	1:A:640:ASP:OD1	2.41	0.59
1:A:688:LEU:HB2	1:A:726:GLY:C	2.22	0.59
1:A:736:GLY:O	1:A:738:GLU:HG3	2.03	0.59
1:B:74:HIS:C	1:B:75:ARG:CG	2.69	0.59
1:B:118:ARG:O	1:B:119:PHE:HB2	2.03	0.59
1:B:584:GLN:C	1:B:586:LEU:HD12	2.23	0.59
1:A:64:ARG:CG	1:A:64:ARG:NH1	2.38	0.59
1:A:688:LEU:CA	1:A:726:GLY:H	2.15	0.59
1:B:321:PHE:O	1:B:325:LYS:HG3	2.03	0.59
1:A:232:MET:CE	1:A:235:LYS:HZ1	2.14	0.59
1:A:316:GLU:CD	1:A:319:ARG:HH12	2.06	0.59
1:B:415:VAL:CG1	1:B:601:PHE:CG	2.85	0.59
1:B:440:GLU:OE2	1:B:463:LYS:HG2	2.03	0.59
1:B:490:GLN:O	1:B:494:ILE:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:OD2	1:A:276:ASP:C	2.40	0.59
1:A:332:ASN:C	1:A:332:ASN:OD1	2.41	0.59
1:A:358:VAL:HG11	1:A:495:ILE:CD1	2.32	0.59
1:A:495:ILE:O	1:A:498:ALA:N	2.31	0.59
1:B:712:GLU:CA	1:B:712:GLU:OE2	2.49	0.59
1:A:408:ARG:CG	1:A:408:ARG:NH1	2.34	0.58
1:A:477:ARG:HD2	1:A:477:ARG:O	2.03	0.58
1:B:174:GLY:O	1:B:175:GLN:HG2	2.02	0.58
1:B:225:VAL:O	1:B:230:LEU:N	2.33	0.58
1:A:128:GLY:HA3	1:A:135:ILE:CG2	2.33	0.58
1:A:482:ARG:CD	1:A:482:ARG:C	2.66	0.58
1:B:418:LEU:CD1	1:B:418:LEU:O	2.52	0.58
1:A:562:ALA:HB1	1:A:597:HIS:CD2	2.37	0.58
1:B:180:MET:O	1:B:198:VAL:CG2	2.48	0.58
1:A:287:ASN:OD1	1:A:288:PHE:N	2.37	0.58
1:A:316:GLU:CD	1:A:319:ARG:NH1	2.57	0.58
1:A:692:LEU:HD13	1:A:723:GLN:O	2.03	0.58
1:B:351:PHE:CD2	1:B:352:LEU:N	2.70	0.58
1:B:711:GLU:O	1:B:714:GLN:N	2.36	0.58
1:B:165:LEU:HB2	1:B:236:HIS:CE1	2.38	0.58
1:B:723:GLN:C	1:B:724:ASN:ND2	2.39	0.58
1:A:64:ARG:HD2	1:A:66:THR:HG22	1.86	0.58
1:A:127:GLU:HB3	1:A:139:ARG:NH2	2.19	0.58
1:B:130:MET:HE3	1:B:133:GLY:CA	2.32	0.58
1:B:488:LEU:O	1:B:491:ALA:N	2.36	0.58
3:P:905:DC:H2'	3:P:906:DT:H73	1.84	0.58
1:A:42:VAL:HG23	1:A:82:TYR:CE1	2.39	0.58
1:A:161:ARG:CB	1:A:314:MET:CE	2.81	0.58
1:B:749:TYR:O	1:B:750:GLU:C	2.41	0.58
2:T:809:DA:C2'	2:T:810:DC:OP2	2.37	0.58
1:A:33:GLN:HB3	1:A:134:THR:HG23	1.86	0.58
1:A:303:GLU:OE1	1:A:303:GLU:N	2.36	0.58
1:A:414:SER:OG	1:A:597:HIS:CE1	2.57	0.58
1:A:692:LEU:HD13	1:A:723:GLN:CA	2.32	0.58
1:A:702:HIS:CD2	1:A:703:VAL:HG23	2.39	0.58
1:B:159:THR:OG1	1:B:163:GLY:CA	2.52	0.58
1:B:179:TYR:CD1	1:B:207:LYS:HD3	2.38	0.58
1:A:351:PHE:HD2	1:A:352:LEU:N	2.02	0.58
1:A:444:GLN:N	1:A:445:PRO:HD3	2.18	0.58
1:A:626:LYS:N	1:A:626:LYS:CD	2.67	0.58
1:A:732:TRP:HB3	1:A:751:HIS:HD2	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:THR:OG1	1:A:738:GLU:HG3	2.04	0.58
1:A:760:VAL:CG2	1:A:761:ALA:N	2.67	0.58
1:B:7:ILE:HD11	1:B:10:ARG:NH1	2.19	0.58
1:B:62:GLY:O	1:B:88:GLN:NE2	2.32	0.58
1:B:193:PHE:HD1	1:B:194:GLU:O	1.86	0.58
1:B:487:PRO:CG	1:B:488:LEU:N	2.66	0.58
1:B:700:PRO:O	1:B:703:VAL:HG12	2.03	0.58
1:A:284:ALA:HB3	1:A:286:TRP:HD1	1.68	0.57
1:A:311:TRP:CB	1:A:312:ASP:OD1	2.48	0.57
1:A:693:SER:O	1:A:696:GLN:OE1	2.22	0.57
1:B:512:ASP:OD1	1:B:513:PRO:HD2	2.03	0.57
2:T:811:DG:H2'	2:T:812:DC:H6	1.68	0.57
1:A:284:ALA:CB	1:A:286:TRP:HD1	2.16	0.57
1:A:378:PHE:HB2	1:A:379:PRO:CD	2.34	0.57
1:B:110:PRO:HB2	1:B:111:PRO:HD3	1.86	0.57
1:B:228:PHE:CE1	1:B:232:MET:HG3	2.40	0.57
1:A:22:SER:HA	1:A:34:VAL:O	2.04	0.57
1:A:42:VAL:CG2	1:A:82:TYR:CE1	2.87	0.57
1:B:413:ASP:N	1:B:413:ASP:OD1	2.34	0.57
1:B:414:SER:HB2	1:B:597:HIS:NE2	2.19	0.57
1:B:525:GLN:HG2	1:B:526:ILE:N	2.19	0.57
1:A:755:ARG:NE	1:A:755:ARG:HA	2.19	0.57
1:B:174:GLY:C	1:B:175:GLN:HG2	2.25	0.57
1:B:431:PHE:CE1	1:B:522:ARG:CZ	2.87	0.57
1:B:561:GLU:OE1	1:B:561:GLU:HA	2.04	0.57
1:B:731:VAL:O	1:B:737:PRO:HA	2.04	0.57
1:A:21:VAL:O	1:A:36:LEU:HD13	1.99	0.57
1:A:692:LEU:CD1	1:A:723:GLN:CA	2.81	0.57
1:B:413:ASP:HA	1:B:600:ARG:HA	1.85	0.57
1:B:431:PHE:CD1	1:B:522:ARG:CZ	2.87	0.57
1:B:455:LEU:O	1:B:456:ASP:HB2	2.05	0.57
1:A:359:ASN:C	1:A:359:ASN:OD1	2.41	0.57
1:B:200:SER:C	1:B:202:PRO:HD2	2.25	0.57
1:B:454:PHE:O	1:B:455:LEU:HB2	2.03	0.57
1:B:484:GLY:HA2	1:B:485:ASN:CB	2.27	0.57
1:B:747:LEU:N	1:B:747:LEU:HD22	2.13	0.57
1:A:121:THR:OG1	1:A:122:SER:N	2.37	0.57
1:B:265:PHE:H	1:B:265:PHE:HD1	1.50	0.57
1:B:634:LEU:HD22	1:B:635:GLU:OE1	2.05	0.57
1:A:2:ALA:HA	1:A:126:VAL:O	2.05	0.57
1:A:83:CYS:HB3	1:A:88:GLN:HE21	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:PRO:C	1:A:703:VAL:N	2.50	0.57
1:B:584:GLN:O	1:B:586:LEU:HD12	2.05	0.57
1:A:159:THR:CB	1:A:164:GLU:O	2.52	0.57
1:B:508:CYS:C	1:B:509:ARG:O	2.37	0.57
1:B:201:ARG:H	1:B:202:PRO:HD3	1.70	0.57
1:B:382:HIS:O	1:B:385:GLY:N	2.27	0.57
1:B:656:ILE:CD1	1:B:764:ILE:HD13	2.35	0.57
1:A:689:ARG:HA	1:A:725:ARG:HD3	1.86	0.56
1:B:381:MET:O	1:B:384:ALA:HB3	2.05	0.56
2:T:819:DC:H2"	2:T:820:DA:C3'	2.35	0.56
1:A:65:LEU:HD22	1:A:79:TYR:HD1	1.71	0.56
1:A:760:VAL:HG23	1:A:761:ALA:N	2.20	0.56
1:B:420:TYR:CD1	1:B:592:LEU:HB2	2.38	0.56
1:B:634:LEU:HD23	1:B:635:GLU:OE1	2.04	0.56
1:A:519:ILE:HG22	1:A:520:THR:N	2.21	0.56
1:A:635:GLU:OE2	1:A:760:VAL:HG12	2.05	0.56
1:B:0:HIS:O	1:B:1:MET:HB2	2.05	0.56
1:B:160:THR:HG23	1:B:164:GLU:C	2.24	0.56
1:B:255:TRP:CD2	1:B:267:ALA:HB2	2.36	0.56
1:B:257:GLU:CG	1:B:265:PHE:CB	2.76	0.56
1:B:413:ASP:HB2	1:B:599:CYS:O	2.06	0.56
1:B:487:PRO:HG2	1:B:488:LEU:H	1.70	0.56
1:B:598:PHE:CD1	1:B:620:LEU:O	2.58	0.56
1:A:248:ARG:NH1	1:A:271:GLY:O	2.37	0.56
1:A:775:LEU:HD23	1:A:777:THR:HG23	1.83	0.56
1:B:72:ASP:OD1	1:B:73:PHE:N	2.38	0.56
1:B:175:GLN:OE1	1:B:215:TYR:CE1	2.54	0.56
1:B:466:LEU:CD1	1:B:466:LEU:C	2.73	0.56
2:T:819:DC:C2'	2:T:820:DA:O4'	2.52	0.56
1:A:348:ILE:HG22	1:A:349:MET:H	1.66	0.56
1:B:91:ASN:O	1:B:94:LYS:HG2	2.06	0.56
1:B:500:TYR:HD2	1:B:500:TYR:O	1.87	0.56
1:B:527:MET:HE2	1:B:549:THR:HG22	1.87	0.56
1:B:601:PHE:CZ	1:B:603:MET:HE2	2.40	0.56
1:A:19:THR:OG1	1:A:84:ARG:O	2.24	0.56
1:A:242:LEU:HD12	1:A:243:PRO:HD2	1.88	0.56
1:A:454:PHE:CB	1:A:455:LEU:HD12	2.35	0.56
1:A:571:GLN:OE1	1:A:571:GLN:C	2.43	0.56
1:B:12:TRP:HB3	1:B:111:PRO:HD3	1.87	0.56
1:B:177:ILE:HG12	1:B:178:VAL:H	1.70	0.56
1:B:466:LEU:CD1	1:B:466:LEU:O	2.51	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:731:VAL:CG1	1:B:732:TRP:N	2.69	0.56
1:A:72:ASP:OD1	1:A:104:TYR:OH	2.17	0.56
1:B:455:LEU:O	1:B:456:ASP:CB	2.53	0.56
1:A:562:ALA:HB3	1:A:597:HIS:HD2	1.68	0.56
1:A:730:TYR:N	1:A:730:TYR:CD2	2.74	0.56
1:B:461:ARG:HH12	1:B:585:ARG:HD3	1.71	0.56
1:B:9:THR:CG2	1:B:10:ARG:N	2.64	0.56
1:B:601:PHE:HE2	1:B:603:MET:CE	2.18	0.56
2:T:813:DT:OP2	2:T:813:DT:H71	2.06	0.56
3:P:910:DG:H2'	3:P:911:DT:H71	1.88	0.56
1:A:716:ARG:O	1:A:718:ARG:HG3	2.06	0.55
1:B:46:PRO:HB2	1:B:49:GLN:HG3	1.89	0.55
1:B:745:SER:CB	1:B:746:PRO:CD	2.82	0.55
1:A:312:ASP:O	1:A:313:ARG:CB	2.49	0.55
1:A:570:VAL:HA	1:A:592:LEU:HD23	1.87	0.55
1:B:413:ASP:HB3	1:B:600:ARG:HH11	1.69	0.55
1:B:636:THR:CG2	1:B:637:VAL:CG2	2.85	0.55
2:T:808:DT:H2"	2:T:809:DA:C8	2.41	0.55
1:A:397:HIS:CD2	1:A:397:HIS:C	2.79	0.55
1:A:495:ILE:HG13	1:A:496:MET:H	1.71	0.55
1:A:640:ASP:OD1	1:A:641:TRP:HD1	1.90	0.55
1:A:686:LYS:O	1:A:727:THR:HA	2.06	0.55
1:A:771:ASN:N	1:A:771:ASN:OD1	2.38	0.55
1:B:382:HIS:C	1:B:384:ALA:N	2.60	0.55
1:A:228:PHE:O	1:A:232:MET:HB2	2.07	0.55
1:A:295:THR:O	1:A:299:GLU:HG3	2.07	0.55
1:A:636:THR:HG23	1:A:650:GLN:OE1	2.06	0.55
1:A:750:GLU:O	1:A:754:THR:OG1	2.23	0.55
1:B:733:THR:CA	1:B:747:LEU:HA	2.18	0.55
3:P:905:DC:H2"	3:P:906:DT:C6	2.41	0.55
1:B:372:ALA:O	1:B:373:PHE:C	2.42	0.55
1:A:581:LEU:HD11	1:A:588:SER:HB2	1.88	0.55
1:A:751:HIS:ND1	1:A:755:ARG:CB	2.70	0.55
1:B:266:PHE:HD2	1:B:267:ALA:N	2.05	0.55
1:A:74:HIS:O	1:A:75:ARG:CB	2.55	0.55
1:A:332:ASN:O	1:A:335:ASN:HB2	2.06	0.55
1:A:434:ASP:OD2	1:A:435:PRO:HD2	2.06	0.55
1:A:642:THR:HG22	1:A:643:PRO:N	2.22	0.55
1:A:692:LEU:CD1	1:A:692:LEU:N	2.39	0.55
1:B:584:GLN:O	1:B:586:LEU:HD11	2.06	0.55
1:B:601:PHE:C	1:B:601:PHE:CD2	2.79	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:PRO:O	1:B:742:TYR:O	2.25	0.55
1:A:89:LEU:O	1:A:93:GLU:CG	2.55	0.55
1:A:647:GLN:OE1	1:A:651:GLU:OE2	2.25	0.55
1:A:731:VAL:CG1	1:A:732:TRP:N	2.70	0.55
1:B:476:GLY:O	1:B:480:ALA:HB3	2.06	0.55
2:T:817:DC:C2'	2:T:818:DA:H1'	2.31	0.55
1:A:276:ASP:OD2	1:A:277:GLY:N	2.41	0.55
1:A:298:GLN:HG3	1:A:298:GLN:O	2.07	0.55
1:A:571:GLN:OE1	1:A:571:GLN:CA	2.54	0.55
1:A:713:ASN:O	1:A:718:ARG:N	2.40	0.55
1:A:737:PRO:O	1:A:738:GLU:HG2	2.07	0.55
1:B:276:ASP:OD1	1:B:279:GLU:HG3	2.06	0.55
1:A:136:VAL:CG1	1:A:137:ASN:N	2.69	0.54
1:B:214:ASN:HB3	1:B:215:TYR:CE2	2.41	0.54
1:B:338:LEU:CD2	1:B:338:LEU:N	2.70	0.54
1:B:346:THR:O	1:B:347:GLU:HB3	2.06	0.54
1:B:355:ARG:O	1:B:359:ASN:OD1	2.26	0.54
1:B:431:PHE:CE2	1:B:522:ARG:CD	2.84	0.54
1:B:642:THR:H	1:B:756:GLN:HE22	1.54	0.54
1:B:642:THR:CG2	1:B:756:GLN:HE21	2.20	0.54
2:T:819:DC:H2"	2:T:820:DA:C1'	2.36	0.54
1:A:7:ILE:HA	1:A:25:LEU:CD2	2.37	0.54
1:A:196:GLU:OE2	1:A:207:LYS:CE	2.52	0.54
1:B:152:TRP:N	1:B:152:TRP:CD1	2.67	0.54
1:A:355:ARG:HG2	1:A:356:ALA:H	1.73	0.54
1:A:502:VAL:O	1:A:505:THR:HG22	2.07	0.54
1:B:176:ARG:HB3	1:B:333:LEU:HD21	1.89	0.54
1:B:332:ASN:O	1:B:335:ASN:HB2	2.08	0.54
1:B:461:ARG:C	1:B:464:HIS:CE1	2.81	0.54
1:B:543:TYR:CD2	1:B:550:PHE:HE2	2.23	0.54
1:A:358:VAL:HG13	1:A:495:ILE:CD1	2.35	0.54
1:A:405:MET:SD	1:A:531:LYS:HD3	2.47	0.54
1:A:639:THR:O	1:A:639:THR:CG2	2.55	0.54
1:B:61:GLN:HG3	1:B:62:GLY:N	2.21	0.54
1:B:107:ASP:C	1:B:107:ASP:OD1	2.45	0.54
1:B:381:MET:HE3	1:B:388:ALA:H	1.66	0.54
1:B:450:SER:HA	1:B:459:PHE:O	2.07	0.54
1:B:749:TYR:HA	1:B:752:TYR:HB2	1.89	0.54
2:T:819:DC:H2'	2:T:820:DA:H2'	1.89	0.54
1:A:695:TYR:CD1	3:P:907:DA:H5'	2.43	0.54
1:A:728:ILE:CG2	1:A:728:ILE:O	2.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:LEU:HD22	1:B:752:TYR:CE1	2.42	0.54
3:P:907:DA:H2"	3:P:908:DG:C5'	2.38	0.54
1:A:117:GLU:OE2	1:A:382:HIS:CD2	2.59	0.54
1:A:722:TYR:OH	1:A:728:ILE:CG1	2.54	0.54
1:B:292:SER:O	1:B:293:LEU:C	2.44	0.54
1:B:629:MET:CE	1:B:657:PHE:HE2	2.21	0.54
1:A:65:LEU:CD2	1:A:79:TYR:HB3	2.37	0.54
1:A:698:ASN:HA	2:T:817:DC:OP1	2.08	0.54
1:A:198:VAL:HG12	1:A:200:SER:H	1.72	0.54
1:A:734:THR:HB	1:A:746:PRO:CG	2.38	0.54
1:B:67:PRO:HG3	1:B:79:TYR:CZ	2.42	0.54
1:B:346:THR:O	1:B:347:GLU:CB	2.54	0.54
1:B:408:ARG:HB2	1:B:542:ILE:CG2	2.38	0.54
1:B:660:GLU:HB3	1:B:661:PRO:CD	2.36	0.54
2:T:813:DT:H2"	2:T:814:DA:C8	2.42	0.54
1:B:130:MET:HE2	1:B:133:GLY:HA2	1.90	0.54
1:B:419:ASP:O	1:B:593:GLU:N	2.37	0.54
1:B:531:LYS:CG	1:B:532:ALA:N	2.67	0.53
1:A:120:ILE:HG22	1:A:121:THR:N	2.23	0.53
1:A:157:ILE:HG13	1:A:157:ILE:O	2.08	0.53
1:A:176:ARG:O	1:A:193:PHE:HB2	2.08	0.53
1:A:351:PHE:CD2	1:A:352:LEU:N	2.75	0.53
1:A:468:GLU:CA	1:A:471:THR:HG23	2.36	0.53
1:A:642:THR:O	1:A:646:GLN:HG3	2.08	0.53
1:A:745:SER:CB	1:A:746:PRO:HD2	2.37	0.53
1:B:636:THR:CG2	1:B:637:VAL:N	2.70	0.53
1:B:733:THR:CA	1:B:746:PRO:O	2.56	0.53
1:A:92:TYR:O	1:A:96:LEU:HD13	2.08	0.53
1:B:8:LEU:HD12	1:B:271:GLY:O	2.09	0.53
1:B:120:ILE:CG2	1:B:121:THR:N	2.70	0.53
2:T:812:DC:C2'	2:T:813:DT:H71	2.38	0.53
1:A:49:GLN:HE22	1:A:102:THR:H	1.55	0.53
1:A:73:PHE:CG	1:A:389:PRO:HG3	2.43	0.53
1:B:224:ASN:HA	1:B:276:ASP:OD2	2.09	0.53
1:B:495:ILE:HG13	1:B:496:MET:N	2.24	0.53
3:P:906:DT:H2"	3:P:907:DA:OP2	2.06	0.53
1:A:3:GLN:O	1:A:126:VAL:HG12	2.08	0.53
1:B:668:GLU:O	1:B:672:LYS:CG	2.37	0.53
1:B:732:TRP:O	1:B:747:LEU:CB	2.56	0.53
1:B:49:GLN:NE2	1:B:102:THR:OG1	2.42	0.53
1:A:72:ASP:OD1	1:A:104:TYR:CZ	2.60	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:HG3	1:A:320:ARG:N	2.14	0.53
1:A:553:LEU:O	1:A:554:LYS:HB2	2.08	0.53
1:B:177:ILE:HD13	1:B:179:TYR:CZ	2.43	0.53
1:B:476:GLY:O	1:B:480:ALA:HB2	2.08	0.53
1:B:598:PHE:HD2	1:B:601:PHE:HD1	1.56	0.53
1:B:121:THR:CG2	1:B:122:SER:N	2.42	0.53
1:B:768:ILE:O	1:B:769:GLU:CB	2.56	0.53
3:P:913:DG:O5'	3:P:913:DG:C2'	2.57	0.53
1:A:336:CYS:O	1:A:340:THR:HG23	2.08	0.53
1:B:697:ARG:O	1:B:698:ASN:CB	2.51	0.53
1:A:294:GLU:N	1:A:294:GLU:CD	2.63	0.53
1:A:710:ASP:OD2	1:A:722:TYR:CB	2.50	0.53
1:B:160:THR:CG2	1:B:164:GLU:O	2.49	0.53
1:B:203:GLN:O	1:B:207:LYS:HG3	2.09	0.53
1:B:570:VAL:HB	1:B:592:LEU:HD22	1.90	0.53
1:B:673:LEU:HD23	1:B:673:LEU:C	2.21	0.53
1:A:410:GLY:HA2	1:A:767:PHE:CE1	2.44	0.52
1:B:415:VAL:HG11	1:B:601:PHE:HB3	1.89	0.52
1:B:524:HIS:C	1:B:528:ARG:HD2	2.28	0.52
1:A:64:ARG:HH11	1:A:64:ARG:HB2	1.66	0.52
1:A:325:LYS:O	1:A:328:LEU:HB3	2.08	0.52
1:A:529:GLN:HE21	1:A:533:LEU:CD1	2.21	0.52
1:A:642:THR:HG23	1:A:681:ARG:O	2.09	0.52
1:B:434:ASP:CG	1:B:436:VAL:HG12	2.30	0.52
1:B:461:ARG:NH2	1:B:584:GLN:O	2.43	0.52
1:B:688:LEU:CD1	1:B:728:ILE:HD13	2.29	0.52
1:A:383:ARG:CG	1:A:383:ARG:NH1	2.59	0.52
1:A:729:LYS:HG3	1:A:729:LYS:O	2.09	0.52
1:B:278:ILE:CG2	1:B:291:PHE:CD1	2.93	0.52
1:B:416:LEU:HD11	1:B:597:HIS:CD2	2.44	0.52
1:A:120:ILE:HG12	1:A:142:PRO:HG3	1.91	0.52
1:A:499:PHE:O	1:A:502:VAL:HG22	2.08	0.52
1:A:756:GLN:O	1:A:760:VAL:HG13	2.09	0.52
2:T:819:DC:H2"	2:T:820:DA:H2'	1.84	0.52
1:A:232:MET:HE1	1:A:235:LYS:HZ1	1.74	0.52
1:A:372:ALA:O	1:A:376:LEU:HD13	2.10	0.52
1:B:255:TRP:CZ3	1:B:267:ALA:CB	2.85	0.52
1:B:446:ASP:HB2	1:B:449:HIS:CE1	2.44	0.52
1:B:644:LEU:HD13	1:B:757:LEU:HD13	1.85	0.52
1:B:687:ARG:HD2	1:B:687:ARG:H	1.74	0.52
1:A:663:GLN:HG2	1:A:774:THR:HG23	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:LEU:CD2	1:A:722:TYR:O	2.57	0.52
1:A:753:LEU:O	1:A:758:GLN:HB2	2.09	0.52
1:B:147:ARG:NH2	1:B:357:THR:HG21	2.23	0.52
1:B:377:TYR:OH	1:B:436:VAL:HG12	2.09	0.52
1:B:466:LEU:HB3	1:B:467:PRO:HD3	1.90	0.52
1:B:510:PHE:O	1:B:515:LEU:HD23	2.10	0.52
1:A:476:GLY:O	1:A:479:GLU:HB3	2.10	0.52
1:A:616:ARG:HB2	1:A:634:LEU:HD13	1.92	0.52
1:B:712:GLU:OE2	1:B:712:GLU:O	2.28	0.52
1:B:765:LEU:HD12	1:B:768:ILE:HD11	1.92	0.52
1:A:416:LEU:HD13	1:A:553:LEU:HD22	1.91	0.52
1:A:688:LEU:HD12	1:A:726:GLY:C	2.31	0.52
1:B:74:HIS:O	1:B:75:ARG:CB	2.58	0.52
1:B:415:VAL:CG2	1:B:416:LEU:N	2.73	0.52
1:B:416:LEU:HD11	1:B:597:HIS:HD2	1.74	0.52
1:B:689:ARG:C	1:B:725:ARG:HG3	2.29	0.52
1:A:174:GLY:C	1:A:175:GLN:HG2	2.30	0.52
1:A:232:MET:CE	1:A:235:LYS:HZ2	2.22	0.52
1:A:732:TRP:HB3	1:A:751:HIS:CD2	2.45	0.52
1:B:180:MET:HG3	1:B:181:LEU:N	2.25	0.52
1:B:418:LEU:HD12	1:B:418:LEU:O	2.10	0.52
1:B:430:THR:HG1	1:B:589:ALA:N	2.05	0.52
1:B:765:LEU:O	1:B:768:ILE:HG12	2.10	0.52
1:A:654:LEU:HD13	1:A:658:ARG:HD3	1.91	0.51
1:A:733:THR:OG1	1:A:736:GLY:O	2.28	0.51
1:B:485:ASN:OD1	1:B:487:PRO:HD3	2.11	0.51
3:P:910:DG:C2'	3:P:911:DT:C6	2.92	0.51
1:A:418:LEU:CD1	1:A:551:VAL:CG2	2.88	0.51
1:A:745:SER:CB	1:A:746:PRO:CD	2.88	0.51
1:B:225:VAL:O	1:B:230:LEU:CB	2.48	0.51
1:A:17:GLN:N	1:A:17:GLN:CD	2.63	0.51
1:A:72:ASP:HB2	1:A:76:GLN:H	1.75	0.51
1:B:436:VAL:HG11	1:B:465:CYS:SG	2.50	0.51
1:A:425:PRO:CB	1:A:496:MET:HE3	2.40	0.51
1:B:389:PRO:O	1:B:390:ASN:OD1	2.29	0.51
1:B:527:MET:CE	1:B:549:THR:CG2	2.89	0.51
1:B:682:LEU:HD22	1:B:752:TYR:CG	2.46	0.51
1:B:711:GLU:O	1:B:714:GLN:CB	2.51	0.51
1:B:760:VAL:HG12	1:B:761:ALA:N	2.21	0.51
1:A:541:VAL:HG13	1:A:549:THR:CG2	2.41	0.51
1:B:682:LEU:CD2	1:B:752:TYR:CD1	2.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:750:GLU:OE1	1:B:754:THR:HG22	2.11	0.51
2:T:811:DG:C2'	2:T:812:DC:O5'	2.58	0.51
1:A:688:LEU:CB	1:A:726:GLY:O	2.58	0.51
1:B:11:HIS:HE1	1:B:24:TRP:HD1	1.57	0.51
1:B:135:ILE:HG22	1:B:138:ALA:HB2	1.93	0.51
1:B:177:ILE:HD13	1:B:179:TYR:CE2	2.45	0.51
1:B:253:LEU:CD1	1:B:269:ALA:HB2	2.41	0.51
1:B:416:LEU:H	1:B:551:VAL:HG13	1.75	0.51
1:A:434:ASP:OD1	1:A:464:HIS:HA	2.11	0.51
1:A:740:LEU:O	1:A:740:LEU:CD2	2.36	0.51
1:B:559:GLU:O	1:B:563:ALA:HB3	2.11	0.51
1:B:731:VAL:HG13	1:B:752:TYR:OH	2.10	0.51
1:A:319:ARG:HG2	1:A:319:ARG:HH11	1.75	0.51
1:B:147:ARG:HE	1:B:354:GLU:CD	2.13	0.51
1:B:160:THR:CG2	1:B:164:GLU:HB3	2.39	0.51
1:B:382:HIS:C	1:B:384:ALA:H	2.14	0.51
1:B:442:MET:HE1	1:B:458:TRP:O	2.11	0.51
1:B:469:ILE:HG22	1:B:470:VAL:N	2.25	0.51
1:A:365:ARG:HG3	1:A:365:ARG:NH1	2.22	0.51
1:B:351:PHE:CE2	1:B:352:LEU:CD2	2.76	0.51
1:B:355:ARG:HG3	1:B:356:ALA:N	2.25	0.51
1:B:464:HIS:O	1:B:468:GLU:OE1	2.29	0.51
1:B:669:THR:O	1:B:672:LYS:CB	2.53	0.51
1:B:284:ALA:HB3	1:B:286:TRP:HD1	1.75	0.51
1:A:703:VAL:O	1:A:704:ARG:C	2.47	0.50
1:B:408:ARG:O	1:B:412:TYR:OH	2.28	0.50
1:B:415:VAL:HG11	1:B:601:PHE:CB	2.41	0.50
1:B:440:GLU:OE2	1:B:463:LYS:CD	2.59	0.50
1:B:488:LEU:O	1:B:492:LEU:N	2.36	0.50
1:B:571:GLN:HA	1:B:574:ASN:HB2	1.92	0.50
1:A:232:MET:HE1	1:A:235:LYS:HZ2	1.76	0.50
1:A:316:GLU:OE1	1:A:316:GLU:O	2.29	0.50
1:A:744:ARG:HH11	1:A:744:ARG:CG	2.17	0.50
1:B:466:LEU:HD11	1:B:470:VAL:CG2	2.36	0.50
1:B:750:GLU:HG3	1:B:751:HIS:N	2.23	0.50
3:P:902:DT:H6	3:P:902:DT:C4'	2.24	0.50
1:A:12:TRP:HB3	1:A:111:PRO:HD3	1.93	0.50
1:A:47:ALA:O	1:A:50:VAL:HB	2.12	0.50
1:A:323:GLU:O	1:A:324:ASP:HB2	2.11	0.50
1:A:709:ALA:HB2	1:A:739:PRO:CG	2.41	0.50
1:B:49:GLN:NE2	1:B:102:THR:H	2.08	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:THR:CG2	1:B:164:GLU:CB	2.89	0.50
1:B:250:ASN:N	1:B:250:ASN:ND2	2.59	0.50
1:A:45:ILE:CG2	1:A:46:PRO:HD2	2.42	0.50
1:A:184:GLU:HA	1:A:197:TYR:CE1	2.47	0.50
1:B:623:GLU:O	1:B:626:LYS:O	2.29	0.50
1:B:625:ASP:O	1:B:626:LYS:HG3	2.10	0.50
1:A:325:LYS:HB2	1:A:326:PRO:HD3	1.92	0.50
1:A:153:VAL:CG2	1:A:211:TRP:CH2	2.95	0.50
1:A:418:LEU:HD11	1:A:551:VAL:CG2	2.41	0.50
1:A:711:GLU:O	1:A:714:GLN:HB3	2.11	0.50
1:B:411:LEU:HD13	1:B:412:TYR:H	1.77	0.50
1:B:414:SER:HA	1:B:599:CYS:O	2.12	0.50
1:B:461:ARG:O	1:B:464:HIS:NE2	2.45	0.50
1:A:136:VAL:O	1:A:137:ASN:C	2.47	0.50
1:A:316:GLU:OE2	1:A:319:ARG:NH1	2.30	0.50
1:A:450:SER:N	1:A:461:ARG:HG3	2.26	0.50
1:A:648:PHE:CD2	1:A:760:VAL:HG21	2.42	0.50
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.76	0.50
1:B:702:HIS:HB3	1:B:730:TYR:CE2	2.46	0.50
1:A:529:GLN:NE2	1:A:533:LEU:CD1	2.75	0.50
1:A:550:PHE:CD2	1:A:550:PHE:N	2.75	0.50
1:A:771:ASN:CA	1:A:773:ALA:HB2	2.42	0.50
1:B:214:ASN:CB	1:B:215:TYR:CD2	2.94	0.50
1:B:640:ASP:OD1	1:B:640:ASP:N	2.38	0.50
1:A:324:ASP:OD2	1:A:324:ASP:O	2.30	0.50
1:A:545:ASP:CG	1:A:546:THR:H	2.15	0.50
1:A:581:LEU:CD1	1:A:588:SER:HB2	2.42	0.50
1:A:725:ARG:NH2	1:A:725:ARG:CG	2.72	0.50
1:B:282:LYS:O	1:B:285:PHE:N	2.31	0.50
1:B:450:SER:CB	1:B:458:TRP:CZ3	2.95	0.50
1:B:600:ARG:HB3	1:B:600:ARG:NH1	2.26	0.50
1:A:319:ARG:O	1:A:322:ALA:HB3	2.12	0.49
1:A:444:GLN:N	1:A:445:PRO:HD2	2.23	0.49
1:A:529:GLN:HE21	1:A:533:LEU:HD12	1.77	0.49
1:A:713:ASN:O	1:A:718:ARG:HB2	2.11	0.49
1:A:23:PHE:CE2	1:A:36:LEU:HD21	2.46	0.49
1:B:157:ILE:O	1:B:157:ILE:HG13	2.12	0.49
1:B:429:ARG:HA	1:B:467:PRO:HB3	1.94	0.49
1:B:701:PRO:HA	1:B:704:ARG:HE	1.77	0.49
1:B:737:PRO:O	1:B:738:GLU:HG2	2.12	0.49
1:A:50:VAL:HG21	1:A:79:TYR:CG	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:VAL:HG12	1:A:137:ASN:CG	2.32	0.49
1:A:156:ASP:OD2	1:A:158:GLU:OE2	2.30	0.49
1:A:245:ARG:NH1	1:A:250:ASN:O	2.45	0.49
1:A:582:GLN:O	1:A:584:GLN:O	2.30	0.49
1:B:103:VAL:O	1:B:103:VAL:HG23	2.12	0.49
1:B:349:MET:CB	1:B:350:PRO:CD	2.81	0.49
1:B:718:ARG:HB2	1:B:719:PRO:HD2	1.95	0.49
1:B:724:ASN:O	1:B:725:ARG:O	2.29	0.49
3:P:909:DC:H2'	3:P:910:DG:C8	2.48	0.49
1:A:212:PHE:CD1	1:A:272:ARG:NH1	2.79	0.49
1:A:234:GLN:O	1:A:238:GLU:CB	2.60	0.49
1:A:394:VAL:HG12	1:A:395:PRO:N	2.27	0.49
1:A:480:ALA:C	1:A:481:LYS:O	2.49	0.49
1:B:408:ARG:O	1:B:542:ILE:HG22	2.12	0.49
1:B:423:LEU:O	1:B:426:SER:OG	2.14	0.49
1:B:686:LYS:HD3	1:B:687:ARG:NH1	2.28	0.49
1:A:49:GLN:CB	1:A:101:VAL:HG13	2.43	0.49
1:A:571:GLN:O	1:A:572:HIS:C	2.48	0.49
1:B:280:ALA:O	1:B:283:SER:OG	2.30	0.49
1:B:667:ARG:O	1:B:668:GLU:C	2.51	0.49
1:B:699:VAL:HG21	1:B:704:ARG:CG	2.41	0.49
1:A:394:VAL:CG1	1:A:395:PRO:N	2.75	0.49
1:B:130:MET:CE	1:B:133:GLY:C	2.81	0.49
1:A:83:CYS:SG	1:A:89:LEU:CG	3.00	0.49
1:A:87:ARG:NH1	4:A:788:HOH:O	2.46	0.49
1:A:383:ARG:HG3	1:A:383:ARG:NH1	2.04	0.49
1:A:688:LEU:HD12	1:A:727:THR:N	2.28	0.49
1:B:278:ILE:HG22	1:B:291:PHE:CD1	2.47	0.49
1:B:413:ASP:OD1	1:B:413:ASP:O	2.31	0.49
1:B:417:VAL:HG12	1:B:417:VAL:O	2.13	0.49
1:B:533:LEU:HD11	1:B:576:TRP:CE3	2.48	0.49
1:B:692:LEU:O	1:B:707:ARG:NH2	2.45	0.49
1:A:358:VAL:HG13	1:A:495:ILE:HD13	1.81	0.49
1:A:393:GLU:O	1:A:394:VAL:HG23	2.12	0.49
1:A:692:LEU:HA	1:A:695:TYR:HD2	1.77	0.49
1:B:153:VAL:O	1:B:153:VAL:HG13	2.12	0.49
2:T:817:DC:H2'	2:T:818:DA:C4'	2.41	0.49
1:A:45:ILE:HG23	1:A:46:PRO:HD2	1.95	0.49
1:A:423:LEU:O	1:A:426:SER:HB2	2.13	0.49
1:B:494:ILE:HG13	1:B:495:ILE:N	2.24	0.49
1:B:601:PHE:HE2	1:B:603:MET:HE3	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:LEU:HD12	1:B:723:GLN:O	2.12	0.49
1:B:732:TRP:HB2	1:B:751:HIS:NE2	2.27	0.49
1:A:147:ARG:NH2	1:A:357:THR:HG21	2.28	0.49
1:B:413:ASP:HB3	1:B:600:ARG:NH1	2.28	0.49
1:B:485:ASN:CA	1:B:487:PRO:HD3	2.39	0.49
1:B:487:PRO:HD2	1:B:488:LEU:N	2.24	0.49
1:A:275:ILE:CG2	1:A:276:ASP:N	2.75	0.48
1:A:732:TRP:CD2	1:A:751:HIS:CD2	3.01	0.48
1:B:72:ASP:OD1	1:B:74:HIS:N	2.25	0.48
1:B:488:LEU:O	1:B:491:ALA:HB3	2.13	0.48
1:B:651:GLU:O	1:B:655:ARG:HG3	2.12	0.48
1:A:48:ASP:O	1:A:51:PRO:CD	2.38	0.48
1:A:76:GLN:O	1:A:77:PRO:C	2.50	0.48
1:A:336:CYS:O	1:A:340:THR:HG22	2.12	0.48
1:A:692:LEU:HD11	1:A:723:GLN:C	2.32	0.48
1:B:346:THR:OG1	1:B:347:GLU:N	2.46	0.48
1:A:193:PHE:CG	1:A:333:LEU:CD1	2.93	0.48
1:A:431:PHE:CE2	1:A:522:ARG:HD3	2.47	0.48
1:A:470:VAL:HG23	1:A:470:VAL:O	2.13	0.48
1:A:625:ASP:C	1:A:626:LYS:CD	2.82	0.48
1:B:625:ASP:C	1:B:626:LYS:CG	2.82	0.48
1:A:103:VAL:O	1:A:103:VAL:HG23	2.14	0.48
1:A:127:GLU:CB	1:A:139:ARG:NH2	2.76	0.48
1:B:146:TYR:O	1:B:147:ARG:NH1	2.39	0.48
1:B:284:ALA:O	1:B:285:PHE:HB2	2.13	0.48
1:A:45:ILE:CG2	1:A:46:PRO:CD	2.91	0.48
1:A:143:HIS:CD2	1:A:146:TYR:HB2	2.49	0.48
1:A:691:PRO:HA	1:A:723:GLN:O	2.13	0.48
1:A:765:LEU:N	1:A:766:PRO:HD2	2.29	0.48
1:B:576:TRP:O	1:B:580:THR:CG2	2.43	0.48
1:B:651:GLU:OE1	1:B:665:TYR:OH	2.29	0.48
1:A:410:GLY:HA2	1:A:767:PHE:CD1	2.49	0.48
1:B:416:LEU:C	1:B:551:VAL:HG12	2.34	0.48
1:B:431:PHE:CD2	1:B:522:ARG:HD3	2.48	0.48
1:A:48:ASP:C	1:A:50:VAL:H	2.16	0.48
1:B:228:PHE:O	1:B:229:ASP:C	2.48	0.48
1:A:466:LEU:O	1:A:467:PRO:C	2.50	0.48
1:B:381:MET:CE	1:B:388:ALA:N	2.59	0.48
1:B:750:GLU:O	1:B:750:GLU:OE1	2.32	0.48
1:A:112:GLU:O	1:A:116:MET:CB	2.56	0.48
1:A:431:PHE:CZ	1:A:522:ARG:HD3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:SER:O	1:A:490:GLN:C	2.52	0.48
1:B:359:ASN:HD22	1:B:361:LEU:CB	2.27	0.48
1:B:378:PHE:HZ	1:B:509:ARG:NH2	2.12	0.48
1:B:419:ASP:O	1:B:593:GLU:HG3	2.13	0.48
1:A:27:THR:OG1	1:A:30:GLY:O	2.28	0.48
1:A:193:PHE:CD2	1:A:333:LEU:HD12	2.49	0.48
1:A:415:VAL:HG21	1:A:601:PHE:HB3	1.96	0.48
1:B:34:VAL:HG11	1:B:140:LEU:HD21	1.95	0.48
1:B:354:GLU:CG	1:B:488:LEU:HB3	2.38	0.48
1:B:703:VAL:HG12	1:B:704:ARG:N	2.29	0.48
1:A:692:LEU:HD13	1:A:723:GLN:C	2.34	0.47
1:B:289:SER:OG	1:B:299:GLU:OE1	2.31	0.47
1:B:529:GLN:O	1:B:533:LEU:HG	2.14	0.47
1:B:762:GLU:O	1:B:766:PRO:HG2	2.14	0.47
1:B:512:ASP:CG	1:B:514:ARG:HG3	2.34	0.47
1:B:757:LEU:HD12	1:B:757:LEU:N	2.29	0.47
2:T:813:DT:H2"	2:T:814:DA:C5'	2.44	0.47
1:A:470:VAL:O	1:A:470:VAL:CG2	2.61	0.47
1:A:625:ASP:HB3	1:A:626:LYS:CD	2.44	0.47
1:B:381:MET:HE3	1:B:388:ALA:CB	2.44	0.47
1:B:486:LYS:N	1:B:487:PRO:CD	2.65	0.47
1:A:94:LYS:HB2	1:A:94:LYS:HE2	1.28	0.47
1:A:529:GLN:HG3	1:A:529:GLN:O	2.10	0.47
1:A:549:THR:CG2	1:A:550:PHE:N	2.76	0.47
1:A:571:GLN:OE1	1:A:571:GLN:N	2.46	0.47
1:A:597:HIS:C	1:A:597:HIS:ND1	2.68	0.47
1:A:734:THR:HG22	1:A:735:ASN:OD1	2.14	0.47
1:B:9:THR:CG2	1:B:11:HIS:NE2	2.74	0.47
1:B:121:THR:HG23	1:B:123:PRO:CD	2.43	0.47
1:B:198:VAL:CG2	1:B:204:LEU:HD21	2.43	0.47
1:B:245:ARG:HA	1:B:251:SER:O	2.15	0.47
1:B:408:ARG:HB2	1:B:542:ILE:HG22	1.95	0.47
1:B:495:ILE:CG1	1:B:496:MET:N	2.77	0.47
1:B:672:LYS:HE2	1:B:678:LEU:HD21	1.97	0.47
1:B:702:HIS:CB	1:B:730:TYR:CE2	2.97	0.47
1:B:733:THR:OG1	1:B:746:PRO:O	2.32	0.47
1:A:278:ILE:HG22	1:A:282:LYS:HE2	1.95	0.47
1:A:319:ARG:CG	1:A:320:ARG:N	2.77	0.47
1:A:674:MET:HA	1:A:749:TYR:CD2	2.50	0.47
1:A:688:LEU:HB2	1:A:726:GLY:O	2.14	0.47
1:B:464:HIS:CA	1:B:468:GLU:OE1	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:GLN:HE22	1:A:783:PHE:HE1	1.63	0.47
1:B:15:THR:O	1:B:18:GLY:O	2.33	0.47
1:B:552:TRP:NE1	1:B:554:LYS:O	2.40	0.47
2:T:819:DC:C2'	2:T:820:DA:C1'	2.92	0.47
1:A:477:ARG:HD3	1:A:489:SER:HB3	1.95	0.47
1:A:531:LYS:HB2	1:A:541:VAL:HG21	1.96	0.47
1:A:691:PRO:O	1:A:694:GLU:N	2.47	0.47
1:A:709:ALA:HB2	1:A:739:PRO:HG2	1.97	0.47
1:B:48:ASP:H	1:B:76:GLN:HE21	1.63	0.47
1:B:112:GLU:O	1:B:116:MET:HB2	2.15	0.47
1:B:209:ASN:ND2	1:B:245:ARG:H	2.12	0.47
1:B:227:GLN:O	1:B:231:ARG:NH1	2.47	0.47
1:B:440:GLU:OE2	1:B:463:LYS:CG	2.63	0.47
1:B:488:LEU:O	1:B:489:SER:C	2.52	0.47
1:B:525:GLN:HA	1:B:528:ARG:CD	2.45	0.47
1:B:525:GLN:HA	1:B:528:ARG:NE	2.29	0.47
1:B:662:TYR:CD1	1:B:662:TYR:C	2.87	0.47
2:T:817:DC:OP1	2:T:817:DC:H4'	2.14	0.47
1:A:11:HIS:CE1	1:A:24:TRP:HD1	2.33	0.47
1:A:692:LEU:HD11	1:A:723:GLN:CA	2.45	0.47
1:B:21:VAL:HG12	1:B:23:PHE:CE2	2.50	0.47
1:B:416:LEU:CD1	1:B:597:HIS:CD2	2.96	0.47
1:B:424:TYR:CD2	1:B:519:ILE:CG2	2.97	0.47
1:B:602:LEU:HG	1:B:603:MET:N	2.30	0.47
1:A:109:ARG:HD3	1:A:109:ARG:HA	1.67	0.47
1:A:183:PRO:O	1:A:325:LYS:HE2	2.15	0.47
1:A:690:ARG:HG2	1:A:695:TYR:CE2	2.50	0.47
1:B:218:ASP:CG	1:B:248:ARG:HH22	2.09	0.47
2:T:820:DA:OP2	2:T:820:DA:C2'	2.62	0.47
3:P:902:DT:H2"	3:P:903:DG:C4'	2.45	0.47
1:A:150:LEU:HD12	1:A:218:ASP:HB3	1.97	0.47
1:A:348:ILE:O	1:A:352:LEU:HD13	2.15	0.47
1:A:395:PRO:HA	1:A:396:PRO:HD3	1.63	0.47
1:A:495:ILE:O	1:A:496:MET:C	2.53	0.47
1:A:688:LEU:C	1:A:726:GLY:H	2.19	0.47
1:B:130:MET:HE3	1:B:133:GLY:C	2.36	0.47
1:B:436:VAL:CG1	1:B:437:GLY:H	2.23	0.47
2:T:820:DA:OP2	2:T:820:DA:H2'	2.15	0.47
1:A:481:LYS:O	1:A:482:ARG:O	2.33	0.46
1:A:725:ARG:HG2	1:A:725:ARG:HH21	1.80	0.46
1:B:418:LEU:O	1:B:418:LEU:HD13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:PRO:O	1:B:490:GLN:HB2	2.14	0.46
1:B:672:LYS:O	1:B:677:GLU:N	2.46	0.46
1:A:29:ASN:N	1:A:29:ASN:OD1	2.46	0.46
1:A:65:LEU:HD23	1:A:79:TYR:HB3	1.97	0.46
1:A:153:VAL:HG23	1:A:211:TRP:CH2	2.50	0.46
1:A:654:LEU:HD12	1:A:655:ARG:CA	2.44	0.46
1:B:11:HIS:NE2	1:B:270:LYS:HG3	2.30	0.46
1:B:68:LEU:HD21	1:B:80:GLY:HA3	1.96	0.46
1:B:591:GLU:O	1:B:591:GLU:CG	2.57	0.46
1:B:710:ASP:O	1:B:711:GLU:C	2.52	0.46
1:B:712:GLU:OE2	1:B:712:GLU:C	2.53	0.46
1:A:25:LEU:O	1:A:31:PRO:HA	2.15	0.46
1:A:116:MET:CE	1:A:378:PHE:CD2	2.98	0.46
1:A:118:ARG:O	1:A:119:PHE:HB2	2.15	0.46
1:A:198:VAL:CG1	1:A:199:ALA:N	2.78	0.46
1:A:326:PRO:O	1:A:330:THR:CG2	2.61	0.46
1:A:755:ARG:HA	1:A:755:ARG:HE	1.79	0.46
1:B:381:MET:HE3	1:B:388:ALA:HB2	1.96	0.46
1:B:474:TRP:O	1:B:478:ASP:OD1	2.32	0.46
1:B:689:ARG:C	1:B:725:ARG:CG	2.84	0.46
3:P:905:DC:C2'	3:P:906:DT:C6	2.98	0.46
1:A:684:TYR:O	1:A:729:LYS:HB2	2.16	0.46
1:B:691:PRO:O	1:B:694:GLU:HG2	2.15	0.46
1:B:735:ASN:OD1	1:B:735:ASN:N	2.35	0.46
1:A:378:PHE:HB2	1:A:379:PRO:HD3	1.97	0.46
1:A:576:TRP:O	1:A:580:THR:HB	2.14	0.46
1:B:9:THR:HG23	1:B:10:ARG:N	2.30	0.46
1:B:200:SER:C	1:B:202:PRO:CD	2.83	0.46
1:B:508:CYS:SG	1:B:509:ARG:O	2.69	0.46
1:B:526:ILE:HG23	1:B:577:TRP:CZ2	2.50	0.46
1:B:664:GLU:O	1:B:668:GLU:HB2	2.15	0.46
2:T:810:DC:H2"	2:T:811:DG:O5'	2.14	0.46
1:A:45:ILE:O	1:A:79:TYR:N	2.36	0.46
1:A:49:GLN:HE21	1:A:101:VAL:CG1	2.15	0.46
1:A:319:ARG:NH1	1:A:319:ARG:HG2	2.30	0.46
1:A:450:SER:HB2	1:A:458:TRP:CE3	2.48	0.46
1:A:600:ARG:HH11	1:A:600:ARG:CB	2.29	0.46
1:A:638:ARG:HA	3:P:910:DG:OP1	2.15	0.46
1:A:710:ASP:CG	1:A:722:TYR:HB2	2.35	0.46
1:B:351:PHE:O	1:B:351:PHE:CG	2.63	0.46
1:B:451:THR:CG2	1:B:586:LEU:HD21	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:ARG:O	1:B:480:ALA:HB3	2.15	0.46
1:B:733:THR:CA	1:B:736:GLY:O	2.63	0.46
1:B:748:ASP:O	1:B:751:HIS:N	2.49	0.46
1:A:398:ALA:O	1:A:399:SER:O	2.34	0.46
1:A:403:TYR:CD1	1:A:404:VAL:N	2.83	0.46
1:A:701:PRO:O	1:A:702:HIS:C	2.52	0.46
1:B:148:PRO:HA	1:B:149:PRO:HD3	1.75	0.46
1:B:175:GLN:CD	1:B:215:TYR:HE1	2.06	0.46
3:P:906:DT:H2"	3:P:907:DA:O5'	2.12	0.46
1:A:515:LEU:HD12	1:A:515:LEU:HA	1.60	0.46
1:B:255:TRP:O	1:B:256:ARG:CG	2.51	0.46
1:B:155:ILE:O	1:B:155:ILE:HG23	2.15	0.46
1:B:191:LEU:N	1:B:191:LEU:HD12	2.31	0.46
1:B:449:HIS:HA	1:B:461:ARG:HG3	1.98	0.46
1:B:477:ARG:N	1:B:492:LEU:HD13	2.30	0.46
1:B:571:GLN:O	1:B:572:HIS:C	2.52	0.46
1:B:601:PHE:CE2	1:B:603:MET:HB3	2.44	0.46
1:A:198:VAL:HG12	1:A:200:SER:N	2.30	0.46
1:B:198:VAL:HG23	1:B:204:LEU:HD21	1.98	0.46
1:B:442:MET:CE	1:B:442:MET:CA	2.94	0.46
1:B:488:LEU:HD12	1:B:492:LEU:HG	1.98	0.46
1:B:491:ALA:O	1:B:495:ILE:CG2	2.64	0.46
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.97	0.45
1:A:686:LYS:NZ	1:A:730:TYR:OH	2.35	0.45
1:A:713:ASN:O	1:A:718:ARG:O	2.34	0.45
1:B:11:HIS:CE1	1:B:24:TRP:HD1	2.34	0.45
1:B:50:VAL:HB	1:B:51:PRO:HD3	1.97	0.45
1:B:72:ASP:OD1	1:B:72:ASP:C	2.54	0.45
1:B:420:TYR:HA	1:B:592:LEU:HA	1.97	0.45
1:B:434:ASP:OD2	1:B:436:VAL:HG12	2.15	0.45
1:B:474:TRP:CB	1:B:496:MET:HE1	2.46	0.45
1:A:184:GLU:HA	1:A:197:TYR:CZ	2.51	0.45
1:A:468:GLU:OE2	1:A:468:GLU:N	2.50	0.45
1:A:746:PRO:O	1:A:746:PRO:CD	2.63	0.45
1:B:571:GLN:O	1:B:575:ALA:N	2.40	0.45
1:A:9:THR:OG1	1:A:11:HIS:HE1	1.98	0.45
1:A:235:LYS:O	1:A:239:ARG:N	2.49	0.45
1:A:365:ARG:NH1	1:A:365:ARG:CG	2.76	0.45
1:A:412:TYR:O	1:A:600:ARG:HA	2.16	0.45
1:A:553:LEU:HD12	1:A:553:LEU:HA	1.60	0.45
1:A:709:ALA:CB	1:A:722:TYR:HE2	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:VAL:O	1:B:137:ASN:C	2.55	0.45
1:B:416:LEU:HD12	1:B:597:HIS:HD2	1.82	0.45
1:B:598:PHE:CD2	1:B:601:PHE:CD1	3.01	0.45
3:P:907:DA:H2"	3:P:908:DG:O4'	2.16	0.45
1:A:219:VAL:CG1	1:A:275:ILE:HD13	2.46	0.45
1:A:454:PHE:O	1:A:455:LEU:CD1	2.65	0.45
1:B:36:LEU:HD12	1:B:36:LEU:HA	1.78	0.45
1:B:143:HIS:CD2	1:B:144:PRO:CD	3.00	0.45
1:B:525:GLN:HA	1:B:528:ARG:HE	1.81	0.45
1:B:601:PHE:HE2	1:B:603:MET:CB	2.25	0.45
1:B:765:LEU:HD12	1:B:765:LEU:HA	1.52	0.45
1:B:765:LEU:N	1:B:766:PRO:HD2	2.32	0.45
2:T:813:DT:C2'	2:T:814:DA:O5'	2.54	0.45
1:A:232:MET:HE3	1:A:235:LYS:NZ	2.30	0.45
1:A:418:LEU:CD1	1:A:551:VAL:HG21	2.47	0.45
1:A:678:LEU:O	1:A:682:LEU:HD13	2.17	0.45
1:A:690:ARG:HB2	1:A:690:ARG:HE	1.55	0.45
1:A:709:ALA:HB1	1:A:722:TYR:HE2	1.82	0.45
1:B:413:ASP:CG	1:B:600:ARG:NH1	2.70	0.45
1:B:585:ARG:C	1:B:586:LEU:HD12	2.33	0.45
1:B:718:ARG:CB	1:B:719:PRO:HD2	2.45	0.45
1:A:49:GLN:NE2	1:A:101:VAL:CG1	2.77	0.45
1:A:714:GLN:C	1:A:716:ARG:N	2.67	0.45
1:B:429:ARG:H	1:B:429:ARG:HG3	1.54	0.45
1:B:711:GLU:HG3	1:B:712:GLU:N	2.32	0.45
1:A:406:ASP:OD1	1:A:406:ASP:O	2.35	0.45
1:A:764:ILE:O	1:A:764:ILE:CG1	2.64	0.45
1:B:362:PRO:O	1:B:365:ARG:HB3	2.16	0.45
1:B:442:MET:N	1:B:442:MET:HE3	2.30	0.45
1:B:446:ASP:C	1:B:448:GLU:N	2.69	0.45
1:B:484:GLY:CA	1:B:485:ASN:HB3	2.40	0.45
1:B:765:LEU:N	1:B:766:PRO:CD	2.79	0.45
1:A:65:LEU:CD2	1:A:79:TYR:HD1	2.29	0.45
1:A:466:LEU:HB3	1:A:467:PRO:HD3	1.99	0.45
1:B:153:VAL:HG23	1:B:211:TRP:CH2	2.51	0.45
1:B:234:GLN:O	1:B:235:LYS:C	2.52	0.45
1:A:66:THR:OG1	1:A:67:PRO:N	2.50	0.45
1:A:529:GLN:O	1:A:533:LEU:HD13	2.16	0.45
1:A:716:ARG:O	1:A:717:GLY:O	2.33	0.45
1:A:734:THR:HB	1:A:746:PRO:HG2	1.99	0.45
1:B:88:GLN:CG	1:B:89:LEU:N	2.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:PRO:O	1:B:124:VAL:HG13	2.16	0.45
1:B:338:LEU:HD23	1:B:338:LEU:N	2.32	0.45
1:B:685:ARG:CZ	1:B:685:ARG:CB	2.90	0.45
2:T:811:DG:H2'	2:T:812:DC:C5	2.49	0.45
2:T:819:DC:C6	2:T:820:DA:C8	3.05	0.45
3:P:908:DG:C2'	3:P:909:DC:O5'	2.63	0.45
3:P:913:DG:P	3:P:913:DG:C2'	2.98	0.45
1:A:479:GLU:OE2	1:A:479:GLU:O	2.35	0.45
1:A:488:LEU:O	1:A:491:ALA:HB3	2.17	0.45
1:A:724:ASN:O	1:A:725:ARG:O	2.34	0.45
1:B:413:ASP:CA	1:B:600:ARG:HA	2.45	0.45
1:A:153:VAL:O	1:A:153:VAL:CG1	2.65	0.44
1:A:237:ALA:HB2	1:A:244:LEU:HD13	1.98	0.44
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.78	0.44
1:A:359:ASN:OD1	1:A:361:LEU:N	2.28	0.44
1:A:529:GLN:O	1:A:532:ALA:HB3	2.18	0.44
1:A:625:ASP:C	1:A:626:LYS:HD3	2.37	0.44
1:B:11:HIS:HE1	1:B:24:TRP:CD1	2.35	0.44
1:B:277:GLY:O	1:B:281:LEU:CB	2.54	0.44
1:B:733:THR:O	1:B:736:GLY:CA	2.65	0.44
1:A:48:ASP:C	1:A:50:VAL:N	2.70	0.44
1:B:55:HIS:O	1:B:58:GLN:HG3	2.14	0.44
1:B:60:GLU:HG3	1:B:92:TYR:OH	2.15	0.44
1:B:84:ARG:HD3	1:B:84:ARG:HA	1.88	0.44
1:B:143:HIS:HD2	1:B:145:ASP:H	1.65	0.44
1:B:354:GLU:HG2	1:B:488:LEU:CB	2.42	0.44
1:B:474:TRP:HB2	1:B:496:MET:HE1	1.99	0.44
1:B:724:ASN:N	1:B:724:ASN:ND2	2.59	0.44
3:P:907:DA:C2'	3:P:908:DG:O5'	2.63	0.44
1:A:90:MET:O	1:A:93:GLU:HG3	2.17	0.44
1:A:130:MET:HE2	1:A:130:MET:HB2	1.84	0.44
1:A:349:MET:O	1:A:350:PRO:C	2.54	0.44
1:A:512:ASP:O	1:A:515:LEU:HB2	2.17	0.44
1:A:728:ILE:O	1:A:728:ILE:HG23	2.15	0.44
1:B:122:SER:H	1:B:123:PRO:CD	2.31	0.44
1:B:130:MET:HE3	1:B:133:GLY:N	2.32	0.44
1:B:426:SER:OG	1:B:427:ILE:N	2.51	0.44
1:B:482:ARG:HG2	1:B:482:ARG:O	2.16	0.44
1:B:692:LEU:HD13	1:B:723:GLN:CA	2.44	0.44
1:A:34:VAL:HG13	1:A:138:ALA:CB	2.48	0.44
1:A:42:VAL:HG21	1:A:82:TYR:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ALA:HB1	1:A:242:LEU:O	2.17	0.44
1:A:725:ARG:CG	1:A:725:ARG:HH21	2.30	0.44
1:B:52:ARG:HH11	1:B:52:ARG:CG	2.30	0.44
1:A:355:ARG:HH22	1:A:366:HIS:HA	1.82	0.44
1:B:60:GLU:OE1	1:B:95:ARG:NH2	2.50	0.44
1:B:240:TYR:O	1:B:241:ARG:HB2	2.18	0.44
1:B:290:SER:HB3	1:B:295:THR:HG21	2.00	0.44
1:B:435:PRO:HG3	1:B:515:LEU:HD21	1.99	0.44
1:B:534:ILE:HA	1:B:534:ILE:HD13	1.71	0.44
1:A:8:LEU:C	1:A:9:THR:CG2	2.85	0.44
1:A:49:GLN:O	1:A:53:ALA:HB2	2.17	0.44
1:A:178:VAL:CG1	1:A:179:TYR:N	2.81	0.44
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.49	0.44
1:A:249:ASP:O	1:A:250:ASN:C	2.54	0.44
1:A:743:GLN:HG2	1:A:744:ARG:N	2.14	0.44
1:B:692:LEU:HA	1:B:695:TYR:HD2	1.83	0.44
1:A:60:GLU:O	1:A:61:GLN:HB3	2.17	0.44
1:A:198:VAL:CG1	1:A:203:GLN:HB2	2.47	0.44
1:A:348:ILE:HG23	1:A:349:MET:N	2.27	0.44
1:B:185:ASN:HB2	1:B:325:LYS:HB2	1.99	0.44
1:B:257:GLU:CB	1:B:265:PHE:HA	2.47	0.44
1:B:394:VAL:HA	1:B:395:PRO:HD3	1.73	0.44
1:B:535:GLU:O	1:B:537:GLN:N	2.50	0.44
1:B:685:ARG:CZ	1:B:685:ARG:HB3	2.48	0.44
1:A:109:ARG:HB3	1:A:112:GLU:OE1	2.17	0.44
1:A:352:LEU:CD1	1:A:352:LEU:N	2.81	0.44
1:A:616:ARG:HB2	1:A:634:LEU:CD1	2.47	0.44
1:B:234:GLN:O	1:B:234:GLN:HG3	2.17	0.44
1:B:734:THR:HB	1:B:746:PRO:CG	2.42	0.44
1:B:756:GLN:O	1:B:759:PRO:HD2	2.18	0.44
1:A:250:ASN:N	1:A:250:ASN:HD22	2.16	0.44
1:A:444:GLN:OE1	1:A:449:HIS:CE1	2.70	0.44
1:A:519:ILE:HD13	1:A:519:ILE:HG21	1.76	0.44
1:A:597:HIS:ND1	1:A:598:PHE:N	2.66	0.44
1:A:625:ASP:C	1:A:626:LYS:HD2	2.38	0.44
1:A:705:ALA:HB1	1:A:739:PRO:HG3	2.00	0.44
1:B:49:GLN:HB3	1:B:101:VAL:HG13	2.00	0.44
1:B:68:LEU:HD23	1:B:80:GLY:N	2.33	0.44
1:B:354:GLU:CG	1:B:488:LEU:CB	2.96	0.44
1:B:638:ARG:CG	1:B:640:ASP:OD1	2.44	0.44
1:B:687:ARG:HA	1:B:726:GLY:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:903:DG:H2'	3:P:904:DC:H5	1.83	0.44
1:A:293:LEU:O	1:A:294:GLU:C	2.55	0.43
1:A:488:LEU:HD23	1:A:488:LEU:HA	1.85	0.43
1:A:733:THR:HB	1:A:745:SER:HB2	1.99	0.43
1:B:297:ALA:O	1:B:301:LEU:HB2	2.18	0.43
1:B:422:SER:HB3	1:B:425:PRO:HG2	2.00	0.43
1:B:577:TRP:O	1:B:580:THR:HG23	2.18	0.43
1:B:622:GLN:HG3	1:B:626:LYS:O	2.17	0.43
1:A:153:VAL:HG21	1:A:211:TRP:CH2	2.54	0.43
1:A:647:GLN:O	1:A:651:GLU:CG	2.62	0.43
1:A:751:HIS:ND1	1:A:755:ARG:HB2	2.33	0.43
1:B:74:HIS:C	1:B:75:ARG:HG3	2.39	0.43
1:B:130:MET:HG3	1:B:131:HIS:N	2.32	0.43
1:B:364:ASP:OD2	1:B:364:ASP:N	2.50	0.43
1:B:442:MET:HE2	1:B:442:MET:HA	2.00	0.43
1:B:495:ILE:HD11	1:B:499:PHE:CZ	2.53	0.43
1:B:602:LEU:O	1:B:618:ALA:O	2.36	0.43
1:B:625:ASP:C	1:B:626:LYS:HG3	2.38	0.43
1:B:692:LEU:HD23	1:B:707:ARG:HG2	1.99	0.43
1:B:122:SER:HB2	1:B:123:PRO:HD3	1.99	0.43
1:B:255:TRP:C	1:B:256:ARG:HG2	2.36	0.43
1:B:430:THR:OG1	1:B:589:ALA:HB2	2.17	0.43
1:B:539:TYR:CZ	1:B:565:ILE:HG21	2.51	0.43
1:B:673:LEU:C	1:B:676:GLY:H	2.18	0.43
1:B:692:LEU:HD12	1:B:722:TYR:O	2.10	0.43
1:A:177:ILE:CG1	1:A:178:VAL:N	2.80	0.43
1:A:772:PHE:CA	1:A:773:ALA:HB2	2.38	0.43
1:B:61:GLN:HG3	1:B:62:GLY:H	1.83	0.43
1:B:264:VAL:O	1:B:264:VAL:HG22	2.17	0.43
1:B:418:LEU:N	1:B:418:LEU:CD1	2.49	0.43
1:B:485:ASN:O	1:B:485:ASN:OD1	2.36	0.43
1:B:577:TRP:CA	1:B:580:THR:HG22	2.48	0.43
1:B:686:LYS:HG3	1:B:687:ARG:HH11	1.83	0.43
1:A:293:LEU:HA	1:A:293:LEU:HD23	1.76	0.43
1:A:467:PRO:HB2	1:A:468:GLU:OE2	2.19	0.43
1:A:692:LEU:HD11	1:A:723:GLN:HA	1.96	0.43
1:A:692:LEU:HA	1:A:695:TYR:CE2	2.53	0.43
1:B:118:ARG:HB3	1:B:120:ILE:HG13	2.00	0.43
1:B:191:LEU:N	1:B:191:LEU:CD1	2.81	0.43
1:B:529:GLN:O	1:B:530:THR:C	2.53	0.43
1:B:568:ALA:O	1:B:571:GLN:HG2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:GLN:H	1:B:759:PRO:HD3	1.80	0.43
3:P:903:DG:H2'	3:P:904:DC:C6	2.54	0.43
1:A:255:TRP:CZ3	1:A:267:ALA:HB2	2.54	0.43
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.16	0.43
1:A:412:TYR:HB3	1:A:552:TRP:CZ3	2.54	0.43
1:B:441:GLY:C	1:B:443:ALA:H	2.22	0.43
1:B:535:GLU:C	1:B:537:GLN:N	2.70	0.43
1:A:83:CYS:SG	1:A:89:LEU:HG	2.59	0.43
1:A:444:GLN:H	1:A:445:PRO:HD3	1.82	0.43
1:A:446:ASP:OD2	1:A:446:ASP:O	2.36	0.43
1:A:702:HIS:O	1:A:706:ALA:CB	2.66	0.43
1:B:123:PRO:O	1:B:124:VAL:CG1	2.67	0.43
1:B:424:TYR:HD2	1:B:519:ILE:HG23	1.83	0.43
1:B:438:LEU:HB2	1:B:459:PHE:CE1	2.53	0.43
1:B:461:ARG:NH1	1:B:585:ARG:HD3	2.33	0.43
1:B:487:PRO:HG2	1:B:488:LEU:N	2.31	0.43
1:B:703:VAL:HG12	1:B:704:ARG:H	1.84	0.43
1:A:321:PHE:O	1:A:321:PHE:CG	2.71	0.43
1:A:454:PHE:HB3	1:A:455:LEU:HD12	2.00	0.43
1:A:557:HIS:C	1:A:558:SER:O	2.54	0.43
1:A:642:THR:CG2	1:A:643:PRO:N	2.82	0.43
1:B:761:ALA:O	1:B:765:LEU:HB2	2.18	0.43
3:P:902:DT:C2'	3:P:903:DG:O4'	2.58	0.43
1:A:36:LEU:CD1	1:A:36:LEU:N	2.40	0.43
1:A:45:ILE:HG22	1:A:46:PRO:N	2.33	0.43
1:A:64:ARG:CB	1:A:64:ARG:CZ	2.95	0.43
1:A:454:PHE:O	1:A:455:LEU:CB	2.58	0.43
1:B:74:HIS:O	1:B:75:ARG:HB2	2.18	0.43
1:B:103:VAL:O	1:B:103:VAL:CG2	2.64	0.43
1:A:316:GLU:OE1	1:A:316:GLU:C	2.58	0.43
1:A:668:GLU:O	1:A:672:LYS:CG	2.54	0.43
1:B:693:SER:O	1:B:695:TYR:N	2.47	0.43
1:B:714:GLN:HE21	1:B:714:GLN:HB2	1.49	0.43
1:A:105:GLU:HG2	1:A:388:ALA:HB3	2.01	0.42
1:A:115:LEU:O	1:A:116:MET:C	2.57	0.42
1:A:323:GLU:O	1:A:324:ASP:CB	2.66	0.42
1:A:449:HIS:C	1:A:461:ARG:HG3	2.40	0.42
1:A:709:ALA:CB	1:A:722:TYR:CE2	3.01	0.42
1:A:709:ALA:HB3	1:A:722:TYR:CE2	2.54	0.42
1:B:15:THR:HB	1:B:16:PRO:HD2	2.01	0.42
1:B:192:ASP:N	1:B:192:ASP:OD1	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:TYR:CE2	1:B:550:PHE:HE2	2.36	0.42
1:B:732:TRP:CD2	1:B:751:HIS:CD2	3.04	0.42
1:A:236:HIS:ND1	1:A:236:HIS:N	2.66	0.42
1:A:379:PRO:O	1:A:383:ARG:HG3	2.18	0.42
1:A:653:TYR:N	1:A:653:TYR:HD1	2.17	0.42
1:A:738:GLU:CD	1:A:745:SER:OG	2.56	0.42
1:B:658:ARG:HE	1:B:658:ARG:HB3	1.67	0.42
1:B:664:GLU:O	1:B:668:GLU:N	2.42	0.42
1:B:704:ARG:O	1:B:705:ALA:C	2.56	0.42
3:P:902:DT:C2'	3:P:903:DG:OP1	2.62	0.42
1:A:325:LYS:N	1:A:326:PRO:CD	2.82	0.42
1:A:438:LEU:O	1:A:442:MET:N	2.52	0.42
1:B:517:SER:O	1:B:518:SER:C	2.55	0.42
1:B:560:GLU:O	1:B:564:LYS:HB2	2.19	0.42
1:B:699:VAL:CG2	1:B:704:ARG:NE	2.83	0.42
3:P:903:DG:C2'	3:P:904:DC:C6	3.02	0.42
3:P:913:DG:O5'	3:P:913:DG:C1'	2.67	0.42
1:A:62:GLY:O	1:A:88:GLN:NE2	2.52	0.42
1:A:268:GLN:HE21	1:A:268:GLN:HB3	1.64	0.42
1:A:397:HIS:HD2	1:A:399:SER:N	2.13	0.42
1:A:687:ARG:HA	1:A:727:THR:HG23	2.02	0.42
1:B:391:LEU:HA	1:B:391:LEU:HD12	1.71	0.42
1:B:414:SER:HA	1:B:598:PHE:O	2.19	0.42
1:B:629:MET:CE	1:B:657:PHE:CE2	2.99	0.42
1:B:720:LEU:HD13	1:B:720:LEU:H	1.84	0.42
1:B:733:THR:O	1:B:736:GLY:N	2.52	0.42
2:T:819:DC:C4	2:T:820:DA:C5	3.08	0.42
3:P:904:DC:H2"	3:P:905:DC:O5'	2.18	0.42
1:A:61:GLN:HB3	1:A:61:GLN:HE21	1.58	0.42
1:A:121:THR:HB	1:A:360:GLY:HA2	2.02	0.42
1:B:93:GLU:OE1	1:B:93:GLU:O	2.37	0.42
1:B:151:LYS:O	1:B:218:ASP:N	2.49	0.42
1:B:342:ILE:HG22	1:B:343:PHE:N	2.33	0.42
1:B:557:HIS:CD2	1:B:557:HIS:H	2.36	0.42
1:B:656:ILE:HD12	1:B:764:ILE:CD1	2.44	0.42
1:A:234:GLN:O	1:A:238:GLU:N	2.38	0.42
1:A:448:GLU:O	1:A:448:GLU:HG2	2.18	0.42
1:A:533:LEU:HD12	1:A:533:LEU:N	2.34	0.42
1:A:653:TYR:N	1:A:653:TYR:CD1	2.87	0.42
3:P:910:DG:H2'	3:P:911:DT:C5	2.54	0.42
1:A:11:HIS:HE1	1:A:24:TRP:HD1	1.66	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:VAL:HG11	1:A:594:TYR:HB2	2.01	0.42
1:A:571:GLN:HA	1:A:574:ASN:HB2	2.01	0.42
1:B:250:ASN:HD22	1:B:250:ASN:N	2.17	0.42
1:B:316:GLU:O	1:B:317:ILE:C	2.53	0.42
1:B:478:ASP:O	1:B:479:GLU:C	2.58	0.42
1:B:535:GLU:O	1:B:538:GLY:N	2.43	0.42
1:B:687:ARG:O	1:B:687:ARG:HD3	2.19	0.42
1:B:690:ARG:O	1:B:691:PRO:C	2.57	0.42
1:A:54:GLN:HG2	1:A:54:GLN:H	1.51	0.42
1:A:70:LEU:HD12	1:A:70:LEU:HA	1.59	0.42
1:A:216:ASP:OD1	1:A:272:ARG:NH2	2.53	0.42
1:A:245:ARG:HA	1:A:251:SER:O	2.20	0.42
1:A:349:MET:HE2	1:A:349:MET:HB3	1.72	0.42
1:A:690:ARG:HG2	1:A:695:TYR:CZ	2.55	0.42
1:B:121:THR:OG1	1:B:357:THR:O	2.30	0.42
1:B:248:ARG:HG3	1:B:270:LYS:O	2.20	0.42
1:B:355:ARG:HA	1:B:491:ALA:HB1	2.01	0.42
1:B:381:MET:CE	1:B:388:ALA:CB	2.96	0.42
1:B:525:GLN:HA	1:B:528:ARG:HD3	2.02	0.42
3:P:910:DG:C8	3:P:911:DT:C7	3.03	0.42
1:A:8:LEU:O	1:A:9:THR:HG22	2.19	0.42
1:A:123:PRO:C	1:A:124:VAL:HG13	2.40	0.42
1:A:242:LEU:HD12	1:A:243:PRO:CD	2.49	0.42
1:A:243:PRO:O	1:A:243:PRO:HG2	2.20	0.42
1:A:281:LEU:HD22	1:A:286:TRP:CD1	2.55	0.42
1:A:665:TYR:O	1:A:669:THR:OG1	2.30	0.42
1:B:11:HIS:HB2	1:B:22:SER:HB3	2.02	0.42
1:B:429:ARG:O	1:B:432:LEU:HD23	2.20	0.42
1:A:64:ARG:HD2	1:A:66:THR:CG2	2.49	0.42
1:A:517:SER:O	1:A:521:MET:CB	2.66	0.42
1:A:700:PRO:HA	1:A:701:PRO:HD3	1.87	0.42
1:B:355:ARG:CG	1:B:356:ALA:N	2.83	0.42
1:B:430:THR:HG22	1:B:431:PHE:CD2	2.55	0.42
1:B:466:LEU:O	1:B:469:ILE:N	2.53	0.42
1:B:513:PRO:O	1:B:517:SER:OG	2.29	0.42
1:B:601:PHE:CE2	1:B:603:MET:HE3	2.53	0.42
1:B:708:LEU:O	1:B:711:GLU:HG2	2.19	0.42
1:A:405:MET:HE3	1:A:405:MET:HB3	1.74	0.41
1:A:430:THR:HG23	1:A:588:SER:HA	2.01	0.41
1:A:11:HIS:NE2	1:A:270:LYS:HB2	2.35	0.41
1:A:228:PHE:HD2	1:A:229:ASP:OD1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:MET:O	1:A:384:ALA:HB3	2.20	0.41
1:A:480:ALA:O	1:A:483:GLN:HB3	2.20	0.41
1:A:686:LYS:O	1:A:727:THR:CA	2.68	0.41
1:B:91:ASN:OD1	1:B:91:ASN:O	2.38	0.41
1:B:282:LYS:C	1:B:284:ALA:N	2.73	0.41
1:B:389:PRO:HD2	1:B:510:PHE:CE1	2.55	0.41
1:B:424:TYR:O	1:B:425:PRO:C	2.57	0.41
1:B:430:THR:HG22	1:B:431:PHE:N	2.35	0.41
1:B:440:GLU:CD	1:B:463:LYS:HG2	2.40	0.41
1:B:577:TRP:HA	1:B:580:THR:HG22	2.03	0.41
1:B:730:TYR:C	1:B:731:VAL:HG23	2.41	0.41
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.71	0.41
1:A:472:ASN:N	1:A:472:ASN:HD22	2.18	0.41
1:A:758:GLN:N	1:A:759:PRO:HD2	2.35	0.41
1:B:36:LEU:C	1:B:37:ALA:O	2.52	0.41
1:B:257:GLU:CG	1:B:265:PHE:HB2	2.46	0.41
2:T:808:DT:H6	2:T:808:DT:H5'	1.86	0.41
1:A:239:ARG:HA	1:A:239:ARG:HD2	1.52	0.41
1:A:495:ILE:H	1:A:495:ILE:HG12	1.57	0.41
1:A:522:ARG:O	1:A:526:ILE:CD1	2.69	0.41
1:B:528:ARG:CD	1:B:528:ARG:H	2.33	0.41
1:B:603:MET:HG3	1:B:604:PRO:N	2.32	0.41
1:A:300:LEU:HD21	1:A:345:LYS:HB3	2.02	0.41
1:A:450:SER:CA	1:A:459:PHE:O	2.66	0.41
1:A:534:ILE:HG22	1:A:535:GLU:N	2.29	0.41
1:A:754:THR:HA	1:A:758:GLN:HB2	2.03	0.41
1:B:36:LEU:HD12	1:B:138:ALA:O	2.21	0.41
1:B:348:ILE:O	1:B:352:LEU:N	2.51	0.41
1:B:486:LYS:O	1:B:486:LYS:CG	2.68	0.41
1:B:598:PHE:HD2	1:B:601:PHE:CD1	2.36	0.41
1:B:682:LEU:O	1:B:752:TYR:CZ	2.72	0.41
1:A:118:ARG:HD3	1:A:118:ARG:HA	1.93	0.41
1:B:209:ASN:HD21	1:B:245:ARG:N	2.19	0.41
1:B:461:ARG:C	1:B:464:HIS:HE1	2.22	0.41
1:A:273:LEU:N	1:A:273:LEU:CD1	2.84	0.41
1:A:346:THR:O	1:A:347:GLU:C	2.56	0.41
1:B:431:PHE:CZ	1:B:522:ARG:NH1	2.88	0.41
1:A:354:GLU:OE1	1:A:488:LEU:HG	2.21	0.41
1:B:42:VAL:HG22	1:B:43:ALA:N	2.35	0.41
1:B:130:MET:HE1	1:B:133:GLY:HA2	1.97	0.41
1:A:52:ARG:NH2	1:A:100:GLY:C	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ARG:HH12	1:A:192:ASP:HB2	1.86	0.41
1:A:378:PHE:CB	1:A:379:PRO:CD	2.95	0.41
1:A:409:PRO:O	1:A:409:PRO:HG2	2.20	0.41
1:A:426:SER:HB3	1:A:590:LEU:CD1	2.50	0.41
1:A:658:ARG:O	1:A:659:ASN:HB2	2.21	0.41
1:A:695:TYR:CE1	3:P:907:DA:H5'	2.56	0.41
1:A:764:ILE:O	1:A:764:ILE:HG12	2.21	0.41
1:B:248:ARG:HH11	1:B:248:ARG:HD3	1.76	0.41
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.55	0.41
1:B:408:ARG:HB2	1:B:542:ILE:HG23	2.02	0.41
1:B:412:TYR:OH	1:B:542:ILE:HG21	2.21	0.41
1:B:431:PHE:CD2	1:B:522:ARG:CD	3.03	0.41
1:B:450:SER:HB2	1:B:458:TRP:CZ3	2.56	0.41
1:B:476:GLY:O	1:B:477:ARG:C	2.58	0.41
1:B:698:ASN:O	1:B:700:PRO:HD3	2.21	0.41
2:T:816:DG:H2"	2:T:817:DC:O5'	2.21	0.41
3:P:913:DG:H2'	3:P:913:DG:O5'	2.20	0.41
1:A:297:ALA:O	1:A:301:LEU:CB	2.67	0.41
1:A:474:TRP:HE3	1:A:496:MET:HE1	1.86	0.41
1:A:552:TRP:CE2	1:A:554:LYS:HA	2.56	0.41
1:A:621:ILE:O	1:A:628:ARG:N	2.52	0.41
1:A:700:PRO:CB	1:A:701:PRO:HD2	2.50	0.41
1:B:175:GLN:NE2	1:B:215:TYR:CE1	2.89	0.41
1:B:215:TYR:H	1:B:215:TYR:HD2	1.69	0.41
1:B:439:VAL:HG12	1:B:440:GLU:N	2.35	0.41
1:B:450:SER:HB3	1:B:458:TRP:CZ3	2.48	0.41
1:B:686:LYS:HG3	1:B:687:ARG:N	2.36	0.41
1:A:184:GLU:HG2	1:A:185:ASN:N	2.24	0.40
1:A:359:ASN:OD1	1:A:360:GLY:N	2.54	0.40
1:B:709:ALA:HB2	1:B:739:PRO:HG3	2.02	0.40
1:B:751:HIS:HD1	1:B:755:ARG:HB2	1.86	0.40
1:B:751:HIS:HD1	1:B:755:ARG:CB	2.34	0.40
1:A:16:PRO:CD	1:A:17:GLN:OE1	2.61	0.40
1:A:145:ASP:O	1:A:145:ASP:OD1	2.39	0.40
1:A:185:ASN:OD1	1:A:185:ASN:O	2.39	0.40
1:A:688:LEU:O	1:A:725:ARG:CA	2.68	0.40
1:A:737:PRO:C	1:A:738:GLU:HG2	2.42	0.40
1:B:107:ASP:OD2	1:B:509:ARG:NH1	2.53	0.40
1:B:177:ILE:CG1	1:B:178:VAL:N	2.83	0.40
1:B:408:ARG:O	1:B:542:ILE:CG2	2.68	0.40
1:B:486:LYS:O	1:B:486:LYS:HG3	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:THR:HG22	1:B:637:VAL:N	2.34	0.40
1:A:372:ALA:O	1:A:373:PHE:C	2.59	0.40
1:A:405:MET:HE2	1:A:405:MET:HB2	1.82	0.40
1:A:772:PHE:O	1:A:775:LEU:CD1	2.70	0.40
1:B:454:PHE:O	1:B:455:LEU:CB	2.69	0.40
1:B:559:GLU:O	1:B:563:ALA:CB	2.69	0.40
1:A:45:ILE:HG23	1:A:46:PRO:CD	2.50	0.40
1:A:201:ARG:N	1:A:202:PRO:HD2	2.36	0.40
1:B:89:LEU:O	1:B:89:LEU:HG	2.21	0.40
1:B:413:ASP:HB3	1:B:600:ARG:HA	2.02	0.40
1:B:493:LYS:CG	1:B:494:ILE:N	2.84	0.40
1:B:559:GLU:O	1:B:560:GLU:C	2.56	0.40
1:A:160:THR:HG23	1:A:161:ARG:H	1.86	0.40
1:A:234:GLN:O	1:A:238:GLU:HB3	2.21	0.40
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.31	0.40
1:A:394:VAL:HG13	1:A:395:PRO:CD	2.47	0.40
1:A:690:ARG:H	1:A:725:ARG:HA	1.86	0.40
1:B:123:PRO:C	1:B:124:VAL:HG13	2.41	0.40
1:B:577:TRP:O	1:B:580:THR:CG2	2.69	0.40
1:B:686:LYS:CD	1:B:687:ARG:HH11	2.35	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:TYR:OH	1:B:671:ASP:OD1[2_554]	1.81	0.39
1:B:79:TYR:OH	1:B:667:ARG:NH1[2_554]	1.85	0.35
1:A:241:ARG:NH2	1:B:585:ARG:NH1[1_556]	2.14	0.06
1:A:201:ARG:NH1	1:B:714:GLN:O[2_555]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	751/786 (96%)	698 (93%)	42 (6%)	11 (2%)	10 41
1	B	728/786 (93%)	678 (93%)	41 (6%)	9 (1%)	13 46
All	All	1479/1572 (94%)	1376 (93%)	83 (6%)	20 (1%)	11 43

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ASP
1	A	483	GLN
1	A	690	ARG
1	A	769	GLU
1	B	1	MET
1	B	698	ASN
1	B	725	ARG
1	B	745	SER
1	A	313	ARG
1	A	717	GLY
1	A	773	ALA
1	B	759	PRO
1	A	414	SER
1	B	389	PRO
1	B	122	SER
1	B	395	PRO
1	B	758	GLN
1	A	122	SER
1	A	395	PRO
1	A	149	PRO

5.3.2 Protein sidechains (i)

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	649/672 (97%)	496 (76%)	153 (24%)	1 3
1	B	632/672 (94%)	493 (78%)	139 (22%)	1 4
All	All	1281/1344 (95%)	989 (77%)	292 (23%)	1 4

All (292) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	22	SER
1	A	36	LEU
1	A	39	GLN
1	A	48	ASP
1	A	54	GLN
1	A	61	GLN
1	A	64	ARG
1	A	66	THR
1	A	72	ASP
1	A	73	PHE
1	A	83	CYS
1	A	84	ARG
1	A	87	ARG
1	A	89	LEU
1	A	93	GLU
1	A	94	LYS
1	A	102	THR
1	A	108	VAL
1	A	109	ARG
1	A	113	ARG
1	A	129	ASP
1	A	141	LYS
1	A	148	PRO
1	A	153	VAL
1	A	161	ARG
1	A	165	LEU
1	A	175	GLN
1	A	184	GLU
1	A	185	ASN
1	A	192	ASP
1	A	200	SER
1	A	205	LEU
1	A	216	ASP
1	A	225	VAL
1	A	226	VAL
1	A	242	LEU
1	A	243	PRO
1	A	268	GLN
1	A	278	ILE
1	A	283	SER
1	A	291	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	293	LEU
1	A	294	GLU
1	A	298	GLN
1	A	300	LEU
1	A	303	GLU
1	A	312	ASP
1	A	313	ARG
1	A	314	MET
1	A	315	ASP
1	A	316	GLU
1	A	319	ARG
1	A	321	PHE
1	A	323	GLU
1	A	330	THR
1	A	333	LEU
1	A	340	THR
1	A	348	ILE
1	A	349	MET
1	A	351	PHE
1	A	355	ARG
1	A	364	ASP
1	A	376	LEU
1	A	383	ARG
1	A	391	LEU
1	A	400	PRO
1	A	408	ARG
1	A	414	SER
1	A	421	LYS
1	A	425	PRO
1	A	429	ARG
1	A	433	ILE
1	A	447	PRO
1	A	449	HIS
1	A	451	THR
1	A	467	PRO
1	A	468	GLU
1	A	469	ILE
1	A	470	VAL
1	A	471	THR
1	A	477	ARG
1	A	481	LYS
1	A	482	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	483	GLN
1	A	488	LEU
1	A	490	GLN
1	A	493	LYS
1	A	495	ILE
1	A	502	VAL
1	A	509	ARG
1	A	515	LEU
1	A	520	THR
1	A	522	ARG
1	A	524	HIS
1	A	527	MET
1	A	540	ASP
1	A	553	LEU
1	A	569	LEU
1	A	571	GLN
1	A	580	THR
1	A	581	LEU
1	A	583	LYS
1	A	590	LEU
1	A	595	GLU
1	A	596	THR
1	A	597	HIS
1	A	599	CYS
1	A	600	ARG
1	A	602	LEU
1	A	605	THR
1	A	622	GLN
1	A	623	GLU
1	A	625	ASP
1	A	626	LYS
1	A	632	LYS
1	A	634	LEU
1	A	635	GLU
1	A	638	ARG
1	A	644	LEU
1	A	647	GLN
1	A	650	GLN
1	A	654	LEU
1	A	667	ARG
1	A	683	VAL
1	A	686	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	690	ARG
1	A	692	LEU
1	A	693	SER
1	A	696	GLN
1	A	702	HIS
1	A	704	ARG
1	A	711	GLU
1	A	713	ASN
1	A	716	ARG
1	A	724	ASN
1	A	725	ARG
1	A	727	THR
1	A	728	ILE
1	A	730	TYR
1	A	734	THR
1	A	743	GLN
1	A	745	SER
1	A	746	PRO
1	A	747	LEU
1	A	751	HIS
1	A	754	THR
1	A	755	ARG
1	A	757	LEU
1	A	762	GLU
1	A	765	LEU
1	A	771	ASN
1	A	772	PHE
1	B	7	ILE
1	B	9	THR
1	B	10	ARG
1	B	19	THR
1	B	25	LEU
1	B	36	LEU
1	B	48	ASP
1	B	54	GLN
1	B	63	PHE
1	B	68	LEU
1	B	72	ASP
1	B	87	ARG
1	B	93	GLU
1	B	94	LYS
1	B	102	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	113	ARG
1	B	115	LEU
1	B	129	ASP
1	B	130	MET
1	B	140	LEU
1	B	141	LYS
1	B	148	PRO
1	B	160	THR
1	B	164	GLU
1	B	175	GLN
1	B	185	ASN
1	B	189	SER
1	B	198	VAL
1	B	200	SER
1	B	204	LEU
1	B	241	ARG
1	B	250	ASN
1	B	257	GLU
1	B	265	PHE
1	B	266	PHE
1	B	278	ILE
1	B	294	GLU
1	B	316	GLU
1	B	326	PRO
1	B	328	LEU
1	B	338	LEU
1	B	348	ILE
1	B	350	PRO
1	B	351	PHE
1	B	354	GLU
1	B	364	ASP
1	B	365	ARG
1	B	376	LEU
1	B	383	ARG
1	B	391	LEU
1	B	393	GLU
1	B	406	ASP
1	B	411	LEU
1	B	412	TYR
1	B	413	ASP
1	B	415	VAL
1	B	418	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	419	ASP
1	B	430	THR
1	B	434	ASP
1	B	439	VAL
1	B	442	MET
1	B	449	HIS
1	B	451	THR
1	B	452	GLU
1	B	454	PHE
1	B	464	HIS
1	B	466	LEU
1	B	472	ASN
1	B	477	ARG
1	B	478	ASP
1	B	479	GLU
1	B	481	LYS
1	B	487	PRO
1	B	488	LEU
1	B	490	GLN
1	B	494	ILE
1	B	495	ILE
1	B	497	ASN
1	B	500	TYR
1	B	505	THR
1	B	509	ARG
1	B	514	ARG
1	B	517	SER
1	B	519	ILE
1	B	520	THR
1	B	527	MET
1	B	528	ARG
1	B	531	LYS
1	B	534	ILE
1	B	542	ILE
1	B	553	LEU
1	B	558	SER
1	B	559	GLU
1	B	561	GLU
1	B	570	VAL
1	B	584	GLN
1	B	586	LEU
1	B	592	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	593	GLU
1	B	599	CYS
1	B	600	ARG
1	B	601	PHE
1	B	603	MET
1	B	621	ILE
1	B	636	THR
1	B	639	THR
1	B	644	LEU
1	B	652	LEU
1	B	661	PRO
1	B	667	ARG
1	B	673	LEU
1	B	677	GLU
1	B	678	LEU
1	B	687	ARG
1	B	693	SER
1	B	695	TYR
1	B	696	GLN
1	B	699	VAL
1	B	708	LEU
1	B	712	GLU
1	B	714	GLN
1	B	718	ARG
1	B	720	LEU
1	B	721	GLN
1	B	724	ASN
1	B	725	ARG
1	B	728	ILE
1	B	734	THR
1	B	735	ASN
1	B	746	PRO
1	B	747	LEU
1	B	750	GLU
1	B	751	HIS
1	B	753	LEU
1	B	754	THR
1	B	762	GLU
1	B	764	ILE
1	B	765	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	49	GLN
1	A	61	GLN
1	A	88	GLN
1	A	143	HIS
1	A	162	HIS
1	A	250	ASN
1	A	268	GLN
1	A	341	GLN
1	A	366	HIS
1	A	382	HIS
1	A	397	HIS
1	A	449	HIS
1	A	464	HIS
1	A	472	ASN
1	A	529	GLN
1	A	537	GLN
1	A	557	HIS
1	A	572	HIS
1	A	597	HIS
1	A	646	GLN
1	A	647	GLN
1	A	713	ASN
1	A	724	ASN
1	A	751	HIS
1	B	0	HIS
1	B	11	HIS
1	B	49	GLN
1	B	76	GLN
1	B	86	HIS
1	B	88	GLN
1	B	143	HIS
1	B	175	GLN
1	B	185	ASN
1	B	209	ASN
1	B	236	HIS
1	B	250	ASN
1	B	341	GLN
1	B	359	ASN
1	B	382	HIS
1	B	464	HIS
1	B	529	GLN
1	B	537	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	582	GLN
1	B	597	HIS
1	B	714	GLN
1	B	721	GLN
1	B	724	ASN
1	B	751	HIS
1	B	756	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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^2)	Q<0.9
1	A	759/786 (96%)	-0.44	4 (0%) 91 86	3, 29, 70, 98	0
1	B	738/786 (93%)	-0.33	2 (0%) 94 92	9, 46, 78, 93	0
2	T	13/20 (65%)	0.30	1 (7%) 13 6	85, 100, 131, 134	0
3	P	13/13 (100%)	0.45	0 100 100	60, 97, 131, 131	0
All	All	1523/1605 (94%)	-0.37	7 (0%) 91 86	3, 36, 78, 134	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	311	TRP	2.9
1	B	688	LEU	2.8
1	A	696	GLN	2.7
1	A	772	PHE	2.5
1	A	698	ASN	2.5
1	B	689	ARG	2.4
2	T	820	DA	2.4

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.