



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:57 AM GMT

PDB ID : 3K70
Title : Crystal structure of the complete initiation complex of RecBCD
Authors : Saikrishnan, K.; Wigley, D.B.
Deposited on : 2009-10-11
Resolution : 3.59 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

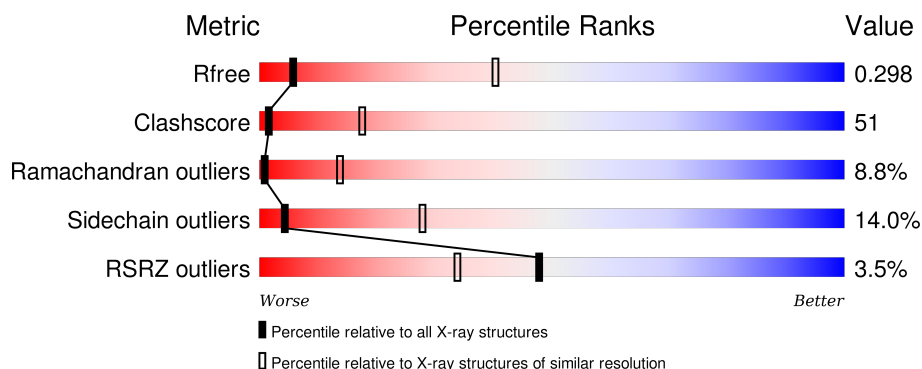
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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

Mol	Chain	Length	Quality of chain
1	B	1180	<div> <div>2%</div> <div>34% 50% 12% ..</div> </div>
1	E	1180	<div> <div>3%</div> <div>34% 51% 12% ..</div> </div>
2	C	1122	<div> <div>%</div> <div>38% 47% 14% .</div> </div>
2	F	1122	<div> <div>%</div> <div>37% 48% 13% .</div> </div>
3	D	608	<div> <div>15%</div> <div>27% 46% 15% . 10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	608	
4	X	51	
4	Y	51	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	5IU	X	2	-	-	X	-
4	5IU	X	3	-	-	X	-
4	5IU	X	46	-	-	X	-
4	5IU	Y	2	-	-	X	-
4	5IU	Y	3	-	-	X	-
4	5IU	Y	46	-	-	X	-
4	5IU	Y	7	-	-	X	-
4	5IU	Y	9	-	-	X	-
5	CA	B	4000	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 46932 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 Exodeoxyribonuclease V beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1155	Total	C	N	O	S	0	0	0
			9236	5823	1638	1736	39			
1	E	1155	Total	C	N	O	S	0	0	0
			9236	5823	1638	1736	39			

- Molecule 2 is a protein called Exodeoxyribonuclease V gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1121	Total	C	N	O	S	0	0	0
			9078	5783	1568	1684	43			
2	F	1121	Total	C	N	O	S	0	0	0
			9078	5783	1568	1684	43			

- Molecule 3 is a protein called Exodeoxyribonuclease V alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	547	Total	C	N	O	S	0	0	0
			4216	2631	771	795	19			
3	G	547	Total	C	N	O	S	0	0	0
			4216	2631	771	795	19			

- Molecule 4 is a DNA chain called DNA (46-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	46	Total	C	I	N	O	P	0	0
			935	442	9	164	276	44		
4	Y	46	Total	C	I	N	O	P	0	0
			935	442	9	164	276	44		

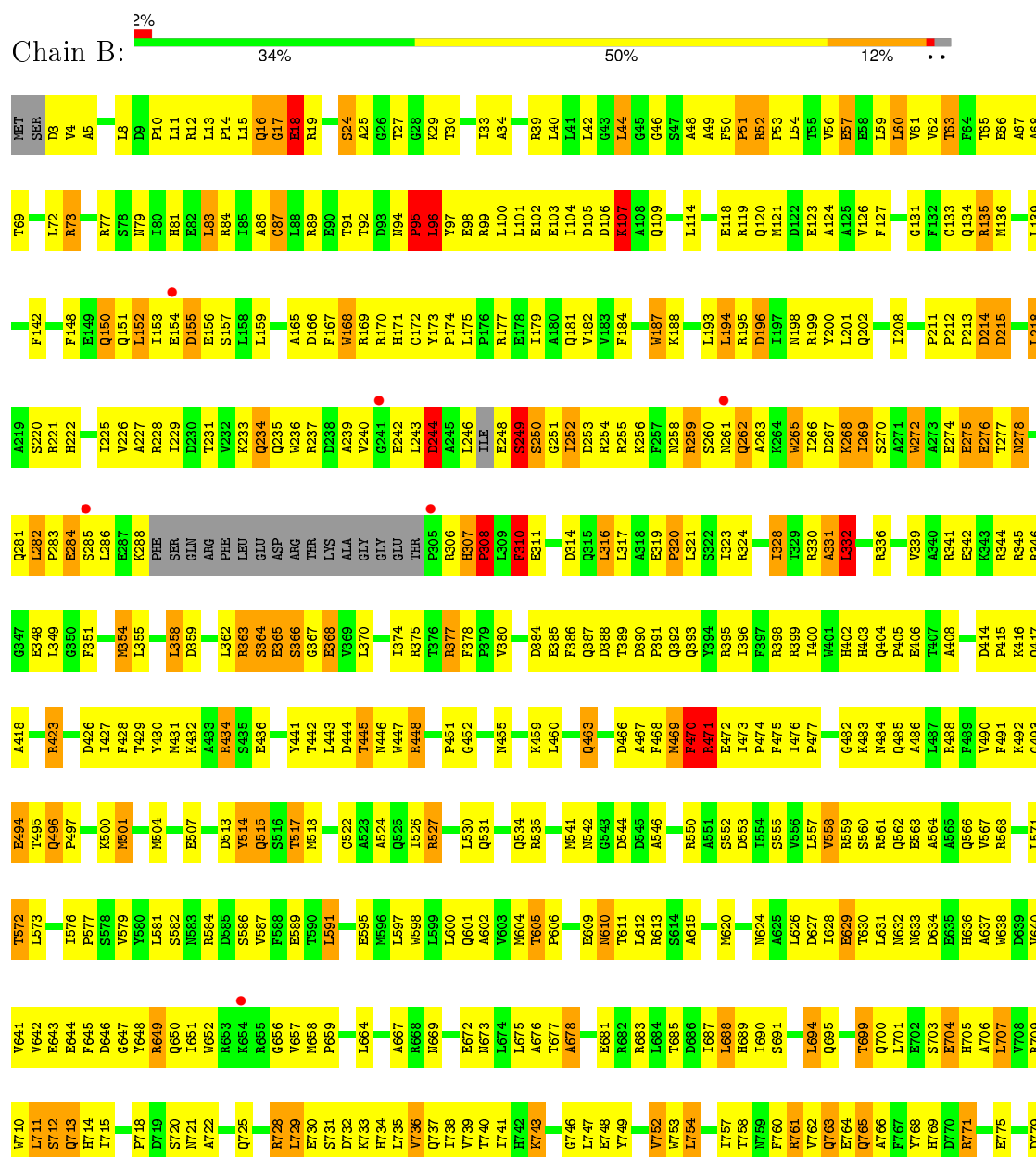
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

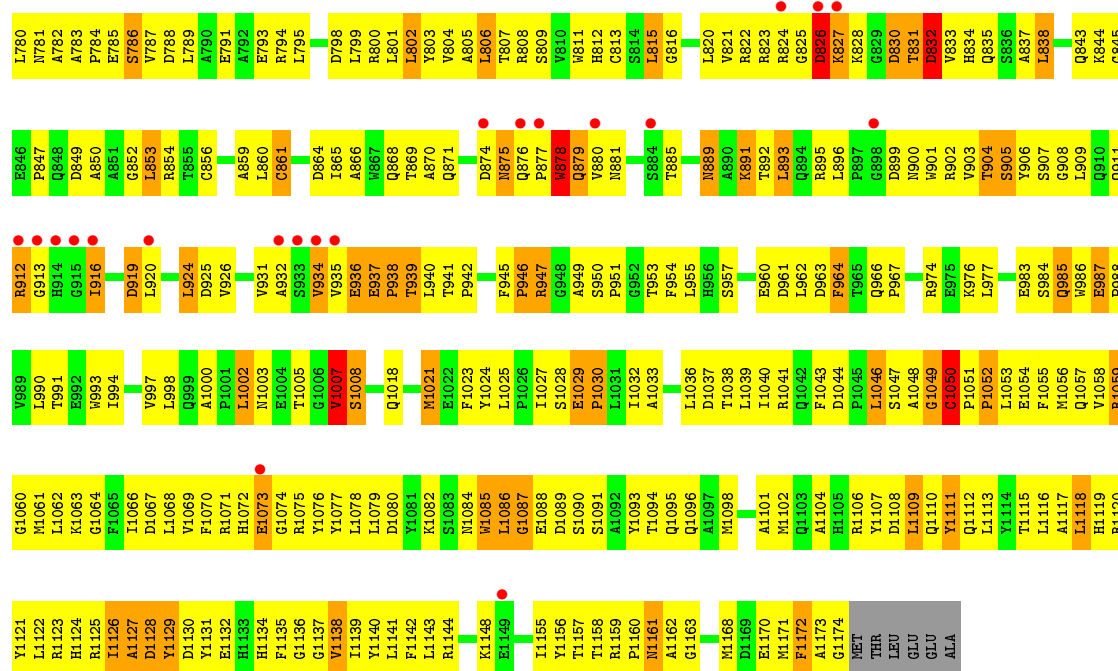
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Ca 1	0	0
5	E	1	Total 1	Ca 1	0	0

3 Residue-property plots

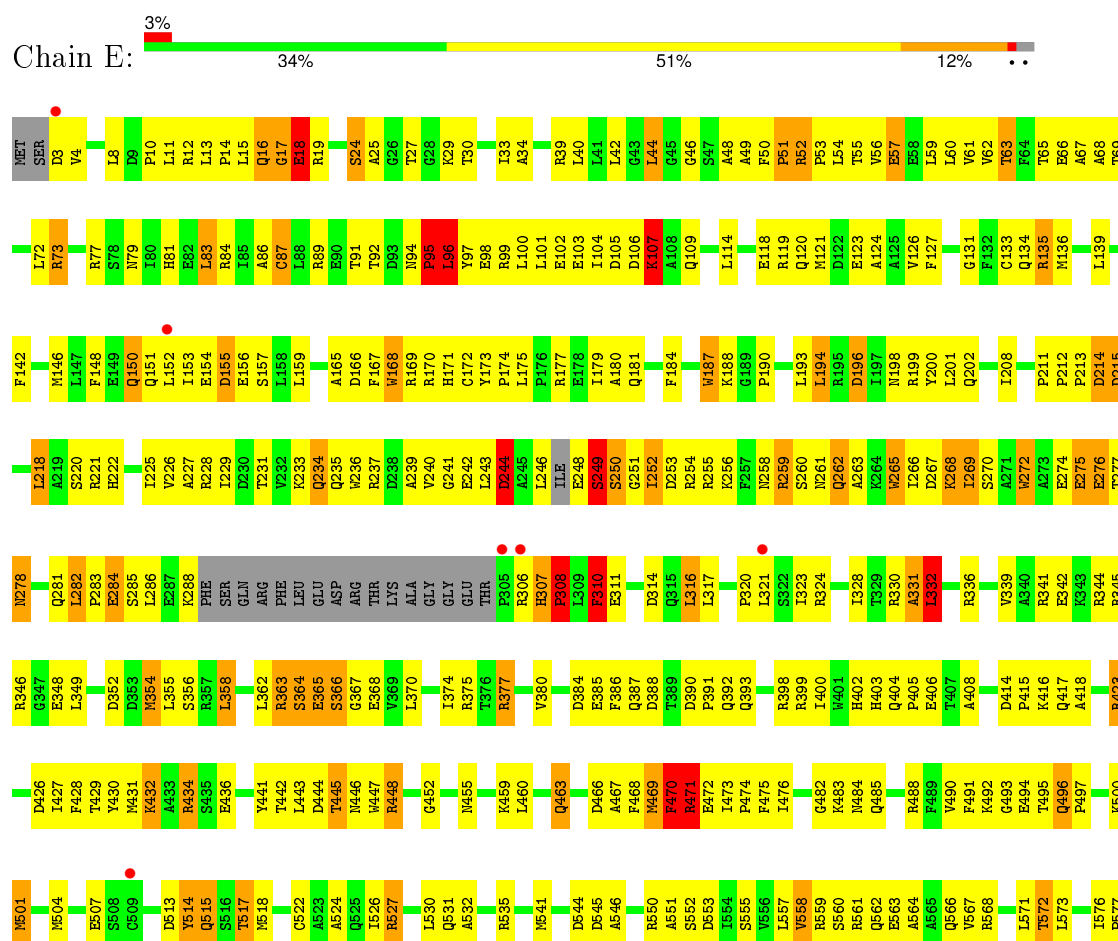
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

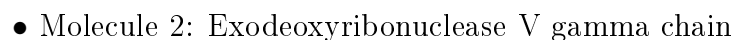
- Molecule 1: Exodeoxyribonuclease V beta chain



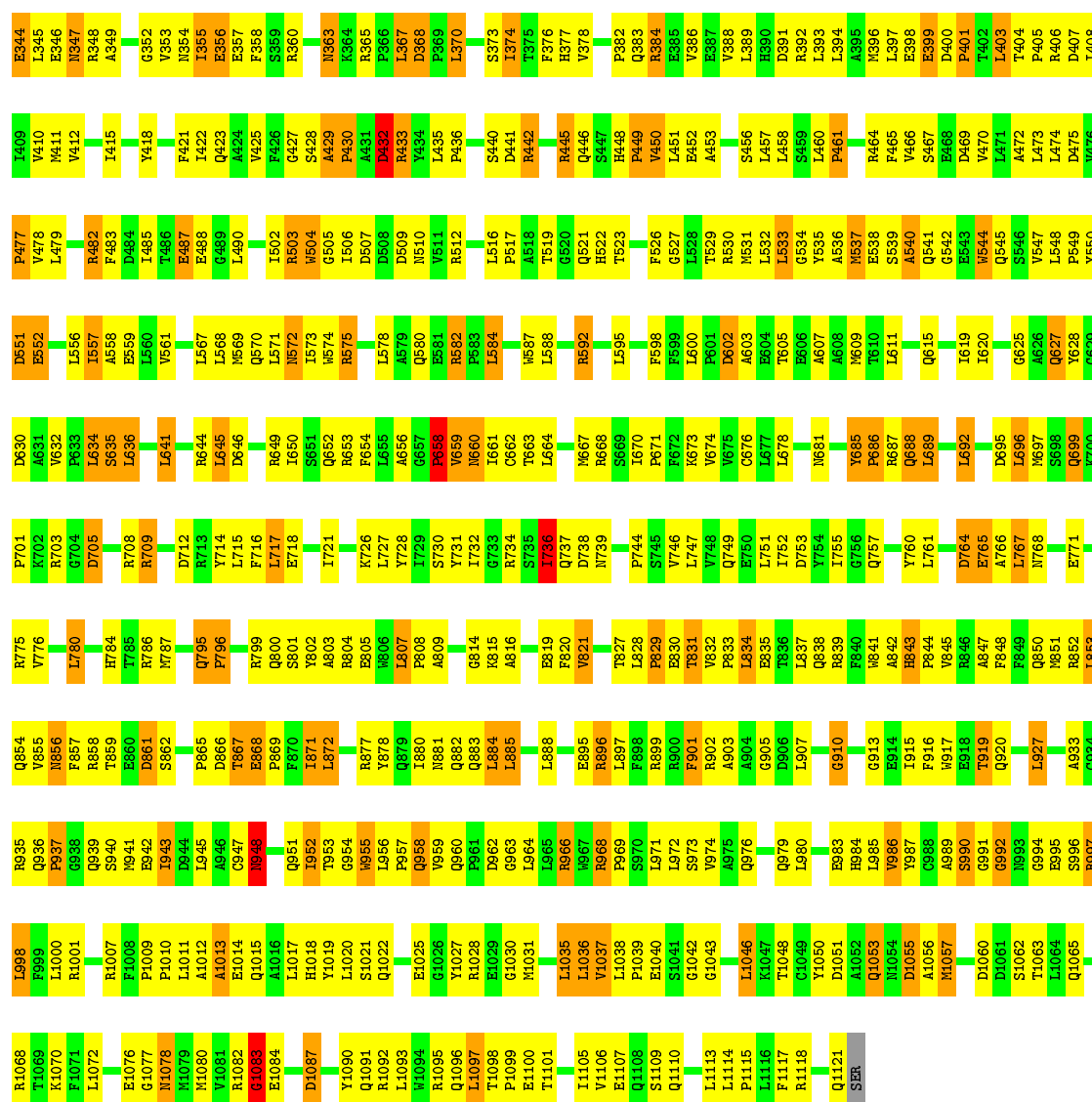


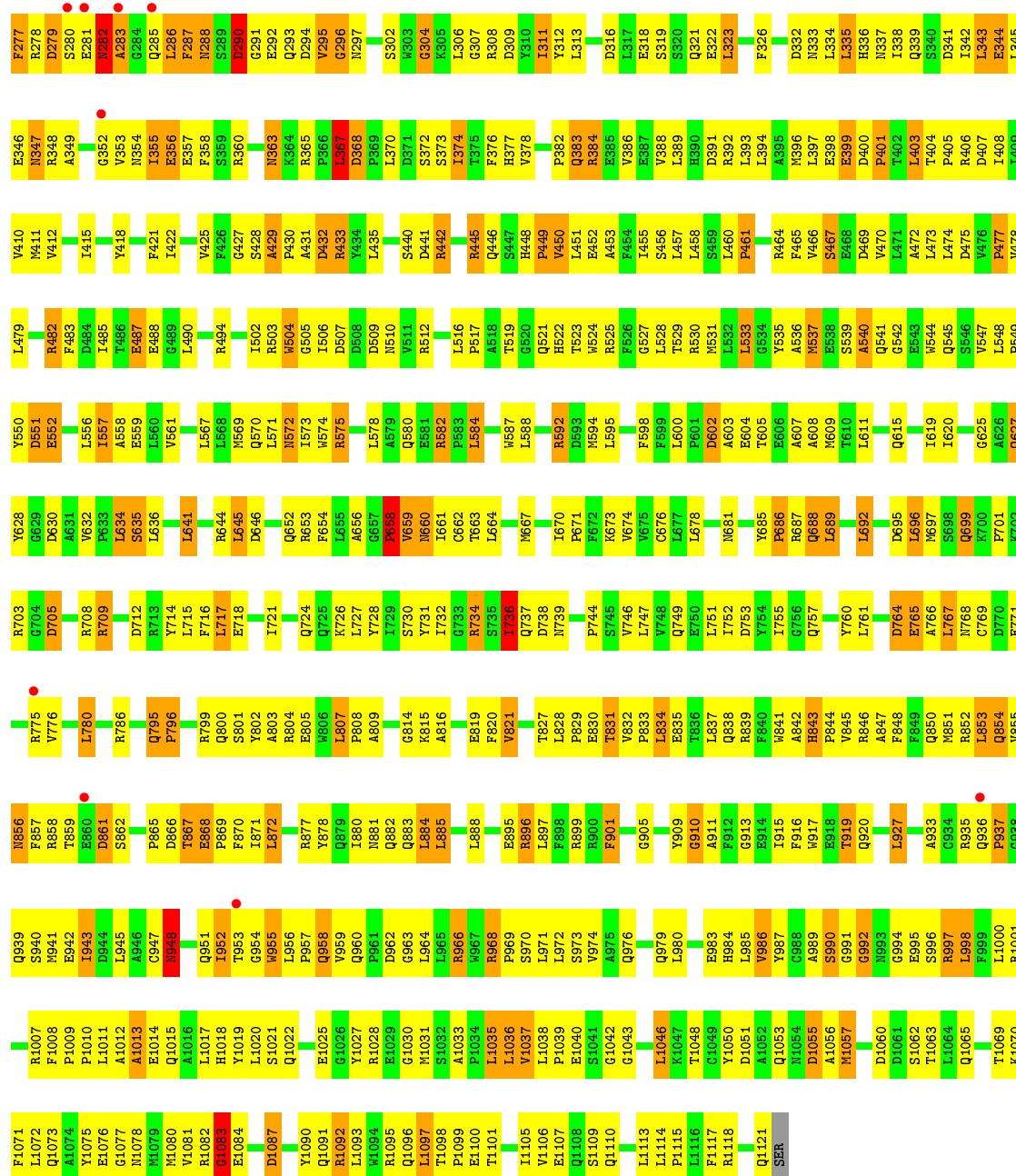
Chain E: Exodeoxyribonuclease V beta chain



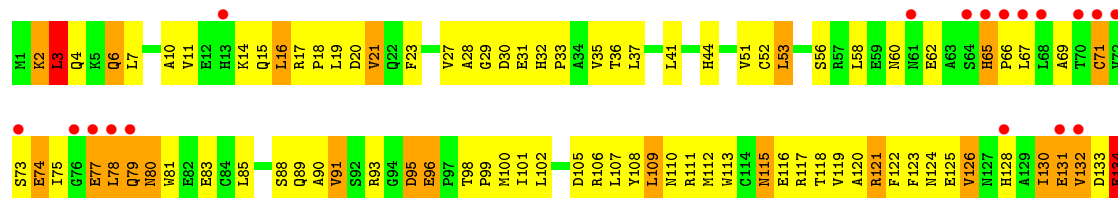


P275	P205	Q137	P65	M1
L277	G206	Y138	W70	L2
R278	L207	L139	D71	R3
D279	S208	Y140	M72	V4
S280	R210	Y141	F73	H6
E281	V211	R142	V74	S7
N282	F212	P143	R75	N8
A283	L213	D144	V76	R9
G284		W145	L77	
Q285	P220	L146	P78	V12
L286			E79	L13
P287	Y223	W149	I80	E14
N288			P81	A15
S289	Q228	V155	K82	L16
D290	A229		E83	M17
G291	L230	G159	S84	E18
E292		E160	A85	F19
Q293	H233	A161	P86	I20
D294	L234	Q162	N87	
V295	E235	A163	K88	R23
G296	L236	W164	Q89	E24
	H237	Q165	S90	R25
	L238	A166	M91	L26
L300	L239	P167		D27
A301	L168	W169	K94	D28
Q302	T241			P29
W303	N242		T97	F30
G304	P243	L172	L98	F31
K305	C244	V173	L99	P32
L306	R245	E174	P100	E33
G307	R246	Y175	Q101	
R308	Y246	T176	L102	L36
D309	Y247	H177	L103	V37
Y310	Y248	Q178	E104	Q38
I311	G249	L179	R105	S39
Y312	D250	G180	E106	
L313	I251	Q181	D107	M42
	D252	P182	F108	A43
D316	D253		L109	Q44
L317	P254	H185	L110	M45
E318	A255	R186	L111	L46
S319	Y256	A187	R112	Q47
S320	L257	N188		
Q321	A258	L189	L115	T49
E322	R259	Y190	T116	L50
L323	L260	Q191	D117	S51
	T261	R192	D118	Q52
F326	D262	F193	S119	K53
	R263	Q264	D120	F54
D332	Q265	E195	K121	G55
N333	R266	T196	F125	I56
L334	E267	L197	Q126	A58
L335	H267	E198	L127	M59
H336	S268	S199	S128	I60
N337	F269	I200	S129	D61
L338	E270	T201	K130	F62
Q339	D271	T202	A131	P63
	R272	C203	I432	L64
	E273	T204		
L342	L274			

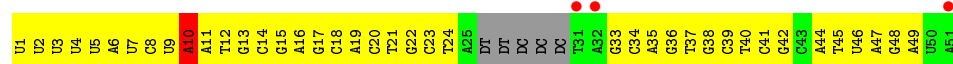




• Molecule 3: Exodeoxyribonuclease V alpha chain







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	133.80Å 192.90Å 334.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.59 29.92 – 3.60	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-3.59) 96.4 (29.92-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.56Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.248 , 0.296 0.253 , 0.298	Depositor DCC
R_{free} test set	4709 reflections (4.84%)	DCC
Wilson B-factor (Å ²)	107.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 93.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 97231 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	46932	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 5IU

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	B	0.29	0/9432	0.67	7/12795 (0.1%)
1	E	0.29	0/9432	0.67	7/12795 (0.1%)
2	C	0.29	0/9305	0.65	3/12644 (0.0%)
2	F	0.29	0/9305	0.64	3/12644 (0.0%)
3	D	0.36	0/4281	0.78	10/5796 (0.2%)
3	G	0.32	0/4281	0.75	9/5796 (0.2%)
4	X	0.45	0/847	0.83	1/1293 (0.1%)
4	Y	0.37	0/847	0.80	1/1293 (0.1%)
All	All	0.31	0/47730	0.68	41/65056 (0.1%)

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
4	Y	0	1

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	10	DA	OP1-P-O3'	8.64	124.22	105.20
3	D	256	HIS	N-CA-C	7.82	132.12	111.00
3	D	239	THR	N-CA-C	-6.73	92.82	111.00
1	B	878	TRP	N-CA-C	-6.66	93.03	111.00
3	G	239	THR	N-CA-C	-6.60	93.18	111.00
3	D	255	HIS	N-CA-C	6.52	128.60	111.00
1	B	308	PRO	N-CA-C	6.46	128.88	112.10
2	C	1083	GLY	N-CA-C	6.42	129.15	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1083	GLY	N-CA-C	6.42	129.14	113.10
1	B	244	ASP	N-CA-C	6.42	128.32	111.00
1	E	244	ASP	N-CA-C	6.40	128.28	111.00
3	D	261	LEU	CB-CG-CD2	-6.37	100.17	111.00
3	G	261	LEU	CB-CG-CD2	-6.23	100.40	111.00
1	E	308	PRO	N-CA-C	6.22	128.27	112.10
3	D	236	ASP	CA-C-N	-6.15	103.68	117.20
3	G	236	ASP	CA-C-N	-6.10	103.77	117.20
1	E	1049	GLY	N-CA-C	-5.78	98.66	113.10
1	B	1049	GLY	N-CA-C	-5.78	98.66	113.10
3	D	109	LEU	N-CA-C	-5.70	95.62	111.00
1	B	913	GLY	N-CA-C	-5.59	99.11	113.10
1	E	913	GLY	N-CA-C	-5.57	99.17	113.10
3	D	531	GLU	N-CA-C	-5.54	96.06	111.00
3	G	109	LEU	N-CA-C	-5.54	96.06	111.00
3	G	531	GLU	N-CA-C	-5.44	96.30	111.00
1	B	1050	CYS	N-CA-C	5.44	125.68	111.00
2	F	861	ASP	N-CA-C	-5.40	96.42	111.00
1	E	1050	CYS	N-CA-C	5.39	125.55	111.00
1	E	332	LEU	CA-CB-CG	5.36	127.62	115.30
3	D	529	GLU	N-CA-C	-5.35	96.55	111.00
2	C	271	ASP	N-CA-C	5.35	125.44	111.00
2	C	861	ASP	N-CA-C	-5.34	96.59	111.00
2	F	271	ASP	N-CA-C	5.33	125.40	111.00
4	Y	10	DA	OP2-P-O3'	5.31	116.88	105.20
3	G	236	ASP	N-CA-C	5.25	125.17	111.00
3	D	236	ASP	N-CA-C	5.21	125.06	111.00
1	B	332	LEU	CA-CB-CG	5.20	127.26	115.30
3	G	528	PRO	N-CA-C	5.13	125.45	112.10
3	G	529	GLU	N-CA-C	-5.00	97.48	111.00
3	D	231	LYS	N-CA-C	-5.00	97.49	111.00
1	E	241	GLY	N-CA-C	-5.00	100.59	113.10
3	G	231	LYS	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	Y	10	DA	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	9236	0	9083	957	0
1	E	9236	0	9083	915	0
2	C	9078	0	8877	849	0
2	F	9078	0	8877	820	0
3	D	4216	0	4261	580	0
3	G	4216	0	4261	568	0
4	X	935	0	498	115	0
4	Y	935	0	498	114	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
All	All	46932	0	45438	4677	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (4677) 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)
3:D:205:THR:HA	4:X:3:5IU:OP1	1.39	1.21
1:B:442:THR:HG21	1:B:476:ILE:HD11	1.24	1.17
4:X:22:DG:C2'	4:X:23:DC:H5''	1.75	1.16
3:D:65:HIS:HB3	3:D:66:PRO:HD2	1.20	1.15
1:E:442:THR:HG21	1:E:476:ILE:HD11	1.28	1.14
4:Y:22:DG:C2'	4:Y:23:DC:H5''	1.76	1.14
4:X:22:DG:H2''	4:X:23:DC:H5''	1.19	1.14
1:B:1051:PRO:N	1:B:1052:PRO:HD2	1.63	1.14
4:X:7:5IU:H3'	4:X:8:DC:H5'	1.26	1.13
3:G:118:THR:HG22	3:G:283:ILE:HD11	1.19	1.12
4:Y:7:5IU:H3'	4:Y:8:DC:H5'	1.27	1.12
3:D:259:ASN:HB3	3:D:260:PRO:HD2	1.17	1.12
3:G:65:HIS:HB3	3:G:66:PRO:HD2	1.19	1.11
3:D:243:LEU:HG	3:D:244:LEU:H	1.01	1.10
4:Y:22:DG:H2''	4:Y:23:DC:H5''	1.19	1.09
3:G:259:ASN:HB3	3:G:260:PRO:HD2	1.12	1.09
1:E:1051:PRO:N	1:E:1052:PRO:HD2	1.63	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:243:LEU:HG	3:G:244:LEU:H	1.11	1.09
1:B:877:PRO:HB2	1:B:879:GLN:HG3	1.12	1.09
3:D:217:GLY:O	3:D:221:ARG:HG3	1.51	1.08
3:G:65:HIS:HB3	3:G:66:PRO:CD	1.82	1.07
1:B:881:ASN:HD22	1:E:883:VAL:HG22	1.18	1.07
3:D:118:THR:HG22	3:D:283:ILE:HD11	1.07	1.07
3:D:65:HIS:HB3	3:D:66:PRO:CD	1.82	1.07
4:X:11:DA:C2'	4:X:12:DT:H5''	1.86	1.06
4:X:46:5IU:H2''	4:X:47:DA:H5'	1.33	1.05
2:C:1055:ASP:HB2	2:C:1118:ARG:HH22	1.12	1.05
2:C:38:GLN:HE21	2:C:667:MET:HG3	1.17	1.05
4:Y:11:DA:C2'	4:Y:12:DT:H5''	1.86	1.05
4:Y:46:5IU:H2''	4:Y:47:DA:H5'	1.33	1.05
1:E:877:PRO:HB2	1:E:879:GLN:HG3	1.35	1.05
1:B:564:ALA:HA	1:B:738:ILE:HD11	1.38	1.04
4:Y:46:5IU:H2''	4:Y:47:DA:C5'	1.88	1.04
3:G:243:LEU:HG	3:G:244:LEU:N	1.69	1.03
4:Y:14:DC:H2''	4:Y:15:DG:H5''	1.41	1.03
2:F:363:ASN:ND2	2:F:363:ASN:H	1.55	1.03
1:B:159:LEU:HD12	1:B:339:VAL:HG13	1.39	1.03
3:D:216:LEU:O	3:D:220:LEU:HB2	1.59	1.03
3:D:240:LEU:HG	3:D:278:MET:SD	1.98	1.02
3:D:244:LEU:HD21	3:D:261:LEU:HG	1.38	1.02
3:D:243:LEU:HG	3:D:244:LEU:N	1.68	1.02
1:E:564:ALA:HA	1:E:738:ILE:HD11	1.38	1.02
3:G:243:LEU:CD1	3:G:261:LEU:HD21	1.90	1.02
1:B:527:ARG:HB3	1:B:576:ILE:HD11	1.42	1.02
1:E:159:LEU:HD12	1:E:339:VAL:HG13	1.42	1.02
2:C:504:TRP:HH2	2:C:516:LEU:HD13	1.21	1.02
3:G:216:LEU:O	3:G:220:LEU:HB2	1.59	1.02
3:D:243:LEU:HD11	3:D:244:LEU:HG	1.37	1.01
1:E:286:LEU:HD13	1:E:306:ARG:HD3	1.38	1.01
4:X:46:5IU:H2''	4:X:47:DA:C5'	1.89	1.01
2:F:363:ASN:HD22	2:F:363:ASN:N	1.55	1.01
1:B:286:LEU:HD13	1:B:306:ARG:HD3	1.39	1.01
1:E:947:ARG:HG3	1:E:1086:LEU:HD11	1.39	1.00
4:X:14:DC:H2''	4:X:15:DG:H5''	1.39	1.00
3:D:243:LEU:CD1	3:D:261:LEU:HD21	1.91	1.00
2:F:38:GLN:HE21	2:F:667:MET:HG3	1.24	1.00
1:B:947:ARG:HG3	1:B:1086:LEU:HD11	1.38	1.00
2:C:1012:ALA:H	2:C:1015:GLN:HE21	1.08	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:248:PRO:HD3	4:Y:4:5IU:H1'	1.43	0.99
3:D:130:ILE:H	3:D:130:ILE:HD12	1.25	0.99
1:E:527:ARG:HB3	1:E:576:ILE:HD11	1.44	0.99
2:C:363:ASN:H	2:C:363:ASN:ND2	1.58	0.99
2:F:347:ASN:ND2	2:F:349:ALA:H	1.61	0.99
4:Y:11:DA:H2''	4:Y:12:DT:H5''	0.99	0.99
3:G:200:ARG:HB2	3:G:263:LEU:HD23	1.45	0.99
2:F:504:TRP:HH2	2:F:516:LEU:HD13	1.22	0.98
3:D:200:ARG:HB2	3:D:263:LEU:HD23	1.42	0.98
2:C:347:ASN:ND2	2:C:349:ALA:H	1.59	0.98
3:G:130:ILE:H	3:G:130:ILE:HD12	1.25	0.98
4:X:11:DA:H2''	4:X:12:DT:C5'	1.94	0.98
2:C:363:ASN:HD22	2:C:363:ASN:N	1.58	0.97
4:Y:3:5IU:H2''	4:Y:4:5IU:H5''	1.43	0.96
3:G:259:ASN:HB3	3:G:260:PRO:CD	1.92	0.96
2:F:104:GLU:H	2:F:112:ARG:HG3	1.31	0.96
4:Y:11:DA:H2''	4:Y:12:DT:C5'	1.94	0.96
1:B:531:GLN:HE21	1:B:879:GLN:HB2	1.31	0.95
4:X:11:DA:H2''	4:X:12:DT:H5''	1.00	0.95
2:C:584:LEU:HD12	2:C:620:ILE:HG23	1.47	0.95
2:F:1055:ASP:HB2	2:F:1118:ARG:HH22	1.30	0.95
4:Y:6:DA:H2'	4:Y:6:DA:N3	1.82	0.95
1:B:286:LEU:HD22	1:B:306:ARG:HH11	1.30	0.95
4:X:3:5IU:H2''	4:X:4:5IU:H5''	1.47	0.94
1:B:877:PRO:CB	1:B:879:GLN:HG3	1.97	0.94
1:E:286:LEU:HD11	1:E:306:ARG:HB3	1.48	0.94
2:F:1012:ALA:H	2:F:1015:GLN:HE21	1.15	0.94
3:D:243:LEU:CD1	3:D:244:LEU:HG	1.97	0.94
3:D:259:ASN:HB3	3:D:260:PRO:CD	1.97	0.94
2:C:77:LEU:HD22	2:C:192:ARG:HD2	1.47	0.94
2:F:971:LEU:HD23	4:Y:10:DA:H5'	1.49	0.94
2:F:850:GLN:HE22	4:Y:7:5IU:HN3	1.13	0.94
2:F:885:LEU:HD12	2:F:969:PRO:HG3	1.46	0.93
3:D:244:LEU:HD21	3:D:261:LEU:CG	1.99	0.93
1:E:286:LEU:HD22	1:E:306:ARG:HH11	1.30	0.93
3:D:460:GLN:HA	3:D:463:GLN:OE1	1.68	0.93
4:X:6:DA:H2'	4:X:6:DA:N3	1.82	0.93
1:E:900:ASN:HD21	1:E:902:ARG:HH21	1.10	0.93
2:C:104:GLU:H	2:C:112:ARG:HG3	1.30	0.93
3:D:367:ILE:N	3:D:393:ILE:HG21	1.82	0.93
1:B:597:LEU:HD12	1:B:715:ILE:HD12	1.50	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:LEU:HB3	1:B:399:ARG:HG2	1.47	0.93
3:D:239:THR:HG21	4:X:4:5IU:OP1	1.68	0.93
4:Y:47:DA:H2''	4:Y:48:DG:O5'	1.69	0.93
1:E:752:VAL:HG13	1:E:809:SER:HB3	1.51	0.92
2:F:557:ILE:HD13	2:F:557:ILE:H	1.34	0.92
2:C:149:TRP:HE1	2:C:162:GLN:HE21	1.09	0.92
3:G:255:HIS:ND1	3:G:256:HIS:N	2.16	0.92
2:C:105:ARG:O	2:C:106:GLU:HB3	1.67	0.92
1:B:598:TRP:CZ2	2:C:857:PHE:HB3	2.04	0.92
1:B:900:ASN:HD21	1:B:902:ARG:HH21	1.10	0.92
3:D:115:ASN:HB3	3:D:276:LEU:HD22	1.50	0.92
1:B:1071:ARG:HH22	2:C:29:PRO:HB2	1.33	0.92
2:C:885:LEU:HD12	2:C:969:PRO:HG3	1.48	0.92
1:B:286:LEU:HD11	1:B:306:ARG:HB3	1.50	0.92
2:F:105:ARG:O	2:F:106:GLU:HB3	1.69	0.92
1:B:987:GLU:HG3	1:B:988:PRO:HD3	1.52	0.92
2:F:584:LEU:HD12	2:F:620:ILE:HG23	1.51	0.91
3:D:304:VAL:HG21	3:D:564:GLU:HG2	1.53	0.91
1:B:925:ASP:H	1:B:953:THR:HG22	1.37	0.90
1:B:236:TRP:O	1:B:240:VAL:HG23	1.72	0.90
2:F:228:GLN:HE22	2:F:318:GLU:H	1.19	0.90
3:D:253:LEU:HB3	3:D:255:HIS:CD2	2.06	0.90
1:E:236:TRP:O	1:E:240:VAL:HG23	1.71	0.90
1:B:824:ARG:HB2	4:X:16:DA:OP2	1.71	0.90
2:F:945:LEU:HB2	2:F:952:ILE:HD11	1.53	0.90
3:D:226:THR:O	3:D:228:GLU:N	2.04	0.90
3:D:255:HIS:HB3	3:D:260:PRO:HG2	1.53	0.90
2:F:149:TRP:HE1	2:F:162:GLN:HE21	1.14	0.90
3:G:62:GLU:HA	3:G:65:HIS:HB2	1.52	0.89
1:E:994:ILE:O	1:E:997:VAL:HG12	1.70	0.89
2:C:433:ARG:HH12	2:C:805:GLU:HG2	1.33	0.89
1:B:86:ALA:HB1	1:B:92:THR:OG1	1.72	0.89
3:D:51:VAL:HG21	3:D:276:LEU:HD12	1.54	0.89
1:B:994:ILE:O	1:B:997:VAL:HG12	1.72	0.89
3:D:62:GLU:HA	3:D:65:HIS:HB2	1.54	0.89
4:X:12:DT:H2''	4:X:13:DG:H5'	1.55	0.89
1:E:86:ALA:HB1	1:E:92:THR:OG1	1.73	0.89
1:E:459:LYS:HE2	1:E:860:LEU:HB2	1.53	0.89
2:C:228:GLN:HE22	2:C:318:GLU:H	1.18	0.89
3:G:226:THR:O	3:G:228:GLU:N	2.06	0.88
1:B:966:GLN:HB3	1:B:967:PRO:HD2	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1037:VAL:HA	2:F:1109:SER:HB3	1.55	0.88
1:E:925:ASP:H	1:E:953:THR:HG22	1.37	0.88
1:B:823:ARG:HG2	1:B:825:GLY:H	1.38	0.88
4:X:6:DA:H2''	4:X:7:5IU:O5'	1.74	0.88
4:Y:12:DT:H2''	4:Y:13:DG:H5'	1.54	0.88
1:E:823:ARG:HG2	1:E:825:GLY:H	1.35	0.88
4:Y:47:DA:H2''	4:Y:48:DG:C5'	2.03	0.88
4:X:47:DA:H2''	4:X:48:DG:O5'	1.71	0.88
1:B:752:VAL:HG13	1:B:809:SER:HB3	1.53	0.88
3:D:17:ARG:HB2	3:D:18:PRO:HD2	1.55	0.88
2:C:482:ARG:O	2:C:482:ARG:HD3	1.74	0.88
1:E:920:LEU:HD11	2:F:448:HIS:CD2	2.09	0.88
2:C:1055:ASP:HB2	2:C:1118:ARG:NH2	1.89	0.87
2:C:828:LEU:HD13	2:C:1028:ARG:HG3	1.55	0.87
4:X:47:DA:H2''	4:X:48:DG:C5'	2.04	0.87
1:B:746:GLY:H	1:B:808:ARG:HH12	1.22	0.87
1:B:459:LYS:HE2	1:B:860:LEU:HB2	1.54	0.87
1:E:597:LEU:HD12	1:E:715:ILE:HD12	1.55	0.87
3:D:345:ALA:HB3	3:D:349:ARG:HG3	1.55	0.87
3:D:255:HIS:HA	3:D:259:ASN:HB3	1.57	0.87
3:G:51:VAL:HG21	3:G:276:LEU:HD12	1.54	0.87
1:E:987:GLU:HG3	1:E:988:PRO:HD3	1.56	0.87
3:G:207:LYS:NZ	3:G:544:SER:HA	1.89	0.87
1:E:175:LEU:HD13	1:E:179:ILE:HG22	1.57	0.87
1:B:307:HIS:CB	1:B:308:PRO:HD2	2.05	0.87
2:C:1118:ARG:HG2	2:C:1118:ARG:HH21	1.39	0.87
1:B:899:ASP:HB3	1:B:1059:ARG:HH12	1.39	0.87
2:C:945:LEU:HB2	2:C:952:ILE:HD11	1.54	0.87
3:D:255:HIS:HA	3:D:259:ASN:CB	2.05	0.86
1:B:175:LEU:HD13	1:B:179:ILE:HG22	1.57	0.86
1:E:11:LEU:HD13	1:E:99:ARG:HD2	1.55	0.86
3:D:253:LEU:HB3	3:D:255:HIS:NE2	1.90	0.86
2:F:28:ASP:H	2:F:29:PRO:CD	1.88	0.86
1:B:658:MET:HB3	1:B:659:PRO:HD3	1.57	0.86
1:E:966:GLN:HB3	1:E:967:PRO:HD2	1.57	0.86
1:B:673:ASN:OD1	2:C:815:LYS:HG2	1.75	0.86
1:E:899:ASP:HB3	1:E:1059:ARG:HH12	1.39	0.86
2:C:504:TRP:CH2	2:C:516:LEU:HD13	2.09	0.86
1:B:200:TYR:O	1:B:201:LEU:HB2	1.74	0.86
2:F:433:ARG:HH12	2:F:805:GLU:HG2	1.40	0.86
2:F:77:LEU:HD22	2:F:192:ARG:HD2	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:678:LEU:HD23	2:F:730:SER:HB3	1.57	0.86
1:E:794:ARG:NH2	1:E:795:LEU:HB3	1.90	0.85
2:F:397:LEU:HD23	2:F:403:LEU:HD13	1.57	0.85
3:G:244:LEU:HD22	3:G:255:HIS:HB3	1.56	0.85
3:G:17:ARG:HB2	3:G:18:PRO:HD2	1.55	0.85
1:E:746:GLY:H	1:E:808:ARG:HH12	1.24	0.85
2:C:557:ILE:HD13	2:C:557:ILE:H	1.40	0.85
3:G:597:ARG:O	3:G:598:SER:HB3	1.74	0.85
2:C:28:ASP:H	2:C:29:PRO:CD	1.88	0.85
1:E:1071:ARG:HH22	2:F:29:PRO:HB2	1.42	0.85
2:C:835:GLU:O	2:C:839:ARG:HG2	1.76	0.85
1:B:900:ASN:HD21	1:B:902:ARG:NH2	1.74	0.85
2:C:1037:VAL:HA	2:C:1109:SER:HB3	1.58	0.85
1:E:947:ARG:HB3	1:E:1086:LEU:HD21	1.57	0.85
1:E:1071:ARG:HD3	1:E:1076:TYR:HE2	1.41	0.85
3:D:165:ARG:HD3	3:D:166:ILE:HD11	1.58	0.84
1:E:307:HIS:ND1	1:E:308:PRO:HD2	1.91	0.84
1:B:1071:ARG:HD3	1:B:1076:TYR:HE2	1.39	0.84
1:E:794:ARG:HH21	1:E:795:LEU:HB3	1.41	0.84
1:E:903:VAL:HG13	1:E:1061:MET:HB2	1.58	0.84
3:G:367:ILE:N	3:G:393:ILE:HG21	1.91	0.84
4:Y:22:DG:H2''	4:Y:23:DC:C5'	2.07	0.84
1:E:307:HIS:CB	1:E:308:PRO:HD2	2.05	0.84
1:E:722:ALA:HA	1:E:725:GLN:HG3	1.58	0.84
1:B:562:GLN:NE2	4:X:46:5IU:I5	2.81	0.84
1:B:541:MET:HG2	1:B:546:ALA:HB2	1.60	0.84
2:F:482:ARG:HD3	2:F:482:ARG:O	1.78	0.84
3:D:80:ASN:HB3	3:D:83:GLU:HB3	1.60	0.84
1:B:488:ARG:HH22	1:E:541:MET:HE1	1.41	0.84
4:Y:46:5IU:C2'	4:Y:47:DA:H5'	2.08	0.84
1:E:200:TYR:O	1:E:201:LEU:HB2	1.76	0.84
1:B:794:ARG:NH2	1:B:795:LEU:HB3	1.93	0.84
4:X:22:DG:H2''	4:X:23:DC:C5'	2.06	0.84
1:E:861:CYS:SG	1:E:866:ALA:HA	2.18	0.84
3:G:174:GLY:O	3:G:357:LYS:HD3	1.77	0.83
3:D:367:ILE:H	3:D:393:ILE:HG21	1.42	0.83
1:B:423:ARG:HG2	4:X:49:DA:C2	2.12	0.83
3:D:597:ARG:O	3:D:598:SER:HB3	1.76	0.83
2:C:872:LEU:HD13	2:C:916:PHE:CE2	2.14	0.83
2:C:16:LEU:O	2:C:20:ILE:HG12	1.78	0.83
2:C:678:LEU:HD23	2:C:730:SER:HB3	1.57	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:213:THR:HG22	3:G:235:GLU:HA	1.61	0.83
2:F:1118:ARG:HH21	2:F:1118:ARG:HG2	1.43	0.83
1:E:900:ASN:HD21	1:E:902:ARG:NH2	1.75	0.83
1:B:722:ALA:HA	1:B:725:GLN:HG3	1.57	0.83
2:F:258:ALA:HA	2:F:261:LEU:HG	1.61	0.83
2:C:397:LEU:HD23	2:C:403:LEU:HD13	1.61	0.83
3:G:244:LEU:HD22	3:G:255:HIS:CB	2.09	0.83
1:B:881:ASN:ND2	1:E:883:VAL:HG22	1.94	0.83
2:F:828:LEU:HD13	2:F:1028:ARG:HG3	1.58	0.83
3:G:392:ASP:O	3:G:576:ARG:HG2	1.78	0.83
1:B:889:ASN:HD22	1:B:889:ASN:N	1.76	0.83
1:B:531:GLN:NE2	1:B:879:GLN:HB2	1.94	0.83
1:E:945:PHE:CE2	1:E:955:LEU:HD21	2.13	0.83
2:C:980:LEU:HD13	2:C:998:LEU:HB2	1.61	0.83
3:D:243:LEU:HD12	3:D:261:LEU:HD21	1.61	0.82
1:E:541:MET:HG2	1:E:546:ALA:HB2	1.61	0.82
4:X:46:5IU:C2'	4:X:47:DA:H5'	2.09	0.82
3:G:398:LEU:H	3:G:398:LEU:HD23	1.43	0.82
2:C:38:GLN:NE2	2:C:667:MET:HG3	1.94	0.82
3:D:280:SER:O	3:D:283:ILE:HG12	1.79	0.82
3:G:165:ARG:HD3	3:G:166:ILE:HD11	1.59	0.82
4:Y:6:DA:H2''	4:Y:7:5IU:O5'	1.77	0.82
1:B:903:VAL:HG13	1:B:1061:MET:HB2	1.62	0.82
2:F:872:LEU:HD13	2:F:916:PHE:CE2	2.14	0.82
3:D:188:LEU:HD21	3:D:291:ARG:NH2	1.93	0.82
1:E:1138:VAL:HB	1:E:1158:THR:O	1.79	0.82
4:X:37:DT:H2''	4:X:38:DG:H5'	1.60	0.82
2:C:685:TYR:O	2:C:687:ARG:N	2.12	0.82
2:F:118:ASP:O	2:F:119:SER:HB2	1.79	0.82
1:E:658:MET:HB3	1:E:659:PRO:HD3	1.61	0.82
2:C:382:PRO:O	2:C:386:VAL:HG23	1.79	0.82
2:C:506:ILE:H	2:C:510:ASN:HD22	1.27	0.82
1:B:307:HIS:ND1	1:B:308:PRO:HD2	1.94	0.82
2:F:504:TRP:CH2	2:F:516:LEU:HD13	2.12	0.82
3:G:80:ASN:HB3	3:G:83:GLU:HB3	1.62	0.82
2:F:466:VAL:HB	2:F:469:ASP:OD2	1.79	0.82
3:G:65:HIS:CB	3:G:66:PRO:HD2	2.08	0.82
2:F:980:LEU:HD13	2:F:998:LEU:HB2	1.61	0.82
2:F:7:SER:HB3	2:F:13:LEU:HG	1.62	0.82
2:C:433:ARG:NH1	2:C:805:GLU:HG2	1.95	0.81
3:D:126:VAL:HG22	3:D:166:ILE:HD13	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:835:GLU:O	2:F:839:ARG:HG2	1.79	0.81
1:B:947:ARG:HB3	1:B:1086:LEU:HD21	1.60	0.81
2:C:192:ARG:O	2:C:196:THR:HG22	1.80	0.81
1:E:807:THR:CG2	1:E:808:ARG:HH21	1.92	0.81
1:B:920:LEU:HD11	2:C:448:HIS:CD2	2.15	0.81
2:C:258:ALA:HA	2:C:261:LEU:HG	1.62	0.81
1:B:945:PHE:CE2	1:B:955:LEU:HD21	2.16	0.81
2:C:104:GLU:O	2:C:104:GLU:HG3	1.80	0.81
3:D:174:GLY:O	3:D:357:LYS:HD3	1.80	0.81
2:F:519:THR:HG23	2:F:521:GLN:H	1.46	0.81
1:B:807:THR:CG2	1:B:808:ARG:HH21	1.93	0.81
2:F:16:LEU:O	2:F:20:ILE:HG12	1.79	0.81
1:B:624:ASN:O	1:B:628:ILE:HG12	1.81	0.81
3:D:243:LEU:CG	3:D:244:LEU:N	2.43	0.81
4:X:2:5IU:C2'	4:X:3:5IU:H5'	2.10	0.81
2:C:466:VAL:HB	2:C:469:ASP:OD2	1.81	0.81
3:D:398:LEU:HD23	3:D:398:LEU:H	1.46	0.81
3:G:115:ASN:HB3	3:G:276:LEU:HD22	1.63	0.81
1:E:624:ASN:O	1:E:628:ILE:HG12	1.81	0.81
3:D:447:GLY:O	3:D:453:GLY:HA3	1.80	0.81
3:D:213:THR:HG22	3:D:235:GLU:HA	1.60	0.80
2:F:685:TYR:O	2:F:687:ARG:N	2.13	0.80
1:B:101:LEU:HD23	1:B:104:ILE:HD12	1.63	0.80
3:G:374:ILE:HA	3:G:590:ILE:HD11	1.64	0.80
1:E:977:LEU:HD21	1:E:990:LEU:HD22	1.63	0.80
2:C:415:ILE:HB	2:C:663:THR:HG23	1.63	0.80
2:F:506:ILE:H	2:F:510:ASN:HD22	1.27	0.80
3:D:230:LYS:HA	3:D:232:ARG:HG3	1.64	0.80
3:D:247:GLN:HE22	4:X:6:DA:H5'	1.46	0.80
2:F:354:ASN:ND2	2:F:357:GLU:H	1.79	0.80
3:G:389:ASP:C	3:G:391:THR:H	1.84	0.80
3:G:247:GLN:O	3:G:251:GLN:HG2	1.81	0.80
2:F:104:GLU:HG3	2:F:104:GLU:O	1.81	0.80
2:F:656:ALA:O	2:F:658:PRO:HD3	1.82	0.80
3:G:204:PRO:HG3	3:G:274:ILE:HD13	1.61	0.80
1:B:1138:VAL:HB	1:B:1158:THR:O	1.81	0.80
3:D:389:ASP:C	3:D:391:THR:H	1.84	0.80
3:G:345:ALA:HB3	3:G:349:ARG:HG3	1.63	0.80
2:C:354:ASN:ND2	2:C:357:GLU:H	1.80	0.80
3:D:247:GLN:HG2	4:X:5:5IU:H5''	1.64	0.80
4:Y:2:5IU:C2'	4:Y:3:5IU:H5'	2.12	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ILE:HG12	1:E:222:HIS:CD2	2.17	0.80
1:E:889:ASN:HD22	1:E:889:ASN:N	1.76	0.80
2:F:112:ARG:O	2:F:116:THR:HG23	1.81	0.80
2:C:681:ASN:HD21	2:C:732:ILE:H	1.29	0.80
3:D:204:PRO:HG3	3:D:274:ILE:HD13	1.64	0.79
2:C:112:ARG:O	2:C:116:THR:HG23	1.82	0.79
2:F:406:ARG:N	2:F:658:PRO:HB3	1.96	0.79
4:Y:37:DT:H2''	4:Y:38:DG:H5'	1.62	0.79
2:C:519:THR:HG23	2:C:521:GLN:H	1.44	0.79
3:G:230:LYS:HA	3:G:232:ARG:HG3	1.64	0.79
3:G:280:SER:O	3:G:283:ILE:HG12	1.83	0.79
1:B:977:LEU:HD21	1:B:990:LEU:HD22	1.64	0.79
2:F:141:TYR:HB2	2:F:697:MET:SD	2.22	0.79
2:C:363:ASN:H	2:C:363:ASN:HD22	0.82	0.79
1:B:900:ASN:ND2	1:B:902:ARG:HH21	1.81	0.79
2:F:257:LEU:HD12	2:F:258:ALA:N	1.98	0.79
2:C:656:ALA:O	2:C:658:PRO:HD3	1.82	0.79
3:G:169:ILE:HB	3:G:295:LEU:HD23	1.65	0.79
3:G:359:TYR:O	3:G:360:ARG:HG2	1.82	0.79
3:G:243:LEU:HD12	3:G:261:LEU:HD21	1.63	0.79
2:C:118:ASP:O	2:C:119:SER:HB2	1.83	0.79
2:F:382:PRO:O	2:F:386:VAL:HG23	1.82	0.79
2:C:8:ASN:HD21	2:C:343:LEU:CG	1.96	0.79
2:F:1055:ASP:HB2	2:F:1118:ARG:NH2	1.97	0.79
3:G:367:ILE:H	3:G:393:ILE:HG21	1.45	0.79
2:C:847:ALA:O	2:C:851:MET:HB2	1.83	0.79
3:G:165:ARG:HA	3:G:291:ARG:HG2	1.64	0.79
2:C:204:PRO:HB3	2:C:233:HIS:HB3	1.64	0.78
1:B:768:TYR:CE2	1:B:786:SER:HB3	2.18	0.78
2:C:7:SER:HB3	2:C:13:LEU:HG	1.63	0.78
2:C:257:LEU:HD12	2:C:258:ALA:N	1.97	0.78
1:E:24:SER:HA	1:E:414:ASP:OD2	1.82	0.78
2:F:376:PHE:CZ	2:F:752:ILE:HG23	2.18	0.78
3:D:169:ILE:HB	3:D:295:LEU:HD23	1.64	0.78
1:E:900:ASN:ND2	1:E:902:ARG:HH21	1.82	0.78
2:F:974:VAL:HG21	2:F:1043:GLY:HA3	1.66	0.78
1:E:673:ASN:OD1	2:F:815:LYS:HG2	1.83	0.78
1:B:1098:MET:O	1:B:1102:MET:HG2	1.84	0.78
1:E:531:GLN:HE21	1:E:879:GLN:HB2	1.48	0.78
2:F:276:LEU:HD22	2:F:279:ASP:HB2	1.65	0.78
2:F:737:GLN:HG3	2:F:738:ASP:H	1.47	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:130:LYS:HD2	2:F:692:LEU:HD21	1.63	0.78
1:B:746:GLY:H	1:B:808:ARG:NH1	1.81	0.78
3:D:157:ALA:HB2	3:D:355:LEU:HD21	1.65	0.78
1:E:1050:CYS:C	1:E:1052:PRO:HD2	2.03	0.78
2:C:737:GLN:HG3	2:C:738:ASP:H	1.48	0.78
2:F:192:ARG:O	2:F:196:THR:HG22	1.83	0.78
1:E:746:GLY:H	1:E:808:ARG:NH1	1.82	0.78
2:C:8:ASN:HD21	2:C:343:LEU:HG	1.49	0.78
2:C:78:PRO:HD2	2:C:192:ARG:NH1	1.99	0.77
2:C:945:LEU:HD21	2:C:990:SER:OG	1.84	0.77
2:F:116:THR:O	2:F:118:ASP:N	2.17	0.77
1:B:104:ILE:HB	1:B:107:LYS:HE2	1.64	0.77
1:B:821:VAL:HA	1:B:832:ASP:OD1	1.84	0.77
1:E:107:LYS:H	1:E:107:LYS:HD2	1.49	0.77
3:D:158:ALA:HA	3:D:184:LEU:HD23	1.63	0.77
3:D:260:PRO:O	3:D:261:LEU:HB2	1.85	0.77
2:F:945:LEU:HD21	2:F:990:SER:OG	1.83	0.77
1:B:11:LEU:HD13	1:B:99:ARG:HD2	1.64	0.77
3:D:17:ARG:HG2	3:D:20:ASP:OD2	1.85	0.77
3:G:370:LEU:O	3:G:374:ILE:HG12	1.85	0.77
1:B:1050:CYS:C	1:B:1052:PRO:HD2	2.04	0.77
3:G:17:ARG:HG2	3:G:20:ASP:OD2	1.85	0.77
3:G:447:GLY:O	3:G:453:GLY:HA3	1.83	0.77
2:C:141:TYR:HB2	2:C:697:MET:SD	2.24	0.77
3:G:367:ILE:HG13	3:G:393:ILE:HG23	1.67	0.77
1:E:104:ILE:HB	1:E:107:LYS:HE2	1.64	0.77
2:C:376:PHE:CZ	2:C:752:ILE:HG23	2.20	0.77
2:C:269:PHE:O	2:C:270:GLU:HG2	1.85	0.77
3:G:255:HIS:HA	3:G:259:ASN:HB2	1.65	0.77
2:F:709:ARG:HH21	2:F:709:ARG:HG2	1.48	0.77
4:X:7:5IU:H3'	4:X:8:DC:C5'	2.12	0.77
1:B:526:ILE:HG22	1:B:576:ILE:HD13	1.67	0.77
1:B:107:LYS:HD2	1:B:107:LYS:H	1.50	0.77
3:G:278:MET:HG3	3:G:279:MET:N	2.00	0.76
2:F:104:GLU:HA	2:F:112:ARG:NH1	2.00	0.76
1:B:1071:ARG:HH22	2:C:29:PRO:CB	1.98	0.76
1:E:101:LEU:HD23	1:E:104:ILE:HD12	1.66	0.76
3:G:385:VAL:HG11	3:G:396:ARG:HD2	1.65	0.76
2:C:116:THR:O	2:C:118:ASP:N	2.18	0.76
1:E:237:ARG:HH21	1:E:266:ILE:HG23	1.50	0.76
3:G:175:THR:HG21	3:G:355:LEU:HB2	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:8:ASN:HD21	2:F:343:LEU:CG	1.99	0.76
1:B:1033:ALA:HB1	1:B:1053:LEU:HA	1.66	0.76
1:B:564:ALA:CA	1:B:738:ILE:HD11	2.14	0.76
1:B:861:CYS:SG	1:B:866:ALA:HA	2.24	0.76
3:G:398:LEU:H	3:G:398:LEU:CD2	1.99	0.76
3:G:158:ALA:HA	3:G:184:LEU:HD23	1.67	0.76
1:E:423:ARG:HG2	4:Y:49:DA:C2	2.21	0.76
1:E:159:LEU:CD1	1:E:339:VAL:HG13	2.15	0.76
1:B:286:LEU:HD22	1:B:306:ARG:NH1	2.00	0.76
2:F:559:GLU:HA	3:G:19:LEU:HD12	1.67	0.76
2:F:415:ILE:HB	2:F:663:THR:HG23	1.67	0.76
3:G:188:LEU:HD21	3:G:291:ARG:NH2	2.00	0.76
1:E:526:ILE:HG22	1:E:576:ILE:HD13	1.68	0.76
3:D:385:VAL:HG11	3:D:396:ARG:HD2	1.66	0.76
3:D:199:ILE:HG12	3:D:265:VAL:HG11	1.66	0.76
1:E:262:GLN:O	1:E:265:TRP:HB3	1.86	0.76
1:E:1075:ARG:HB3	1:E:1135:PHE:O	1.86	0.76
3:G:126:VAL:HG22	3:G:166:ILE:HD13	1.68	0.76
3:G:243:LEU:CG	3:G:244:LEU:N	2.47	0.76
1:B:794:ARG:HH21	1:B:795:LEU:HB3	1.50	0.76
1:E:610:ASN:HD22	1:E:613:ARG:HH12	1.30	0.76
1:B:119:ARG:HD3	2:C:302:SER:HB3	1.67	0.76
3:D:228:GLU:HA	3:D:228:GLU:OE1	1.85	0.76
1:E:562:GLN:NE2	4:Y:46:5IU:I5	2.89	0.75
1:B:262:GLN:O	1:B:265:TRP:HB3	1.87	0.75
1:E:821:VAL:HA	1:E:832:ASP:OD1	1.86	0.75
3:G:199:ILE:HG12	3:G:265:VAL:HG11	1.68	0.75
1:E:286:LEU:HD22	1:E:306:ARG:NH1	2.00	0.75
1:E:307:HIS:CG	1:E:308:PRO:HD2	2.22	0.75
2:C:347:ASN:HD22	2:C:349:ALA:H	1.33	0.75
1:B:1075:ARG:HB3	1:B:1135:PHE:O	1.86	0.75
2:F:347:ASN:HD22	2:F:347:ASN:C	1.90	0.75
1:B:488:ARG:HH12	1:E:544:ASP:HA	1.52	0.75
1:B:467:ALA:O	1:B:799:LEU:HD13	1.85	0.75
2:F:269:PHE:O	2:F:270:GLU:HG2	1.87	0.75
1:B:24:SER:HA	1:B:414:ASP:OD2	1.87	0.75
3:D:204:PRO:HB3	4:X:2:5IU:H6	1.69	0.75
1:E:1051:PRO:N	1:E:1052:PRO:CD	2.48	0.75
1:B:881:ASN:HD21	1:E:883:VAL:HA	1.51	0.75
1:E:362:LEU:HB3	1:E:399:ARG:HG2	1.68	0.75
2:F:347:ASN:HD22	2:F:349:ALA:H	1.34	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1132:GLU:HG3	1:B:1159:ARG:HH22	1.52	0.75
2:F:752:ILE:HD12	2:F:753:ASP:N	2.01	0.75
1:E:768:TYR:CE2	1:E:786:SER:HB3	2.22	0.75
3:D:261:LEU:HD13	3:D:286:LEU:HD23	1.68	0.75
3:G:241:HIS:CG	4:Y:3:5IU:H4'	2.22	0.75
3:D:526:ARG:HE	3:D:526:ARG:HA	1.51	0.75
1:B:652:TRP:NE1	1:B:657:VAL:HG22	2.01	0.75
1:B:179:ILE:HG12	1:B:222:HIS:CD2	2.22	0.75
3:G:157:ALA:HB2	3:G:355:LEU:HD21	1.68	0.75
3:D:247:GLN:NE2	4:X:6:DA:H5'	2.02	0.75
2:C:971:LEU:HD23	4:X:10:DA:H5'	1.68	0.75
1:B:1109:LEU:HD22	1:B:1113:LEU:HG	1.69	0.75
1:E:1109:LEU:HD22	1:E:1113:LEU:HG	1.68	0.75
3:G:228:GLU:HA	3:G:228:GLU:OE1	1.86	0.75
3:D:175:THR:HG21	3:D:355:LEU:HB2	1.68	0.75
1:E:1098:MET:O	1:E:1102:MET:HG2	1.86	0.75
3:G:260:PRO:O	3:G:261:LEU:HB2	1.86	0.74
4:X:46:5IU:H2''	4:X:47:DA:C4'	2.17	0.74
3:D:536:MET:SD	3:D:540:LYS:HD2	2.27	0.74
2:C:752:ILE:HD12	2:C:753:ASP:N	2.02	0.74
3:D:370:LEU:O	3:D:374:ILE:HG12	1.87	0.74
1:B:758:THR:HG22	1:B:820:LEU:HD12	1.69	0.74
3:D:65:HIS:CB	3:D:66:PRO:HD2	2.08	0.74
3:G:253:LEU:HB3	3:G:255:HIS:NE2	2.01	0.74
3:G:261:LEU:HD13	3:G:286:LEU:HD23	1.69	0.74
3:D:366:GLY:HA3	3:D:393:ILE:CD1	2.17	0.74
1:B:571:LEU:HD21	1:B:736:VAL:HG21	1.68	0.74
3:G:244:LEU:HD11	3:G:285:ALA:CB	2.17	0.74
1:E:467:ALA:O	1:E:799:LEU:HD13	1.86	0.74
1:E:1039:LEU:H	1:E:1039:LEU:HD23	1.52	0.74
1:B:1003:ASN:HD22	1:B:1157:THR:HG21	1.52	0.74
4:Y:47:DA:H2''	4:Y:48:DG:H5''	1.69	0.74
1:E:306:ARG:O	1:E:307:HIS:HB2	1.85	0.74
2:C:347:ASN:HD22	2:C:347:ASN:C	1.89	0.74
2:F:433:ARG:NH1	2:F:805:GLU:HG2	2.01	0.74
2:F:506:ILE:N	2:F:510:ASN:HD22	1.86	0.74
1:E:482:GLY:HA2	1:E:485:GLN:HG2	1.68	0.74
4:Y:46:5IU:H2''	4:Y:47:DA:C4'	2.17	0.74
1:B:488:ARG:NH1	1:E:544:ASP:HA	2.02	0.74
2:F:533:LEU:HD11	2:F:537:MET:HE3	1.69	0.74
3:G:316:TYR:HE1	3:G:604:PHE:HB2	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:GLU:HB2	2:C:786:ARG:HD2	1.67	0.74
2:F:681:ASN:HD21	2:F:732:ILE:H	1.32	0.74
4:X:22:DG:C3'	4:X:23:DC:H5"	2.18	0.74
2:C:1046:LEU:HD21	2:C:1110:GLN:HG3	1.69	0.74
4:Y:8:DC:H2"	4:Y:9:5IU:H5"	1.68	0.74
1:E:1033:ALA:HB1	1:E:1053:LEU:HA	1.69	0.74
1:B:159:LEU:CD1	1:B:339:VAL:HG13	2.18	0.74
2:C:104:GLU:HA	2:C:112:ARG:NH1	2.02	0.74
1:B:925:ASP:H	1:B:953:THR:CG2	2.01	0.74
1:B:799:LEU:HD23	1:B:837:ALA:HB1	1.69	0.74
3:D:528:PRO:O	3:D:529:GLU:HB2	1.87	0.74
3:D:165:ARG:NH2	3:D:288:ASP:HA	2.02	0.74
1:E:1132:GLU:HG3	1:E:1159:ARG:HH22	1.52	0.74
2:F:506:ILE:HG23	2:F:507:ASP:N	2.02	0.74
1:E:1003:ASN:HD22	1:E:1157:THR:HG21	1.53	0.74
2:C:335:LEU:HA	2:C:374:ILE:HD11	1.70	0.74
2:F:968:ARG:NH2	4:Y:9:5IU:OP1	2.19	0.74
1:B:237:ARG:HH21	1:B:266:ILE:HG23	1.53	0.74
2:C:709:ARG:HG2	2:C:709:ARG:HH21	1.50	0.74
1:B:142:PHE:HB3	2:C:110:LEU:HD22	1.68	0.74
4:X:47:DA:H2"	4:X:48:DG:H5"	1.68	0.74
1:B:587:VAL:HG21	1:B:689:HIS:ND1	2.02	0.74
1:E:65:THR:HB	1:E:68:ALA:HB2	1.70	0.74
2:C:834:LEU:HD12	2:C:838:GLN:NE2	2.02	0.73
1:E:758:THR:HG22	1:E:820:LEU:HD12	1.70	0.73
3:D:460:GLN:HA	3:D:463:GLN:CD	2.08	0.73
2:C:273:GLU:OE2	2:C:274:LEU:HD23	1.86	0.73
1:E:281:GLN:O	1:E:282:LEU:HB2	1.89	0.73
3:D:367:ILE:HG13	3:D:393:ILE:HG23	1.71	0.73
1:E:652:TRP:NE1	1:E:657:VAL:HG22	2.04	0.73
2:C:989:ALA:C	2:C:991:GLY:H	1.92	0.73
2:C:406:ARG:N	2:C:658:PRO:HB3	2.03	0.73
1:B:248:GLU:HG3	1:B:288:LYS:O	1.88	0.73
3:G:301:LEU:H	3:G:568:THR:CG2	2.01	0.73
1:B:761:ARG:HG3	1:B:822:ARG:HH22	1.52	0.73
2:C:276:LEU:HD22	2:C:279:ASP:HB2	1.70	0.73
1:E:809:SER:OG	1:E:813:CYS:HB2	1.88	0.73
3:D:370:LEU:HB2	3:D:394:GLU:OE2	1.89	0.73
3:D:562:THR:HB	3:D:594:THR:H	1.53	0.73
2:C:714:TYR:O	2:C:718:GLU:HG3	1.88	0.73
2:F:321:GLN:O	2:F:323:LEU:HD23	1.88	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:THR:CG2	2:C:804:ARG:HE	2.01	0.73
1:E:564:ALA:CA	1:E:738:ILE:HD11	2.16	0.73
1:E:233:LYS:NZ	1:E:269:ILE:HG12	2.04	0.73
1:E:471:ARG:HD2	1:E:471:ARG:N	2.02	0.73
2:F:506:ILE:CG2	2:F:507:ASP:N	2.50	0.73
1:E:610:ASN:ND2	1:E:613:ARG:HH12	1.87	0.73
1:B:307:HIS:CG	1:B:308:PRO:HD2	2.23	0.73
2:C:142:ARG:N	2:C:142:ARG:HD3	2.02	0.73
2:C:70:TRP:CH2	2:C:84:SER:HB2	2.24	0.73
1:B:281:GLN:HB3	1:B:283:PRO:HD2	1.69	0.73
2:C:951:GLN:O	2:C:952:ILE:HG23	1.87	0.73
1:B:471:ARG:N	1:B:471:ARG:HD2	2.04	0.73
2:C:550:TYR:CE2	2:C:552:GLU:HB2	2.23	0.72
1:B:561:ARG:HH22	1:B:584:ARG:H	1.35	0.72
1:E:281:GLN:HB3	1:E:283:PRO:HD2	1.69	0.72
1:B:488:ARG:HH22	1:E:541:MET:CE	2.01	0.72
1:E:799:LEU:HD23	1:E:837:ALA:HB1	1.71	0.72
3:D:398:LEU:CD2	3:D:398:LEU:H	2.01	0.72
3:G:526:ARG:HA	3:G:526:ARG:HE	1.54	0.72
1:B:658:MET:HB2	1:B:695:GLN:HG2	1.71	0.72
2:C:974:VAL:HG21	2:C:1043:GLY:HA3	1.71	0.72
3:D:307:GLY:CA	3:D:597:ARG:HH21	2.00	0.72
4:X:39:DC:H2''	4:X:40:DT:OP2	1.88	0.72
3:D:121:ARG:CB	3:D:121:ARG:HH11	2.03	0.72
3:G:241:HIS:HB3	4:Y:3:5IU:O3'	1.89	0.72
3:G:244:LEU:HD11	3:G:285:ALA:HB3	1.72	0.72
3:G:207:LYS:HZ1	3:G:544:SER:HA	1.53	0.72
1:B:286:LEU:CD1	1:B:306:ARG:HB3	2.19	0.72
3:D:223:LEU:HB2	3:D:224:PRO:HD2	1.71	0.72
2:F:87:ASN:HD21	2:F:90:SER:H	1.37	0.72
4:Y:22:DG:C3'	4:Y:23:DC:H5''	2.18	0.72
1:B:306:ARG:O	1:B:307:HIS:HB2	1.87	0.72
2:F:273:GLU:OE2	2:F:274:LEU:HD23	1.88	0.72
3:G:304:VAL:HG21	3:G:564:GLU:HG2	1.70	0.72
1:B:610:ASN:HD22	1:B:613:ARG:HH12	1.35	0.72
1:E:561:ARG:HH12	1:E:584:ARG:HB2	1.55	0.72
1:E:286:LEU:CD1	1:E:306:ARG:HB3	2.18	0.72
2:C:664:LEU:HD22	2:C:685:TYR:CE1	2.25	0.72
2:C:506:ILE:HG23	2:C:507:ASP:N	2.03	0.72
2:C:251:ILE:HD13	2:C:252:LYS:H	1.55	0.72
2:C:87:ASN:HD21	2:C:90:SER:H	1.37	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:548:LEU:HB2	2:C:903:ALA:CB	2.19	0.72
2:F:155:VAL:H	2:F:162:GLN:HE22	1.37	0.72
2:C:506:ILE:CG2	2:C:507:ASP:N	2.52	0.72
1:B:249:SER:OG	1:B:250:SER:N	2.22	0.72
2:F:304:GLY:HA2	2:F:714:TYR:HD1	1.55	0.72
3:D:234:PRO:C	3:D:236:ASP:N	2.40	0.72
1:B:1051:PRO:N	1:B:1052:PRO:CD	2.48	0.72
2:C:550:TYR:CZ	2:C:552:GLU:HB2	2.24	0.72
3:G:121:ARG:HH11	3:G:121:ARG:CB	2.02	0.72
3:G:255:HIS:HA	3:G:259:ASN:CB	2.19	0.72
1:B:283:PRO:HD3	1:B:314:ASP:HB2	1.70	0.72
1:B:947:ARG:HD3	1:B:947:ARG:H	1.54	0.72
2:C:347:ASN:HD21	2:C:349:ALA:HB3	1.55	0.72
1:B:252:ILE:O	1:B:255:ARG:HB2	1.90	0.72
2:F:169:TRP:O	2:F:173:VAL:HG23	1.90	0.72
3:D:526:ARG:HH22	3:D:533:THR:CG2	2.03	0.72
3:D:226:THR:HA	3:D:229:GLN:HB3	1.72	0.72
1:B:763:GLN:HE22	1:B:765:GLN:H	1.35	0.72
1:B:65:THR:HB	1:B:68:ALA:HB2	1.70	0.72
2:F:834:LEU:HD12	2:F:838:GLN:NE2	2.04	0.72
3:D:16:LEU:HD12	3:D:16:LEU:O	1.90	0.72
1:E:249:SER:OG	1:E:250:SER:N	2.22	0.72
1:B:281:GLN:O	1:B:282:LEU:HB2	1.89	0.71
1:E:947:ARG:HD3	1:E:947:ARG:H	1.55	0.71
1:E:925:ASP:H	1:E:953:THR:CG2	2.03	0.71
1:B:233:LYS:NZ	1:B:269:ILE:HG12	2.04	0.71
2:F:664:LEU:HD22	2:F:685:TYR:CE1	2.25	0.71
3:G:536:MET:SD	3:G:540:LYS:HD2	2.30	0.71
1:B:34:ALA:HB1	1:B:79:ASN:HD22	1.53	0.71
2:F:550:TYR:CE2	2:F:552:GLU:HB2	2.25	0.71
3:D:526:ARG:HH22	3:D:533:THR:HG22	1.53	0.71
1:B:987:GLU:HG3	1:B:988:PRO:CD	2.20	0.71
4:X:37:DT:H2''	4:X:38:DG:C5'	2.19	0.71
2:C:539:SER:HB2	2:C:551:ASP:OD1	1.90	0.71
2:C:169:TRP:O	2:C:173:VAL:HG23	1.90	0.71
1:B:251:GLY:HA3	1:B:255:ARG:CZ	2.19	0.71
3:G:165:ARG:NH2	3:G:288:ASP:HA	2.04	0.71
1:E:1071:ARG:HH22	2:F:29:PRO:CB	2.03	0.71
1:B:889:ASN:HA	2:C:807:LEU:HD11	1.73	0.71
1:E:587:VAL:HG21	1:E:689:HIS:ND1	2.05	0.71
2:F:550:TYR:CZ	2:F:552:GLU:HB2	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:LEU:HD11	1:B:808:ARG:HG3	1.73	0.71
2:C:506:ILE:N	2:C:510:ASN:HD22	1.88	0.71
1:E:418:ALA:O	1:E:800:ARG:HD2	1.90	0.71
2:C:265:ARG:O	2:C:323:LEU:HB2	1.90	0.71
2:F:253:ASP:C	2:F:255:ALA:H	1.93	0.71
2:F:502:ILE:CG1	2:F:527:GLY:HA3	2.20	0.71
2:F:551:ASP:HB3	3:G:111:ARG:NH2	2.06	0.71
4:Y:7:5IU:H3'	4:Y:8:DC:C5'	2.13	0.71
4:X:14:DC:C2'	4:X:15:DG:H5''	2.18	0.71
2:F:506:ILE:CG2	2:F:507:ASP:H	2.03	0.71
2:C:304:GLY:HA2	2:C:714:TYR:HD1	1.56	0.71
2:C:736:ILE:H	2:C:736:ILE:HD12	1.56	0.71
3:G:121:ARG:HB2	3:G:121:ARG:HH11	1.56	0.71
1:B:560:SER:HB3	4:X:47:DA:N3	2.05	0.71
3:D:213:THR:CG2	3:D:235:GLU:HA	2.21	0.71
3:D:75:ILE:HB	3:D:78:LEU:HD13	1.72	0.71
1:E:658:MET:HB2	1:E:695:GLN:CG	2.20	0.71
1:E:763:GLN:HE22	1:E:765:GLN:H	1.36	0.71
1:E:252:ILE:O	1:E:255:ARG:HB2	1.90	0.71
3:G:243:LEU:CD1	3:G:244:LEU:HG	2.20	0.71
1:E:739:VAL:HG22	1:E:740:THR:N	2.06	0.71
2:C:347:ASN:HD22	2:C:348:ARG:N	1.89	0.71
2:F:951:GLN:O	2:F:952:ILE:HG23	1.90	0.71
3:D:78:LEU:O	3:D:80:ASN:N	2.22	0.71
1:B:380:VAL:HG23	1:B:408:ALA:HB3	1.70	0.71
1:E:729:LEU:HD22	1:E:729:LEU:H	1.54	0.71
2:F:70:TRP:CH2	2:F:84:SER:HB2	2.25	0.71
3:D:199:ILE:HG12	3:D:265:VAL:CG1	2.21	0.71
1:E:283:PRO:HD3	1:E:314:ASP:HB2	1.71	0.71
3:G:226:THR:HA	3:G:229:GLN:HB3	1.72	0.71
2:C:321:GLN:O	2:C:323:LEU:HD23	1.90	0.71
2:F:265:ARG:O	2:F:323:LEU:HB2	1.90	0.71
1:B:891:LYS:HD2	2:C:802:TYR:CZ	2.25	0.71
4:Y:2:5IU:C3'	4:Y:3:5IU:H5'	2.21	0.71
2:C:80:ILE:HD12	2:C:189:LEU:HD21	1.73	0.71
3:D:462:MET:HE1	3:D:534:TRP:HE1	1.54	0.71
4:Y:37:DT:H2''	4:Y:38:DG:C5'	2.20	0.71
3:G:16:LEU:O	3:G:16:LEU:HD12	1.90	0.71
1:E:1130:ASP:H	1:E:1134:HIS:HD2	1.38	0.71
3:G:213:THR:CG2	3:G:235:GLU:HA	2.21	0.70
1:B:1071:ARG:HB3	1:B:1076:TYR:CD2	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:386:VAL:HG12	2:F:425:VAL:HG21	1.72	0.70
4:Y:39:DC:H2''	4:Y:40:DT:OP2	1.89	0.70
1:B:658:MET:HB2	1:B:695:GLN:CG	2.21	0.70
1:B:1039:LEU:HD23	1:B:1039:LEU:H	1.53	0.70
1:E:483:LYS:HG3	1:E:484:ASN:ND2	2.05	0.70
3:G:135:ALA:O	3:G:139:GLN:HG3	1.90	0.70
1:B:809:SER:OG	1:B:813:CYS:HB2	1.91	0.70
2:C:828:LEU:HD22	2:C:1028:ARG:CD	2.22	0.70
1:E:1071:ARG:HB3	1:E:1076:TYR:CD2	2.26	0.70
1:E:25:ALA:HB1	1:E:807:THR:CG2	2.21	0.70
3:D:58:LEU:HD13	3:D:81:TRP:CZ3	2.26	0.70
2:F:142:ARG:N	2:F:142:ARG:HD3	2.05	0.70
1:B:676:ALA:O	2:C:816:ALA:HB2	1.91	0.70
3:G:529:GLU:OE2	3:G:529:GLU:HA	1.91	0.70
3:G:373:ALA:HB1	3:G:380:THR:HB	1.72	0.70
1:B:497:PRO:O	1:B:812:HIS:HD2	1.75	0.70
2:C:506:ILE:CG2	2:C:507:ASP:H	2.04	0.70
3:G:78:LEU:O	3:G:80:ASN:N	2.23	0.70
2:C:269:PHE:N	2:C:269:PHE:HD2	1.90	0.70
1:E:936:GLU:HG2	1:E:936:GLU:O	1.89	0.70
2:F:989:ALA:C	2:F:991:GLY:H	1.94	0.70
2:C:1055:ASP:CB	2:C:1118:ARG:HH22	1.98	0.70
1:E:925:ASP:N	1:E:953:THR:HG22	2.07	0.70
1:E:924:LEU:HD23	1:E:953:THR:HG21	1.72	0.70
1:B:892:THR:HG22	2:C:804:ARG:NE	2.06	0.70
4:Y:8:DC:H2''	4:Y:9:5IU:C5'	2.22	0.70
1:B:739:VAL:HG22	1:B:740:THR:N	2.07	0.70
1:E:949:ALA:O	1:E:953:THR:HG23	1.92	0.70
1:E:920:LEU:HD21	2:F:448:HIS:CE1	2.27	0.70
3:G:465:LYS:O	3:G:466:ARG:HB2	1.90	0.70
1:B:729:LEU:H	1:B:729:LEU:HD22	1.55	0.70
2:F:752:ILE:HD12	2:F:753:ASP:H	1.55	0.70
1:E:761:ARG:HG3	1:E:822:ARG:HH22	1.56	0.70
1:E:620:MET:CE	1:E:687:ILE:HD13	2.21	0.70
1:E:380:VAL:HG23	1:E:408:ALA:HB3	1.73	0.70
4:X:8:DC:H2''	4:X:9:5IU:H5''	1.74	0.70
1:E:1052:PRO:C	1:E:1053:LEU:HD23	2.12	0.70
2:C:584:LEU:CD1	2:C:620:ILE:HG23	2.20	0.70
3:D:2:LYS:O	3:D:3:LEU:HB2	1.91	0.70
2:F:506:ILE:H	2:F:510:ASN:ND2	1.90	0.70
2:F:269:PHE:HD2	2:F:269:PHE:N	1.89	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:300:GLN:HG3	3:G:568:THR:HG22	1.74	0.70
3:D:201:LEU:HB3	3:D:212:LEU:HD13	1.74	0.69
3:D:130:ILE:O	3:D:132:VAL:N	2.25	0.69
2:F:1:MET:HG2	2:F:3:ARG:HE	1.57	0.69
3:D:121:ARG:HB2	3:D:121:ARG:HH11	1.56	0.69
1:B:620:MET:CE	1:B:687:ILE:HD13	2.22	0.69
2:C:828:LEU:HD22	2:C:1028:ARG:HD2	1.74	0.69
2:C:386:VAL:HG12	2:C:425:VAL:HG21	1.72	0.69
2:F:137:GLN:HG2	2:F:697:MET:HE1	1.72	0.69
3:G:234:PRO:C	3:G:236:ASP:N	2.40	0.69
1:E:218:LEU:HD23	1:E:323:ILE:HD11	1.72	0.69
1:B:936:GLU:HG2	1:B:936:GLU:O	1.90	0.69
1:E:282:LEU:N	1:E:283:PRO:HD2	2.08	0.69
3:D:134:GLU:OE1	3:D:331:ARG:HD2	1.92	0.69
1:B:924:LEU:HD23	1:B:953:THR:HG21	1.72	0.69
1:B:807:THR:HG22	1:B:808:ARG:HH21	1.58	0.69
2:C:1:MET:HG2	2:C:3:ARG:HE	1.57	0.69
1:B:1052:PRO:C	1:B:1053:LEU:HD23	2.12	0.69
1:E:497:PRO:O	1:E:812:HIS:HD2	1.76	0.69
2:F:828:LEU:HD22	2:F:1028:ARG:CD	2.22	0.69
2:C:980:LEU:CD1	2:C:998:LEU:HB2	2.22	0.69
2:C:502:ILE:CG1	2:C:527:GLY:HA3	2.23	0.69
1:B:482:GLY:HA2	1:B:485:GLN:HG2	1.72	0.69
4:X:2:5IU:C3'	4:X:3:5IU:H5'	2.23	0.69
1:B:925:ASP:N	1:B:953:THR:HG22	2.06	0.69
2:C:559:GLU:HA	3:D:19:LEU:HD12	1.74	0.69
3:D:550:ALA:HA	3:D:578:SER:O	1.91	0.69
3:D:261:LEU:HD12	3:D:285:ALA:O	1.92	0.69
3:G:259:ASN:CB	3:G:260:PRO:HD2	2.06	0.69
3:D:135:ALA:O	3:D:139:GLN:HG3	1.92	0.69
1:B:683:ARG:NE	2:C:1095:ARG:HH12	1.90	0.69
3:D:230:LYS:C	3:D:232:ARG:H	1.96	0.69
1:E:987:GLU:HG3	1:E:988:PRO:CD	2.22	0.69
1:B:148:PHE:H	2:C:126:GLN:HE22	1.41	0.69
1:B:875:ASN:C	1:B:877:PRO:HD2	2.13	0.69
2:F:363:ASN:HD22	2:F:363:ASN:H	0.77	0.69
3:D:465:LYS:O	3:D:466:ARG:HB2	1.91	0.69
2:C:253:ASP:C	2:C:255:ALA:H	1.94	0.69
1:E:248:GLU:HG3	1:E:288:LYS:O	1.93	0.69
2:F:347:ASN:HD21	2:F:349:ALA:HB3	1.56	0.69
1:B:1071:ARG:HH12	2:C:29:PRO:HA	1.58	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LYS:HD2	1:E:107:LYS:N	2.08	0.69
2:C:548:LEU:HB2	2:C:903:ALA:HB3	1.73	0.69
1:B:218:LEU:HD23	1:B:323:ILE:HD11	1.74	0.69
1:E:1073:GLU:OE2	1:E:1073:GLU:HA	1.93	0.69
1:B:985:GLN:CD	1:B:985:GLN:H	1.96	0.69
2:F:654:PHE:O	2:F:660:ASN:ND2	2.26	0.69
3:G:550:ALA:HA	3:G:578:SER:O	1.92	0.69
1:E:251:GLY:HA3	1:E:255:ARG:CZ	2.22	0.69
3:G:256:HIS:CG	3:G:257:ALA:H	2.10	0.69
1:B:527:ARG:CB	1:B:576:ILE:HD11	2.21	0.69
1:B:25:ALA:HB1	1:B:807:THR:CG2	2.23	0.69
1:E:620:MET:HE2	1:E:687:ILE:HD13	1.73	0.69
2:F:847:ALA:O	2:F:851:MET:HB2	1.92	0.69
2:C:968:ARG:NH2	4:X:9:5IU:OP1	2.26	0.69
3:G:130:ILE:O	3:G:132:VAL:N	2.23	0.69
2:F:588:LEU:HG	2:F:620:ILE:HG21	1.73	0.69
3:D:229:GLN:CG	3:D:229:GLN:O	2.41	0.69
1:B:541:MET:HG2	1:B:546:ALA:CB	2.23	0.69
2:F:714:TYR:O	2:F:718:GLU:HG3	1.93	0.69
3:D:234:PRO:C	3:D:236:ASP:H	1.94	0.69
1:B:771:ARG:N	1:B:771:ARG:HD2	2.08	0.69
4:X:19:DA:H1'	4:X:20:DC:H5'	1.75	0.69
1:B:483:LYS:HG3	1:B:484:ASN:ND2	2.08	0.69
2:C:850:GLN:HE22	4:X:7:5IU:HN3	1.40	0.68
3:G:229:GLN:CG	3:G:229:GLN:O	2.40	0.68
3:G:58:LEU:HD13	3:G:81:TRP:CZ3	2.27	0.68
1:B:375:ARG:HD3	1:B:400:ILE:O	1.93	0.68
1:B:167:PHE:O	1:B:171:HIS:HB2	1.93	0.68
3:G:2:LYS:O	3:G:3:LEU:HB2	1.93	0.68
2:F:942:GLU:OE1	3:G:196:ARG:NH1	2.26	0.68
2:F:736:ILE:HD12	2:F:736:ILE:H	1.58	0.68
3:G:201:LEU:HB3	3:G:212:LEU:HD13	1.76	0.68
2:F:38:GLN:NE2	2:F:667:MET:HG3	2.03	0.68
3:D:3:LEU:HD23	3:D:6:GLN:HG3	1.75	0.68
1:E:985:GLN:CD	1:E:985:GLN:H	1.95	0.68
1:B:13:LEU:HD12	1:B:14:PRO:HD2	1.76	0.68
1:E:875:ASN:C	1:E:877:PRO:HD2	2.13	0.68
2:F:347:ASN:HD22	2:F:348:ARG:N	1.89	0.68
3:G:134:GLU:OE1	3:G:331:ARG:HD2	1.92	0.68
3:D:374:ILE:HA	3:D:590:ILE:HD11	1.74	0.68
3:D:98:THR:HG22	3:D:100:MET:H	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HD21	1:B:114:LEU:HG	1.75	0.68
1:E:240:VAL:O	1:E:240:VAL:HG12	1.93	0.68
3:G:199:ILE:HG12	3:G:265:VAL:CG1	2.23	0.68
1:E:561:ARG:HH22	1:E:584:ARG:H	1.41	0.68
1:B:240:VAL:HG12	1:B:240:VAL:O	1.92	0.68
1:E:225:ILE:HG22	1:E:229:ILE:HD11	1.76	0.68
1:E:11:LEU:CD1	1:E:99:ARG:HD2	2.22	0.68
1:E:1136:GLY:HA2	1:E:1159:ARG:HD3	1.74	0.68
3:G:462:MET:HE1	3:G:534:TRP:HE1	1.58	0.68
1:E:771:ARG:N	1:E:771:ARG:HD2	2.08	0.68
3:D:204:PRO:HB3	4:X:2:5IU:I5	2.63	0.68
3:D:254:ARG:O	3:D:260:PRO:CG	2.42	0.68
1:B:159:LEU:HD21	1:B:342:GLU:HG2	1.75	0.68
1:B:282:LEU:N	1:B:283:PRO:HD2	2.08	0.68
1:B:225:ILE:HG22	1:B:229:ILE:HD11	1.76	0.68
2:F:771:GLU:O	2:F:775:ARG:HG3	1.92	0.68
1:E:947:ARG:CB	1:E:1086:LEU:HD21	2.23	0.68
1:B:488:ARG:NH2	1:E:541:MET:HE1	2.09	0.68
2:C:997:ARG:HG3	2:C:1007:ARG:HG3	1.76	0.68
2:F:1046:LEU:HD21	2:F:1110:GLN:HG3	1.73	0.68
3:D:261:LEU:HD12	3:D:285:ALA:C	2.14	0.68
3:D:526:ARG:HH12	3:D:536:MET:CE	2.07	0.68
2:F:273:GLU:OE2	2:F:274:LEU:N	2.27	0.68
2:F:619:ILE:HD11	2:F:644:ARG:HD2	1.76	0.68
1:E:1089:ASP:O	1:E:1091:SER:N	2.27	0.68
2:C:771:GLU:O	2:C:775:ARG:HG3	1.93	0.68
1:E:658:MET:HB2	1:E:695:GLN:HG2	1.75	0.68
1:B:1130:ASP:H	1:B:1134:HIS:HD2	1.39	0.68
2:F:335:LEU:HA	2:F:374:ILE:HD11	1.76	0.68
3:G:261:LEU:HD12	3:G:285:ALA:C	2.14	0.68
1:E:541:MET:HG2	1:E:546:ALA:CB	2.23	0.68
1:B:675:LEU:HD12	2:C:809:ALA:HB1	1.75	0.68
3:D:300:GLN:HG3	3:D:568:THR:HG22	1.75	0.68
3:D:165:ARG:HA	3:D:291:ARG:HG2	1.73	0.68
3:G:234:PRO:C	3:G:236:ASP:H	1.94	0.68
4:Y:19:DA:H1'	4:Y:20:DC:H5'	1.76	0.68
2:F:418:TYR:O	2:F:422:ILE:HG12	1.94	0.68
2:F:997:ARG:HG3	2:F:1007:ARG:HG3	1.76	0.68
2:F:251:ILE:HD13	2:F:252:LYS:H	1.58	0.68
2:C:418:TYR:O	2:C:422:ILE:HG12	1.93	0.68
3:G:261:LEU:HD12	3:G:285:ALA:O	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:366:GLY:HA3	3:D:393:ILE:HG21	1.76	0.67
1:B:107:LYS:HD2	1:B:107:LYS:N	2.09	0.67
3:G:75:ILE:HB	3:G:78:LEU:HD13	1.75	0.67
1:E:513:ASP:O	1:E:515:GLN:N	2.27	0.67
3:G:132:VAL:HG12	3:G:133:ASP:N	2.09	0.67
1:E:823:ARG:HG2	1:E:825:GLY:N	2.09	0.67
2:F:78:PRO:HD2	2:F:192:ARG:NH1	2.09	0.67
2:F:7:SER:CB	2:F:13:LEU:HG	2.24	0.67
2:C:619:ILE:HD11	2:C:644:ARG:HD2	1.75	0.67
1:B:1089:ASP:O	1:B:1091:SER:N	2.28	0.67
3:D:165:ARG:HB3	3:D:166:ILE:HD12	1.75	0.67
1:E:807:THR:HG22	1:E:808:ARG:HH21	1.58	0.67
2:F:8:ASN:HD21	2:F:343:LEU:HG	1.57	0.67
3:D:123:PHE:HB2	3:D:604:PHE:CE2	2.29	0.67
1:B:964:PHE:HD2	1:B:964:PHE:H	1.42	0.67
4:Y:2:5IU:H3'	4:Y:3:5IU:H5'	1.76	0.67
2:F:405:PRO:HG2	2:F:658:PRO:CB	2.25	0.67
2:F:980:LEU:CD1	2:F:998:LEU:HB2	2.24	0.67
1:B:624:ASN:HB2	1:B:627:ASP:OD2	1.94	0.67
3:D:301:LEU:H	3:D:568:THR:CG2	2.06	0.67
4:Y:9:5IU:H2''	4:Y:10:DA:O5'	1.95	0.67
1:E:159:LEU:HD21	1:E:342:GLU:HG2	1.75	0.67
1:B:1136:GLY:HA2	1:B:1159:ARG:HD3	1.77	0.67
1:B:213:PRO:O	1:B:215:ASP:N	2.28	0.67
1:B:1078:LEU:CD1	1:B:1118:LEU:HD12	2.25	0.67
3:G:440:LEU:O	3:G:441:LEU:HD23	1.95	0.67
1:B:442:THR:CG2	1:B:476:ILE:HD11	2.15	0.67
1:B:243:LEU:HD22	1:B:259:ARG:NH1	2.10	0.67
2:F:405:PRO:HB2	2:F:659:VAL:HG23	1.77	0.67
2:C:506:ILE:H	2:C:510:ASN:ND2	1.92	0.67
1:B:426:ASP:O	1:B:429:THR:HG22	1.94	0.67
1:E:426:ASP:O	1:E:429:THR:HG22	1.95	0.67
2:F:435:LEU:HD12	2:F:435:LEU:O	1.95	0.67
3:G:254:ARG:CG	3:G:259:ASN:ND2	2.58	0.67
3:G:274:ILE:HG23	3:G:278:MET:HG2	1.75	0.67
3:D:366:GLY:HA3	3:D:393:ILE:HD12	1.76	0.67
2:C:1036:LEU:O	2:C:1037:VAL:HB	1.94	0.67
3:G:301:LEU:HD22	3:G:565:LEU:HA	1.76	0.67
1:B:892:THR:HG22	2:C:804:ARG:HE	1.59	0.67
1:B:18:GLU:HG2	1:B:18:GLU:O	1.94	0.67
2:C:97:THR:HG23	2:C:628:TYR:CE1	2.29	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:964:PHE:H	1:E:964:PHE:HD2	1.43	0.67
1:B:1043:PHE:HB3	1:B:1161:ASN:CG	2.15	0.67
3:D:529:GLU:OE2	3:D:529:GLU:HA	1.93	0.67
2:F:834:LEU:HD21	2:F:986:VAL:HG21	1.77	0.67
2:C:502:ILE:HG13	2:C:527:GLY:HA3	1.76	0.67
3:D:200:ARG:HB2	3:D:263:LEU:CD2	2.22	0.66
3:G:230:LYS:C	3:G:232:ARG:H	1.96	0.66
1:E:1078:LEU:CD1	1:E:1118:LEU:HD12	2.24	0.66
1:B:423:ARG:HG2	4:X:49:DA:H2	1.57	0.66
3:G:398:LEU:HD23	3:G:398:LEU:N	2.10	0.66
3:D:85:LEU:HD13	3:D:107:LEU:HD13	1.77	0.66
3:G:561:VAL:HG12	3:G:589:ALA:HB2	1.76	0.66
1:E:148:PHE:H	2:F:126:GLN:HE22	1.43	0.66
1:E:1071:ARG:HH12	2:F:29:PRO:HA	1.60	0.66
1:E:557:LEU:HD11	1:E:808:ARG:HG3	1.77	0.66
1:E:893:LEU:O	1:E:893:LEU:HD13	1.96	0.66
1:B:636:HIS:O	1:B:640:VAL:HG23	1.95	0.66
2:C:28:ASP:H	2:C:29:PRO:HD2	1.60	0.66
2:F:28:ASP:H	2:F:29:PRO:HD2	1.60	0.66
3:G:344:GLU:HG3	3:G:345:ALA:N	2.08	0.66
1:E:571:LEU:HD21	1:E:736:VAL:HG21	1.77	0.66
1:E:81:HIS:HA	1:E:118:GLU:OE2	1.95	0.66
3:D:278:MET:SD	4:X:2:5IU:I5	3.24	0.66
2:F:584:LEU:CD1	2:F:620:ILE:HG23	2.24	0.66
2:C:664:LEU:HB3	2:C:715:LEU:HD13	1.77	0.66
1:B:920:LEU:HD11	2:C:448:HIS:NE2	2.11	0.66
2:F:539:SER:HB2	2:F:551:ASP:OD1	1.95	0.66
3:D:286:LEU:HD13	3:D:292:VAL:HG21	1.77	0.66
3:D:207:LYS:NZ	3:D:544:SER:HA	2.10	0.66
1:B:610:ASN:ND2	1:B:613:ARG:HH12	1.93	0.66
2:F:172:LEU:O	2:F:176:THR:HG22	1.94	0.66
1:B:919:ASP:OD1	2:C:652:GLN:HB2	1.95	0.66
1:E:558:VAL:HG22	1:E:563:GLU:HB3	1.77	0.66
3:D:526:ARG:HE	3:D:526:ARG:CA	2.09	0.66
2:F:1037:VAL:HG22	2:F:1109:SER:HA	1.77	0.66
2:F:354:ASN:ND2	2:F:356:GLU:HB3	2.10	0.66
3:D:179:THR:O	3:D:182:ALA:HB3	1.95	0.66
4:X:8:DC:OP2	4:X:9:5IU:I5	2.84	0.66
3:G:204:PRO:HG3	3:G:274:ILE:CD1	2.24	0.66
1:B:947:ARG:CB	1:B:1086:LEU:HD21	2.25	0.66
2:C:347:ASN:HD21	2:C:349:ALA:H	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:THR:HG23	1:E:544:ASP:O	1.96	0.66
3:G:526:ARG:HH22	3:G:533:THR:CG2	2.08	0.66
1:E:13:LEU:HD12	1:E:14:PRO:HD2	1.77	0.66
1:B:1121:TYR:CD1	2:C:58:ALA:HB3	2.31	0.66
1:E:741:ILE:HD12	1:E:805:ALA:HB2	1.78	0.66
3:G:179:THR:O	3:G:182:ALA:HB3	1.96	0.66
1:B:1073:GLU:OE2	1:B:1073:GLU:HA	1.93	0.66
1:E:530:LEU:HB3	1:E:878:TRP:CZ3	2.31	0.66
3:G:207:LYS:HZ3	3:G:544:SER:HA	1.59	0.66
3:D:344:GLU:HG3	3:D:345:ALA:N	2.10	0.66
2:F:265:ARG:O	2:F:323:LEU:CB	2.43	0.66
1:E:167:PHE:O	1:E:171:HIS:HB2	1.96	0.66
1:E:636:HIS:O	1:E:640:VAL:HG23	1.96	0.66
1:B:513:ASP:O	1:B:515:GLN:N	2.27	0.66
1:B:530:LEU:HB3	1:B:878:TRP:CZ3	2.31	0.66
3:D:233:ILE:C	3:D:235:GLU:H	1.99	0.66
3:D:233:ILE:O	3:D:235:GLU:N	2.28	0.66
3:D:229:GLN:HG3	3:D:229:GLN:O	1.96	0.66
2:C:269:PHE:C	2:C:270:GLU:HG2	2.16	0.66
2:F:269:PHE:C	2:F:270:GLU:HG2	2.17	0.66
1:B:34:ALA:HB1	1:B:79:ASN:ND2	2.11	0.66
3:D:244:LEU:HB3	3:D:255:HIS:CD2	2.31	0.66
2:F:112:ARG:HG3	2:F:112:ARG:HH11	1.62	0.66
3:D:58:LEU:HD13	3:D:81:TRP:HZ3	1.60	0.66
2:C:752:ILE:HD12	2:C:753:ASP:H	1.59	0.66
2:F:269:PHE:CD2	2:F:269:PHE:N	2.62	0.66
3:D:562:THR:HG21	3:D:594:THR:HG23	1.77	0.66
3:D:300:GLN:NE2	3:D:568:THR:HG22	2.10	0.66
3:G:425:ARG:O	3:G:427:GLU:N	2.29	0.66
2:F:828:LEU:HD22	2:F:1028:ARG:HD2	1.77	0.65
2:C:685:TYR:O	2:C:687:ARG:HG3	1.95	0.65
2:F:972:LEU:HA	2:F:1000:LEU:HD13	1.78	0.65
2:C:172:LEU:O	2:C:176:THR:HG22	1.94	0.65
2:C:111:LEU:HD13	2:C:127:LEU:HD21	1.78	0.65
1:B:139:LEU:CD2	1:B:377:ARG:HH12	2.09	0.65
3:G:229:GLN:HG3	3:G:229:GLN:O	1.96	0.65
1:B:746:GLY:N	1:B:808:ARG:HH12	1.93	0.65
3:D:597:ARG:HH11	3:D:598:SER:HB2	1.61	0.65
3:G:389:ASP:O	3:G:391:THR:N	2.30	0.65
2:C:354:ASN:ND2	2:C:356:GLU:HB3	2.11	0.65
2:F:273:GLU:CD	2:F:274:LEU:HD23	2.17	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:14:DC:C2'	4:Y:15:DG:H5"	2.20	0.65
2:C:834:LEU:HD21	2:C:986:VAL:HG21	1.78	0.65
1:B:221:ARG:O	1:B:225:ILE:HG12	1.97	0.65
3:G:366:GLY:HA3	3:G:393:ILE:CD1	2.26	0.65
4:X:41:DC:H2"	4:X:42:DG:OP2	1.97	0.65
1:E:1079:LEU:HD11	1:E:1141:LEU:HG	1.78	0.65
3:D:201:LEU:HB3	3:D:212:LEU:CD1	2.25	0.65
1:E:423:ARG:HG2	4:Y:49:DA:H2	1.60	0.65
2:F:1036:LEU:O	2:F:1037:VAL:HB	1.95	0.65
1:B:119:ARG:HD3	2:C:302:SER:CB	2.25	0.65
3:D:378:ASP:O	3:D:382:VAL:HG23	1.96	0.65
1:E:550:ARG:HH11	1:E:550:ARG:HG2	1.61	0.65
2:F:776:VAL:O	2:F:780:LEU:HD22	1.96	0.65
3:G:244:LEU:HD21	3:G:261:LEU:HG	1.77	0.65
1:E:947:ARG:H	1:E:947:ARG:CD	2.09	0.65
2:C:588:LEU:HG	2:C:620:ILE:HG21	1.78	0.65
1:B:924:LEU:HD11	2:C:607:ALA:HA	1.79	0.65
1:E:1043:PHE:HB3	1:E:1161:ASN:CG	2.17	0.65
3:G:177:LYS:O	3:G:181:VAL:HG23	1.97	0.65
2:C:545:GLN:O	2:C:547:VAL:HG23	1.97	0.65
2:F:502:ILE:HG13	2:F:527:GLY:HA3	1.77	0.65
1:B:893:LEU:O	1:B:893:LEU:HD13	1.97	0.65
1:E:243:LEU:HD22	1:E:259:ARG:NH1	2.11	0.65
3:G:233:ILE:O	3:G:235:GLU:N	2.29	0.65
3:D:51:VAL:CG2	3:D:276:LEU:HD12	2.25	0.65
1:B:226:VAL:HA	1:B:229:ILE:HD12	1.78	0.65
1:B:1003:ASN:ND2	1:B:1157:THR:HG21	2.12	0.65
1:E:649:ARG:HG3	1:E:650:GLN:N	2.12	0.65
2:F:832:VAL:HG23	2:F:832:VAL:O	1.96	0.65
2:F:442:ARG:HH11	2:F:442:ARG:HG3	1.61	0.65
3:G:233:ILE:C	3:G:235:GLU:H	2.00	0.65
3:D:255:HIS:HA	3:D:259:ASN:HB2	1.77	0.65
4:X:8:DC:H2"	4:X:9:5IU:C5'	2.27	0.65
1:B:823:ARG:HG2	1:B:825:GLY:N	2.10	0.65
2:C:273:GLU:OE2	2:C:274:LEU:N	2.27	0.65
4:Y:41:DC:H2"	4:Y:42:DG:OP2	1.96	0.65
1:E:390:ASP:HB2	1:E:391:PRO:HD2	1.79	0.65
2:F:161:ALA:HA	2:F:164:TRP:CD1	2.32	0.65
1:B:541:MET:O	1:B:811:TRP:HZ3	1.80	0.65
4:Y:36:DG:H2"	4:Y:37:DT:OP2	1.97	0.65
2:F:753:ASP:O	2:F:757:GLN:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:891:LYS:HD2	2:F:802:TYR:CZ	2.31	0.65
3:G:28:ALA:O	3:G:30:ASP:N	2.30	0.65
1:B:889:ASN:ND2	1:B:889:ASN:N	2.45	0.65
1:B:903:VAL:HG23	2:C:656:ALA:HA	1.79	0.65
2:C:72:MET:HE1	2:C:208:PRO:HD2	1.78	0.65
2:C:265:ARG:O	2:C:323:LEU:CB	2.45	0.65
1:E:649:ARG:HH11	1:E:649:ARG:HB2	1.62	0.65
3:G:98:THR:HG22	3:G:100:MET:H	1.61	0.65
2:C:776:VAL:O	2:C:780:LEU:HD22	1.97	0.65
3:D:254:ARG:O	3:D:260:PRO:HG3	1.96	0.64
3:D:530:HIS:C	3:D:532:THR:H	1.99	0.64
3:G:370:LEU:HB2	3:G:394:GLU:OE2	1.97	0.64
2:C:753:ASP:O	2:C:757:GLN:HG3	1.97	0.64
2:C:569:MET:O	2:C:573:ILE:HG13	1.95	0.64
2:C:435:LEU:HD12	2:C:435:LEU:O	1.97	0.64
3:G:85:LEU:HD13	3:G:107:LEU:HD13	1.79	0.64
1:B:645:PHE:HA	1:B:648:TYR:CD2	2.33	0.64
1:B:1033:ALA:HB1	1:B:1053:LEU:CA	2.27	0.64
3:G:165:ARG:HB3	3:G:166:ILE:HD12	1.79	0.64
3:G:243:LEU:HD11	3:G:244:LEU:HG	1.77	0.64
3:G:254:ARG:HG3	3:G:259:ASN:ND2	2.13	0.64
2:F:166:ALA:HB3	2:F:167:PRO:HD3	1.77	0.64
1:B:747:LEU:HD23	1:B:749:TYR:OH	1.97	0.64
3:D:398:LEU:N	3:D:398:LEU:HD23	2.12	0.64
2:F:948:ASN:C	2:F:948:ASN:HD22	2.01	0.64
3:D:165:ARG:HD3	3:D:166:ILE:CD1	2.27	0.64
2:C:28:ASP:N	2:C:29:PRO:CD	2.60	0.64
2:F:584:LEU:CD2	2:F:632:VAL:HG21	2.27	0.64
3:D:389:ASP:O	3:D:391:THR:N	2.30	0.64
3:G:412:LEU:HD13	3:G:462:MET:HG2	1.80	0.64
4:Y:8:DC:OP2	4:Y:9:5IU:I5	2.85	0.64
1:E:1033:ALA:HB1	1:E:1053:LEU:CA	2.28	0.64
1:E:561:ARG:NH2	1:E:584:ARG:H	1.95	0.64
2:C:405:PRO:HB2	2:C:659:VAL:HG23	1.80	0.64
2:C:273:GLU:CD	2:C:274:LEU:HD23	2.17	0.64
3:D:244:LEU:HD11	3:D:285:ALA:HB3	1.80	0.64
3:G:165:ARG:HD3	3:G:166:ILE:CD1	2.27	0.64
1:B:282:LEU:HD21	1:B:307:HIS:HB2	1.80	0.64
2:C:166:ALA:HB3	2:C:167:PRO:HD3	1.79	0.64
2:F:80:ILE:HD12	2:F:189:LEU:HD21	1.79	0.64
1:B:390:ASP:HB2	1:B:391:PRO:HD2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ARG:HG3	1:B:650:GLN:N	2.12	0.64
2:C:112:ARG:HG3	2:C:112:ARG:HH11	1.62	0.64
1:E:747:LEU:HD23	1:E:749:TYR:OH	1.98	0.64
1:B:746:GLY:N	1:B:808:ARG:NH1	2.46	0.64
2:C:207:LEU:HB3	2:C:208:PRO:HD2	1.79	0.64
3:D:201:LEU:HD21	3:D:233:ILE:HG21	1.79	0.64
3:G:200:ARG:HB2	3:G:263:LEU:CD2	2.24	0.64
1:B:253:ASP:C	1:B:255:ARG:H	2.01	0.64
1:E:226:VAL:HA	1:E:229:ILE:HD12	1.80	0.64
2:C:1037:VAL:HG22	2:C:1109:SER:HA	1.79	0.64
2:C:7:SER:CB	2:C:13:LEU:HG	2.26	0.64
1:B:81:HIS:HA	1:B:118:GLU:OE2	1.97	0.64
1:E:213:PRO:O	1:E:215:ASP:N	2.28	0.64
2:F:207:LEU:HD12	2:F:234:ILE:HD13	1.78	0.64
3:D:28:ALA:O	3:D:30:ASP:N	2.28	0.64
3:D:132:VAL:HG12	3:D:133:ASP:N	2.11	0.64
2:C:832:VAL:HG23	2:C:832:VAL:O	1.96	0.64
1:B:222:HIS:HE1	1:B:226:VAL:HG21	1.63	0.64
3:D:177:LYS:O	3:D:181:VAL:HG23	1.97	0.64
1:E:1130:ASP:H	1:E:1134:HIS:CD2	2.15	0.64
4:Y:2:5IU:C2'	4:Y:3:5IU:C5'	2.76	0.64
1:B:881:ASN:ND2	1:E:882:ASP:O	2.31	0.64
3:G:366:GLY:HA3	3:G:393:ILE:HG21	1.79	0.64
2:C:269:PHE:N	2:C:269:PHE:CD2	2.62	0.64
3:G:426:ALA:C	3:G:428:PRO:HD2	2.17	0.64
2:F:602:ASP:OD1	2:F:603:ALA:N	2.31	0.64
4:X:2:5IU:H3'	4:X:3:5IU:H5'	1.80	0.63
2:C:109:THR:HG23	2:C:112:ARG:NH2	2.14	0.63
1:B:1018:GLN:HA	1:B:1018:GLN:OE1	1.96	0.63
1:B:25:ALA:HB1	1:B:807:THR:HG23	1.79	0.63
1:E:889:ASN:ND2	1:E:889:ASN:N	2.45	0.63
1:E:65:THR:HG22	1:E:66:GLU:N	2.12	0.63
2:F:954:GLY:O	2:F:955:TRP:HE3	1.81	0.63
2:C:935:ARG:O	2:C:937:PRO:HD3	1.98	0.63
1:B:1079:LEU:HD11	1:B:1141:LEU:HG	1.79	0.63
1:E:709:ARG:NH1	2:F:475:ASP:OD1	2.32	0.63
1:E:18:GLU:HG2	1:E:18:GLU:O	1.98	0.63
2:C:945:LEU:CB	2:C:952:ILE:HD11	2.27	0.63
3:D:58:LEU:HD22	3:D:81:TRP:CH2	2.33	0.63
3:D:300:GLN:CG	3:D:568:THR:HG22	2.28	0.63
2:C:676:CYS:HA	2:C:728:TYR:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:2:5IU:C2'	4:X:3:5IU:C5'	2.76	0.63
3:G:51:VAL:HG11	3:G:276:LEU:CD1	2.29	0.63
2:C:155:VAL:H	2:C:162:GLN:HE22	1.44	0.63
2:C:954:GLY:O	2:C:955:TRP:HE3	1.80	0.63
1:E:1018:GLN:HA	1:E:1018:GLN:OE1	1.97	0.63
3:G:526:ARG:CA	3:G:526:ARG:HE	2.10	0.63
3:D:254:ARG:O	3:D:255:HIS:HB3	1.99	0.63
1:B:1071:ARG:HD3	1:B:1076:TYR:CE2	2.30	0.63
3:G:597:ARG:HH11	3:G:598:SER:HB2	1.63	0.63
3:D:91:VAL:HA	3:D:100:MET:O	1.99	0.63
1:B:208:ILE:O	1:B:211:PRO:HD3	1.97	0.63
1:B:98:GLU:O	1:B:102:GLU:HG3	1.98	0.63
1:E:500:LYS:HA	1:E:866:ALA:O	1.99	0.63
2:C:228:GLN:NE2	2:C:318:GLU:H	1.93	0.63
1:E:945:PHE:HE2	1:E:955:LEU:HD21	1.60	0.63
3:D:426:ALA:C	3:D:428:PRO:HD2	2.18	0.63
3:G:89:GLN:HA	3:G:89:GLN:OE1	1.98	0.63
2:F:347:ASN:HD21	2:F:349:ALA:CB	2.12	0.63
1:B:1078:LEU:HD22	1:B:1115:THR:HG22	1.80	0.63
2:F:228:GLN:NE2	2:F:318:GLU:H	1.94	0.63
1:E:221:ARG:O	1:E:225:ILE:HG12	1.99	0.63
1:B:771:ARG:HG2	1:B:771:ARG:HH11	1.64	0.63
1:B:878:TRP:O	1:B:880:VAL:N	2.31	0.63
1:E:550:ARG:HG2	1:E:550:ARG:NH1	2.13	0.63
2:F:207:LEU:HB3	2:F:208:PRO:HD2	1.79	0.63
1:E:253:ASP:C	1:E:255:ARG:H	2.02	0.63
2:C:161:ALA:HA	2:C:164:TRP:CD1	2.34	0.63
3:G:366:GLY:HA3	3:G:393:ILE:HD12	1.81	0.63
3:G:385:VAL:HG21	3:G:396:ARG:CZ	2.28	0.63
3:G:201:LEU:HD21	3:G:233:ILE:HG21	1.80	0.63
2:F:405:PRO:C	2:F:658:PRO:HB3	2.19	0.63
1:E:807:THR:HG21	1:E:808:ARG:HH21	1.64	0.63
4:X:36:DG:H2''	4:X:37:DT:OP2	1.98	0.63
3:G:58:LEU:HD22	3:G:81:TRP:CH2	2.34	0.63
1:B:148:PHE:N	2:C:126:GLN:HE22	1.95	0.63
4:X:2:5IU:H2'	4:X:3:5IU:H5'	1.80	0.63
1:B:741:ILE:HD12	1:B:805:ALA:HB2	1.80	0.63
1:E:233:LYS:HZ1	1:E:269:ILE:HG12	1.63	0.63
2:C:539:SER:HB2	2:C:551:ASP:CG	2.18	0.63
2:F:539:SER:HB2	2:F:551:ASP:CG	2.19	0.63
2:F:895:GLU:HG3	2:F:899:ARG:NH2	2.14	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:TYR:O	2:F:909:TYR:HE2	1.81	0.63
3:D:243:LEU:HD12	3:D:244:LEU:CD2	2.29	0.62
3:G:201:LEU:HB3	3:G:212:LEU:CD1	2.29	0.62
3:D:440:LEU:O	3:D:441:LEU:HD23	1.99	0.62
1:B:597:LEU:O	1:B:601:GLN:HG3	1.99	0.62
1:B:267:ASP:C	1:B:269:ILE:H	2.01	0.62
1:E:1115:THR:HG21	1:E:1160:PRO:HG2	1.81	0.62
1:E:1003:ASN:ND2	1:E:1157:THR:HG21	2.13	0.62
3:D:562:THR:OG1	3:D:594:THR:HG23	1.99	0.62
1:B:1130:ASP:H	1:B:1134:HIS:CD2	2.17	0.62
1:E:892:THR:HG22	2:F:804:ARG:HE	1.64	0.62
3:G:326:ALA:O	3:G:337:VAL:HB	1.99	0.62
3:G:582:ASP:C	3:G:584:ARG:H	2.03	0.62
3:G:255:HIS:CG	3:G:256:HIS:H	2.18	0.62
4:Y:44:DA:H2"	4:Y:45:DT:OP2	1.98	0.62
2:C:347:ASN:HD21	2:C:349:ALA:CB	2.11	0.62
2:C:943:ILE:HD12	2:C:956:LEU:HG	1.81	0.62
1:B:469:MET:SD	1:B:795:LEU:CD1	2.87	0.62
3:G:58:LEU:HD13	3:G:81:TRP:HZ3	1.62	0.62
2:F:685:TYR:O	2:F:687:ARG:HG3	1.98	0.62
2:C:853:LEU:O	2:C:855:VAL:HG23	1.98	0.62
1:E:856:CYS:O	1:E:859:ALA:HB3	2.00	0.62
2:C:602:ASP:OD1	2:C:603:ALA:N	2.32	0.62
1:B:50:PHE:CD1	1:B:51:PRO:HD2	2.34	0.62
3:G:246:ALA:HB1	3:G:251:GLN:NE2	2.14	0.62
1:B:501:MET:HG3	1:B:815:LEU:HD21	1.82	0.62
1:E:1102:MET:HE3	1:E:1107:TYR:HB2	1.81	0.62
3:D:562:THR:CG2	3:D:594:THR:HG23	2.29	0.62
2:F:935:ARG:O	2:F:937:PRO:HD3	1.99	0.62
2:F:384:ARG:HD3	2:F:786:ARG:O	2.00	0.62
4:X:2:5IU:H2"	4:X:3:5IU:O5'	2.00	0.62
3:G:239:THR:HG23	3:G:242:ARG:HB2	1.81	0.62
1:E:282:LEU:HD21	1:E:307:HIS:HB2	1.81	0.62
3:D:531:GLU:H	3:D:533:THR:HG23	1.65	0.62
1:E:1078:LEU:HD22	1:E:1115:THR:HG22	1.80	0.62
1:B:1102:MET:CE	1:B:1107:TYR:HB2	2.30	0.62
3:G:301:LEU:H	3:G:568:THR:HG23	1.64	0.62
3:D:425:ARG:O	3:D:427:GLU:N	2.32	0.62
1:B:856:CYS:O	1:B:859:ALA:HB3	2.00	0.62
1:B:1127:ALA:HB2	2:C:25:ARG:HD2	1.82	0.62
1:E:98:GLU:O	1:E:102:GLU:HG3	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:239:THR:C	3:G:241:HIS:H	2.01	0.62
1:B:949:ALA:O	1:B:953:THR:HG23	1.99	0.62
2:C:382:PRO:HB2	2:C:421:PHE:CE1	2.35	0.62
2:C:384:ARG:HD3	2:C:786:ARG:O	1.99	0.62
3:G:234:PRO:O	3:G:236:ASP:N	2.33	0.62
1:B:139:LEU:HD21	1:B:377:ARG:HH12	1.65	0.62
2:F:1099:PRO:HG2	2:F:1100:GLU:OE1	1.99	0.62
2:F:569:MET:O	2:F:573:ILE:HG13	2.00	0.62
2:F:853:LEU:O	2:F:855:VAL:HG23	1.99	0.62
3:D:89:GLN:OE1	3:D:89:GLN:HA	2.00	0.62
3:D:205:THR:CA	4:X:3:5IU:OP1	2.32	0.62
2:C:207:LEU:HD12	2:C:234:ILE:HD13	1.82	0.62
1:E:893:LEU:HB3	2:F:802:TYR:CE2	2.35	0.62
1:E:577:PRO:HB2	1:E:735:LEU:HD22	1.82	0.62
3:G:562:THR:HB	3:G:594:THR:H	1.63	0.62
2:F:952:ILE:N	2:F:952:ILE:HD13	2.14	0.62
2:F:678:LEU:CD2	2:F:730:SER:HB3	2.28	0.62
1:E:746:GLY:N	1:E:808:ARG:NH1	2.46	0.62
3:D:308:ALA:O	3:D:597:ARG:NH2	2.33	0.62
3:D:177:LYS:O	3:D:180:THR:HG22	2.00	0.62
1:B:1040:ILE:HD11	1:B:1168:MET:CE	2.29	0.62
3:G:330:SER:HB3	3:G:337:VAL:HG23	1.80	0.62
3:D:397:LEU:HD13	3:D:580:TYR:HE2	1.65	0.62
3:D:244:LEU:HD11	3:D:285:ALA:CB	2.30	0.62
3:G:271:ALA:O	3:G:274:ILE:HG12	1.99	0.62
4:Y:15:DG:H1'	4:Y:16:DA:OP1	1.99	0.62
1:B:246:LEU:HD23	1:B:307:HIS:HE2	1.65	0.62
1:B:1098:MET:HE3	1:B:1142:PHE:HD1	1.65	0.62
1:E:1102:MET:CE	1:E:1107:TYR:HB2	2.30	0.62
3:G:530:HIS:C	3:G:532:THR:H	2.01	0.62
1:E:802:LEU:HD22	1:E:806:LEU:HD22	1.81	0.62
2:C:948:ASN:HD22	2:C:948:ASN:C	2.02	0.62
3:D:106:ARG:HB3	3:D:108:TYR:CE1	2.35	0.62
1:E:676:ALA:O	2:F:816:ALA:HB2	1.98	0.62
2:C:442:ARG:HG3	2:C:442:ARG:HH11	1.65	0.62
3:D:204:PRO:HG3	3:D:274:ILE:CD1	2.28	0.62
4:X:44:DA:H2''	4:X:45:DT:OP2	1.99	0.62
1:B:558:VAL:HG22	1:B:563:GLU:HB3	1.82	0.62
3:D:366:GLY:CA	3:D:393:ILE:HG21	2.30	0.62
1:E:920:LEU:HD11	2:F:448:HIS:NE2	2.15	0.62
1:E:25:ALA:HB1	1:E:807:THR:HG21	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:GLU:HG2	1:B:648:TYR:CE2	2.35	0.62
2:C:26:LEU:HD22	2:C:210:ARG:HH12	1.65	0.62
2:C:60:ILE:HD12	2:C:60:ILE:N	2.15	0.62
1:B:8:LEU:HD13	1:B:10:PRO:HD3	1.82	0.62
1:E:1121:TYR:CD1	2:F:58:ALA:HB3	2.35	0.62
2:F:61:ASP:C	2:F:63:PRO:HD3	2.18	0.62
3:D:275:ASP:OD1	4:X:2:5IU:O4	2.18	0.62
1:B:947:ARG:CD	1:B:947:ARG:H	2.08	0.62
1:E:527:ARG:CB	1:E:576:ILE:HD11	2.23	0.62
2:F:347:ASN:HD21	2:F:349:ALA:H	1.46	0.62
1:E:893:LEU:HB3	2:F:802:TYR:HE2	1.65	0.62
2:F:464:ARG:O	2:F:505:GLY:HA2	2.00	0.62
1:B:562:GLN:OE1	4:X:46:5IU:I5	2.88	0.61
2:C:1055:ASP:CB	2:C:1118:ARG:NH2	2.60	0.61
1:B:924:LEU:CD2	1:B:949:ALA:HB1	2.30	0.61
1:E:1062:LEU:HD21	1:E:1113:LEU:HD22	1.82	0.61
3:G:531:GLU:H	3:G:533:THR:HG23	1.64	0.61
3:D:234:PRO:O	3:D:236:ASP:N	2.32	0.61
1:E:771:ARG:HG2	1:E:771:ARG:HH11	1.64	0.61
2:F:676:CYS:HA	2:F:728:TYR:HB3	1.82	0.61
4:Y:2:5IU:H2''	4:Y:3:5IU:O5'	1.99	0.61
3:D:526:ARG:HH12	3:D:536:MET:HE2	1.64	0.61
1:B:11:LEU:CD1	1:B:99:ARG:HD2	2.29	0.61
1:B:233:LYS:O	1:B:237:ARG:HG3	1.99	0.61
3:D:307:GLY:C	3:D:597:ARG:HH21	2.03	0.61
1:B:916:ILE:HG21	2:C:448:HIS:NE2	2.15	0.61
2:F:382:PRO:HB2	2:F:421:PHE:CE1	2.35	0.61
2:C:250:ASP:OD1	2:C:291:GLY:HA3	2.00	0.61
1:B:649:ARG:HB2	1:B:649:ARG:HH11	1.65	0.61
1:B:56:VAL:CG1	1:B:124:ALA:HA	2.30	0.61
3:G:255:HIS:CA	3:G:259:ASN:HB2	2.28	0.61
1:B:947:ARG:CG	1:B:1086:LEU:HD21	2.29	0.61
1:B:1071:ARG:HB3	1:B:1076:TYR:HD2	1.65	0.61
1:E:267:ASP:C	1:E:269:ILE:H	2.03	0.61
1:E:795:LEU:HA	1:E:798:ASP:HB2	1.82	0.61
3:G:365:SER:HB3	3:G:390:PHE:CE2	2.35	0.61
2:C:681:ASN:ND2	2:C:732:ILE:H	1.97	0.61
1:B:1102:MET:HE3	1:B:1107:TYR:HB2	1.80	0.61
3:D:256:HIS:CG	3:D:257:ALA:H	2.19	0.61
3:D:247:GLN:HE22	4:X:6:DA:C5'	2.14	0.61
1:B:1132:GLU:HG3	1:B:1159:ARG:NH2	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:160:GLU:C	2:F:162:GLN:H	2.04	0.61
2:C:952:ILE:N	2:C:952:ILE:HD13	2.16	0.61
1:B:795:LEU:HA	1:B:798:ASP:HB2	1.82	0.61
2:C:678:LEU:CD2	2:C:730:SER:HB3	2.29	0.61
2:F:941:MET:HE3	2:F:959:VAL:HG11	1.83	0.61
3:G:278:MET:HG2	4:Y:2:5IU:I5	2.71	0.61
1:B:924:LEU:HD23	1:B:953:THR:CG2	2.30	0.61
1:B:807:THR:HG21	1:B:808:ARG:HH21	1.66	0.61
1:E:1098:MET:HE3	1:E:1142:PHE:HD1	1.65	0.61
2:F:146:LEU:HB3	2:F:169:TRP:NE1	2.16	0.61
1:E:604:MET:SD	1:E:704:GLU:HB2	2.41	0.61
1:B:61:VAL:HB	1:B:126:VAL:HG13	1.81	0.61
2:F:60:ILE:HD12	2:F:60:ILE:N	2.15	0.61
1:B:1056:MET:O	1:B:1058:VAL:HG23	2.00	0.61
2:C:895:GLU:HG3	2:C:899:ARG:NH2	2.15	0.61
1:B:275:GLU:OE1	1:B:276:GLU:HG2	2.00	0.61
3:D:223:LEU:CB	3:D:224:PRO:HD2	2.31	0.61
1:E:924:LEU:HD23	1:E:953:THR:CG2	2.30	0.61
2:F:545:GLN:O	2:F:547:VAL:HG23	2.00	0.61
3:G:528:PRO:O	3:G:529:GLU:HB2	1.99	0.61
2:F:25:ARG:HH11	2:F:25:ARG:HG3	1.65	0.61
3:D:392:ASP:O	3:D:576:ARG:HG2	2.00	0.61
1:E:834:HIS:CE1	1:E:847:PRO:HB3	2.35	0.61
3:D:31:GLU:CD	3:D:88:SER:HB2	2.20	0.61
3:G:253:LEU:HD22	3:G:255:HIS:HE2	1.66	0.61
3:G:259:ASN:O	3:G:260:PRO:O	2.18	0.61
3:G:286:LEU:HD13	3:G:292:VAL:HG21	1.83	0.61
3:G:62:GLU:HB2	3:G:66:PRO:HG2	1.83	0.61
1:E:947:ARG:CG	1:E:1086:LEU:HD21	2.30	0.61
3:D:115:ASN:O	3:D:119:VAL:HG23	2.01	0.61
2:C:440:SER:O	2:C:441:ASP:HB2	2.01	0.61
2:F:519:THR:HG23	2:F:521:GLN:N	2.16	0.61
1:E:624:ASN:HB2	1:E:627:ASP:OD2	2.01	0.61
1:B:1062:LEU:HD21	1:B:1113:LEU:HD22	1.83	0.61
2:C:286:LEU:H	2:C:292:GLU:HA	1.66	0.61
2:F:250:ASP:OD1	2:F:291:GLY:HA3	1.99	0.61
2:F:25:ARG:HH11	2:F:25:ARG:CG	2.14	0.61
1:E:275:GLU:HG3	1:E:276:GLU:N	2.15	0.61
1:E:598:TRP:CZ2	2:F:857:PHE:HB3	2.35	0.61
1:E:265:TRP:O	1:E:265:TRP:CD1	2.53	0.61
1:B:908:GLY:O	1:B:1055:PHE:HB3	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:584:LEU:CD2	2:C:632:VAL:HG21	2.31	0.61
1:E:831:THR:C	1:E:833:VAL:H	2.03	0.61
2:F:433:ARG:NH1	2:F:803:ALA:HA	2.15	0.61
3:D:326:ALA:O	3:D:337:VAL:HB	2.00	0.61
2:C:1082:ARG:NH1	2:C:1082:ARG:HB2	2.16	0.61
1:E:306:ARG:O	1:E:307:HIS:CB	2.48	0.61
1:E:597:LEU:O	1:E:601:GLN:HG3	2.01	0.61
3:D:597:ARG:HD2	3:D:597:ARG:C	2.21	0.61
1:B:42:LEU:HB2	1:B:44:LEU:HD13	1.82	0.61
1:B:634:ASP:OD1	1:B:636:HIS:ND1	2.34	0.61
2:F:62:PHE:N	2:F:63:PRO:HD3	2.16	0.61
1:E:275:GLU:O	1:E:277:THR:HG23	2.01	0.61
2:C:654:PHE:O	2:C:660:ASN:ND2	2.33	0.61
1:E:52:ARG:HB2	1:E:53:PRO:HD2	1.83	0.61
3:G:51:VAL:CG2	3:G:276:LEU:HD12	2.30	0.61
1:B:562:GLN:CD	4:X:46:5IU:I5	3.09	0.61
3:G:106:ARG:HB3	3:G:108:TYR:CE1	2.36	0.61
1:E:1040:ILE:HD11	1:E:1168:MET:CE	2.30	0.61
3:D:91:VAL:HG12	3:D:100:MET:CB	2.30	0.61
2:F:161:ALA:HA	2:F:164:TRP:NE1	2.16	0.61
2:C:25:ARG:HG3	2:C:25:ARG:HH11	1.66	0.61
1:E:641:VAL:O	1:E:644:GLU:HB3	2.01	0.61
1:E:645:PHE:HA	1:E:648:TYR:CD2	2.35	0.61
2:F:37:VAL:HG21	2:F:42:MET:HB3	1.83	0.61
1:E:405:PRO:O	1:E:406:GLU:HB2	2.01	0.61
4:X:15:DG:H1'	4:X:16:DA:OP1	2.00	0.60
3:D:134:GLU:HB3	3:D:332:LEU:CD2	2.31	0.60
1:E:924:LEU:CD2	1:E:949:ALA:HB1	2.30	0.60
1:B:831:THR:C	1:B:833:VAL:H	2.05	0.60
1:E:233:LYS:O	1:E:237:ARG:HG3	2.01	0.60
1:E:1071:ARG:HD3	1:E:1076:TYR:CE2	2.31	0.60
3:G:177:LYS:O	3:G:180:THR:HG22	2.01	0.60
2:C:146:LEU:HB3	2:C:169:TRP:NE1	2.15	0.60
2:C:62:PHE:N	2:C:63:PRO:HD3	2.16	0.60
1:E:56:VAL:CG1	1:E:124:ALA:HA	2.30	0.60
1:E:908:GLY:O	1:E:1055:PHE:HB3	2.01	0.60
3:D:56:SER:C	3:D:58:LEU:H	2.04	0.60
1:E:65:THR:HG22	1:E:67:ALA:H	1.65	0.60
1:B:52:ARG:HB2	1:B:53:PRO:HD2	1.83	0.60
3:D:239:THR:C	3:D:241:HIS:H	2.03	0.60
2:C:989:ALA:O	2:C:991:GLY:N	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:664:LEU:HB3	2:F:715:LEU:HD13	1.83	0.60
3:G:524:PRO:HD2	3:G:527:LEU:HD12	1.84	0.60
1:E:8:LEU:HD13	1:E:10:PRO:HD3	1.82	0.60
4:Y:46:5IU:OP1	4:Y:46:5IU:H4'	2.00	0.60
1:B:306:ARG:O	1:B:307:HIS:CB	2.48	0.60
1:E:860:LEU:O	1:E:861:CYS:HB2	2.01	0.60
2:C:376:PHE:CE2	2:C:752:ILE:HG23	2.37	0.60
3:D:385:VAL:HG21	3:D:396:ARG:CZ	2.30	0.60
2:C:251:ILE:HD13	2:C:252:LYS:N	2.17	0.60
1:B:641:VAL:O	1:B:644:GLU:HB3	2.01	0.60
1:E:42:LEU:HB2	1:E:44:LEU:HD13	1.82	0.60
2:C:503:ARG:HD3	2:C:867:THR:O	2.01	0.60
3:D:95:ASP:OD2	3:D:96:GLU:HG3	2.01	0.60
3:D:253:LEU:CB	3:D:255:HIS:NE2	2.63	0.60
3:D:62:GLU:HB2	3:D:66:PRO:HG2	1.81	0.60
3:G:278:MET:O	3:G:279:MET:C	2.39	0.60
4:X:46:5IU:OP1	4:X:46:5IU:H4'	2.00	0.60
2:F:347:ASN:ND2	2:F:349:ALA:N	2.43	0.60
1:E:469:MET:SD	1:E:795:LEU:CD1	2.89	0.60
3:D:562:THR:HG21	3:D:594:THR:HA	1.83	0.60
2:C:533:LEU:HD11	2:C:537:MET:HE3	1.84	0.60
1:E:892:THR:CG2	2:F:804:ARG:HE	2.14	0.60
3:D:163:THR:OG1	3:D:325:ARG:NH2	2.35	0.60
3:G:405:ILE:H	3:G:405:ILE:HD12	1.66	0.60
2:C:971:LEU:HD23	4:X:10:DA:C5'	2.30	0.60
2:C:1118:ARG:NH2	2:C:1118:ARG:HG2	2.10	0.60
3:D:130:ILE:N	3:D:130:ILE:HD12	2.08	0.60
2:C:160:GLU:C	2:C:162:GLN:H	2.05	0.60
1:B:265:TRP:CD1	1:B:265:TRP:O	2.54	0.60
1:E:821:VAL:HG22	1:E:831:THR:HA	1.83	0.60
2:C:389:LEU:HD22	2:C:678:LEU:HD11	1.83	0.60
2:F:440:SER:O	2:F:441:ASP:HB2	2.01	0.60
2:C:207:LEU:CB	2:C:208:PRO:HD2	2.32	0.60
1:E:1127:ALA:HB2	2:F:25:ARG:HD2	1.83	0.60
1:B:275:GLU:HG3	1:B:276:GLU:N	2.15	0.60
1:E:275:GLU:OE1	1:E:276:GLU:HG2	2.02	0.60
2:F:309:ASP:O	2:F:313:LEU:HG	2.01	0.60
2:F:228:GLN:HG3	2:F:319:SER:HB3	1.83	0.60
3:D:225:LEU:O	3:D:229:GLN:HB2	2.01	0.60
2:C:972:LEU:HA	2:C:1000:LEU:HD13	1.82	0.60
2:F:8:ASN:HD21	2:F:343:LEU:CD1	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:997:ARG:HH11	2:C:997:ARG:HG2	1.66	0.60
2:F:197:LEU:HD13	2:F:230:LEU:HA	1.82	0.60
3:G:163:THR:OG1	3:G:325:ARG:NH2	2.35	0.60
2:F:1009:PRO:O	2:F:1011:LEU:HD22	2.02	0.60
1:E:1056:MET:O	1:E:1058:VAL:HG23	2.01	0.60
1:B:282:LEU:HD21	1:B:307:HIS:CB	2.31	0.60
1:B:307:HIS:HB3	1:B:308:PRO:HD2	1.83	0.60
1:E:705:HIS:CD2	2:F:487:GLU:HG3	2.36	0.60
3:G:156:VAL:O	3:G:160:VAL:HG23	2.01	0.60
1:E:702:GLU:HB2	2:F:449:PRO:CG	2.32	0.60
2:C:130:LYS:HD2	2:C:692:LEU:HD21	1.84	0.60
3:D:201:LEU:HD13	3:D:216:LEU:HD12	1.84	0.60
1:E:931:VAL:HG12	1:E:932:ALA:H	1.65	0.60
2:C:161:ALA:HA	2:C:164:TRP:NE1	2.17	0.60
1:E:1071:ARG:HB3	1:E:1076:TYR:HD2	1.67	0.60
2:C:61:ASP:C	2:C:63:PRO:HD3	2.22	0.60
2:C:1099:PRO:HG2	2:C:1100:GLU:OE1	2.01	0.60
3:D:188:LEU:HD21	3:D:291:ARG:HH22	1.67	0.60
3:G:246:ALA:HA	3:G:253:LEU:HD23	1.84	0.60
4:Y:2:5IU:H2'	4:Y:3:5IU:H5'	1.84	0.60
1:B:879:GLN:HB3	1:E:883:VAL:HG11	1.84	0.60
1:B:821:VAL:HG22	1:B:831:THR:HA	1.84	0.60
1:B:459:LYS:CE	1:B:860:LEU:HB2	2.29	0.60
2:C:519:THR:HG23	2:C:521:GLN:N	2.15	0.60
2:F:533:LEU:CD1	2:F:537:MET:HE3	2.31	0.60
1:B:65:THR:HG22	1:B:66:GLU:N	2.16	0.60
2:F:943:ILE:HD12	2:F:956:LEU:HG	1.83	0.60
3:G:3:LEU:HD23	3:G:6:GLN:HG3	1.84	0.60
1:E:634:ASP:OD1	1:E:636:HIS:ND1	2.35	0.60
2:F:1082:ARG:HB2	2:F:1082:ARG:NH1	2.17	0.59
1:B:881:ASN:ND2	1:E:883:VAL:HA	2.17	0.59
1:B:931:VAL:HG12	1:B:932:ALA:H	1.67	0.59
1:B:227:ALA:O	1:B:231:THR:HG23	2.01	0.59
1:B:86:ALA:HB1	1:B:92:THR:HG1	1.67	0.59
2:C:943:ILE:HG12	2:C:954:GLY:N	2.17	0.59
1:B:802:LEU:HD22	1:B:806:LEU:HD22	1.82	0.59
2:C:1009:PRO:O	2:C:1011:LEU:HD22	2.02	0.59
3:G:243:LEU:HD13	3:G:261:LEU:HD21	1.82	0.59
4:X:16:DA:H2''	4:X:17:DG:O5'	2.02	0.59
1:B:761:ARG:HG3	1:B:822:ARG:NH2	2.18	0.59
1:E:282:LEU:HD21	1:E:307:HIS:CB	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:56:SER:C	3:G:58:LEU:H	2.05	0.59
1:B:275:GLU:O	1:B:277:THR:HG23	2.02	0.59
1:E:50:PHE:CD1	1:E:51:PRO:HD2	2.37	0.59
2:F:540:ALA:C	2:F:542:GLY:H	2.05	0.59
1:E:246:LEU:HD23	1:E:307:HIS:HE2	1.68	0.59
2:C:78:PRO:HD2	2:C:192:ARG:HH11	1.64	0.59
1:E:225:ILE:O	1:E:229:ILE:HG13	2.02	0.59
3:G:75:ILE:O	3:G:78:LEU:HD13	2.02	0.59
2:F:294:ASP:O	2:F:296:GLY:N	2.34	0.59
3:G:423:GLN:C	3:G:425:ARG:H	2.06	0.59
1:E:702:GLU:HB2	2:F:449:PRO:HG2	1.83	0.59
3:D:444:LEU:HD21	3:D:558:THR:HG21	1.83	0.59
3:D:71:CYS:HB3	3:D:74:GLU:HB3	1.85	0.59
1:B:901:TRP:CZ3	1:B:1060:GLY:HA2	2.37	0.59
2:C:1072:LEU:O	2:C:1076:GLU:HG2	2.02	0.59
3:D:239:THR:HG23	3:D:242:ARG:HB2	1.83	0.59
3:D:267:VAL:HG22	3:D:293:ILE:HB	1.83	0.59
3:D:62:GLU:O	3:D:69:ALA:HB2	2.03	0.59
2:F:77:LEU:CD2	2:F:192:ARG:HD2	2.31	0.59
3:G:178:THR:HG23	3:G:179:THR:HG23	1.84	0.59
1:E:448:ARG:HG3	1:E:748:GLU:OE1	2.01	0.59
3:D:243:LEU:HD12	3:D:244:LEU:HD23	1.84	0.59
3:D:259:ASN:O	3:D:260:PRO:O	2.20	0.59
2:F:850:GLN:NE2	4:Y:7:5IU:HN3	1.92	0.59
1:B:831:THR:OG1	1:B:831:THR:O	2.21	0.59
1:E:222:HIS:HE1	1:E:226:VAL:HG21	1.67	0.59
2:C:8:ASN:HD21	2:C:343:LEU:CD1	2.16	0.59
3:G:31:GLU:CD	3:G:88:SER:HB2	2.23	0.59
2:C:819:GLU:CD	2:C:821:VAL:HG13	2.22	0.59
1:B:1115:THR:HG21	1:B:1160:PRO:HG2	1.83	0.59
1:B:1132:GLU:HA	1:B:1159:ARG:NH2	2.18	0.59
1:B:175:LEU:HD13	1:B:179:ILE:CG2	2.31	0.59
2:F:266:ARG:NH1	2:F:269:PHE:CD1	2.70	0.59
3:G:316:TYR:HE1	3:G:604:PHE:CB	2.14	0.59
1:B:645:PHE:HA	1:B:648:TYR:HD2	1.68	0.59
1:B:779:ASP:C	1:B:781:ASN:H	2.05	0.59
3:D:271:ALA:O	3:D:274:ILE:HG12	2.03	0.59
3:G:115:ASN:O	3:G:119:VAL:HG23	2.02	0.59
1:B:879:GLN:O	1:E:883:VAL:HG21	2.02	0.59
4:Y:16:DA:H2''	4:Y:17:DG:O5'	2.02	0.59
1:E:560:SER:HB2	4:Y:48:DG:OP1	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:134:GLU:HB3	3:G:332:LEU:CD2	2.33	0.59
2:C:228:GLN:HG3	2:C:319:SER:HB3	1.84	0.59
2:F:376:PHE:CE2	2:F:752:ILE:HG23	2.37	0.59
1:B:248:GLU:CG	1:B:288:LYS:O	2.50	0.59
1:B:893:LEU:HB3	2:C:802:TYR:CE2	2.38	0.59
2:F:764:ASP:HB2	2:F:767:LEU:HD21	1.84	0.59
2:C:764:ASP:HB2	2:C:767:LEU:HD21	1.85	0.59
2:C:941:MET:HE3	2:C:959:VAL:HG11	1.85	0.59
1:B:568:ARG:O	1:B:572:THR:HB	2.03	0.59
2:C:37:VAL:HG21	2:C:42:MET:HB3	1.84	0.59
2:F:1114:LEU:N	2:F:1115:PRO:HD2	2.18	0.59
3:G:256:HIS:CD2	3:G:257:ALA:H	2.21	0.59
1:B:500:LYS:HA	1:B:866:ALA:O	2.03	0.59
2:C:943:ILE:HD13	2:C:943:ILE:N	2.18	0.59
1:E:1109:LEU:CD2	1:E:1113:LEU:HG	2.32	0.59
1:B:248:GLU:HG3	1:B:288:LYS:C	2.23	0.59
3:D:52:CYS:HB3	3:D:108:TYR:CD2	2.38	0.59
2:F:367:LEU:O	2:F:368:ASP:CB	2.51	0.59
2:C:309:ASP:O	2:C:313:LEU:HG	2.03	0.59
3:D:405:ILE:H	3:D:405:ILE:HD12	1.68	0.59
3:D:130:ILE:CD1	3:D:130:ILE:H	2.00	0.59
1:E:501:MET:HG3	1:E:815:LEU:HD21	1.83	0.59
2:C:736:ILE:H	2:C:736:ILE:CD1	2.13	0.59
2:C:25:ARG:CG	2:C:25:ARG:HH11	2.16	0.59
1:B:550:ARG:HH11	1:B:550:ARG:HG2	1.67	0.59
4:Y:47:DA:C2'	4:Y:48:DG:O5'	2.48	0.59
3:D:526:ARG:NE	3:D:526:ARG:HA	2.17	0.59
2:F:945:LEU:CB	2:F:952:ILE:HD11	2.28	0.59
1:B:966:GLN:HB3	1:B:967:PRO:CD	2.32	0.59
1:E:762:VAL:HG13	1:E:791:GLU:CG	2.33	0.59
3:D:389:ASP:C	3:D:391:THR:N	2.53	0.59
2:F:834:LEU:HD12	2:F:838:GLN:CD	2.23	0.59
2:C:253:ASP:C	2:C:255:ALA:N	2.56	0.59
1:E:984:SER:HB2	1:E:985:GLN:NE2	2.17	0.59
3:D:423:GLN:C	3:D:425:ARG:H	2.06	0.59
1:B:418:ALA:O	1:B:800:ARG:HD2	2.03	0.59
1:B:1148:LYS:HD2	1:B:1148:LYS:H	1.67	0.59
1:B:1023:PHE:CZ	1:B:1064:GLY:HA3	2.38	0.59
1:E:227:ALA:O	1:E:231:THR:HG23	2.03	0.58
2:C:433:ARG:NH1	2:C:803:ALA:HA	2.18	0.58
1:E:541:MET:O	1:E:811:TRP:HZ3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:PHE:HE2	1:B:955:LEU:HD21	1.66	0.58
3:D:301:LEU:H	3:D:568:THR:HG23	1.68	0.58
3:G:91:VAL:HA	3:G:100:MET:O	2.03	0.58
1:E:56:VAL:HG12	1:E:124:ALA:HA	1.84	0.58
1:B:405:PRO:O	1:B:406:GLU:HB2	2.03	0.58
1:B:63:THR:OG1	1:B:69:THR:HG22	2.03	0.58
3:G:239:THR:C	3:G:241:HIS:N	2.53	0.58
3:G:201:LEU:HD13	3:G:216:LEU:HD12	1.84	0.58
2:C:828:LEU:HD13	2:C:1028:ARG:CG	2.30	0.58
1:E:746:GLY:N	1:E:808:ARG:HH12	1.95	0.58
3:G:367:ILE:HG13	3:G:393:ILE:CG2	2.32	0.58
2:F:257:LEU:HD13	2:F:281:GLU:OE1	2.03	0.58
2:F:26:LEU:HD22	2:F:210:ARG:HH12	1.68	0.58
2:C:994:GLY:O	2:C:1010:PRO:HB3	2.03	0.58
1:E:675:LEU:HD12	2:F:809:ALA:HB1	1.83	0.58
2:F:717:LEU:O	2:F:717:LEU:HD22	2.03	0.58
1:E:265:TRP:O	1:E:265:TRP:HD1	1.86	0.58
2:F:1080:MET:HG3	4:Y:11:DA:C4	2.39	0.58
3:D:461:PHE:C	3:D:463:GLN:H	2.07	0.58
2:C:292:GLU:O	2:C:295:VAL:HG23	2.02	0.58
1:E:248:GLU:HG3	1:E:288:LYS:C	2.24	0.58
2:F:292:GLU:O	2:F:295:VAL:HG23	2.03	0.58
3:D:417:ARG:NH2	3:D:576:ARG:NH2	2.51	0.58
1:E:175:LEU:HD13	1:E:179:ILE:CG2	2.31	0.58
2:C:834:LEU:HD12	2:C:838:GLN:CD	2.23	0.58
2:F:681:ASN:ND2	2:F:732:ILE:H	2.01	0.58
1:B:65:THR:HG22	1:B:67:ALA:H	1.67	0.58
1:B:375:ARG:HD2	1:B:404:GLN:HG2	1.85	0.58
1:E:644:GLU:HG2	1:E:648:TYR:CE2	2.38	0.58
3:G:271:ALA:C	3:G:273:MET:H	2.07	0.58
1:E:281:GLN:OE1	1:E:317:LEU:HD12	2.03	0.58
2:C:77:LEU:CD2	2:C:192:ARG:HD2	2.27	0.58
1:E:831:THR:O	1:E:831:THR:OG1	2.20	0.58
2:F:972:LEU:HD23	2:F:973:SER:N	2.19	0.58
2:C:767:LEU:O	2:C:768:ASN:HB2	2.03	0.58
2:C:393:LEU:HD22	2:C:408:ILE:HD13	1.84	0.58
2:F:1051:ASP:HB3	2:F:1056:ALA:HB3	1.86	0.58
1:E:1148:LYS:H	1:E:1148:LYS:HD2	1.68	0.58
1:B:233:LYS:HZ1	1:B:269:ILE:HG12	1.67	0.58
2:C:974:VAL:HB	2:C:1039:PRO:O	2.03	0.58
2:F:506:ILE:HG22	2:F:507:ASP:H	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1046:LEU:HD12	2:C:1117:PHE:CD2	2.39	0.58
2:F:838:GLN:HB3	2:F:979:GLN:NE2	2.19	0.58
4:Y:20:DC:H2"	4:Y:21:DT:OP2	2.03	0.58
1:B:964:PHE:HD2	1:B:964:PHE:N	2.00	0.58
1:B:550:ARG:NH1	1:B:550:ARG:HG2	2.18	0.58
2:C:540:ALA:C	2:C:542:GLY:H	2.05	0.58
3:D:253:LEU:HD13	3:D:255:HIS:NE2	2.18	0.58
1:B:286:LEU:HD21	1:B:306:ARG:O	2.03	0.58
2:F:1118:ARG:NH2	2:F:1118:ARG:HG2	2.14	0.58
1:B:683:ARG:NE	2:C:1095:ARG:NH1	2.51	0.58
3:G:225:LEU:O	3:G:229:GLN:HB2	2.04	0.58
2:F:1109:SER:O	2:F:1113:LEU:HB2	2.03	0.58
2:C:1109:SER:O	2:C:1113:LEU:HB2	2.04	0.58
1:B:1082:LYS:HE2	1:B:1107:TYR:CZ	2.38	0.58
2:F:207:LEU:CB	2:F:208:PRO:HD2	2.33	0.58
1:E:730:GLU:HB2	2:F:786:ARG:HD2	1.86	0.58
1:E:591:LEU:O	1:E:595:GLU:HG3	2.04	0.58
2:F:312:TYR:HD1	2:F:313:LEU:HD23	1.66	0.58
2:C:717:LEU:O	2:C:717:LEU:HD22	2.03	0.58
4:X:1:5IU:O2	4:X:1:5IU:O4'	2.20	0.58
3:D:225:LEU:C	3:D:225:LEU:HD23	2.23	0.58
1:E:823:ARG:HH22	1:E:828:LYS:NZ	2.02	0.58
1:B:860:LEU:O	1:B:861:CYS:HB2	2.04	0.58
3:D:75:ILE:O	3:D:78:LEU:HD13	2.03	0.58
1:E:1082:LYS:HE2	1:E:1107:TYR:CZ	2.39	0.58
2:F:943:ILE:HG12	2:F:954:GLY:N	2.19	0.58
1:E:964:PHE:N	1:E:964:PHE:HD2	2.01	0.58
3:D:417:ARG:HH11	3:D:437:GLU:HB3	1.68	0.58
1:E:42:LEU:HD21	1:E:114:LEU:HG	1.86	0.58
2:C:342:ILE:HG21	2:C:721:ILE:HD11	1.84	0.58
3:D:207:LYS:HZ3	3:D:544:SER:HA	1.65	0.58
1:B:924:LEU:HD21	1:B:949:ALA:HB1	1.86	0.58
1:B:823:ARG:HH22	1:B:828:LYS:NZ	2.00	0.58
3:G:597:ARG:HD2	3:G:597:ARG:C	2.23	0.58
1:E:683:ARG:NE	2:F:1095:ARG:HH12	2.01	0.58
2:F:373:SER:HA	2:F:726:LYS:HD3	1.86	0.58
1:E:892:THR:HG22	2:F:804:ARG:NE	2.18	0.58
2:F:185:HIS:H	2:F:188:ASN:HD21	1.51	0.58
1:E:568:ARG:O	1:E:572:THR:HB	2.04	0.58
1:E:631:LEU:O	1:E:631:LEU:HD23	2.04	0.58
3:G:253:LEU:CD1	3:G:281:ARG:HG2	2.34	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:201:LEU:CG	3:G:233:ILE:HG21	2.34	0.58
1:E:1132:GLU:HA	1:E:1159:ARG:NH2	2.18	0.58
2:F:712:ASP:O	2:F:715:LEU:HB2	2.03	0.58
1:B:984:SER:HB2	1:B:985:GLN:NE2	2.19	0.58
1:E:779:ASP:C	1:E:781:ASN:H	2.07	0.58
3:D:255:HIS:CB	3:D:260:PRO:HG2	2.31	0.57
1:B:652:TRP:HA	1:B:656:GLY:O	2.04	0.57
1:B:234:GLN:C	1:B:236:TRP:H	2.08	0.57
1:E:924:LEU:HD21	1:E:949:ALA:HB1	1.86	0.57
1:B:222:HIS:CE1	1:B:226:VAL:HG21	2.38	0.57
2:C:689:LEU:HD22	2:C:708:ARG:HD2	1.86	0.57
1:E:657:VAL:HG21	1:E:707:LEU:CD1	2.34	0.57
2:C:294:ASP:O	2:C:296:GLY:N	2.36	0.57
2:F:736:ILE:CD1	2:F:736:ILE:H	2.15	0.57
2:F:819:GLU:CD	2:F:821:VAL:HG13	2.24	0.57
3:D:201:LEU:CG	3:D:233:ILE:HG21	2.34	0.57
1:E:281:GLN:CB	1:E:283:PRO:HD2	2.34	0.57
3:D:134:GLU:HB3	3:D:332:LEU:HD23	1.84	0.57
1:E:459:LYS:CE	1:E:860:LEU:HB2	2.28	0.57
1:E:1132:GLU:HG3	1:E:1159:ARG:NH2	2.17	0.57
2:F:397:LEU:CD2	2:F:403:LEU:HD13	2.33	0.57
3:D:79:GLN:C	3:D:81:TRP:H	2.08	0.57
2:C:551:ASP:HB3	3:D:111:ARG:NH2	2.19	0.57
1:E:771:ARG:H	1:E:771:ARG:HD2	1.65	0.57
2:F:251:ILE:HD13	2:F:256:TYR:HD2	1.69	0.57
2:C:312:TYR:HD1	2:C:313:LEU:HD23	1.69	0.57
1:B:131:GLY:O	1:B:135:ARG:HB2	2.03	0.57
1:E:139:LEU:CD2	1:E:377:ARG:HH12	2.16	0.57
1:E:131:GLY:O	1:E:135:ARG:HB2	2.04	0.57
1:E:234:GLN:C	1:E:236:TRP:H	2.06	0.57
1:B:1033:ALA:HA	1:B:1055:PHE:CZ	2.40	0.57
3:G:278:MET:CG	4:Y:2:5IU:I5	3.22	0.57
2:C:347:ASN:ND2	2:C:349:ALA:N	2.41	0.57
2:F:109:THR:HG23	2:F:112:ARG:NH2	2.19	0.57
2:F:1055:ASP:O	2:F:1055:ASP:CG	2.42	0.57
1:B:225:ILE:O	1:B:229:ILE:HG13	2.04	0.57
1:B:762:VAL:HG13	1:B:791:GLU:CG	2.34	0.57
3:G:175:THR:HG22	3:G:176:GLY:N	2.20	0.57
1:B:964:PHE:CD2	1:B:964:PHE:N	2.69	0.57
2:C:464:ARG:O	2:C:505:GLY:HA2	2.03	0.57
1:E:253:ASP:O	1:E:256:LYS:HD2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:739:VAL:HG22	1:E:740:THR:H	1.69	0.57
1:E:307:HIS:HB3	1:E:308:PRO:HD2	1.85	0.57
3:D:418:TYR:OH	3:D:530:HIS:HE1	1.87	0.57
1:E:652:TRP:HA	1:E:656:GLY:O	2.04	0.57
2:C:251:ILE:HB	2:C:286:LEU:HD13	1.87	0.57
3:D:91:VAL:HG13	3:D:100:MET:HE3	1.86	0.57
1:B:494:GLU:HB3	1:E:545:ASP:OD1	2.04	0.57
1:E:365:GLU:HG3	1:E:366:SER:N	2.19	0.57
2:C:338:ILE:HD11	2:C:755:ILE:HD13	1.85	0.57
1:B:631:LEU:O	1:B:631:LEU:HD23	2.04	0.57
1:E:476:ILE:HG13	1:E:476:ILE:O	2.03	0.57
1:E:255:ARG:O	1:E:258:ASN:HB2	2.05	0.57
1:E:752:VAL:HG13	1:E:809:SER:CB	2.31	0.57
1:B:253:ASP:O	1:B:256:LYS:HD2	2.05	0.57
1:B:265:TRP:HD1	1:B:265:TRP:O	1.88	0.57
2:C:141:TYR:O	2:C:142:ARG:HG2	2.04	0.57
3:G:301:LEU:H	3:G:568:THR:HG21	1.68	0.57
3:G:526:ARG:HA	3:G:526:ARG:NE	2.18	0.57
2:F:767:LEU:HD23	2:F:767:LEU:N	2.20	0.57
2:F:286:LEU:H	2:F:292:GLU:HA	1.67	0.57
3:D:330:SER:HB3	3:D:337:VAL:HG23	1.85	0.57
1:B:341:ARG:HA	1:B:344:ARG:HD2	1.87	0.57
3:D:253:LEU:HD13	3:D:255:HIS:CE1	2.39	0.57
3:G:267:VAL:HG22	3:G:293:ILE:HB	1.87	0.57
1:E:558:VAL:CG2	1:E:563:GLU:HB3	2.35	0.57
1:E:278:ASN:O	1:E:284:GLU:HG2	2.05	0.57
2:F:104:GLU:HA	2:F:112:ARG:HH11	1.68	0.57
1:B:501:MET:HG3	1:B:815:LEU:CD2	2.33	0.57
2:C:963:GLY:HA2	2:C:987:TYR:OH	2.04	0.57
2:C:137:GLN:HG2	2:C:697:MET:HE1	1.84	0.57
2:F:422:ILE:HD12	2:F:661:ILE:HG21	1.86	0.57
3:D:239:THR:C	3:D:241:HIS:N	2.55	0.57
3:D:259:ASN:CB	3:D:260:PRO:HD2	2.11	0.57
1:E:1033:ALA:HA	1:E:1055:PHE:CZ	2.40	0.57
2:C:1080:MET:HG3	4:X:11:DA:C4	2.40	0.57
1:B:281:GLN:OE1	1:B:317:LEU:HD12	2.04	0.57
1:E:25:ALA:HB1	1:E:807:THR:HG23	1.85	0.57
2:C:266:ARG:NH1	2:C:269:PHE:CD1	2.72	0.57
1:E:763:GLN:HE21	1:E:763:GLN:HA	1.69	0.57
1:B:771:ARG:H	1:B:771:ARG:HD2	1.69	0.57
2:F:251:ILE:HD13	2:F:252:LYS:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:365:GLU:HG3	1:E:366:SER:H	1.70	0.57
2:F:994:GLY:O	2:F:1010:PRO:HB3	2.04	0.57
1:B:1172:PHE:CG	1:B:1173:ALA:N	2.73	0.57
2:C:367:LEU:O	2:C:368:ASP:CB	2.53	0.57
3:D:199:ILE:HA	3:D:265:VAL:HG13	1.85	0.57
4:Y:2:5IU:C3'	4:Y:3:5IU:C5'	2.82	0.57
3:G:62:GLU:O	3:G:69:ALA:HB2	2.04	0.57
1:B:620:MET:HE3	1:B:687:ILE:HD13	1.85	0.57
1:E:501:MET:HG3	1:E:815:LEU:CD2	2.35	0.57
2:C:506:ILE:HG22	2:C:507:ASP:H	1.70	0.57
2:C:263:ARG:HA	2:C:273:GLU:HG2	1.87	0.57
2:C:5:TYR:HE2	2:C:267:HIS:HD2	1.52	0.57
2:F:1046:LEU:HD12	2:F:1117:PHE:CD2	2.39	0.57
3:D:41:LEU:O	3:D:44:HIS:HB3	2.05	0.57
1:E:341:ARG:HA	1:E:344:ARG:HD2	1.87	0.57
3:D:243:LEU:HD12	3:D:261:LEU:CD2	2.33	0.57
1:E:286:LEU:HD21	1:E:306:ARG:O	2.04	0.57
1:B:278:ASN:O	1:B:284:GLU:HG2	2.05	0.57
2:F:28:ASP:N	2:F:29:PRO:CD	2.60	0.57
3:G:455:ASN:ND2	3:G:532:THR:O	2.37	0.57
1:E:761:ARG:HG3	1:E:822:ARG:NH2	2.20	0.57
1:E:83:LEU:HD13	1:E:114:LEU:HD11	1.85	0.57
2:F:185:HIS:H	2:F:188:ASN:ND2	2.03	0.57
2:C:246:TYR:CE2	2:C:275:PRO:HD3	2.40	0.57
3:D:243:LEU:CD1	3:D:244:LEU:CG	2.79	0.57
2:F:1012:ALA:O	2:F:1014:GLU:N	2.38	0.57
1:B:657:VAL:HG21	1:B:707:LEU:CD1	2.35	0.57
3:G:366:GLY:CA	3:G:393:ILE:HG21	2.35	0.57
3:G:79:GLN:C	3:G:81:TRP:H	2.09	0.57
2:F:767:LEU:O	2:F:768:ASN:HB2	2.04	0.57
1:E:1027:ILE:HA	1:E:1172:PHE:CD1	2.40	0.57
2:F:939:GLN:HE21	2:F:940:SER:H	1.52	0.57
3:D:243:LEU:HD13	3:D:261:LEU:HD21	1.83	0.56
1:B:739:VAL:HG22	1:B:740:THR:H	1.70	0.56
2:C:1012:ALA:O	2:C:1014:GLU:N	2.38	0.56
1:B:604:MET:SD	1:B:704:GLU:HB2	2.45	0.56
2:C:160:GLU:O	2:C:162:GLN:N	2.35	0.56
2:C:401:PRO:C	2:C:403:LEU:H	2.08	0.56
3:G:77:GLU:HG2	3:G:79:GLN:H	1.70	0.56
1:E:977:LEU:HD21	1:E:990:LEU:CD2	2.33	0.56
1:E:248:GLU:CG	1:E:288:LYS:O	2.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LEU:HD13	1:E:40:LEU:CD2	2.34	0.56
2:C:185:HIS:H	2:C:188:ASN:HD21	1.53	0.56
1:E:901:TRP:CZ3	1:E:1060:GLY:HA2	2.40	0.56
3:D:201:LEU:HG	3:D:233:ILE:CG2	2.35	0.56
1:E:107:LYS:H	1:E:107:LYS:CD	2.17	0.56
2:C:251:ILE:HD13	2:C:256:TYR:HD2	1.69	0.56
1:B:763:GLN:HA	1:B:763:GLN:HE21	1.70	0.56
1:E:148:PHE:N	2:F:126:GLN:HE22	2.03	0.56
1:E:208:ILE:O	1:E:211:PRO:HD3	2.06	0.56
2:F:367:LEU:HB3	2:F:761:LEU:HD23	1.87	0.56
2:C:367:LEU:HB3	2:C:761:LEU:HD23	1.85	0.56
1:E:184:PHE:CE1	1:E:188:LYS:HG2	2.40	0.56
2:F:199:SER:O	2:F:200:ALA:C	2.43	0.56
3:G:397:LEU:HD13	3:G:580:TYR:HE2	1.70	0.56
3:D:274:ILE:HA	4:X:2:5IU:I5	2.75	0.56
4:X:2:5IU:C3'	4:X:3:5IU:C5'	2.84	0.56
2:C:1055:ASP:O	2:C:1055:ASP:CG	2.42	0.56
3:D:530:HIS:CE1	3:D:534:TRP:HZ3	2.23	0.56
2:C:104:GLU:HA	2:C:112:ARG:HH11	1.70	0.56
3:D:366:GLY:C	3:D:393:ILE:HG21	2.26	0.56
4:Y:1:5IU:O4'	4:Y:1:5IU:O2	2.24	0.56
2:F:974:VAL:HB	2:F:1039:PRO:O	2.05	0.56
1:E:269:ILE:O	1:E:270:SER:HB2	2.06	0.56
2:C:405:PRO:HG2	2:C:658:PRO:CB	2.35	0.56
3:G:387:GLN:O	3:G:389:ASP:N	2.38	0.56
2:F:141:TYR:O	2:F:142:ARG:HG2	2.04	0.56
1:B:83:LEU:HD13	1:B:114:LEU:HD11	1.86	0.56
2:C:410:VAL:HG13	2:C:676:CYS:HB2	1.86	0.56
2:F:895:GLU:HG3	2:F:899:ARG:HH22	1.70	0.56
2:C:25:ARG:O	2:C:26:LEU:HB3	2.05	0.56
1:E:604:MET:HG3	1:E:705:HIS:CE1	2.40	0.56
2:F:338:ILE:HD11	2:F:755:ILE:HD13	1.86	0.56
3:G:95:ASP:OD2	3:G:96:GLU:HG3	2.04	0.56
2:F:1072:LEU:O	2:F:1076:GLU:HG2	2.05	0.56
2:F:12:VAL:O	2:F:15:ALA:HB3	2.05	0.56
1:E:153:ILE:HB	1:E:348:GLU:HB3	1.87	0.56
3:G:71:CYS:HB3	3:G:74:GLU:HB3	1.87	0.56
1:E:1023:PHE:CZ	1:E:1064:GLY:HA3	2.40	0.56
2:C:257:LEU:HD13	2:C:281:GLU:OE1	2.05	0.56
2:F:72:MET:HE1	2:F:207:LEU:HB3	1.87	0.56
1:B:1068:LEU:HD23	1:B:1079:LEU:HD23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:555:SER:O	3:D:585:ILE:HG13	2.06	0.56
2:F:342:ILE:HG21	2:F:721:ILE:HD11	1.87	0.56
2:C:373:SER:HA	2:C:726:LYS:HD3	1.87	0.56
2:C:751:LEU:O	2:C:755:ILE:HG12	2.05	0.56
1:B:834:HIS:CE1	1:B:847:PRO:HB3	2.41	0.56
2:C:1051:ASP:HB3	2:C:1056:ALA:HB3	1.88	0.56
1:E:375:ARG:HD2	1:E:404:GLN:HG2	1.88	0.56
3:G:213:THR:HG21	3:G:235:GLU:O	2.06	0.56
2:F:155:VAL:H	2:F:162:GLN:NE2	2.02	0.56
1:E:507:GLU:HA	1:E:850:ALA:CB	2.35	0.56
2:F:943:ILE:CD1	2:F:956:LEU:HG	2.35	0.56
3:D:365:SER:HB3	3:D:390:PHE:CE2	2.40	0.56
2:F:98:LEU:HD21	2:F:175:TYR:CG	2.40	0.56
1:B:448:ARG:HG3	1:B:748:GLU:OE1	2.03	0.56
1:B:739:VAL:CG2	1:B:740:THR:N	2.69	0.56
1:E:826:ASP:O	1:E:828:LYS:HG3	2.06	0.56
2:F:389:LEU:HD22	2:F:678:LEU:HD11	1.86	0.56
2:C:87:ASN:C	2:C:87:ASN:HD22	2.08	0.56
2:F:963:GLY:HA2	2:F:987:TYR:OH	2.05	0.56
2:F:997:ARG:HH11	2:F:997:ARG:HG2	1.70	0.56
1:E:577:PRO:HB2	1:E:735:LEU:CD2	2.35	0.56
3:D:390:PHE:O	3:D:392:ASP:N	2.39	0.56
2:F:751:LEU:O	2:F:755:ILE:HG12	2.05	0.56
2:C:1101:THR:O	2:C:1105:ILE:HG13	2.05	0.56
3:D:271:ALA:C	3:D:273:MET:H	2.09	0.56
3:D:286:LEU:CD1	3:D:292:VAL:HG21	2.35	0.56
3:D:184:LEU:HD11	3:D:293:ILE:HD13	1.86	0.56
2:C:856:ASN:O	2:C:858:ARG:N	2.38	0.56
3:G:245:GLY:O	3:G:253:LEU:HA	2.05	0.56
1:B:920:LEU:HD23	2:C:650:ILE:CD1	2.36	0.56
2:F:263:ARG:HA	2:F:273:GLU:HG2	1.87	0.56
1:E:1024:TYR:O	2:F:51:SER:HB2	2.06	0.56
1:E:34:ALA:HB1	1:E:79:ASN:HD22	1.71	0.56
2:F:213:ILE:HB	2:F:238:LEU:HA	1.87	0.56
3:D:266:LEU:HD12	3:D:267:VAL:H	1.71	0.56
2:C:77:LEU:CD1	2:C:189:LEU:HG	2.35	0.56
3:D:367:ILE:N	3:D:393:ILE:CG2	2.62	0.56
3:D:304:VAL:CG2	3:D:564:GLU:HG2	2.33	0.56
2:F:160:GLU:O	2:F:162:GLN:N	2.34	0.56
1:B:507:GLU:HA	1:B:850:ALA:CB	2.36	0.56
2:F:656:ALA:O	2:F:658:PRO:CD	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:MET:HE3	1:B:514:TYR:HA	1.88	0.56
2:F:795:GLN:HB3	2:F:796:PRO:HD2	1.85	0.56
2:F:587:TRP:CH2	2:F:634:LEU:HG	2.39	0.56
1:B:699:THR:HG21	2:C:423:GLN:HE22	1.70	0.56
1:B:935:VAL:O	1:B:935:VAL:HG12	2.06	0.56
2:F:856:ASN:O	2:F:858:ARG:N	2.35	0.56
1:B:488:ARG:NH1	1:E:544:ASP:CA	2.68	0.56
2:F:689:LEU:HD22	2:F:708:ARG:HD2	1.86	0.56
3:G:530:HIS:CE1	3:G:534:TRP:HZ3	2.23	0.56
2:F:943:ILE:HD13	2:F:943:ILE:N	2.21	0.56
4:Y:40:DT:H1'	4:Y:41:DC:H5'	1.88	0.56
4:X:20:DC:H2''	4:X:21:DT:OP2	2.05	0.56
2:F:895:GLU:OE1	2:F:895:GLU:HA	2.05	0.56
1:B:854:ARG:HH11	1:B:854:ARG:HG2	1.71	0.56
2:C:838:GLN:HB3	2:C:979:GLN:NE2	2.20	0.56
2:F:5:TYR:HE2	2:F:267:HIS:HD2	1.53	0.56
3:G:440:LEU:HB2	3:G:535:ALA:HA	1.88	0.56
2:F:87:ASN:C	2:F:87:ASN:HD22	2.10	0.56
1:E:29:LYS:HD3	1:E:33:ILE:HD11	1.88	0.56
1:B:544:ASP:OD1	1:E:488:ARG:NH1	2.39	0.56
3:D:156:VAL:O	3:D:160:VAL:HG23	2.05	0.56
1:B:476:ILE:O	1:B:476:ILE:HG13	2.04	0.55
3:G:201:LEU:HG	3:G:233:ILE:CG2	2.36	0.55
1:B:947:ARG:N	1:B:947:ARG:CD	2.69	0.55
1:B:269:ILE:O	1:B:270:SER:HB2	2.07	0.55
1:B:1061:MET:HE3	2:C:48:MET:HA	1.88	0.55
2:C:712:ASP:O	2:C:715:LEU:HB2	2.06	0.55
2:C:335:LEU:HA	2:C:374:ILE:CD1	2.36	0.55
2:F:989:ALA:C	2:F:991:GLY:N	2.60	0.55
1:B:936:GLU:O	1:B:937:GLU:C	2.45	0.55
1:B:1021:MET:CE	1:B:1069:VAL:HG21	2.35	0.55
2:C:334:LEU:HD11	2:C:755:ILE:HG23	1.88	0.55
1:B:121:MET:C	1:B:123:GLU:H	2.08	0.55
2:C:795:GLN:HB3	2:C:796:PRO:HD2	1.87	0.55
1:B:709:ARG:NH2	2:C:487:GLU:OE2	2.40	0.55
3:D:151:ILE:O	3:D:151:ILE:HG23	2.05	0.55
1:B:46:GLY:N	1:B:49:ALA:HB2	2.21	0.55
3:D:247:GLN:HG2	4:X:5:5IU:C5'	2.34	0.55
1:E:739:VAL:CG2	1:E:740:THR:N	2.68	0.55
3:G:134:GLU:HB3	3:G:332:LEU:HD23	1.86	0.55
3:D:367:ILE:HG13	3:D:393:ILE:CG2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:ALA:HB3	3:D:349:ARG:CG	2.32	0.55
2:C:989:ALA:C	2:C:991:GLY:N	2.57	0.55
3:G:77:GLU:C	3:G:79:GLN:H	2.10	0.55
2:F:539:SER:HA	2:F:549:PRO:HG2	1.88	0.55
2:C:767:LEU:N	2:C:767:LEU:HD23	2.22	0.55
2:C:895:GLU:OE1	2:C:895:GLU:HA	2.06	0.55
3:D:417:ARG:HH21	3:D:576:ARG:NH2	2.03	0.55
2:C:213:ILE:HB	2:C:238:LEU:HA	1.87	0.55
1:E:119:ARG:HD3	2:F:302:SER:HB3	1.89	0.55
3:G:255:HIS:HB2	3:G:285:ALA:HB1	1.87	0.55
3:G:243:LEU:HD12	3:G:261:LEU:CD2	2.34	0.55
2:C:164:TRP:C	2:C:167:PRO:HD2	2.27	0.55
2:F:989:ALA:O	2:F:991:GLY:N	2.39	0.55
1:B:148:PHE:H	2:C:126:GLN:NE2	2.04	0.55
1:E:514:TYR:CG	1:E:514:TYR:O	2.59	0.55
1:E:647:GLY:O	1:E:651:ILE:HG12	2.06	0.55
2:C:12:VAL:O	2:C:15:ALA:HB3	2.06	0.55
1:B:40:LEU:HD13	1:B:59:LEU:HD22	1.88	0.55
4:X:47:DA:C2'	4:X:48:DG:O5'	2.50	0.55
2:F:104:GLU:N	2:F:112:ARG:HG3	2.13	0.55
1:E:1131:TYR:OH	1:E:1160:PRO:HB2	2.06	0.55
3:D:19:LEU:HD23	3:D:19:LEU:O	2.06	0.55
2:F:137:GLN:CG	2:F:697:MET:HE1	2.37	0.55
1:B:685:THR:HG21	1:B:729:LEU:HD12	1.89	0.55
3:D:300:GLN:CD	3:D:568:THR:HG22	2.27	0.55
2:F:442:ARG:NH1	2:F:442:ARG:HG3	2.21	0.55
3:G:151:ILE:HG23	3:G:151:ILE:O	2.05	0.55
2:F:26:LEU:HB2	2:F:210:ARG:HH22	1.70	0.55
2:C:895:GLU:HG3	2:C:899:ARG:HH22	1.71	0.55
3:D:256:HIS:CD2	3:D:257:ALA:H	2.24	0.55
3:D:213:THR:HG21	3:D:235:GLU:O	2.07	0.55
3:D:455:ASN:ND2	3:D:532:THR:O	2.40	0.55
1:B:107:LYS:CD	1:B:107:LYS:H	2.18	0.55
2:F:401:PRO:C	2:F:403:LEU:H	2.09	0.55
1:B:920:LEU:HD21	2:C:448:HIS:CE1	2.42	0.55
3:G:316:TYR:CE1	3:G:604:PHE:CB	2.90	0.55
2:F:838:GLN:HB3	2:F:979:GLN:HE22	1.69	0.55
4:X:18:DC:H4'	4:X:19:DA:OP1	2.07	0.55
3:D:301:LEU:H	3:D:568:THR:HG21	1.72	0.55
2:F:204:PRO:HB3	2:F:233:HIS:HB3	1.89	0.55
1:E:377:ARG:HH11	1:E:377:ARG:HG3	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1114:LEU:N	2:C:1115:PRO:HD2	2.21	0.55
3:G:199:ILE:HA	3:G:265:VAL:HG13	1.88	0.55
1:B:561:ARG:NH2	1:B:584:ARG:H	2.01	0.55
1:E:558:VAL:HG22	1:E:563:GLU:CB	2.35	0.55
1:B:826:ASP:O	1:B:828:LYS:HG3	2.07	0.55
1:B:752:VAL:HG13	1:B:809:SER:CB	2.32	0.55
1:E:645:PHE:HA	1:E:648:TYR:HD2	1.71	0.55
1:E:34:ALA:HB1	1:E:79:ASN:ND2	2.20	0.55
2:F:465:PHE:CE1	2:F:575:ARG:HD2	2.42	0.55
2:C:522:HIS:HE1	2:C:905:GLY:O	1.90	0.55
1:B:284:GLU:HG3	1:B:285:SER:N	2.22	0.55
2:F:584:LEU:HD22	2:F:632:VAL:HG21	1.88	0.55
1:E:222:HIS:CD2	1:E:272:TRP:HH2	2.23	0.55
3:G:390:PHE:O	3:G:392:ASP:N	2.39	0.55
2:C:664:LEU:N	2:C:664:LEU:HD12	2.22	0.55
1:B:1109:LEU:CD2	1:B:1113:LEU:HG	2.35	0.55
3:G:91:VAL:HG12	3:G:100:MET:CB	2.36	0.55
1:E:1172:PHE:CG	1:E:1173:ALA:N	2.74	0.55
2:C:572:ASN:HD22	2:C:575:ARG:HG2	1.71	0.55
3:D:312:ASP:OD1	3:D:596:ARG:HD3	2.06	0.55
1:B:184:PHE:CE1	1:B:188:LYS:HG2	2.42	0.55
3:D:166:ILE:HD12	3:D:166:ILE:N	2.21	0.55
1:E:561:ARG:O	1:E:564:ALA:HB3	2.07	0.55
1:B:555:SER:HB2	1:B:749:TYR:CD2	2.42	0.55
2:F:972:LEU:HA	2:F:1000:LEU:CD1	2.37	0.55
2:F:8:ASN:HD21	2:F:343:LEU:HD11	1.72	0.55
3:D:524:PRO:HD2	3:D:527:LEU:HD12	1.89	0.55
2:F:539:SER:HB2	2:F:551:ASP:OD2	2.06	0.55
1:B:649:ARG:HG3	1:B:650:GLN:H	1.70	0.55
3:G:31:GLU:O	3:G:32:HIS:C	2.45	0.55
2:C:641:LEU:HD22	2:C:645:LEU:HD22	1.88	0.55
2:C:199:SER:O	2:C:200:ALA:C	2.45	0.55
1:B:444:ASP:OD2	1:B:445:THR:HG22	2.07	0.55
1:B:1032:ILE:N	1:B:1032:ILE:HD12	2.21	0.55
3:D:279:MET:O	3:D:282:LEU:N	2.40	0.55
1:B:1131:TYR:CZ	1:B:1135:PHE:HD1	2.24	0.55
1:E:966:GLN:HB3	1:E:967:PRO:CD	2.34	0.55
3:D:387:GLN:O	3:D:389:ASP:N	2.39	0.55
3:D:157:ALA:CB	3:D:355:LEU:HD21	2.37	0.55
3:D:91:VAL:CA	3:D:98:THR:HG21	2.37	0.55
2:F:396:MET:HE2	2:F:674:VAL:CG2	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:MET:HE2	2:C:674:VAL:CG2	2.37	0.55
3:D:164:ARG:HG3	3:D:351:SER:HB3	1.88	0.55
3:D:244:LEU:HD21	3:D:261:LEU:CD2	2.37	0.55
2:C:347:ASN:C	2:C:347:ASN:ND2	2.58	0.55
3:G:225:LEU:C	3:G:225:LEU:HD23	2.28	0.55
1:E:1131:TYR:CZ	1:E:1135:PHE:HD1	2.24	0.55
3:D:123:PHE:HB2	3:D:604:PHE:HE2	1.72	0.55
1:B:1027:ILE:HA	1:B:1172:PHE:CD1	2.42	0.55
2:C:465:PHE:CE1	2:C:575:ARG:HD2	2.42	0.55
3:G:417:ARG:HH11	3:G:437:GLU:HB3	1.72	0.55
3:G:164:ARG:HG3	3:G:351:SER:HB3	1.87	0.55
1:B:153:ILE:HG22	1:B:349:LEU:C	2.27	0.55
3:D:27:VAL:CG1	3:D:90:ALA:HB1	2.37	0.55
4:Y:6:DA:C2'	4:Y:6:DA:N3	2.65	0.54
3:D:526:ARG:HH11	3:D:536:MET:HG2	1.71	0.54
1:B:222:HIS:CD2	1:B:272:TRP:HH2	2.24	0.54
2:C:52:GLN:O	2:C:54:PHE:N	2.36	0.54
2:F:8:ASN:ND2	2:F:343:LEU:HD11	2.23	0.54
1:B:153:ILE:HB	1:B:348:GLU:HB3	1.88	0.54
2:C:1027:TYR:O	2:C:1031:MET:HG2	2.07	0.54
1:E:121:MET:C	1:E:123:GLU:H	2.10	0.54
3:G:184:LEU:HD11	3:G:293:ILE:HD13	1.87	0.54
3:D:201:LEU:CD2	3:D:233:ILE:HG21	2.37	0.54
1:E:500:LYS:NZ	1:E:868:GLN:HG3	2.22	0.54
1:B:954:PHE:O	1:B:957:SER:HB3	2.08	0.54
1:B:799:LEU:HA	1:B:837:ALA:HB1	1.89	0.54
1:B:136:MET:CE	1:B:374:ILE:HG12	2.37	0.54
2:F:393:LEU:HD22	2:F:408:ILE:HD13	1.88	0.54
1:B:426:ASP:OD1	1:B:428:PHE:HB2	2.07	0.54
3:G:41:LEU:O	3:G:44:HIS:HB3	2.07	0.54
3:G:93:ARG:HH11	3:G:93:ARG:HG2	1.71	0.54
3:D:118:THR:HG22	3:D:283:ILE:CD1	2.04	0.54
2:F:971:LEU:HD23	4:Y:10:DA:C5'	2.33	0.54
1:E:947:ARG:CD	1:E:947:ARG:N	2.69	0.54
1:E:222:HIS:CE1	1:E:226:VAL:HG21	2.42	0.54
1:B:916:ILE:CG2	2:C:448:HIS:NE2	2.70	0.54
2:F:382:PRO:HB2	2:F:421:PHE:CD1	2.41	0.54
3:D:175:THR:HG22	3:D:176:GLY:N	2.22	0.54
3:D:178:THR:HG23	3:D:179:THR:HG23	1.88	0.54
1:B:332:LEU:O	1:B:336:ARG:HG3	2.07	0.54
2:F:611:LEU:HD23	2:F:611:LEU:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:HA	2:C:517:PRO:HG2	1.89	0.54
1:B:365:GLU:HG3	1:B:366:SER:N	2.21	0.54
1:E:869:THR:O	1:E:871:GLN:N	2.41	0.54
1:E:150:GLN:HA	1:E:150:GLN:HE21	1.72	0.54
4:X:6:DA:N3	4:X:6:DA:C2'	2.64	0.54
4:X:13:DG:H2''	4:X:14:DC:OP2	2.07	0.54
1:B:924:LEU:CD1	2:C:607:ALA:HA	2.37	0.54
1:E:799:LEU:HA	1:E:837:ALA:HB1	1.89	0.54
3:D:75:ILE:HB	3:D:78:LEU:CD1	2.37	0.54
2:F:277:PHE:CE1	2:F:278:ARG:HG3	2.42	0.54
4:X:40:DT:H1'	4:X:41:DC:H5'	1.88	0.54
2:C:530:ARG:NE	2:C:548:LEU:O	2.35	0.54
1:B:365:GLU:C	1:B:367:GLY:H	2.11	0.54
2:C:55:GLY:O	2:C:56:ILE:HB	2.06	0.54
2:F:1077:GLY:H	2:F:1083:GLY:H	1.55	0.54
2:F:910:GLY:O	2:F:913:GLY:N	2.40	0.54
3:G:361:PHE:C	3:G:361:PHE:CD1	2.80	0.54
1:E:854:ARG:HH11	1:E:854:ARG:HG2	1.72	0.54
3:G:208:ALA:HB2	3:G:270:GLU:HG3	1.88	0.54
4:X:46:5IU:H2''	4:X:47:DA:O4'	2.07	0.54
1:B:159:LEU:HD21	1:B:342:GLU:CG	2.37	0.54
2:F:347:ASN:ND2	2:F:347:ASN:C	2.59	0.54
3:D:533:THR:O	3:D:535:ALA:N	2.34	0.54
1:B:459:LYS:HD3	1:B:865:ILE:HD12	1.90	0.54
3:G:370:LEU:HD22	3:G:394:GLU:OE2	2.07	0.54
3:D:307:GLY:C	3:D:597:ARG:NH2	2.61	0.54
2:F:537:MET:HA	3:G:110:ASN:HB3	1.90	0.54
3:G:300:GLN:CG	3:G:568:THR:HG22	2.37	0.54
2:F:4:VAL:O	2:F:322:GLU:HA	2.07	0.54
1:B:187:TRP:HZ3	1:B:196:ASP:OD2	1.91	0.54
2:F:194:ILE:HG23	2:F:229:ALA:HB2	1.89	0.54
3:D:247:GLN:O	3:D:251:GLN:HG2	2.07	0.54
4:Y:13:DG:H2''	4:Y:14:DC:OP2	2.07	0.54
2:C:943:ILE:CD1	2:C:956:LEU:HG	2.36	0.54
1:B:423:ARG:O	1:B:423:ARG:CD	2.56	0.54
3:G:526:ARG:HH12	3:G:536:MET:CE	2.20	0.54
2:F:25:ARG:O	2:F:26:LEU:HB3	2.07	0.54
1:B:29:LYS:O	1:B:33:ILE:HG13	2.08	0.54
1:E:259:ARG:O	1:E:262:GLN:NE2	2.40	0.54
1:B:281:GLN:CB	1:B:283:PRO:HD2	2.35	0.54
2:C:828:LEU:HD22	2:C:1028:ARG:HD3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:ASP:N	2:F:29:PRO:HD2	2.22	0.54
1:B:488:ARG:HH12	1:E:544:ASP:CA	2.20	0.54
2:C:469:ASP:O	2:C:472:ALA:HB3	2.07	0.54
2:F:304:GLY:HA2	2:F:714:TYR:CD1	2.40	0.54
1:E:763:GLN:NE2	1:E:765:GLN:H	2.03	0.54
1:B:675:LEU:CD1	2:C:809:ALA:HB1	2.37	0.54
2:F:199:SER:O	2:F:201:THR:N	2.41	0.54
2:F:795:GLN:HB3	2:F:796:PRO:CD	2.38	0.54
3:D:554:PRO:HD2	3:D:561:VAL:HG21	1.88	0.54
1:B:1044:ASP:HB3	1:B:1047:SER:OG	2.06	0.54
2:C:1040:GLU:HB2	2:C:1084:GLU:OE1	2.06	0.54
2:F:1055:ASP:CB	2:F:1118:ARG:NH2	2.69	0.54
2:C:155:VAL:H	2:C:162:GLN:NE2	2.06	0.54
1:B:1018:GLN:NE2	2:C:30:PHE:O	2.40	0.54
2:F:258:ALA:HA	2:F:261:LEU:CG	2.36	0.54
2:F:828:LEU:HD22	2:F:1028:ARG:HD3	1.87	0.54
1:B:763:GLN:NE2	1:B:765:GLN:H	2.02	0.54
2:F:1013:ALA:O	2:F:1017:LEU:HD23	2.07	0.54
3:G:561:VAL:HG12	3:G:589:ALA:CB	2.37	0.54
1:B:869:THR:O	1:B:871:GLN:N	2.40	0.54
2:C:17:MET:HG3	2:C:212:PHE:CE2	2.43	0.54
1:B:647:GLY:O	1:B:651:ILE:HG12	2.08	0.54
1:E:935:VAL:HG12	1:E:935:VAL:O	2.07	0.54
1:E:909:LEU:HD22	1:E:1054:GLU:CD	2.27	0.54
1:E:740:THR:OG1	4:Y:49:DA:OP1	2.13	0.54
2:C:104:GLU:CA	2:C:112:ARG:NH1	2.70	0.54
1:E:459:LYS:HD3	1:E:865:ILE:HD12	1.89	0.54
2:C:59:ASN:O	2:C:60:ILE:O	2.26	0.54
1:B:365:GLU:HG3	1:B:366:SER:H	1.72	0.54
2:F:246:TYR:CE2	2:F:275:PRO:HD3	2.43	0.54
2:C:94:LYS:O	2:C:98:LEU:HG	2.08	0.54
1:E:398:ARG:HB2	1:E:402:HIS:HB2	1.90	0.54
3:D:246:ALA:HA	3:D:253:LEU:HD23	1.90	0.54
2:F:881:ASN:O	2:F:885:LEU:HB2	2.08	0.54
3:G:220:LEU:HA	3:G:223:LEU:HD21	1.90	0.54
2:F:155:VAL:N	2:F:162:GLN:HE22	2.06	0.54
1:E:86:ALA:HB1	1:E:92:THR:HG1	1.73	0.54
2:C:1039:PRO:HA	2:C:1113:LEU:HD11	1.90	0.54
2:C:52:GLN:C	2:C:54:PHE:H	2.12	0.54
1:B:577:PRO:HB2	1:B:735:LEU:CD2	2.39	0.54
3:G:526:ARG:HH22	3:G:533:THR:HG21	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:763:GLN:NE2	1:B:764:GLU:N	2.56	0.54
1:E:139:LEU:HD21	1:E:377:ARG:HH12	1.72	0.54
2:C:17:MET:HG3	2:C:212:PHE:CD2	2.43	0.54
1:E:1044:ASP:HB3	1:E:1047:SER:OG	2.07	0.54
3:D:208:ALA:HB2	3:D:270:GLU:HG3	1.88	0.53
3:G:188:LEU:HD21	3:G:291:ARG:HH22	1.73	0.53
3:G:213:THR:HG21	3:G:235:GLU:C	2.27	0.53
1:B:236:TRP:O	1:B:240:VAL:CG2	2.53	0.53
2:C:989:ALA:HB1	2:C:1017:LEU:HD22	1.90	0.53
2:F:253:ASP:C	2:F:255:ALA:N	2.55	0.53
2:C:422:ILE:HD12	2:C:661:ILE:HG21	1.90	0.53
3:G:554:PRO:CD	3:G:561:VAL:HG21	2.38	0.53
3:G:562:THR:HG21	3:G:594:THR:HA	1.90	0.53
2:F:410:VAL:HG13	2:F:676:CYS:HB2	1.90	0.53
2:F:699:GLN:O	2:F:701:PRO:HD3	2.08	0.53
1:B:150:GLN:HA	1:B:150:GLN:HE21	1.71	0.53
2:F:306:LEU:HD23	2:F:306:LEU:C	2.28	0.53
2:F:971:LEU:CD2	4:Y:10:DA:H5'	2.31	0.53
2:F:1055:ASP:CB	2:F:1118:ARG:HH22	2.13	0.53
2:C:951:GLN:C	2:C:952:ILE:HD13	2.29	0.53
2:F:536:ALA:O	2:F:537:MET:C	2.46	0.53
2:C:335:LEU:HD22	2:C:339:GLN:OE1	2.08	0.53
1:E:936:GLU:O	1:E:937:GLU:C	2.45	0.53
1:B:390:ASP:HA	1:B:429:THR:HG21	1.90	0.53
2:C:33:GLU:O	2:C:60:ILE:HA	2.08	0.53
1:B:56:VAL:HG12	1:B:124:ALA:HA	1.90	0.53
1:E:40:LEU:HD13	1:E:59:LEU:HD22	1.91	0.53
1:E:29:LYS:O	1:E:33:ILE:HG13	2.07	0.53
2:C:795:GLN:HB3	2:C:796:PRO:CD	2.37	0.53
2:C:796:PRO:HA	2:C:800:GLN:NE2	2.22	0.53
2:C:1077:GLY:H	2:C:1083:GLY:H	1.55	0.53
3:G:50:HIS:CE1	3:G:306:ALA:HB2	2.43	0.53
3:D:256:HIS:O	3:D:285:ALA:HA	2.09	0.53
1:B:558:VAL:O	1:B:740:THR:HA	2.08	0.53
3:D:213:THR:HG21	3:D:235:GLU:C	2.28	0.53
1:B:957:SER:O	1:B:960:GLU:HB2	2.08	0.53
1:B:233:LYS:HZ2	1:B:269:ILE:HG12	1.71	0.53
1:B:377:ARG:HH11	1:B:377:ARG:HG3	1.71	0.53
1:E:1021:MET:CE	1:E:1069:VAL:HG21	2.38	0.53
1:E:365:GLU:C	1:E:367:GLY:H	2.11	0.53
1:E:700:GLN:O	1:E:701:LEU:HD23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1101:THR:O	2:F:1105:ILE:HG13	2.09	0.53
1:B:16:GLN:O	1:B:16:GLN:HG3	2.09	0.53
3:G:255:HIS:HB3	3:G:260:PRO:HG2	1.89	0.53
4:Y:46:5IU:H2''	4:Y:47:DA:O4'	2.08	0.53
1:E:423:ARG:O	1:E:423:ARG:CD	2.56	0.53
2:F:77:LEU:CD2	2:F:196:THR:HG21	2.37	0.53
3:G:52:CYS:HB3	3:G:108:TYR:CD2	2.43	0.53
1:E:1061:MET:HE1	2:F:52:GLN:HG3	1.91	0.53
3:D:77:GLU:C	3:D:79:GLN:H	2.10	0.53
1:B:1061:MET:HG3	2:C:48:MET:CE	2.39	0.53
2:F:966:ARG:HH11	2:F:983:GLU:CD	2.11	0.53
3:D:181:VAL:HG21	3:D:295:LEU:HD13	1.90	0.53
2:C:251:ILE:HD13	2:C:256:TYR:CD2	2.43	0.53
2:C:537:MET:HE3	2:C:544:TRP:HB2	1.90	0.53
2:F:200:ALA:O	2:F:202:THR:N	2.42	0.53
2:F:572:ASN:HD22	2:F:575:ARG:HG2	1.73	0.53
2:C:939:GLN:HE21	2:C:940:SER:H	1.57	0.53
1:B:363:ARG:HG3	1:B:364:SER:N	2.24	0.53
2:C:584:LEU:HD22	2:C:632:VAL:HG21	1.91	0.53
2:C:28:ASP:H	2:C:29:PRO:HD3	1.71	0.53
1:E:1168:MET:O	1:E:1171:MET:HB3	2.08	0.53
3:G:462:MET:O	3:G:466:ARG:HA	2.09	0.53
2:F:86:PHE:CZ	2:F:176:THR:HG21	2.44	0.53
3:G:91:VAL:CA	3:G:98:THR:HG21	2.38	0.53
1:E:704:GLU:CD	1:E:704:GLU:H	2.10	0.53
1:B:1172:PHE:CZ	1:B:1173:ALA:HB2	2.43	0.53
3:G:354:LEU:HD12	3:G:354:LEU:H	1.74	0.53
2:C:1060:ASP:OD2	2:C:1062:SER:OG	2.25	0.53
1:E:61:VAL:HB	1:E:126:VAL:HG13	1.90	0.53
3:D:321:PHE:CE2	3:D:329:LEU:HD11	2.43	0.53
3:D:243:LEU:CD1	3:D:261:LEU:CD2	2.79	0.53
3:G:271:ALA:O	3:G:273:MET:N	2.42	0.53
1:B:876:GLN:N	1:B:877:PRO:HD2	2.24	0.53
1:B:527:ARG:HG2	1:B:527:ARG:HH11	1.73	0.53
2:C:972:LEU:HD23	2:C:973:SER:N	2.23	0.53
1:E:658:MET:HB2	1:E:695:GLN:HG3	1.90	0.53
3:G:77:GLU:O	3:G:79:GLN:N	2.42	0.53
2:F:265:ARG:HG2	2:F:266:ARG:O	2.08	0.53
2:F:251:ILE:HD13	2:F:256:TYR:CD2	2.43	0.53
3:G:554:PRO:HD2	3:G:561:VAL:HG21	1.91	0.53
2:C:947:CYS:SG	2:C:1021:SER:OG	2.67	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:781:ASN:O	1:E:783:ALA:N	2.39	0.53
3:D:554:PRO:CD	3:D:561:VAL:HG21	2.38	0.53
1:E:190:PRO:HG3	2:F:870:PHE:CE1	2.43	0.53
3:D:242:ARG:O	3:D:245:GLY:N	2.42	0.53
1:E:739:VAL:CG2	1:E:740:THR:H	2.21	0.53
1:E:159:LEU:HD21	1:E:342:GLU:CG	2.39	0.53
3:G:201:LEU:CD2	3:G:233:ILE:HG21	2.39	0.53
3:D:412:LEU:CD1	3:D:461:PHE:HD2	2.21	0.53
1:B:591:LEU:O	1:B:595:GLU:HG3	2.08	0.53
3:D:77:GLU:HG2	3:D:79:GLN:H	1.72	0.53
2:C:278:ARG:O	2:C:280:SER:N	2.41	0.53
3:D:91:VAL:HG12	3:D:100:MET:HB3	1.90	0.53
2:F:396:MET:HE3	2:F:726:LYS:HG3	1.89	0.53
3:G:562:THR:OG1	3:G:594:THR:HG23	2.08	0.53
1:E:50:PHE:HE2	1:E:52:ARG:HD3	1.73	0.53
2:F:1027:TYR:O	2:F:1031:MET:HG2	2.09	0.53
4:X:7:5IU:C3'	4:X:8:DC:H5'	2.18	0.53
3:G:240:LEU:HD21	3:G:274:ILE:HD12	1.90	0.53
1:B:739:VAL:CG2	1:B:740:THR:H	2.21	0.53
3:D:526:ARG:NH1	3:D:536:MET:HG2	2.24	0.53
1:E:1076:TYR:HD1	1:E:1122:LEU:HD13	1.74	0.53
2:C:966:ARG:HH11	2:C:983:GLU:CD	2.11	0.53
2:C:239:LEU:HD12	2:C:239:LEU:N	2.23	0.53
3:D:181:VAL:HG21	3:D:295:LEU:CD1	2.38	0.53
1:B:732:ASP:OD1	1:B:735:LEU:HD12	2.08	0.53
3:G:330:SER:HB3	3:G:337:VAL:N	2.24	0.53
1:B:15:LEU:HD13	1:B:40:LEU:CD2	2.39	0.53
3:G:321:PHE:CE2	3:G:329:LEU:HD11	2.44	0.53
2:F:17:MET:HG3	2:F:212:PHE:CD2	2.44	0.53
2:F:17:MET:HG3	2:F:212:PHE:CE2	2.44	0.53
1:E:46:GLY:N	1:E:49:ALA:HB2	2.24	0.53
1:E:602:ALA:HB2	1:E:615:ALA:HB2	1.91	0.53
1:B:558:VAL:HG22	1:B:563:GLU:CB	2.38	0.53
1:E:423:ARG:O	1:E:423:ARG:HD2	2.09	0.53
1:B:25:ALA:HB1	1:B:807:THR:HG21	1.90	0.53
1:B:807:THR:HG22	1:B:808:ARG:NH2	2.23	0.53
1:E:987:GLU:O	1:E:991:THR:HG22	2.08	0.53
3:G:109:LEU:O	3:G:110:ASN:C	2.47	0.53
2:F:245:ARG:HD3	2:F:344:GLU:OE2	2.08	0.53
2:F:483:PHE:CE2	2:F:567:LEU:HA	2.43	0.53
1:E:491:PHE:O	1:E:493:GLY:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:PRO:HG3	2:C:182:PRO:CB	2.38	0.53
1:E:16:GLN:O	1:E:16:GLN:HG3	2.09	0.53
3:D:93:ARG:HH11	3:D:93:ARG:HG2	1.72	0.53
1:E:1032:ILE:HD12	1:E:1032:ILE:N	2.23	0.53
3:D:264:ASP:O	3:D:291:ARG:N	2.41	0.53
1:B:442:THR:HG22	1:B:443:LEU:N	2.23	0.53
2:C:881:ASN:O	2:C:885:LEU:HB2	2.09	0.53
1:B:342:GLU:HA	1:B:342:GLU:OE2	2.09	0.53
1:E:823:ARG:HH22	1:E:828:LYS:HZ3	1.55	0.53
1:B:1168:MET:O	1:B:1171:MET:HB3	2.09	0.53
3:G:593:ARG:O	3:G:594:THR:C	2.48	0.53
1:B:494:GLU:CB	1:E:545:ASP:OD1	2.57	0.53
2:C:199:SER:OG	2:C:200:ALA:N	2.42	0.53
2:C:580:GLN:O	2:C:582:ARG:HD2	2.09	0.53
2:C:964:LEU:O	2:C:996:SER:HA	2.09	0.53
3:D:266:LEU:HD12	3:D:267:VAL:N	2.24	0.52
3:D:207:LYS:HE2	3:D:211:ARG:NH2	2.24	0.52
1:E:555:SER:HB2	1:E:749:TYR:CD2	2.44	0.52
3:D:17:ARG:HB2	3:D:18:PRO:CD	2.35	0.52
1:B:198:ASN:O	1:B:200:TYR:O	2.26	0.52
1:B:490:VAL:HG12	1:B:495:THR:CG2	2.38	0.52
1:B:1109:LEU:HA	1:B:1112:GLN:OE1	2.08	0.52
2:F:278:ARG:O	2:F:280:SER:N	2.42	0.52
1:E:65:THR:HG22	1:E:67:ALA:N	2.24	0.52
2:C:536:ALA:O	2:C:537:MET:C	2.47	0.52
1:B:893:LEU:HB3	2:C:802:TYR:HE2	1.73	0.52
2:C:97:THR:HG23	2:C:628:TYR:CD1	2.44	0.52
2:F:97:THR:HG23	2:F:628:TYR:CE1	2.44	0.52
3:D:274:ILE:HG21	3:D:279:MET:HG2	1.91	0.52
3:G:254:ARG:HG2	3:G:259:ASN:ND2	2.24	0.52
2:F:839:ARG:HB3	4:Y:7:5IU:I5	2.79	0.52
1:E:558:VAL:O	1:E:740:THR:HA	2.09	0.52
2:F:38:GLN:OE1	2:F:65:PRO:HG2	2.08	0.52
2:F:104:GLU:CA	2:F:112:ARG:NH1	2.70	0.52
2:F:557:ILE:HG23	4:Y:1:5IU:I5	2.79	0.52
1:B:815:LEU:HD13	1:B:815:LEU:H	1.74	0.52
1:E:470:PHE:O	1:E:472:GLU:N	2.42	0.52
1:E:815:LEU:H	1:E:815:LEU:HD13	1.74	0.52
2:F:664:LEU:N	2:F:664:LEU:HD12	2.24	0.52
1:B:730:GLU:HB2	2:C:786:ARG:CD	2.37	0.52
2:C:292:GLU:HB3	2:C:295:VAL:HG22	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:763:GLN:NE2	1:E:764:GLU:N	2.57	0.52
3:D:91:VAL:CG1	3:D:100:MET:HB2	2.39	0.52
2:F:580:GLN:O	2:F:582:ARG:HD2	2.09	0.52
2:F:344:GLU:HB3	2:F:346:GLU:HG2	1.92	0.52
1:E:677:THR:O	1:E:678:ALA:O	2.27	0.52
2:C:244:CYS:SG	2:C:345:LEU:HB2	2.49	0.52
1:E:342:GLU:HA	1:E:342:GLU:OE2	2.09	0.52
1:B:281:GLN:HE21	1:B:283:PRO:HG2	1.75	0.52
1:B:1076:TYR:HD1	1:B:1122:LEU:HD13	1.73	0.52
1:B:1131:TYR:OH	1:B:1160:PRO:HB2	2.08	0.52
1:E:804:VAL:O	1:E:808:ARG:HG2	2.09	0.52
1:B:799:LEU:HD23	1:B:837:ALA:CB	2.39	0.52
2:F:254:PRO:HA	2:F:257:LEU:HD23	1.90	0.52
2:F:469:ASP:O	2:F:472:ALA:HB3	2.08	0.52
3:G:385:VAL:CG2	3:G:396:ARG:CZ	2.86	0.52
1:E:1098:MET:HE1	1:E:1156:TYR:HB2	1.91	0.52
2:C:768:ASN:HB3	2:C:771:GLU:HB2	1.91	0.52
1:E:878:TRP:O	1:E:878:TRP:CE3	2.62	0.52
1:E:649:ARG:HG3	1:E:650:GLN:H	1.73	0.52
2:F:505:GLY:O	2:F:523:THR:HB	2.10	0.52
1:E:39:ARG:HG3	1:E:39:ARG:HH11	1.73	0.52
2:C:185:HIS:H	2:C:188:ASN:ND2	2.06	0.52
1:B:46:GLY:H	1:B:49:ALA:HB2	1.74	0.52
1:B:398:ARG:HB2	1:B:402:HIS:HB2	1.91	0.52
2:C:306:LEU:C	2:C:306:LEU:HD23	2.30	0.52
3:D:286:LEU:HD13	3:D:292:VAL:CG2	2.39	0.52
1:E:236:TRP:O	1:E:240:VAL:CG2	2.52	0.52
4:Y:15:DG:C1'	4:Y:16:DA:OP1	2.56	0.52
1:E:281:GLN:HE21	1:E:283:PRO:HG2	1.75	0.52
1:E:524:ALA:O	1:E:527:ARG:HG3	2.09	0.52
1:E:527:ARG:HH11	1:E:527:ARG:HG2	1.73	0.52
2:F:104:GLU:CA	2:F:112:ARG:HH11	2.22	0.52
1:B:600:LEU:O	1:B:604:MET:HB2	2.09	0.52
1:B:255:ARG:O	1:B:258:ASN:HB2	2.09	0.52
1:B:977:LEU:HD21	1:B:990:LEU:CD2	2.36	0.52
1:E:233:LYS:HZ2	1:E:269:ILE:HG12	1.74	0.52
2:C:838:GLN:HB3	2:C:979:GLN:HE22	1.75	0.52
2:C:989:ALA:CB	2:C:1017:LEU:HD22	2.39	0.52
2:F:482:ARG:HG2	2:F:482:ARG:HH11	1.74	0.52
2:C:699:GLN:C	2:C:701:PRO:HD3	2.30	0.52
3:G:385:VAL:HG11	3:G:396:ARG:CD	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:301:LEU:N	3:G:568:THR:HG21	2.24	0.52
2:C:551:ASP:OD2	2:C:551:ASP:N	2.33	0.52
2:F:335:LEU:HD22	2:F:339:GLN:OE1	2.09	0.52
1:B:153:ILE:HD12	1:B:154:GLU:OE2	2.09	0.52
2:F:1060:ASP:OD2	2:F:1062:SER:OG	2.27	0.52
3:G:207:LYS:O	3:G:210:ALA:HB3	2.10	0.52
1:E:581:LEU:HD11	1:E:737:GLN:OE1	2.10	0.52
3:G:19:LEU:O	3:G:19:LEU:HD23	2.10	0.52
2:C:28:ASP:N	2:C:29:PRO:HD2	2.22	0.52
3:D:157:ALA:HB1	3:D:169:ILE:HD12	1.92	0.52
2:C:265:ARG:HG2	2:C:266:ARG:O	2.09	0.52
1:B:65:THR:HB	1:B:68:ALA:CB	2.38	0.52
1:E:985:GLN:CD	1:E:985:GLN:N	2.63	0.52
3:D:91:VAL:HG12	3:D:100:MET:HB2	1.91	0.52
3:D:568:THR:O	3:D:572:ARG:HG2	2.09	0.52
1:E:426:ASP:OD1	1:E:428:PHE:HB2	2.10	0.52
1:E:18:GLU:O	1:E:19:ARG:HD3	2.09	0.52
3:G:582:ASP:O	3:G:584:ARG:N	2.43	0.52
3:D:147:VAL:HG12	3:D:147:VAL:O	2.10	0.52
3:G:126:VAL:HA	3:G:166:ILE:HD13	1.91	0.52
2:F:1035:LEU:O	2:F:1036:LEU:O	2.28	0.52
1:B:754:LEU:HB2	1:B:815:LEU:HB3	1.92	0.52
2:F:52:GLN:C	2:F:54:PHE:H	2.13	0.52
3:D:77:GLU:O	3:D:79:GLN:N	2.42	0.52
2:C:382:PRO:HB2	2:C:421:PHE:CD1	2.44	0.52
2:C:252:LYS:HB2	2:C:256:TYR:CD2	2.45	0.52
2:C:539:SER:HB2	2:C:551:ASP:OD2	2.10	0.52
2:F:989:ALA:HB1	2:F:1017:LEU:HD22	1.91	0.52
2:F:736:ILE:HD12	2:F:736:ILE:N	2.24	0.52
2:F:199:SER:OG	2:F:200:ALA:N	2.43	0.52
1:E:490:VAL:HG12	1:E:495:THR:CG2	2.39	0.52
3:D:109:LEU:O	3:D:110:ASN:C	2.47	0.52
2:F:55:GLY:O	2:F:56:ILE:HB	2.09	0.52
2:C:360:ARG:CZ	2:C:766:ALA:HB2	2.39	0.52
1:E:496:GLN:NE2	1:E:496:GLN:N	2.57	0.52
3:D:118:THR:HA	3:D:121:ARG:NH1	2.25	0.52
3:D:260:PRO:O	3:D:261:LEU:CB	2.56	0.52
3:D:270:GLU:OE1	3:D:273:MET:HE2	2.09	0.52
2:C:850:GLN:HG2	2:C:856:ASN:OD1	2.10	0.52
1:E:284:GLU:HG3	1:E:285:SER:N	2.23	0.52
1:E:307:HIS:ND1	1:E:308:PRO:CD	2.70	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:130:ILE:N	3:G:130:ILE:HD12	2.08	0.52
1:B:358:LEU:HD13	1:B:396:ILE:HD13	1.91	0.52
1:B:237:ARG:HE	1:B:266:ILE:CG2	2.22	0.52
1:E:957:SER:O	1:E:960:GLU:HB2	2.09	0.52
3:G:157:ALA:HB1	3:G:169:ILE:HD12	1.91	0.52
2:C:699:GLN:O	2:C:701:PRO:HD3	2.10	0.52
2:C:260:LEU:C	2:C:262:THR:H	2.13	0.52
1:B:771:ARG:HH21	1:B:793:GLU:HG3	1.75	0.52
2:C:964:LEU:HB2	2:C:996:SER:CB	2.40	0.52
1:E:363:ARG:HG3	1:E:364:SER:N	2.23	0.52
1:B:60:LEU:HB2	1:B:378:PHE:HB3	1.91	0.52
1:E:142:PHE:HB3	2:F:110:LEU:HD22	1.92	0.52
2:C:355:ILE:HD12	2:C:355:ILE:N	2.25	0.52
3:D:207:LYS:O	3:D:210:ALA:HB3	2.09	0.52
3:G:132:VAL:HG12	3:G:133:ASP:H	1.74	0.52
2:C:77:LEU:CD2	2:C:196:THR:HG21	2.40	0.52
3:D:462:MET:CE	3:D:534:TRP:HE1	2.20	0.52
2:C:830:GLU:O	2:C:831:THR:OG1	2.20	0.52
2:C:955:TRP:O	2:C:957:PRO:HD3	2.10	0.52
1:E:807:THR:HG22	1:E:808:ARG:NH2	2.23	0.52
1:E:198:ASN:O	1:E:200:TYR:O	2.28	0.52
3:G:568:THR:O	3:G:572:ARG:HG2	2.09	0.52
2:C:277:PHE:CE1	2:C:278:ARG:HG3	2.45	0.52
2:C:86:PHE:CZ	2:C:176:THR:HG21	2.45	0.52
2:F:252:LYS:HB2	2:F:256:TYR:CD2	2.45	0.52
2:C:570:GLN:HA	2:C:573:ILE:HD12	1.92	0.52
1:E:626:LEU:C	1:E:626:LEU:HD13	2.30	0.52
2:F:99:LEU:N	2:F:100:PRO:HD2	2.24	0.52
2:F:1040:GLU:HB2	2:F:1084:GLU:OE1	2.10	0.52
1:B:602:ALA:HB2	1:B:615:ALA:HB2	1.92	0.52
3:G:556:GLN:O	3:G:557:ARG:CB	2.58	0.52
3:G:378:ASP:O	3:G:382:VAL:HG23	2.09	0.52
2:F:964:LEU:O	2:F:996:SER:HA	2.09	0.52
3:G:126:VAL:HG13	3:G:166:ILE:H	1.73	0.52
2:C:1080:MET:HG3	4:X:11:DA:N3	2.24	0.52
4:X:15:DG:C1'	4:X:16:DA:OP1	2.57	0.52
1:E:874:ASP:O	1:E:875:ASN:HB2	2.10	0.52
3:D:440:LEU:HD22	3:D:552:ILE:CD1	2.40	0.52
1:E:861:CYS:HA	1:E:865:ILE:HB	1.91	0.52
1:E:754:LEU:HB2	1:E:815:LEU:HB3	1.91	0.52
2:C:880:ILE:HG23	2:C:901:PHE:CE1	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:383:LYS:O	3:D:387:GLN:HB2	2.10	0.52
3:G:181:VAL:HG21	3:G:295:LEU:CD1	2.40	0.52
1:E:416:LYS:HE2	1:E:803:TYR:CE2	2.45	0.52
1:E:1002:LEU:HD22	1:E:1007:VAL:HG12	1.91	0.52
1:B:136:MET:HE2	1:B:374:ILE:HG12	1.92	0.52
2:F:335:LEU:HA	2:F:374:ILE:CD1	2.40	0.52
3:G:27:VAL:CG1	3:G:90:ALA:HB1	2.40	0.52
2:F:203:CYS:HB2	2:F:204:PRO:HD2	1.91	0.52
2:C:442:ARG:HG3	2:C:442:ARG:NH1	2.24	0.52
2:F:59:ASN:O	2:F:60:ILE:O	2.27	0.52
3:D:582:ASP:C	3:D:584:ARG:H	2.14	0.52
1:E:375:ARG:HD3	1:E:400:ILE:O	2.10	0.52
2:C:509:ASP:HA	2:C:512:ARG:NH1	2.25	0.52
1:B:359:ASP:OD1	1:B:395:ARG:HD2	2.09	0.52
3:D:248:PRO:HD3	4:X:4:5IU:H1'	1.90	0.52
1:E:256:LYS:HA	1:E:259:ARG:HD2	1.92	0.52
1:B:947:ARG:CD	1:B:1086:LEU:HD21	2.40	0.52
2:F:1050:TYR:HD1	2:F:1057:MET:HE2	1.75	0.52
2:C:77:LEU:HD23	2:C:196:THR:HG21	1.92	0.52
1:E:823:ARG:C	1:E:825:GLY:H	2.14	0.52
2:C:254:PRO:HA	2:C:257:LEU:HD23	1.92	0.52
1:B:732:ASP:C	1:B:734:HIS:H	2.14	0.52
2:F:548:LEU:HD22	2:F:549:PRO:HD2	1.92	0.52
4:Y:18:DC:H4'	4:Y:19:DA:OP1	2.08	0.52
1:B:514:TYR:CG	1:B:514:TYR:O	2.60	0.52
3:D:52:CYS:HB3	3:D:108:TYR:CE2	2.45	0.52
2:F:26:LEU:HD22	2:F:33:GLU:OE1	2.10	0.52
1:E:52:ARG:CG	1:E:52:ARG:HH21	2.23	0.52
3:D:556:GLN:O	3:D:557:ARG:HG3	2.10	0.52
1:E:444:ASP:OD2	1:E:445:THR:HG22	2.10	0.52
2:F:239:LEU:N	2:F:239:LEU:HD12	2.25	0.52
1:B:838:LEU:HD22	1:B:838:LEU:O	2.09	0.52
3:G:256:HIS:CG	3:G:257:ALA:N	2.78	0.51
3:G:266:LEU:HD12	3:G:267:VAL:H	1.73	0.51
1:B:561:ARG:O	1:B:564:ALA:HB3	2.10	0.51
1:B:243:LEU:HD22	1:B:259:ARG:HH12	1.74	0.51
2:F:228:GLN:NE2	2:F:319:SER:H	2.07	0.51
1:B:815:LEU:HD13	1:B:815:LEU:N	2.25	0.51
3:G:367:ILE:N	3:G:393:ILE:CG2	2.68	0.51
3:G:175:THR:HG21	3:G:355:LEU:CB	2.40	0.51
1:E:1098:MET:CE	1:E:1156:TYR:HB2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:593:ARG:O	3:D:594:THR:C	2.48	0.51
1:B:985:GLN:CD	1:B:985:GLN:N	2.63	0.51
1:E:771:ARG:HH21	1:E:793:GLU:HG3	1.75	0.51
3:D:52:CYS:SG	3:D:106:ARG:HG2	2.49	0.51
3:D:437:GLU:O	3:D:548:HIS:N	2.34	0.51
2:C:910:GLY:O	2:C:913:GLY:N	2.42	0.51
2:F:592:ARG:HH11	2:F:592:ARG:HB2	1.74	0.51
3:G:286:LEU:HD13	3:G:292:VAL:CG2	2.39	0.51
1:B:558:VAL:CG2	1:B:563:GLU:HB3	2.40	0.51
1:E:584:ARG:HH11	1:E:584:ARG:HG2	1.75	0.51
2:F:348:ARG:HG3	2:F:365:ARG:NH1	2.25	0.51
1:B:823:ARG:HH22	1:B:828:LYS:HZ3	1.57	0.51
1:B:754:LEU:HB3	1:B:757:ILE:HB	1.91	0.51
2:F:74:VAL:HA	2:F:80:ILE:HB	1.92	0.51
3:D:385:VAL:CG2	3:D:396:ARG:CZ	2.88	0.51
1:E:1040:ILE:HG23	1:E:1112:GLN:NE2	2.26	0.51
1:B:65:THR:HG22	1:B:67:ALA:N	2.25	0.51
1:B:769:HIS:HD2	1:B:793:GLU:OE1	1.93	0.51
1:B:769:HIS:HA	1:B:775:GLU:O	2.10	0.51
2:C:997:ARG:NH1	2:C:997:ARG:HG2	2.24	0.51
1:B:213:PRO:C	1:B:215:ASP:H	2.12	0.51
1:E:1068:LEU:HD23	1:E:1079:LEU:HD23	1.90	0.51
1:B:781:ASN:O	1:B:783:ALA:N	2.39	0.51
1:E:1172:PHE:CZ	1:E:1173:ALA:HB2	2.44	0.51
2:C:199:SER:O	2:C:201:THR:N	2.43	0.51
2:F:842:ALA:O	2:F:843:HIS:HB2	2.10	0.51
2:C:344:GLU:HB3	2:C:346:GLU:HG2	1.92	0.51
2:F:360:ARG:CZ	2:F:766:ALA:HB2	2.40	0.51
3:D:279:MET:O	3:D:281:ARG:N	2.44	0.51
3:D:462:MET:HE1	3:D:534:TRP:NE1	2.25	0.51
2:F:28:ASP:H	2:F:29:PRO:HD3	1.69	0.51
1:E:815:LEU:HD13	1:E:815:LEU:N	2.25	0.51
2:C:1038:LEU:HD23	2:C:1038:LEU:N	2.25	0.51
1:E:889:ASN:HA	2:F:807:LEU:HD11	1.91	0.51
2:F:551:ASP:HB3	3:G:111:ARG:HH22	1.75	0.51
2:F:334:LEU:HD11	2:F:755:ILE:HG23	1.93	0.51
1:E:136:MET:CE	1:E:374:ILE:HG12	2.41	0.51
2:C:842:ALA:O	2:C:843:HIS:CB	2.59	0.51
3:D:373:ALA:HB1	3:D:380:THR:HB	1.91	0.51
2:F:867:THR:OG1	2:F:868:GLU:N	2.44	0.51
3:D:240:LEU:HD21	3:D:274:ILE:HD12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:255:HIS:ND1	3:G:285:ALA:HB2	2.26	0.51
1:E:824:ARG:HB2	4:Y:16:DA:OP2	2.11	0.51
1:E:282:LEU:N	1:E:283:PRO:CD	2.73	0.51
2:C:104:GLU:CA	2:C:112:ARG:HH11	2.22	0.51
2:F:951:GLN:C	2:F:952:ILE:HD13	2.31	0.51
2:F:406:ARG:HB3	2:F:658:PRO:HG3	1.93	0.51
1:B:1111:TYR:HD1	1:B:1111:TYR:H	1.59	0.51
1:E:610:ASN:HD22	1:E:613:ARG:NH1	2.04	0.51
1:E:1109:LEU:HA	1:E:1112:GLN:OE1	2.10	0.51
2:F:530:ARG:NE	2:F:548:LEU:O	2.37	0.51
2:C:736:ILE:HD12	2:C:736:ILE:N	2.23	0.51
2:F:292:GLU:HB3	2:F:295:VAL:HG22	1.92	0.51
1:B:514:TYR:O	1:B:515:GLN:CG	2.59	0.51
2:C:478:VAL:HG21	2:C:605:THR:HG21	1.92	0.51
1:E:133:CYS:HA	1:E:358:LEU:HD12	1.92	0.51
2:F:460:LEU:N	2:F:461:PRO:HD2	2.25	0.51
1:B:1051:PRO:CD	1:B:1052:PRO:HD2	2.38	0.51
1:B:362:LEU:HD23	1:B:370:LEU:HD23	1.91	0.51
1:B:823:ARG:C	1:B:825:GLY:H	2.14	0.51
4:X:36:DG:C8	4:X:37:DT:H72	2.46	0.51
2:F:354:ASN:HD22	2:F:356:GLU:HB3	1.74	0.51
1:E:667:ALA:C	1:E:669:ASN:H	2.13	0.51
2:F:295:VAL:O	2:F:295:VAL:HG12	2.11	0.51
2:C:33:GLU:OE2	2:C:210:ARG:NH1	2.43	0.51
1:E:153:ILE:HD12	1:E:154:GLU:OE2	2.10	0.51
2:C:571:LEU:HD23	2:C:598:PHE:CE2	2.46	0.51
2:F:611:LEU:HD22	2:F:645:LEU:HD11	1.93	0.51
3:D:354:LEU:H	3:D:354:LEU:HD12	1.75	0.51
1:B:95:PRO:O	1:B:96:LEU:C	2.49	0.51
2:C:457:LEU:O	2:C:460:LEU:HG	2.11	0.51
4:Y:16:DA:C2'	4:Y:17:DG:C8	2.94	0.51
2:C:74:VAL:HA	2:C:80:ILE:HB	1.92	0.51
1:B:591:LEU:HB3	2:C:1095:ARG:HH21	1.74	0.51
1:B:620:MET:HE2	1:B:687:ILE:HD13	1.90	0.51
3:D:228:GLU:C	3:D:230:LYS:H	2.14	0.51
2:C:228:GLN:NE2	2:C:319:SER:H	2.09	0.51
1:B:672:GLU:HG2	2:C:808:PRO:HG2	1.93	0.51
1:E:471:ARG:HH11	1:E:472:GLU:CD	2.14	0.51
1:B:470:PHE:O	1:B:472:GLU:N	2.44	0.51
1:B:471:ARG:H	1:B:471:ARG:HD2	1.75	0.51
3:G:383:LYS:O	3:G:387:GLN:HB2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:394:LEU:HD23	2:C:802:TYR:CB	2.41	0.51
1:E:1072:HIS:O	1:E:1073:GLU:C	2.48	0.51
3:D:417:ARG:NH1	3:D:437:GLU:HB3	2.24	0.51
2:C:865:PRO:C	2:C:867:THR:H	2.13	0.51
1:E:136:MET:HE2	1:E:374:ILE:HG12	1.92	0.51
2:C:81:PRO:HG3	2:C:182:PRO:HB2	1.93	0.51
1:B:626:LEU:C	1:B:626:LEU:HD13	2.31	0.51
1:B:909:LEU:HD22	1:B:1054:GLU:CD	2.29	0.51
3:D:242:ARG:O	3:D:243:LEU:C	2.49	0.51
3:D:244:LEU:HD13	3:D:255:HIS:ND1	2.25	0.51
1:E:442:THR:HG22	1:E:443:LEU:N	2.26	0.51
3:G:286:LEU:CD1	3:G:292:VAL:HG21	2.41	0.51
1:B:584:ARG:HH11	1:B:584:ARG:HG2	1.75	0.51
3:G:233:ILE:N	3:G:233:ILE:HD13	2.25	0.51
1:E:283:PRO:HB3	1:E:314:ASP:OD1	2.10	0.51
3:G:130:ILE:H	3:G:130:ILE:CD1	2.00	0.51
1:B:951:PRO:O	1:B:954:PHE:HB3	2.11	0.51
3:G:229:GLN:HG2	3:G:230:LYS:HD2	1.92	0.51
2:F:1039:PRO:HA	2:F:1113:LEU:HD11	1.92	0.51
2:F:884:LEU:HG	2:F:917:TRP:CH2	2.46	0.51
2:C:688:GLN:O	2:C:689:LEU:HB3	2.11	0.51
2:F:687:ARG:O	2:F:708:ARG:HG2	2.10	0.51
1:E:951:PRO:O	1:E:954:PHE:HB3	2.11	0.51
3:G:344:GLU:HG3	3:G:345:ALA:H	1.75	0.51
2:C:295:VAL:O	2:C:295:VAL:HG12	2.10	0.51
2:F:164:TRP:C	2:F:167:PRO:HD2	2.31	0.51
1:E:732:ASP:OD1	1:E:735:LEU:HD12	2.11	0.51
3:G:562:THR:CB	3:G:594:THR:H	2.22	0.51
2:F:26:LEU:HB2	2:F:210:ARG:NH2	2.25	0.51
2:C:611:LEU:HD23	2:C:611:LEU:O	2.11	0.51
1:E:95:PRO:O	1:E:96:LEU:C	2.49	0.51
1:B:496:GLN:N	1:B:496:GLN:NE2	2.58	0.51
3:D:185:LEU:HD13	3:D:199:ILE:HG21	1.93	0.51
4:Y:2:5IU:H3'	4:Y:3:5IU:C5'	2.40	0.51
1:E:507:GLU:HB3	1:E:827:LYS:HE3	1.92	0.51
3:G:75:ILE:HB	3:G:78:LEU:CD1	2.39	0.51
3:D:570:VAL:HG13	3:D:577:LEU:HD22	1.93	0.51
2:F:989:ALA:CB	2:F:1017:LEU:HD22	2.40	0.51
1:E:514:TYR:O	1:E:515:GLN:CG	2.59	0.51
2:F:33:GLU:O	2:F:60:ILE:HA	2.11	0.51
2:C:717:LEU:HD22	2:C:721:ILE:HG12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:VAL:HG12	1:E:495:THR:HG22	1.93	0.51
2:C:578:LEU:HB3	2:C:634:LEU:HD12	1.93	0.51
2:C:842:ALA:O	2:C:843:HIS:HB2	2.09	0.51
1:E:177:ARG:HE	1:E:181:GLN:HE21	1.58	0.51
3:D:298:ARG:HD3	3:D:314:CYS:HB3	1.93	0.51
3:D:271:ALA:O	3:D:273:MET:N	2.44	0.51
1:E:254:ARG:NH2	4:Y:22:DG:OP1	2.44	0.51
3:G:207:LYS:HE2	3:G:211:ARG:NH2	2.25	0.51
3:G:216:LEU:O	3:G:220:LEU:CB	2.46	0.51
2:F:103:LEU:HD22	2:F:112:ARG:HA	1.92	0.51
1:B:222:HIS:CE1	1:B:272:TRP:HH2	2.29	0.51
2:C:1035:LEU:O	2:C:1036:LEU:O	2.29	0.51
2:C:1037:VAL:C	2:C:1038:LEU:HD23	2.31	0.51
1:B:39:ARG:HG3	1:B:39:ARG:HH11	1.76	0.51
2:F:251:ILE:HB	2:F:286:LEU:HD13	1.92	0.51
3:G:178:THR:HG23	3:G:179:THR:N	2.25	0.51
2:C:26:LEU:HD22	2:C:33:GLU:OE1	2.11	0.51
2:C:445:ARG:NH1	2:C:452:GLU:OE1	2.44	0.51
3:G:255:HIS:CG	3:G:256:HIS:N	2.75	0.51
3:D:233:ILE:HD13	3:D:233:ILE:N	2.26	0.51
1:B:987:GLU:O	1:B:991:THR:HG22	2.10	0.51
3:D:226:THR:C	3:D:228:GLU:N	2.61	0.51
1:E:92:THR:HG21	1:E:97:TYR:HB2	1.93	0.51
3:D:79:GLN:O	3:D:81:TRP:N	2.43	0.51
1:B:762:VAL:HG13	1:B:791:GLU:CD	2.30	0.51
2:C:8:ASN:ND2	2:C:343:LEU:HD11	2.26	0.51
1:E:1142:PHE:O	1:E:1144:ARG:O	2.29	0.51
2:F:87:ASN:O	2:F:87:ASN:ND2	2.43	0.51
1:E:685:THR:HG21	1:E:729:LEU:HD12	1.93	0.51
1:E:119:ARG:HD3	2:F:302:SER:CB	2.41	0.51
2:C:611:LEU:HD22	2:C:645:LEU:HD11	1.93	0.51
2:C:344:GLU:HB3	2:C:346:GLU:OE2	2.11	0.51
2:F:428:SER:O	2:F:429:ALA:C	2.50	0.51
2:C:1078:ASN:OD1	4:X:11:DA:N7	2.45	0.50
1:B:1161:ASN:O	1:B:1162:ALA:HB3	2.11	0.50
2:F:1038:LEU:N	2:F:1038:LEU:HD23	2.25	0.50
1:B:861:CYS:HA	1:B:865:ILE:HB	1.93	0.50
1:B:415:PRO:HB3	1:B:430:TYR:CE2	2.47	0.50
1:B:1172:PHE:CD1	1:B:1172:PHE:C	2.84	0.50
2:F:578:LEU:HB3	2:F:634:LEU:HD12	1.93	0.50
2:C:995:GLU:HG2	2:C:996:SER:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1087:ASP:O	2:C:1091:GLN:HG2	2.11	0.50
3:D:526:ARG:NH1	3:D:536:MET:CE	2.72	0.50
3:D:229:GLN:HG2	3:D:230:LYS:HD2	1.92	0.50
1:B:92:THR:HG21	1:B:97:TYR:HB2	1.92	0.50
1:E:172:CYS:HA	1:E:175:LEU:HG	1.93	0.50
1:E:899:ASP:CB	1:E:1059:ARG:HH12	2.17	0.50
2:C:749:GLN:OE1	2:C:752:ILE:HD11	2.11	0.50
1:B:385:GLU:HG3	1:B:387:GLN:HE22	1.76	0.50
1:E:763:GLN:CA	1:E:763:GLN:HE21	2.24	0.50
2:F:33:GLU:OE2	2:F:210:ARG:NH1	2.44	0.50
1:E:496:GLN:N	1:E:496:GLN:HE21	2.08	0.50
2:F:509:ASP:HA	2:F:512:ARG:NH1	2.26	0.50
3:D:271:ALA:C	3:D:273:MET:N	2.65	0.50
3:G:260:PRO:O	3:G:261:LEU:CB	2.57	0.50
3:G:277:PRO:O	3:G:280:SER:OG	2.30	0.50
2:F:885:LEU:HD12	2:F:969:PRO:CG	2.32	0.50
2:F:971:LEU:HD21	2:F:1001:ARG:NH2	2.27	0.50
2:C:971:LEU:CD2	4:X:10:DA:H5'	2.39	0.50
1:E:531:GLN:NE2	1:E:879:GLN:HB2	2.23	0.50
3:D:233:ILE:C	3:D:235:GLU:N	2.65	0.50
1:B:804:VAL:O	1:B:808:ARG:HG2	2.11	0.50
1:B:200:TYR:C	1:B:202:GLN:H	2.15	0.50
3:G:106:ARG:NH2	3:G:598:SER:O	2.44	0.50
2:F:828:LEU:HD13	2:F:1028:ARG:CG	2.35	0.50
2:C:972:LEU:HA	2:C:1000:LEU:CD1	2.41	0.50
1:B:920:LEU:HD23	2:C:650:ILE:HG13	1.92	0.50
3:D:562:THR:HG21	3:D:594:THR:CG2	2.39	0.50
3:G:533:THR:C	3:G:535:ALA:H	2.14	0.50
3:D:550:ALA:CB	3:D:578:SER:HB2	2.42	0.50
2:F:2:LEU:HD23	2:F:236:ILE:CG2	2.41	0.50
1:B:52:ARG:CG	1:B:52:ARG:HH21	2.24	0.50
3:D:397:LEU:HD13	3:D:580:TYR:CE2	2.45	0.50
1:E:600:LEU:O	1:E:604:MET:HB2	2.11	0.50
3:D:31:GLU:O	3:D:32:HIS:C	2.49	0.50
2:C:867:THR:OG1	2:C:868:GLU:N	2.44	0.50
3:D:556:GLN:O	3:D:557:ARG:CB	2.59	0.50
2:F:1077:GLY:H	2:F:1083:GLY:CA	2.24	0.50
2:F:699:GLN:C	2:F:701:PRO:HD3	2.31	0.50
3:D:414:GLY:C	3:D:416:GLY:H	2.14	0.50
4:X:45:DT:H2''	4:X:46:5IU:H5'	1.94	0.50
1:B:524:ALA:O	1:B:527:ARG:HG3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:186:ALA:HB2	3:G:223:LEU:HD11	1.93	0.50
2:F:103:LEU:HD11	2:F:115:LEU:CD1	2.41	0.50
1:E:900:ASN:ND2	1:E:902:ARG:HG3	2.26	0.50
2:F:556:LEU:HB3	4:Y:1:5IU:I5	2.82	0.50
3:G:226:THR:HG22	3:G:226:THR:O	2.11	0.50
2:F:872:LEU:HD22	2:F:880:ILE:HD12	1.92	0.50
1:E:1102:MET:HA	1:E:1102:MET:HE3	1.94	0.50
1:B:375:ARG:CZ	1:B:404:GLN:NE2	2.73	0.50
1:B:355:LEU:HD11	1:B:392:GLN:NE2	2.27	0.50
1:E:390:ASP:HA	1:E:429:THR:HG21	1.92	0.50
1:E:732:ASP:C	1:E:734:HIS:H	2.13	0.50
3:D:330:SER:HB3	3:D:337:VAL:N	2.26	0.50
1:E:42:LEU:CB	1:E:44:LEU:HD13	2.42	0.50
2:C:505:GLY:O	2:C:523:THR:HB	2.11	0.50
2:F:98:LEU:HD21	2:F:175:TYR:CD2	2.46	0.50
3:G:556:GLN:HA	3:G:585:ILE:HD12	1.94	0.50
2:F:102:LEU:HD11	2:F:171:ALA:CB	2.41	0.50
1:E:199:ARG:HH11	1:E:199:ARG:HG3	1.76	0.50
1:B:199:ARG:HH11	1:B:199:ARG:HG3	1.76	0.50
2:F:850:GLN:HG2	2:F:856:ASN:OD1	2.11	0.50
1:E:931:VAL:HG12	1:E:932:ALA:N	2.27	0.50
1:B:1118:LEU:O	1:B:1122:LEU:HG	2.12	0.50
2:C:482:ARG:HH11	2:C:482:ARG:HG2	1.75	0.50
1:E:469:MET:O	1:E:470:PHE:CD2	2.65	0.50
2:C:258:ALA:HA	2:C:261:LEU:CG	2.37	0.50
2:F:955:TRP:O	2:F:957:PRO:HD3	2.11	0.50
2:F:717:LEU:HD22	2:F:721:ILE:HG12	1.94	0.50
3:G:417:ARG:NH1	3:G:437:GLU:HB3	2.27	0.50
1:E:942:PRO:HB3	1:E:993:TRP:CE2	2.47	0.50
2:C:470:VAL:O	2:C:473:LEU:HB2	2.10	0.50
1:E:838:LEU:O	1:E:838:LEU:HD22	2.12	0.50
3:G:243:LEU:CD1	3:G:261:LEU:CD2	2.77	0.50
2:F:970:SER:HB2	4:Y:10:DA:OP2	2.12	0.50
3:D:218:LYS:HA	3:D:221:ARG:HD2	1.93	0.50
1:B:704:GLU:CD	1:B:704:GLU:H	2.12	0.50
1:B:362:LEU:O	1:B:399:ARG:HD3	2.12	0.50
1:E:497:PRO:HG3	1:E:866:ALA:HB3	1.93	0.50
2:C:138:TYR:HE1	2:C:165:GLN:NE2	2.10	0.50
1:B:1043:PHE:HD2	1:B:1161:ASN:CB	2.25	0.50
1:B:256:LYS:HA	1:B:259:ARG:HD2	1.92	0.50
1:B:259:ARG:O	1:B:262:GLN:NE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1013:ALA:O	2:C:1017:LEU:HD23	2.12	0.50
2:F:29:PRO:O	2:F:30:PHE:HB2	2.12	0.50
1:E:471:ARG:CD	1:E:471:ARG:H	2.24	0.50
1:E:417:GLN:HG2	1:E:804:VAL:HG22	1.94	0.50
3:G:106:ARG:CZ	3:G:598:SER:O	2.60	0.50
1:E:65:THR:HB	1:E:68:ALA:CB	2.40	0.50
1:E:769:HIS:HD2	1:E:793:GLU:OE1	1.94	0.50
1:B:170:ARG:HA	2:C:517:PRO:CG	2.42	0.50
2:F:108:PHE:CD1	2:F:108:PHE:N	2.80	0.50
2:C:920:GLN:OE1	2:C:920:GLN:HA	2.12	0.50
3:D:274:ILE:CG2	3:D:279:MET:HG2	2.42	0.50
3:G:243:LEU:HD12	3:G:244:LEU:HG	1.92	0.50
1:B:283:PRO:HB3	1:B:314:ASP:OD1	2.12	0.50
1:E:222:HIS:CE1	1:E:272:TRP:HH2	2.30	0.50
1:E:200:TYR:C	1:E:202:GLN:H	2.15	0.50
1:B:577:PRO:HB2	1:B:735:LEU:HD22	1.94	0.50
2:F:834:LEU:CD2	2:F:986:VAL:HG21	2.41	0.50
2:F:997:ARG:HG2	2:F:997:ARG:NH1	2.27	0.50
1:B:1072:HIS:O	1:B:1073:GLU:C	2.50	0.50
1:E:878:TRP:O	1:E:880:VAL:N	2.45	0.50
2:F:25:ARG:CG	2:F:25:ARG:NH1	2.73	0.50
1:E:375:ARG:CZ	1:E:404:GLN:NE2	2.75	0.50
1:E:626:LEU:O	1:E:630:THR:HG23	2.12	0.50
2:C:460:LEU:N	2:C:461:PRO:HD2	2.26	0.50
2:C:108:PHE:CD1	2:C:108:PHE:N	2.80	0.50
1:B:1101:ALA:HA	1:B:1104:ALA:HB3	1.94	0.50
1:B:177:ARG:HE	1:B:181:GLN:HE21	1.58	0.50
1:E:876:GLN:N	1:E:877:PRO:HD2	2.27	0.50
1:E:1043:PHE:O	1:E:1161:ASN:ND2	2.43	0.50
2:F:52:GLN:O	2:F:54:PHE:N	2.41	0.50
1:E:187:TRP:HZ3	1:E:196:ASP:OD2	1.94	0.50
2:C:406:ARG:HB3	2:C:658:PRO:HG3	1.94	0.50
2:C:687:ARG:O	2:C:708:ARG:HG2	2.12	0.50
3:G:463:GLN:C	3:G:465:LYS:H	2.14	0.50
2:C:87:ASN:ND2	2:C:90:SER:H	2.08	0.50
2:C:200:ALA:O	2:C:202:THR:N	2.43	0.50
2:F:995:GLU:HG2	2:F:996:SER:H	1.76	0.50
3:G:266:LEU:HD12	3:G:267:VAL:N	2.27	0.50
1:B:282:LEU:N	1:B:283:PRO:CD	2.74	0.50
3:G:157:ALA:HB2	3:G:355:LEU:CD2	2.38	0.50
3:G:181:VAL:HG21	3:G:295:LEU:HD13	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:157:ALA:CB	3:G:355:LEU:HD21	2.39	0.50
3:D:175:THR:HG21	3:D:355:LEU:CB	2.39	0.50
3:G:533:THR:O	3:G:535:ALA:N	2.34	0.50
2:C:529:THR:O	2:C:533:LEU:HB2	2.12	0.50
2:C:1082:ARG:HH11	2:C:1082:ARG:HB2	1.76	0.50
1:E:1172:PHE:C	1:E:1172:PHE:CD1	2.85	0.50
2:F:457:LEU:O	2:F:460:LEU:HG	2.12	0.50
1:E:180:ALA:HB3	2:F:911:ALA:HB1	1.93	0.50
1:E:332:LEU:O	1:E:336:ARG:HG3	2.12	0.50
1:E:473:ILE:HG22	1:E:473:ILE:O	2.11	0.50
3:D:304:VAL:HG21	3:D:564:GLU:CG	2.34	0.49
1:E:237:ARG:HE	1:E:266:ILE:CG2	2.24	0.49
1:B:791:GLU:OE2	1:B:794:ARG:HD3	2.11	0.49
2:F:709:ARG:NH2	2:F:709:ARG:HG2	2.21	0.49
1:B:1102:MET:HA	1:B:1102:MET:HE3	1.94	0.49
3:G:525:SER:C	3:G:527:LEU:H	2.14	0.49
1:B:681:GLU:O	1:B:685:THR:HG23	2.10	0.49
2:F:358:PHE:CZ	2:F:768:ASN:OD1	2.65	0.49
1:B:8:LEU:HB2	1:B:441:TYR:HB3	1.92	0.49
1:E:711:LEU:O	1:E:712:SER:C	2.50	0.49
3:D:71:CYS:CB	3:D:74:GLU:HB3	2.41	0.49
2:F:842:ALA:O	2:F:843:HIS:CB	2.60	0.49
2:C:107:ASP:HB3	2:C:108:PHE:CD1	2.47	0.49
1:B:700:GLN:O	1:B:701:LEU:HD23	2.12	0.49
3:G:51:VAL:HG13	3:G:112:MET:SD	2.52	0.49
1:E:947:ARG:CD	1:E:1086:LEU:HD21	2.42	0.49
1:B:931:VAL:HG12	1:B:932:ALA:N	2.27	0.49
1:B:362:LEU:CD1	1:B:396:ILE:HG23	2.41	0.49
3:G:228:GLU:C	3:G:230:LYS:H	2.14	0.49
1:B:497:PRO:HG3	1:B:866:ALA:HB3	1.93	0.49
2:F:78:PRO:HD2	2:F:192:ARG:HH11	1.77	0.49
2:F:405:PRO:HG2	2:F:658:PRO:HB2	1.93	0.49
1:B:423:ARG:O	1:B:423:ARG:HD2	2.10	0.49
2:F:519:THR:CG2	2:F:521:GLN:H	2.21	0.49
1:E:385:GLU:HG3	1:E:387:GLN:HE22	1.76	0.49
2:F:262:THR:O	2:F:273:GLU:HG3	2.13	0.49
1:E:1111:TYR:H	1:E:1111:TYR:HD1	1.60	0.49
3:D:178:THR:HG23	3:D:179:THR:N	2.27	0.49
2:F:948:ASN:ND2	2:F:948:ASN:C	2.65	0.49
1:B:1068:LEU:HD12	1:B:1069:VAL:H	1.77	0.49
2:F:344:GLU:HB3	2:F:346:GLU:OE2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:112:ARG:CG	2:C:112:ARG:HH11	2.26	0.49
1:B:133:CYS:HA	1:B:358:LEU:HD12	1.93	0.49
1:B:900:ASN:ND2	1:B:902:ARG:HG3	2.27	0.49
2:C:29:PRO:O	2:C:30:PHE:HB2	2.12	0.49
1:E:1131:TYR:CE2	1:E:1162:ALA:HB2	2.48	0.49
2:C:397:LEU:CD2	2:C:403:LEU:HD13	2.37	0.49
1:E:54:LEU:HD13	1:E:380:VAL:CG1	2.43	0.49
2:F:161:ALA:O	2:F:165:GLN:HG3	2.13	0.49
2:C:185:HIS:CE1	2:C:188:ASN:HD22	2.30	0.49
3:G:397:LEU:HD13	3:G:580:TYR:CE2	2.48	0.49
3:G:71:CYS:CB	3:G:74:GLU:HB3	2.42	0.49
2:F:81:PRO:HG3	2:F:182:PRO:CB	2.42	0.49
1:E:243:LEU:HD22	1:E:259:ARG:HH12	1.76	0.49
3:G:166:ILE:HD12	3:G:166:ILE:N	2.27	0.49
2:C:971:LEU:HD21	2:C:1001:ARG:NH2	2.28	0.49
3:D:216:LEU:O	3:D:220:LEU:CB	2.48	0.49
2:C:832:VAL:O	2:C:833:PRO:C	2.51	0.49
1:E:762:VAL:HG13	1:E:791:GLU:CD	2.32	0.49
1:B:628:ILE:O	1:B:632:ASN:ND2	2.46	0.49
2:C:203:CYS:HB2	2:C:204:PRO:HD2	1.94	0.49
3:D:562:THR:CB	3:D:594:THR:H	2.23	0.49
3:G:15:GLN:O	3:G:16:LEU:HB3	2.11	0.49
3:D:550:ALA:HB2	3:D:578:SER:HB2	1.94	0.49
3:D:326:ALA:HB1	3:D:337:VAL:O	2.12	0.49
1:E:675:LEU:CD1	2:F:809:ALA:HB1	2.43	0.49
1:B:905:SER:HB3	1:B:1063:LYS:HB2	1.94	0.49
3:G:147:VAL:O	3:G:147:VAL:HG12	2.12	0.49
3:D:244:LEU:HD13	3:D:255:HIS:CG	2.48	0.49
3:D:65:HIS:O	3:D:66:PRO:C	2.51	0.49
3:G:185:LEU:HD13	3:G:199:ILE:HG21	1.95	0.49
1:B:172:CYS:HA	1:B:175:LEU:HG	1.94	0.49
2:C:405:PRO:C	2:C:658:PRO:HB3	2.32	0.49
1:E:954:PHE:O	1:E:957:SER:HB3	2.12	0.49
2:F:130:LYS:CD	2:F:692:LEU:HD21	2.38	0.49
2:F:412:VAL:O	2:F:663:THR:HG22	2.12	0.49
3:G:178:THR:HG23	3:G:179:THR:H	1.76	0.49
1:E:213:PRO:C	1:E:215:ASP:H	2.14	0.49
2:F:571:LEU:HD23	2:F:598:PHE:CE2	2.48	0.49
2:C:1077:GLY:H	2:C:1083:GLY:CA	2.26	0.49
2:C:587:TRP:CH2	2:C:634:LEU:HG	2.47	0.49
2:F:716:PHE:CB	2:F:747:LEU:HD13	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ALA:O	1:B:169:ARG:HG3	2.12	0.49
1:B:1024:TYR:O	2:C:51:SER:HB2	2.13	0.49
3:G:253:LEU:HB3	3:G:255:HIS:CD2	2.47	0.49
2:C:1055:ASP:CG	2:C:1118:ARG:NH2	2.65	0.49
1:B:507:GLU:HA	1:B:850:ALA:HB1	1.95	0.49
1:B:581:LEU:HD11	1:B:737:GLN:OE1	2.12	0.49
2:C:412:VAL:O	2:C:663:THR:HG22	2.11	0.49
2:F:749:GLN:OE1	2:F:752:ILE:HD11	2.12	0.49
2:F:277:PHE:CD1	2:F:278:ARG:HG3	2.47	0.49
3:G:525:SER:O	3:G:527:LEU:N	2.45	0.49
2:F:768:ASN:HB3	2:F:771:GLU:HB2	1.95	0.49
1:E:964:PHE:N	1:E:964:PHE:CD2	2.69	0.49
3:G:553:LEU:HB3	3:G:554:PRO:HD2	1.94	0.49
2:F:832:VAL:O	2:F:832:VAL:CG2	2.61	0.49
2:F:1077:GLY:H	2:F:1083:GLY:N	2.09	0.49
1:B:1046:LEU:C	1:B:1048:ALA:H	2.16	0.49
2:C:428:SER:O	2:C:429:ALA:C	2.50	0.49
1:E:134:GLN:HB3	1:E:354:MET:SD	2.53	0.49
3:G:271:ALA:C	3:G:273:MET:N	2.64	0.49
3:G:244:LEU:CD1	3:G:285:ALA:CB	2.88	0.49
3:G:233:ILE:C	3:G:235:GLU:N	2.65	0.49
2:C:103:LEU:HD22	2:C:112:ARG:HA	1.94	0.49
1:B:1132:GLU:HA	1:B:1159:ARG:HH22	1.78	0.49
2:F:1037:VAL:C	2:F:1038:LEU:HD23	2.33	0.49
3:D:349:ARG:HH11	3:D:349:ARG:CB	2.26	0.49
1:E:1118:LEU:O	1:E:1122:LEU:HG	2.12	0.49
3:D:56:SER:C	3:D:58:LEU:N	2.65	0.49
3:D:597:ARG:O	3:D:598:SER:CB	2.52	0.49
2:C:884:LEU:O	2:C:888:LEU:HG	2.13	0.49
1:B:610:ASN:HD22	1:B:613:ARG:NH1	2.07	0.49
2:F:832:VAL:O	2:F:833:PRO:C	2.51	0.49
1:B:646:ASP:O	1:B:649:ARG:CG	2.61	0.49
1:B:29:LYS:HD3	1:B:33:ILE:HD11	1.95	0.49
1:B:173:TYR:N	1:B:174:PRO:HD2	2.28	0.49
3:G:414:GLY:C	3:G:416:GLY:H	2.15	0.49
2:F:391:ASP:OD2	2:F:801:SER:HA	2.12	0.49
3:G:270:GLU:OE1	3:G:273:MET:HE2	2.12	0.49
4:Y:45:DT:H2''	4:Y:46:5IU:H5'	1.95	0.49
3:G:597:ARG:O	3:G:598:SER:CB	2.52	0.49
1:B:471:ARG:H	1:B:471:ARG:CD	2.25	0.49
2:F:411:MET:HB3	2:F:664:LEU:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:672:GLU:HG2	2:F:808:PRO:HG2	1.95	0.49
3:D:157:ALA:HB2	3:D:355:LEU:CD2	2.39	0.49
2:F:260:LEU:C	2:F:262:THR:H	2.16	0.49
1:B:763:GLN:CA	1:B:763:GLN:HE21	2.25	0.49
2:F:947:CYS:O	2:F:948:ASN:ND2	2.45	0.49
1:E:173:TYR:N	1:E:174:PRO:HD2	2.27	0.49
2:C:941:MET:HG2	2:C:942:GLU:N	2.27	0.49
2:F:865:PRO:C	2:F:867:THR:H	2.16	0.49
2:F:1048:THR:OG1	2:F:1070:LYS:HG3	2.13	0.49
2:F:355:ILE:N	2:F:355:ILE:HD12	2.27	0.49
3:D:204:PRO:CB	4:X:2:5IU:H6	2.42	0.49
2:C:858:ARG:HB2	2:C:858:ARG:CZ	2.42	0.49
3:G:185:LEU:HA	3:G:188:LEU:HB2	1.95	0.49
3:G:185:LEU:HD23	3:G:188:LEU:HD12	1.95	0.49
3:G:211:ARG:HA	3:G:214:GLU:CG	2.43	0.49
1:B:237:ARG:HH21	1:B:266:ILE:CG2	2.25	0.49
2:F:482:ARG:NH1	2:F:482:ARG:HG2	2.27	0.49
3:D:91:VAL:HA	3:D:98:THR:HG21	1.93	0.49
1:E:365:GLU:CG	1:E:366:SER:N	2.76	0.49
1:B:491:PHE:O	1:B:493:GLY:N	2.46	0.49
2:C:99:LEU:N	2:C:100:PRO:HD2	2.28	0.49
1:E:692:GLU:HG2	2:F:383:GLN:HG3	1.95	0.49
2:C:483:PHE:CE2	2:C:567:LEU:HA	2.47	0.49
1:B:604:MET:HG3	1:B:705:HIS:CE1	2.48	0.49
3:D:226:THR:O	3:D:226:THR:HG22	2.13	0.49
1:B:221:ARG:HG2	1:B:221:ARG:HH11	1.77	0.49
3:G:79:GLN:O	3:G:81:TRP:N	2.45	0.49
3:G:349:ARG:CB	3:G:349:ARG:HH11	2.26	0.49
1:E:672:GLU:O	2:F:814:GLY:HA3	2.13	0.49
2:C:239:LEU:N	2:C:239:LEU:CD1	2.76	0.49
2:F:5:TYR:CD2	2:F:323:LEU:HD11	2.48	0.49
1:E:1139:ILE:HD13	1:E:1157:THR:HG23	1.95	0.49
2:F:87:ASN:ND2	2:F:90:SER:H	2.08	0.49
2:F:539:SER:CB	2:F:551:ASP:OD1	2.61	0.49
1:B:771:ARG:HD3	1:B:789:LEU:HD22	1.94	0.49
2:F:250:ASP:CG	2:F:291:GLY:HA3	2.34	0.49
3:D:117:ARG:HA	3:D:603:LEU:HD13	1.95	0.49
1:E:148:PHE:H	2:F:126:GLN:NE2	2.09	0.49
3:G:150:GLU:O	3:G:151:ILE:C	2.51	0.49
2:F:388:VAL:HG22	2:F:799:ARG:NH1	2.28	0.49
3:D:359:TYR:O	3:D:360:ARG:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:212:LEU:HD22	3:D:216:LEU:CD1	2.43	0.48
2:C:80:ILE:CD1	2:C:189:LEU:HD21	2.41	0.48
2:C:103:LEU:HD11	2:C:115:LEU:CD1	2.43	0.48
1:B:598:TRP:CH2	2:C:857:PHE:HB3	2.46	0.48
2:F:77:LEU:HD23	2:F:196:THR:HG21	1.95	0.48
1:E:799:LEU:HD23	1:E:837:ALA:CB	2.41	0.48
1:E:754:LEU:HB3	1:E:757:ILE:HB	1.93	0.48
3:G:570:VAL:HG13	3:G:577:LEU:HD22	1.95	0.48
2:F:254:PRO:O	2:F:257:LEU:HG	2.13	0.48
2:C:973:SER:OG	2:C:976:GLN:HB2	2.13	0.48
2:F:408:ILE:HG23	2:F:674:VAL:CG1	2.43	0.48
3:D:300:GLN:NE2	3:D:568:THR:HA	2.28	0.48
1:E:1066:ILE:HG21	1:E:1069:VAL:CG2	2.42	0.48
3:G:556:GLN:O	3:G:557:ARG:HG3	2.13	0.48
2:F:920:GLN:HA	2:F:920:GLN:OE1	2.13	0.48
3:G:278:MET:CG	3:G:279:MET:N	2.73	0.48
1:B:874:ASP:O	1:B:875:ASN:HB2	2.11	0.48
4:Y:15:DG:H2''	4:Y:16:DA:C8	2.48	0.48
4:Y:47:DA:C2'	4:Y:48:DG:H5''	2.42	0.48
1:B:500:LYS:NZ	1:B:868:GLN:HG3	2.28	0.48
1:E:791:GLU:OE2	1:E:794:ARG:HD3	2.14	0.48
4:Y:36:DG:C8	4:Y:37:DT:H72	2.48	0.48
1:B:1098:MET:CE	1:B:1156:TYR:HB2	2.43	0.48
1:E:1098:MET:HE3	1:E:1142:PHE:CD1	2.47	0.48
3:G:91:VAL:CG1	3:G:100:MET:HB2	2.42	0.48
3:D:28:ALA:HB1	3:D:35:VAL:HG23	1.95	0.48
1:B:1066:ILE:HG21	1:B:1069:VAL:CG2	2.43	0.48
2:F:61:ASP:HB3	2:F:63:PRO:HD3	1.94	0.48
1:B:447:TRP:O	1:B:448:ARG:HB2	2.13	0.48
4:X:34:DC:H1'	4:X:35:DA:C5'	2.43	0.48
1:B:552:SER:HB3	1:B:733:LYS:O	2.13	0.48
1:B:268:LYS:HA	1:B:268:LYS:CE	2.43	0.48
1:E:231:THR:O	1:E:234:GLN:HB2	2.14	0.48
3:G:246:ALA:HB1	3:G:251:GLN:HE22	1.79	0.48
1:B:1085:TRP:HD1	1:B:1087:GLY:HA3	1.78	0.48
1:E:1161:ASN:C	1:E:1163:GLY:H	2.17	0.48
2:C:685:TYR:O	2:C:686:PRO:C	2.51	0.48
1:B:1139:ILE:HD13	1:B:1157:THR:HG23	1.96	0.48
2:F:529:THR:O	2:F:533:LEU:HB2	2.13	0.48
3:D:562:THR:HG21	3:D:594:THR:CA	2.43	0.48
2:C:304:GLY:HA2	2:C:714:TYR:CD1	2.41	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:462:MET:HE1	3:G:534:TRP:NE1	2.27	0.48
2:C:250:ASP:CG	2:C:291:GLY:HA3	2.34	0.48
2:C:294:ASP:C	2:C:296:GLY:N	2.67	0.48
1:E:769:HIS:HA	1:E:775:GLU:O	2.12	0.48
2:F:2:LEU:HD23	2:F:236:ILE:HB	1.94	0.48
2:C:948:ASN:ND2	2:C:948:ASN:C	2.66	0.48
2:C:61:ASP:HB3	2:C:63:PRO:HD3	1.94	0.48
3:G:449:PHE:O	3:G:450:GLY:O	2.30	0.48
2:C:670:ILE:CG2	2:C:671:PRO:HD2	2.43	0.48
2:C:535:TYR:HD1	2:C:558:ALA:HB1	1.78	0.48
1:B:1052:PRO:HD3	1:B:1106:ARG:NH1	2.28	0.48
3:G:279:MET:O	3:G:282:LEU:N	2.46	0.48
4:X:16:DA:C2'	4:X:17:DG:C8	2.96	0.48
1:B:281:GLN:NE2	1:B:283:PRO:HG2	2.29	0.48
3:D:412:LEU:HD13	3:D:462:MET:HG2	1.95	0.48
3:D:440:LEU:HD22	3:D:552:ILE:HD11	1.94	0.48
1:B:1071:ARG:NH1	2:C:29:PRO:HA	2.26	0.48
2:F:318:GLU:OE1	2:F:318:GLU:N	2.46	0.48
1:B:752:VAL:CG1	1:B:809:SER:HB3	2.34	0.48
3:G:549:ALA:O	3:G:577:LEU:HA	2.14	0.48
2:C:709:ARG:NH2	2:C:709:ARG:HG2	2.22	0.48
2:C:304:GLY:O	2:C:307:GLY:N	2.47	0.48
1:E:8:LEU:HB2	1:E:441:TYR:HB3	1.95	0.48
1:E:153:ILE:HG22	1:E:349:LEU:C	2.33	0.48
2:F:796:PRO:HA	2:F:800:GLN:NE2	2.28	0.48
1:E:1119:HIS:ND1	1:E:1129:TYR:OH	2.46	0.48
3:D:137:LEU:HD22	3:D:141:LEU:CD1	2.43	0.48
3:D:261:LEU:CB	3:D:287:PRO:HD3	2.44	0.48
3:D:211:ARG:O	3:D:212:LEU:C	2.52	0.48
1:E:947:ARG:HG3	1:E:1086:LEU:CD1	2.27	0.48
1:B:947:ARG:HG3	1:B:1086:LEU:CD1	2.27	0.48
2:F:556:LEU:O	2:F:559:GLU:HB2	2.13	0.48
1:B:507:GLU:HB3	1:B:827:LYS:HE3	1.96	0.48
1:E:507:GLU:HA	1:E:850:ALA:HB1	1.95	0.48
1:E:1043:PHE:HD2	1:E:1161:ASN:CB	2.26	0.48
1:B:471:ARG:HH11	1:B:472:GLU:CD	2.17	0.48
2:C:441:ASP:O	2:C:649:ARG:NH1	2.46	0.48
1:B:920:LEU:HD23	2:C:650:ILE:HD11	1.96	0.48
2:F:688:GLN:O	2:F:689:LEU:HB3	2.13	0.48
3:G:567:TYR:O	3:G:571:THR:HG23	2.13	0.48
2:C:277:PHE:CD1	2:C:278:ARG:HG3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:THR:HG21	2:C:804:ARG:HE	1.76	0.48
2:C:539:SER:CB	2:C:551:ASP:OD1	2.60	0.48
2:C:25:ARG:CG	2:C:25:ARG:NH1	2.75	0.48
2:F:540:ALA:C	2:F:542:GLY:N	2.67	0.48
2:F:245:ARG:HA	2:F:326:PHE:CZ	2.48	0.48
1:E:919:ASP:OD1	2:F:652:GLN:HB2	2.14	0.48
3:D:270:GLU:HB3	3:D:273:MET:CE	2.43	0.48
1:B:1049:GLY:C	1:B:1051:PRO:HD3	2.34	0.48
1:B:310:PHE:CD2	1:B:310:PHE:C	2.87	0.48
1:B:1043:PHE:O	1:B:1161:ASN:ND2	2.44	0.48
1:B:1131:TYR:CE2	1:B:1162:ALA:HB2	2.48	0.48
2:C:318:GLU:OE1	2:C:318:GLU:N	2.46	0.48
1:E:1074:GLY:C	1:E:1075:ARG:HG2	2.34	0.48
2:C:966:ARG:O	2:C:998:LEU:HA	2.13	0.48
2:C:261:LEU:HD11	2:C:281:GLU:OE1	2.13	0.48
3:G:375:ASN:O	3:G:376:ARG:HG2	2.14	0.48
3:G:418:TYR:OH	3:G:530:HIS:HE1	1.95	0.48
1:E:683:ARG:O	1:E:687:ILE:HG13	2.13	0.48
1:E:771:ARG:HD3	1:E:789:LEU:HD22	1.94	0.48
1:E:14:PRO:HA	1:E:48:ALA:HB1	1.96	0.48
3:G:91:VAL:HG12	3:G:100:MET:HB2	1.94	0.48
1:B:711:LEU:O	1:B:712:SER:C	2.51	0.48
2:C:155:VAL:N	2:C:162:GLN:HE22	2.12	0.48
1:B:237:ARG:NH2	1:B:266:ILE:HG23	2.25	0.48
1:B:669:ASN:HB3	1:B:672:GLU:OE2	2.14	0.48
2:F:77:LEU:HB3	2:F:78:PRO:HD2	1.96	0.48
1:B:490:VAL:HG12	1:B:495:THR:HG22	1.95	0.48
2:F:976:GLN:HG3	2:F:998:LEU:HD11	1.95	0.48
2:F:664:LEU:HD22	2:F:685:TYR:CZ	2.49	0.48
2:C:2:LEU:HD23	2:C:236:ILE:CG2	2.43	0.48
2:C:539:SER:HA	2:C:549:PRO:HG2	1.96	0.48
1:E:760:PHE:CZ	1:E:822:ARG:HG3	2.49	0.48
3:D:567:TYR:O	3:D:571:THR:HG23	2.13	0.48
2:F:138:TYR:HE1	2:F:165:GLN:NE2	2.12	0.48
3:D:556:GLN:HA	3:D:585:ILE:HD12	1.95	0.48
1:B:901:TRP:CE3	1:B:1060:GLY:HA2	2.49	0.48
1:B:496:GLN:N	1:B:496:GLN:HE21	2.12	0.48
1:E:328:ILE:O	1:E:332:LEU:CD2	2.62	0.48
1:E:905:SER:HB3	1:E:1063:LYS:HB2	1.95	0.48
1:B:84:ARG:O	1:B:87:CYS:HB2	2.14	0.48
3:G:242:ARG:C	3:G:242:ARG:HD3	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:GLN:O	1:E:282:LEU:CB	2.60	0.48
1:B:281:GLN:O	1:B:282:LEU:CB	2.61	0.48
3:G:130:ILE:O	3:G:132:VAL:HG23	2.14	0.48
2:C:834:LEU:CD2	2:C:986:VAL:HG21	2.42	0.48
1:B:763:GLN:HE21	1:B:764:GLU:N	2.12	0.48
3:G:550:ALA:CB	3:G:578:SER:HB2	2.44	0.48
1:B:504:MET:CE	1:B:514:TYR:HA	2.43	0.48
1:B:1068:LEU:HD12	1:B:1069:VAL:N	2.29	0.48
3:G:326:ALA:HB1	3:G:337:VAL:O	2.13	0.48
2:C:334:LEU:HD11	2:C:755:ILE:HD12	1.94	0.48
1:B:155:ASP:O	1:B:157:SER:N	2.45	0.48
4:X:15:DG:H2''	4:X:16:DA:C8	2.49	0.48
1:E:826:ASP:O	1:E:827:LYS:C	2.52	0.48
2:C:986:VAL:HG12	2:C:987:TYR:N	2.29	0.48
1:B:667:ALA:C	1:B:669:ASN:H	2.16	0.48
2:C:441:ASP:OD2	2:C:662:CYS:HB2	2.14	0.48
3:G:56:SER:C	3:G:58:LEU:N	2.67	0.48
1:E:954:PHE:CZ	1:E:977:LEU:HD23	2.49	0.48
1:B:1040:ILE:HD11	1:B:1168:MET:HE1	1.96	0.48
3:D:385:VAL:HG11	3:D:396:ARG:CD	2.41	0.48
1:B:24:SER:HB2	1:B:27:THR:HG21	1.95	0.48
2:C:294:ASP:O	2:C:295:VAL:C	2.52	0.48
3:D:6:GLN:HE21	3:D:6:GLN:HB3	1.55	0.48
2:F:294:ASP:C	2:F:296:GLY:N	2.65	0.48
2:F:394:LEU:HD23	2:F:802:TYR:CB	2.44	0.48
1:E:46:GLY:H	1:E:49:ALA:HB2	1.78	0.48
2:F:107:ASP:HB3	2:F:108:PHE:CD1	2.49	0.48
1:E:895:ARG:HG2	1:E:896:LEU:H	1.79	0.48
4:Y:34:DC:H1'	4:Y:35:DA:C5'	2.43	0.48
1:E:1046:LEU:C	1:E:1048:ALA:H	2.18	0.48
3:D:274:ILE:HG23	3:D:278:MET:HG2	1.96	0.48
2:F:1082:ARG:HH11	2:F:1082:ARG:HB2	1.79	0.48
1:B:368:GLU:OE1	1:B:399:ARG:NH1	2.45	0.48
1:B:1077:TYR:CD2	1:B:1137:GLY:HA2	2.49	0.48
1:B:1136:GLY:HA2	1:B:1159:ARG:NH1	2.28	0.48
1:E:1077:TYR:CD2	1:E:1137:GLY:HA2	2.49	0.48
1:E:1136:GLY:HA2	1:E:1159:ARG:NH1	2.28	0.48
2:C:872:LEU:HD13	2:C:916:PHE:CZ	2.47	0.48
2:C:884:LEU:HG	2:C:917:TRP:CH2	2.49	0.48
1:B:387:GLN:HG3	1:B:414:ASP:O	2.14	0.48
1:E:65:THR:CG2	1:E:66:GLU:N	2.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:294:ASP:O	2:F:295:VAL:C	2.52	0.48
1:B:18:GLU:O	1:B:19:ARG:HD3	2.14	0.48
1:B:901:TRP:CH2	1:B:1060:GLY:HA2	2.49	0.48
2:F:185:HIS:CE1	2:F:188:ASN:HD22	2.32	0.48
1:E:905:SER:O	1:E:906:TYR:C	2.52	0.48
1:B:677:THR:O	1:B:678:ALA:O	2.31	0.48
3:D:65:HIS:CB	3:D:66:PRO:CD	2.72	0.47
3:G:211:ARG:O	3:G:212:LEU:C	2.52	0.47
1:B:1084:ASN:O	1:B:1085:TRP:O	2.31	0.47
3:D:132:VAL:HG12	3:D:133:ASP:H	1.79	0.47
1:E:522:CYS:O	1:E:526:ILE:HD13	2.14	0.47
3:D:461:PHE:CZ	3:D:465:LYS:HE3	2.49	0.47
2:F:830:GLU:O	2:F:831:THR:OG1	2.20	0.47
1:E:269:ILE:HG22	1:E:270:SER:N	2.29	0.47
1:B:899:ASP:CB	1:B:1059:ARG:HH12	2.18	0.47
1:E:1132:GLU:HA	1:E:1159:ARG:HH22	1.79	0.47
3:D:597:ARG:HH11	3:D:598:SER:CB	2.27	0.47
2:F:685:TYR:O	2:F:686:PRO:C	2.51	0.47
2:C:354:ASN:HD22	2:C:356:GLU:HB3	1.75	0.47
1:B:1040:ILE:HG23	1:B:1112:GLN:NE2	2.28	0.47
2:C:262:THR:O	2:C:273:GLU:HG3	2.13	0.47
2:C:1042:GLY:O	2:C:1046:LEU:HB2	2.13	0.47
3:D:178:THR:HG23	3:D:179:THR:H	1.78	0.47
3:D:150:GLU:O	3:D:151:ILE:C	2.52	0.47
2:C:571:LEU:O	2:C:575:ARG:HB3	2.15	0.47
1:B:365:GLU:CG	1:B:366:SER:N	2.77	0.47
1:E:452:GLY:HA2	1:E:864:ASP:OD1	2.15	0.47
1:E:84:ARG:O	1:E:87:CYS:HB2	2.14	0.47
1:E:268:LYS:HA	1:E:268:LYS:CE	2.44	0.47
2:C:731:TYR:CZ	2:C:744:PRO:HB3	2.49	0.47
3:G:118:THR:HA	3:G:121:ARG:NH1	2.29	0.47
2:C:348:ARG:HG3	2:C:365:ARG:NH1	2.29	0.47
1:B:1074:GLY:C	1:B:1075:ARG:HG2	2.33	0.47
1:B:469:MET:SD	1:B:795:LEU:HD11	2.54	0.47
1:E:646:ASP:O	1:E:649:ARG:CG	2.62	0.47
2:F:233:HIS:O	2:F:234:ILE:HD12	2.14	0.47
1:B:153:ILE:HG13	1:B:154:GLU:N	2.29	0.47
1:B:328:ILE:O	1:B:332:LEU:CD2	2.62	0.47
2:C:1077:GLY:H	2:C:1083:GLY:N	2.11	0.47
2:C:848:PHE:O	2:C:852:ARG:HB3	2.14	0.47
1:B:434:ARG:HH21	1:B:474:PRO:HD2	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:403:ASP:O	3:D:406:ALA:HB3	2.14	0.47
2:F:120:ASP:O	2:F:121:LYS:HB2	2.14	0.47
3:G:403:ASP:O	3:G:406:ALA:HB3	2.13	0.47
1:E:1126:ILE:HD12	1:E:1126:ILE:N	2.29	0.47
3:G:261:LEU:HD23	3:G:261:LEU:HA	1.35	0.47
3:G:199:ILE:HG23	3:G:265:VAL:HG22	1.96	0.47
4:Y:16:DA:C2'	4:Y:17:DG:H8	2.27	0.47
1:E:1084:ASN:O	1:E:1085:TRP:O	2.32	0.47
2:C:104:GLU:N	2:C:112:ARG:HH11	2.12	0.47
1:B:747:LEU:HB3	1:B:749:TYR:CE1	2.49	0.47
1:B:809:SER:HG	1:B:813:CYS:HB2	1.77	0.47
1:E:1070:PHE:CE1	1:E:1077:TYR:HB2	2.49	0.47
1:B:469:MET:O	1:B:470:PHE:CD2	2.66	0.47
2:F:277:PHE:CD1	2:F:278:ARG:N	2.82	0.47
1:B:416:LYS:HE2	1:B:803:TYR:CE2	2.49	0.47
3:D:525:SER:C	3:D:527:LEU:H	2.18	0.47
3:G:300:GLN:NE2	3:G:568:THR:HG22	2.29	0.47
3:D:98:THR:HG23	3:D:99:PRO:HD2	1.96	0.47
1:B:50:PHE:HE2	1:B:52:ARG:HD3	1.77	0.47
1:B:802:LEU:HD22	1:B:806:LEU:CD2	2.45	0.47
3:G:397:LEU:HB2	3:G:580:TYR:CE2	2.49	0.47
2:C:45:TRP:HB2	2:C:670:ILE:HD13	1.96	0.47
3:D:375:ASN:O	3:D:376:ARG:HG2	2.14	0.47
2:F:14:GLU:HG3	2:F:49:THR:HG21	1.95	0.47
1:E:434:ARG:HH21	1:E:474:PRO:HD2	1.79	0.47
4:X:47:DA:C2'	4:X:48:DG:H5''	2.42	0.47
3:D:211:ARG:HA	3:D:214:GLU:CG	2.44	0.47
1:E:286:LEU:CD1	1:E:306:ARG:HD3	2.28	0.47
3:D:230:LYS:C	3:D:232:ARG:N	2.66	0.47
2:C:482:ARG:NH1	2:C:482:ARG:HG2	2.28	0.47
3:G:343:THR:O	3:G:344:GLU:HB2	2.14	0.47
2:C:8:ASN:HD21	2:C:343:LEU:HD11	1.79	0.47
2:C:394:LEU:HD23	2:C:802:TYR:HB2	1.96	0.47
2:C:615:GLN:OE1	2:C:644:ARG:HD3	2.14	0.47
1:B:1007:VAL:HG22	1:B:1072:HIS:CD2	2.49	0.47
2:F:313:LEU:HD21	2:F:703:ARG:HB3	1.97	0.47
1:E:374:ILE:HG21	1:E:400:ILE:HD13	1.97	0.47
3:D:553:LEU:HB3	3:D:554:PRO:HD2	1.97	0.47
1:B:268:LYS:CA	1:B:268:LYS:HE3	2.45	0.47
3:G:11:VAL:HG21	3:G:21:VAL:HG11	1.96	0.47
2:C:716:PHE:CB	2:C:747:LEU:HD13	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:5:5IU:H2'	4:Y:5:5IU:H6	1.47	0.47
3:G:184:LEU:HD11	3:G:293:ILE:CD1	2.45	0.47
3:G:253:LEU:HD13	3:G:255:HIS:HE2	1.79	0.47
1:B:760:PHE:CZ	1:B:822:ARG:HG3	2.50	0.47
3:G:212:LEU:HD22	3:G:216:LEU:CD1	2.44	0.47
1:E:861:CYS:SG	1:E:866:ALA:CA	3.00	0.47
2:C:556:LEU:O	2:C:559:GLU:HB2	2.15	0.47
1:B:689:HIS:HE1	1:B:725:GLN:O	1.97	0.47
2:C:411:MET:HB3	2:C:664:LEU:HD12	1.95	0.47
2:F:142:ARG:O	2:F:145:TRP:HB2	2.14	0.47
1:B:1142:PHE:O	1:B:1144:ARG:O	2.31	0.47
1:B:414:ASP:OD1	1:B:416:LYS:N	2.46	0.47
1:E:355:LEU:HD11	1:E:392:GLN:NE2	2.30	0.47
2:C:540:ALA:C	2:C:542:GLY:N	2.68	0.47
2:C:378:VAL:HG22	2:C:731:TYR:CZ	2.50	0.47
1:B:1119:HIS:ND1	1:B:1129:TYR:OH	2.48	0.47
2:C:388:VAL:HG22	2:C:799:ARG:NH1	2.28	0.47
2:C:915:ILE:O	2:C:919:THR:CG2	2.63	0.47
3:D:256:HIS:CG	3:D:257:ALA:N	2.82	0.47
4:X:2:5IU:H3'	4:X:3:5IU:C5'	2.43	0.47
3:D:440:LEU:HB2	3:D:535:ALA:HA	1.96	0.47
3:D:412:LEU:HD11	3:D:461:PHE:HD2	1.80	0.47
3:D:533:THR:C	3:D:535:ALA:H	2.17	0.47
1:B:902:ARG:HH21	1:B:902:ARG:HG3	1.80	0.47
3:D:51:VAL:HG13	3:D:112:MET:SD	2.54	0.47
1:B:417:GLN:HG2	1:B:804:VAL:HG22	1.96	0.47
2:C:989:ALA:HB1	2:C:1017:LEU:CD2	2.45	0.47
1:B:658:MET:HB2	1:B:695:GLN:HG3	1.95	0.47
3:G:308:ALA:O	3:G:597:ARG:NH2	2.48	0.47
2:C:142:ARG:O	2:C:145:TRP:HB2	2.15	0.47
1:E:362:LEU:HD23	1:E:370:LEU:HD23	1.96	0.47
2:C:87:ASN:ND2	2:C:87:ASN:C	2.67	0.47
1:E:504:MET:HE3	1:E:514:TYR:HA	1.97	0.47
1:E:1068:LEU:HD12	1:E:1069:VAL:H	1.80	0.47
2:F:312:TYR:CD1	2:F:313:LEU:HD23	2.49	0.47
1:E:177:ARG:HE	1:E:181:GLN:NE2	2.12	0.47
2:C:308:ARG:O	2:C:311:ILE:HG22	2.14	0.47
1:E:106:ASP:OD2	1:E:109:GLN:HB2	2.15	0.47
1:B:455:ASN:HD22	1:B:455:ASN:N	2.11	0.47
3:D:185:LEU:HD23	3:D:188:LEU:HD12	1.97	0.47
3:D:242:ARG:O	3:D:242:ARG:HD3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:244:LEU:CD1	3:D:285:ALA:CB	2.93	0.47
2:C:882:GLN:HA	2:C:969:PRO:HG2	1.97	0.47
3:G:254:ARG:HG3	3:G:259:ASN:HD21	1.77	0.47
1:E:1052:PRO:HD3	1:E:1106:ARG:NH1	2.30	0.47
1:B:246:LEU:HD23	1:B:307:HIS:NE2	2.30	0.47
1:E:947:ARG:HD3	1:E:947:ARG:N	2.28	0.47
2:C:160:GLU:C	2:C:162:GLN:N	2.68	0.47
2:C:30:PHE:O	2:C:32:PRO:HD3	2.15	0.47
2:F:1030:GLY:HA2	2:F:1035:LEU:HB2	1.97	0.47
1:B:826:ASP:O	1:B:827:LYS:C	2.52	0.47
2:C:832:VAL:CG2	2:C:832:VAL:O	2.59	0.47
3:G:52:CYS:SG	3:G:106:ARG:HG2	2.54	0.47
3:G:108:TYR:HB2	3:G:113:TRP:HB2	1.96	0.47
2:F:880:ILE:HG23	2:F:901:PHE:CE1	2.50	0.47
4:X:37:DT:H1'	4:X:38:DG:H5''	1.97	0.47
2:C:254:PRO:O	2:C:257:LEU:HG	2.15	0.47
2:F:749:GLN:HA	2:F:752:ILE:HD11	1.97	0.47
1:E:610:ASN:ND2	1:E:613:ARG:NH1	2.59	0.47
1:B:416:LYS:HE2	1:B:803:TYR:CZ	2.50	0.47
2:F:87:ASN:C	2:F:87:ASN:ND2	2.68	0.47
2:C:545:GLN:C	2:C:547:VAL:H	2.17	0.47
2:F:393:LEU:HD22	2:F:408:ILE:HG21	1.96	0.47
3:D:120:ALA:HA	3:D:604:PHE:CE2	2.50	0.47
3:G:91:VAL:HA	3:G:98:THR:HG21	1.95	0.47
1:B:646:ASP:O	1:B:649:ARG:HG3	2.14	0.47
2:F:478:VAL:HG13	2:F:600:LEU:O	2.14	0.47
2:C:947:CYS:O	2:C:948:ASN:ND2	2.45	0.47
2:F:239:LEU:N	2:F:239:LEU:CD1	2.78	0.47
1:E:181:GLN:HB2	2:F:915:ILE:HD11	1.97	0.47
1:E:199:ARG:HG3	1:E:199:ARG:NH1	2.29	0.47
1:B:629:GLU:CD	2:C:852:ARG:HH12	2.18	0.47
3:G:137:LEU:HD22	3:G:141:LEU:CD1	2.44	0.47
1:E:1101:ALA:HA	1:E:1104:ALA:HB3	1.95	0.47
1:E:415:PRO:HB3	1:E:430:TYR:CE2	2.50	0.47
3:G:547:ASP:HA	3:G:574:ARG:HB2	1.97	0.47
2:C:4:VAL:O	2:C:322:GLU:HA	2.14	0.47
2:F:470:VAL:O	2:F:473:LEU:HB2	2.14	0.47
2:C:592:ARG:HH11	2:C:592:ARG:HB2	1.80	0.47
1:B:1050:CYS:C	1:B:1052:PRO:CD	2.81	0.47
3:G:161:ALA:HB3	3:G:184:LEU:HD21	1.96	0.47
4:Y:7:5IU:C3'	4:Y:8:DC:H5'	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:GLN:NE2	1:E:283:PRO:HG2	2.29	0.47
1:B:262:GLN:HA	1:B:265:TRP:HB3	1.95	0.47
1:E:1093:TYR:CE2	1:E:1144:ARG:HB2	2.50	0.47
2:C:87:ASN:ND2	2:C:87:ASN:O	2.47	0.47
1:B:66:GLU:HA	1:B:66:GLU:OE1	2.14	0.47
2:F:545:GLN:C	2:F:547:VAL:H	2.17	0.47
2:F:941:MET:HG2	2:F:942:GLU:N	2.29	0.47
1:E:504:MET:CE	1:E:514:TYR:HA	2.45	0.47
1:E:568:ARG:HG3	1:E:568:ARG:HH11	1.80	0.47
2:F:360:ARG:NH1	2:F:766:ALA:HB2	2.29	0.47
1:B:1101:ALA:O	1:B:1104:ALA:HB3	2.15	0.47
1:E:268:LYS:CA	1:E:268:LYS:HE3	2.45	0.47
1:B:57:GLU:HG3	1:B:57:GLU:H	1.36	0.47
3:G:259:ASN:CB	3:G:260:PRO:CD	2.78	0.47
2:F:858:ARG:HB2	2:F:858:ARG:CZ	2.43	0.47
2:C:1050:TYR:HD1	2:C:1057:MET:HE2	1.80	0.47
1:E:531:GLN:O	1:E:535:ARG:HD3	2.15	0.47
3:D:201:LEU:HG	3:D:233:ILE:HG21	1.96	0.47
1:B:522:CYS:O	1:B:526:ILE:HD13	2.15	0.47
3:G:219:ALA:O	3:G:223:LEU:HD22	2.14	0.47
1:E:1085:TRP:HD1	1:E:1087:GLY:HA3	1.79	0.47
2:F:104:GLU:N	2:F:112:ARG:HH11	2.13	0.47
3:D:455:ASN:O	3:D:459:GLU:HG3	2.14	0.47
3:D:459:GLU:O	3:D:463:GLN:HG3	2.15	0.47
2:F:159:GLY:O	2:F:160:GLU:O	2.33	0.47
2:C:519:THR:CG2	2:C:521:GLN:H	2.21	0.47
2:C:197:LEU:HD13	2:C:230:LEU:HA	1.97	0.47
2:F:737:GLN:HG3	2:F:738:ASP:N	2.25	0.47
2:C:1076:GLU:O	2:C:1076:GLU:HG3	2.14	0.47
3:D:409:GLU:C	3:D:411:ALA:H	2.17	0.47
1:B:907:SER:C	1:B:909:LEU:N	2.68	0.47
3:D:261:LEU:HB3	3:D:287:PRO:HD3	1.97	0.47
1:E:262:GLN:HA	1:E:265:TRP:HB3	1.96	0.47
3:G:246:ALA:CA	3:G:253:LEU:HD23	2.44	0.47
3:G:261:LEU:HB3	3:G:287:PRO:HD3	1.96	0.47
3:G:240:LEU:CD2	3:G:274:ILE:HD12	2.45	0.47
3:G:51:VAL:HG11	3:G:276:LEU:HD12	1.96	0.47
1:B:282:LEU:HD23	1:B:310:PHE:HE2	1.80	0.47
1:E:902:ARG:HH21	1:E:902:ARG:HG3	1.80	0.47
3:D:51:VAL:HG11	3:D:276:LEU:CD1	2.45	0.47
1:B:236:TRP:CZ2	1:B:262:GLN:NE2	2.82	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:984:HIS:O	2:C:987:TYR:HB3	2.14	0.47
2:F:872:LEU:HD13	2:F:916:PHE:CZ	2.49	0.47
3:G:343:THR:OG1	3:G:344:GLU:N	2.48	0.47
1:B:1036:LEU:O	1:B:1040:ILE:HG12	2.15	0.47
1:E:729:LEU:HD22	1:E:729:LEU:N	2.26	0.47
2:C:26:LEU:HB2	2:C:210:ARG:HH22	1.80	0.47
2:F:570:GLN:HA	2:F:573:ILE:HD12	1.97	0.47
2:F:308:ARG:O	2:F:311:ILE:HG22	2.14	0.47
1:B:785:GLU:N	1:B:785:GLU:OE1	2.45	0.47
1:B:473:ILE:HG22	1:B:473:ILE:O	2.15	0.47
3:D:184:LEU:HD13	3:D:184:LEU:C	2.35	0.46
3:D:244:LEU:O	3:D:253:LEU:HD22	2.15	0.46
4:X:22:DG:C3'	4:X:23:DC:C5'	2.91	0.46
2:C:971:LEU:N	2:C:971:LEU:HD22	2.30	0.46
2:F:557:ILE:HD13	2:F:557:ILE:N	2.17	0.46
1:B:252:ILE:HG12	1:B:254:ARG:HG2	1.97	0.46
1:E:237:ARG:NH2	1:E:266:ILE:HG23	2.24	0.46
1:B:221:ARG:HG2	1:B:221:ARG:NH1	2.31	0.46
3:G:52:CYS:HB3	3:G:108:TYR:CE2	2.50	0.46
2:F:973:SER:OG	2:F:976:GLN:HB2	2.15	0.46
3:D:549:ALA:O	3:D:577:LEU:HA	2.15	0.46
3:G:550:ALA:HB2	3:G:578:SER:HB2	1.98	0.46
2:F:358:PHE:HA	2:F:769:CYS:SG	2.55	0.46
1:B:904:THR:OG1	1:B:1058:VAL:HG11	2.15	0.46
2:C:393:LEU:CD2	2:C:408:ILE:HG21	2.45	0.46
2:F:175:TYR:CZ	2:F:179:LEU:HD11	2.50	0.46
1:B:199:ARG:NH1	1:B:199:ARG:HG3	2.29	0.46
1:B:905:SER:O	1:B:906:TYR:C	2.52	0.46
2:C:1063:THR:C	2:C:1065:GLN:N	2.69	0.46
3:D:264:ASP:OD1	3:D:289:HIS:NE2	2.47	0.46
3:G:270:GLU:HB3	3:G:273:MET:HE2	1.97	0.46
3:D:366:GLY:HA3	3:D:393:ILE:HD13	1.97	0.46
1:E:471:ARG:HD2	1:E:471:ARG:H	1.74	0.46
3:G:17:ARG:HB2	3:G:18:PRO:CD	2.36	0.46
2:F:966:ARG:O	2:F:998:LEU:HA	2.16	0.46
2:F:689:LEU:CD2	2:F:708:ARG:HD2	2.45	0.46
2:C:415:ILE:CB	2:C:663:THR:HG23	2.42	0.46
2:C:233:HIS:O	2:C:234:ILE:HD12	2.14	0.46
1:B:17:GLY:HA2	1:B:408:ALA:HA	1.97	0.46
3:D:449:PHE:HZ	3:D:555:SER:HB2	1.80	0.46
3:G:556:GLN:O	3:G:557:ARG:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:ARG:HA	1:B:1129:TYR:CD1	2.50	0.46
2:F:1087:ASP:O	2:F:1091:GLN:HG2	2.15	0.46
2:C:282:ASN:HB3	2:C:283:ALA:H	1.36	0.46
3:G:272:SER:HB3	3:G:310:LEU:HD23	1.96	0.46
2:F:731:TYR:CE2	2:F:744:PRO:HB3	2.51	0.46
2:F:731:TYR:CZ	2:F:744:PRO:HB3	2.50	0.46
3:D:272:SER:HB3	3:D:310:LEU:HD23	1.96	0.46
1:B:1126:ILE:HD12	1:B:1126:ILE:N	2.30	0.46
3:D:282:LEU:O	3:D:286:LEU:HG	2.15	0.46
1:E:265:TRP:CD1	1:E:265:TRP:C	2.89	0.46
1:E:747:LEU:HB3	1:E:749:TYR:CE1	2.50	0.46
2:C:164:TRP:O	2:C:167:PRO:HD2	2.15	0.46
1:B:683:ARG:O	1:B:687:ILE:HG13	2.14	0.46
1:B:104:ILE:HB	1:B:107:LYS:CE	2.42	0.46
2:C:807:LEU:N	2:C:808:PRO:HD2	2.30	0.46
2:C:998:LEU:HD22	2:C:1000:LEU:CD2	2.45	0.46
4:Y:37:DT:H1'	4:Y:38:DG:H5''	1.97	0.46
1:B:65:THR:CG2	1:B:66:GLU:N	2.79	0.46
1:E:763:GLN:HE21	1:E:764:GLU:N	2.13	0.46
2:F:478:VAL:HG21	2:F:605:THR:HG21	1.97	0.46
2:C:1021:SER:O	2:C:1025:GLU:N	2.47	0.46
1:E:600:LEU:HD12	1:E:711:LEU:HD12	1.97	0.46
3:G:409:GLU:C	3:G:411:ALA:H	2.18	0.46
2:C:408:ILE:HG23	2:C:674:VAL:CG1	2.45	0.46
1:B:177:ARG:HE	1:B:181:GLN:NE2	2.14	0.46
2:C:388:VAL:HA	2:C:799:ARG:NH1	2.30	0.46
2:C:18:GLU:OE2	2:C:53:LYS:HB2	2.16	0.46
2:F:971:LEU:N	2:F:971:LEU:HD22	2.31	0.46
2:F:846:ARG:HH12	4:Y:7:5IU:H2'	1.79	0.46
3:G:65:HIS:O	3:G:66:PRO:C	2.51	0.46
3:D:531:GLU:HG3	3:D:531:GLU:O	2.15	0.46
1:E:920:LEU:HD13	2:F:608:ALA:HA	1.97	0.46
2:C:957:PRO:O	2:C:958:GLN:C	2.53	0.46
1:E:469:MET:SD	1:E:795:LEU:HD12	2.55	0.46
1:B:469:MET:HG3	1:B:469:MET:O	2.16	0.46
1:B:1093:TYR:CE2	1:B:1144:ARG:HB2	2.51	0.46
1:B:1098:MET:HE1	1:B:1156:TYR:HB2	1.95	0.46
3:G:316:TYR:CE1	3:G:604:PHE:HB2	2.41	0.46
1:B:14:PRO:HA	1:B:48:ALA:HB1	1.98	0.46
2:F:615:GLN:OE1	2:F:644:ARG:HD3	2.16	0.46
3:D:301:LEU:N	3:D:568:THR:HG21	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:637:ALA:O	1:B:640:VAL:HB	2.16	0.46
1:E:646:ASP:HA	1:E:649:ARG:HG2	1.97	0.46
2:C:393:LEU:HD22	2:C:408:ILE:HG21	1.96	0.46
3:D:93:ARG:NH1	3:D:93:ARG:HG2	2.31	0.46
2:C:360:ARG:NH1	2:C:766:ALA:HB2	2.30	0.46
3:G:449:PHE:HZ	3:G:555:SER:HB2	1.81	0.46
1:E:1123:ARG:HA	1:E:1129:TYR:CD1	2.49	0.46
1:E:63:THR:OG1	1:E:69:THR:HG22	2.15	0.46
1:E:688:LEU:O	1:E:691:SER:HB2	2.16	0.46
3:G:317:ALA:C	3:G:319:ALA:H	2.19	0.46
3:D:279:MET:O	3:D:280:SER:C	2.52	0.46
2:C:1055:ASP:OD1	2:C:1118:ARG:NH2	2.49	0.46
2:F:228:GLN:HE22	2:F:318:GLU:N	2.00	0.46
3:G:226:THR:C	3:G:228:GLU:N	2.61	0.46
2:C:943:ILE:O	2:C:953:THR:HA	2.14	0.46
1:B:222:HIS:CE1	1:B:226:VAL:CG2	2.98	0.46
1:B:469:MET:SD	1:B:795:LEU:HD12	2.56	0.46
2:C:976:GLN:HG3	2:C:998:LEU:HD11	1.97	0.46
3:G:73:SER:O	3:G:75:ILE:HG13	2.16	0.46
2:C:72:MET:HG3	2:C:230:LEU:HD11	1.97	0.46
3:G:462:MET:CE	3:G:534:TRP:HE1	2.23	0.46
1:B:937:GLU:HA	1:B:938:PRO:HD2	1.69	0.46
1:E:983:GLU:HB3	1:E:985:GLN:OE1	2.15	0.46
2:F:767:LEU:HD23	2:F:767:LEU:H	1.79	0.46
1:E:390:ASP:OD1	1:E:393:GLN:HG3	2.16	0.46
1:E:637:ALA:O	1:E:640:VAL:HB	2.15	0.46
1:E:705:HIS:CG	2:F:487:GLU:HG3	2.51	0.46
1:E:904:THR:OG1	1:E:1058:VAL:HG11	2.16	0.46
3:D:449:PHE:O	3:D:450:GLY:O	2.33	0.46
1:E:871:GLN:HA	1:E:871:GLN:OE1	2.15	0.46
2:C:582:ARG:HD3	2:C:587:TRP:CZ2	2.51	0.46
1:B:629:GLU:CD	2:C:852:ARG:NH1	2.69	0.46
2:F:670:ILE:CG2	2:F:671:PRO:HD2	2.46	0.46
3:D:240:LEU:CD2	3:D:274:ILE:CD1	2.93	0.46
3:D:278:MET:O	3:D:279:MET:C	2.54	0.46
1:E:252:ILE:HG12	1:E:254:ARG:HG2	1.97	0.46
3:G:240:LEU:CD2	3:G:274:ILE:CD1	2.94	0.46
1:B:307:HIS:ND1	1:B:308:PRO:CD	2.73	0.46
1:B:1161:ASN:C	1:B:1163:GLY:H	2.19	0.46
2:F:831:THR:HG22	2:F:951:GLN:HB2	1.97	0.46
1:E:237:ARG:HH21	1:E:266:ILE:CG2	2.25	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1137:GLY:O	1:E:1138:VAL:HB	2.15	0.46
2:F:386:VAL:HG12	2:F:425:VAL:CG2	2.44	0.46
1:E:387:GLN:HG3	1:E:414:ASP:O	2.15	0.46
2:F:957:PRO:O	2:F:958:GLN:C	2.54	0.46
2:F:551:ASP:OD2	2:F:551:ASP:N	2.35	0.46
1:E:937:GLU:O	1:E:939:THR:N	2.44	0.46
1:E:1007:VAL:HG22	1:E:1072:HIS:CD2	2.50	0.46
1:B:42:LEU:CB	1:B:44:LEU:HD13	2.44	0.46
3:G:562:THR:HG21	3:G:594:THR:HG23	1.97	0.46
1:E:802:LEU:HD22	1:E:806:LEU:CD2	2.45	0.46
1:E:648:TYR:CE2	1:E:664:LEU:HD13	2.51	0.46
1:B:166:ASP:O	1:B:170:ARG:HG2	2.15	0.46
2:C:731:TYR:CE2	2:C:744:PRO:HB3	2.51	0.46
1:E:606:PRO:HB2	1:E:642:VAL:HG13	1.98	0.46
2:C:220:PRO:HD2	2:C:223:TYR:CD1	2.51	0.46
1:B:573:LEU:HD23	1:B:573:LEU:O	2.16	0.46
3:D:242:ARG:C	3:D:242:ARG:HD3	2.34	0.46
3:G:292:VAL:HG11	3:G:294:PHE:CZ	2.51	0.46
3:G:201:LEU:HG	3:G:233:ILE:HG22	1.97	0.46
3:D:526:ARG:NE	3:D:526:ARG:CA	2.77	0.46
1:B:265:TRP:CD1	1:B:265:TRP:C	2.89	0.46
1:B:262:GLN:C	1:B:265:TRP:HB3	2.36	0.46
3:D:343:THR:O	3:D:344:GLU:HB2	2.15	0.46
1:E:1161:ASN:O	1:E:1162:ALA:HB3	2.15	0.46
1:E:945:PHE:CD1	1:E:946:PRO:HD2	2.51	0.46
3:G:316:TYR:CE1	3:G:604:PHE:HB3	2.51	0.46
1:B:148:PHE:HD1	2:C:126:GLN:HE21	1.64	0.46
1:B:771:ARG:CG	1:B:771:ARG:HH11	2.28	0.46
3:D:123:PHE:HB3	3:D:348:LEU:HG	1.96	0.46
2:C:377:HIS:NE2	2:C:728:TYR:CE1	2.84	0.46
1:E:15:LEU:HD13	1:E:40:LEU:HD23	1.96	0.46
2:F:94:LYS:O	2:F:98:LEU:HG	2.16	0.46
3:G:93:ARG:HG2	3:G:93:ARG:NH1	2.30	0.46
1:B:319:GLU:HA	1:B:320:PRO:HD2	1.61	0.46
2:C:190:TYR:CE1	2:C:191:GLN:HG3	2.51	0.46
2:C:885:LEU:HD11	2:C:927:LEU:HD13	1.98	0.46
3:G:242:ARG:O	3:G:242:ARG:HD3	2.15	0.46
3:G:274:ILE:CG2	3:G:279:MET:HG2	2.45	0.46
3:G:282:LEU:O	3:G:286:LEU:HG	2.16	0.46
3:G:118:THR:O	3:G:283:ILE:CD1	2.64	0.46
3:G:122:PHE:HB2	3:G:283:ILE:HD12	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1049:GLY:C	1:E:1051:PRO:HD3	2.35	0.46
1:E:282:LEU:HD23	1:E:310:PHE:HE2	1.81	0.46
3:G:393:ILE:O	3:G:577:LEU:N	2.44	0.46
1:B:945:PHE:CD1	1:B:946:PRO:HD2	2.51	0.46
2:C:844:PRO:O	2:C:847:ALA:HB3	2.16	0.46
3:D:15:GLN:O	3:D:16:LEU:HB3	2.15	0.46
1:B:380:VAL:CG2	1:B:408:ALA:HB3	2.42	0.46
2:F:352:GLY:HA3	2:F:358:PHE:HB2	1.98	0.46
2:F:1021:SER:O	2:F:1025:GLU:N	2.47	0.46
1:E:39:ARG:NH1	1:E:39:ARG:HG3	2.30	0.46
1:B:1027:ILE:O	1:B:1027:ILE:HG13	2.16	0.46
2:F:334:LEU:HD11	2:F:755:ILE:HD12	1.97	0.46
2:F:245:ARG:HA	2:F:326:PHE:CE1	2.51	0.46
1:E:906:TYR:CG	1:E:906:TYR:O	2.69	0.46
1:E:582:SER:OG	1:E:743:LYS:HG3	2.16	0.46
3:D:7:LEU:O	3:D:10:ALA:HB3	2.15	0.46
2:C:450:VAL:O	2:C:453:ALA:HB3	2.15	0.46
3:G:279:MET:O	3:G:280:SER:C	2.53	0.46
3:G:279:MET:O	3:G:281:ARG:N	2.48	0.46
1:E:932:ALA:HB2	1:E:947:ARG:CG	2.46	0.46
3:D:263:LEU:O	3:D:263:LEU:HD12	2.16	0.46
1:B:1070:PHE:CE1	1:B:1077:TYR:HB2	2.51	0.46
1:B:252:ILE:HG12	1:B:254:ARG:H	1.81	0.46
1:B:263:ALA:O	1:B:266:ILE:HG12	2.16	0.46
1:E:587:VAL:CG1	1:E:690:ILE:HG13	2.46	0.46
2:F:884:LEU:O	2:F:888:LEU:HG	2.15	0.46
1:B:1098:MET:HE3	1:B:1142:PHE:CD1	2.47	0.46
3:G:455:ASN:HD21	3:G:532:THR:C	2.20	0.46
1:B:83:LEU:HD22	1:B:83:LEU:O	2.15	0.46
2:F:393:LEU:CD2	2:F:408:ILE:HG21	2.46	0.46
1:E:165:ALA:O	1:E:169:ARG:HG3	2.16	0.46
1:E:169:ARG:O	1:E:173:TYR:HB2	2.16	0.46
2:C:246:TYR:CD2	2:C:275:PRO:HD3	2.51	0.46
1:E:155:ASP:O	1:E:157:SER:N	2.48	0.46
2:F:571:LEU:O	2:F:575:ARG:HB3	2.15	0.46
1:E:190:PRO:HG3	2:F:870:PHE:CZ	2.51	0.46
2:F:1027:TYR:CD1	2:F:1027:TYR:C	2.88	0.46
2:C:429:ALA:HA	2:C:430:PRO:HD2	1.83	0.46
1:E:166:ASP:O	1:E:170:ARG:HG2	2.16	0.46
1:B:1038:THR:O	1:B:1041:ARG:HB3	2.16	0.46
2:F:18:GLU:OE2	2:F:53:LYS:HB2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:985:LEU:HB2	2:C:1020:LEU:HD13	1.97	0.46
2:C:474:LEU:HD21	2:C:485:ILE:HD12	1.98	0.46
3:D:185:LEU:HA	3:D:188:LEU:HB2	1.98	0.46
2:C:850:GLN:NE2	4:X:7:5IU:HN3	2.10	0.46
3:G:264:ASP:O	3:G:291:ARG:N	2.47	0.46
3:G:261:LEU:HD12	3:G:286:LEU:HA	1.98	0.46
1:E:283:PRO:CD	1:E:314:ASP:HB2	2.44	0.46
1:B:597:LEU:O	1:B:597:LEU:HD23	2.16	0.46
1:E:728:ARG:CB	1:E:728:ARG:HH21	2.29	0.46
2:C:159:GLY:O	2:C:160:GLU:O	2.34	0.46
1:B:226:VAL:HG13	1:B:269:ILE:HD13	1.98	0.46
1:E:683:ARG:NE	2:F:1095:ARG:NH1	2.64	0.46
1:B:646:ASP:HA	1:B:649:ARG:HG2	1.98	0.46
1:B:544:ASP:OD2	1:E:495:THR:HG23	2.15	0.46
2:C:1027:TYR:CD1	2:C:1027:TYR:C	2.88	0.46
1:B:895:ARG:HG2	1:B:896:LEU:H	1.81	0.46
3:G:7:LEU:O	3:G:10:ALA:HB3	2.16	0.46
2:C:871:ILE:HD13	2:C:871:ILE:HA	1.79	0.46
3:D:184:LEU:HD11	3:D:293:ILE:CD1	2.46	0.45
1:E:236:TRP:CZ2	1:E:262:GLN:NE2	2.84	0.45
3:G:115:ASN:OD1	3:G:277:PRO:HA	2.16	0.45
1:E:907:SER:C	1:E:909:LEU:N	2.69	0.45
3:G:201:LEU:HG	3:G:233:ILE:HG21	1.97	0.45
3:D:537:THR:OG1	3:D:540:LYS:HG3	2.16	0.45
1:B:707:LEU:O	1:B:710:TRP:HB3	2.16	0.45
1:E:728:ARG:HE	2:F:739:ASN:HB2	1.81	0.45
2:F:160:GLU:C	2:F:162:GLN:N	2.67	0.45
3:D:344:GLU:HG3	3:D:345:ALA:H	1.77	0.45
1:E:1071:ARG:NH1	2:F:29:PRO:HA	2.30	0.45
2:F:404:THR:HB	2:F:405:PRO:HD2	1.97	0.45
1:E:1124:HIS:HE1	2:F:54:PHE:CD1	2.34	0.45
2:C:901:PHE:HD1	2:C:917:TRP:CZ3	2.34	0.45
2:F:828:LEU:HB2	2:F:1028:ARG:HD2	1.98	0.45
1:E:416:LYS:HD2	1:E:468:PHE:CZ	2.51	0.45
1:E:1082:LYS:HD2	1:E:1140:TYR:CE1	2.50	0.45
2:F:989:ALA:HB1	2:F:1017:LEU:CD2	2.45	0.45
1:E:380:VAL:CG2	1:E:408:ALA:HB3	2.43	0.45
3:G:91:VAL:HG12	3:G:100:MET:HB3	1.98	0.45
1:E:600:LEU:HD11	1:E:694:LEU:HD21	1.98	0.45
1:E:1148:LYS:HD2	1:E:1148:LYS:N	2.30	0.45
2:F:821:VAL:O	2:F:821:VAL:HG22	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:645:LEU:HD12	2:F:645:LEU:HA	1.79	0.45
2:C:102:LEU:HD13	2:C:108:PHE:CZ	2.51	0.45
2:F:388:VAL:HA	2:F:799:ARG:NH1	2.31	0.45
3:D:361:PHE:C	3:D:361:PHE:CD1	2.89	0.45
1:B:1051:PRO:O	1:B:1052:PRO:O	2.34	0.45
2:C:968:ARG:HA	2:C:969:PRO:HD3	1.82	0.45
3:G:244:LEU:HD22	3:G:255:HIS:CG	2.50	0.45
2:F:885:LEU:HD11	2:F:927:LEU:HD13	1.98	0.45
1:B:582:SER:OG	1:B:743:LYS:HG3	2.16	0.45
2:F:228:GLN:HE21	2:F:319:SER:H	1.63	0.45
1:E:221:ARG:HG2	1:E:221:ARG:HH11	1.81	0.45
3:G:366:GLY:C	3:G:393:ILE:HG21	2.35	0.45
1:B:467:ALA:C	1:B:469:MET:H	2.20	0.45
2:F:998:LEU:HD22	2:F:1000:LEU:CD2	2.46	0.45
2:C:545:GLN:C	2:C:547:VAL:N	2.69	0.45
2:F:984:HIS:O	2:F:987:TYR:HB3	2.16	0.45
1:B:983:GLU:HB3	1:B:985:GLN:OE1	2.16	0.45
2:F:207:LEU:CB	2:F:208:PRO:CD	2.93	0.45
2:C:24:GLU:O	2:C:210:ARG:NH2	2.50	0.45
2:C:26:LEU:HB2	2:C:210:ARG:NH2	2.31	0.45
3:D:108:TYR:HB2	3:D:113:TRP:HB2	1.97	0.45
1:B:1148:LYS:HD2	1:B:1148:LYS:N	2.30	0.45
2:C:334:LEU:O	2:C:338:ILE:HG12	2.16	0.45
1:E:55:THR:HG21	1:E:57:GLU:OE2	2.15	0.45
1:E:586:SER:O	1:E:589:GLU:OE1	2.34	0.45
1:E:345:ARG:NH1	1:E:346:ARG:HG2	2.31	0.45
2:F:36:LEU:HD21	2:F:68:PHE:CD1	2.50	0.45
3:G:131:GLU:O	3:G:131:GLU:HG2	2.16	0.45
1:B:942:PRO:HB3	1:B:993:TRP:CE2	2.51	0.45
2:C:552:GLU:OE2	3:D:251:GLN:N	2.49	0.45
3:G:270:GLU:HB3	3:G:273:MET:CE	2.47	0.45
3:G:278:MET:SD	4:Y:2:5IU:I5	3.44	0.45
2:F:968:ARG:HA	2:F:969:PRO:HD3	1.81	0.45
1:E:246:LEU:HD23	1:E:307:HIS:NE2	2.32	0.45
1:E:310:PHE:C	1:E:310:PHE:CD2	2.89	0.45
2:F:1118:ARG:NH2	2:F:1118:ARG:CG	2.79	0.45
1:B:1018:GLN:NE2	2:C:32:PRO:HG3	2.31	0.45
2:C:943:ILE:CG2	2:C:986:VAL:HG13	2.45	0.45
2:C:991:GLY:O	2:C:992:GLY:C	2.55	0.45
1:B:269:ILE:HG22	1:B:270:SER:N	2.31	0.45
1:E:469:MET:O	1:E:469:MET:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1036:LEU:O	2:C:1037:VAL:CB	2.60	0.45
1:E:1108:ASP:O	1:E:1111:TYR:HB2	2.16	0.45
3:G:526:ARG:HH22	3:G:533:THR:HG22	1.81	0.45
1:B:374:ILE:HG21	1:B:400:ILE:HD13	1.96	0.45
2:C:775:ARG:HB3	2:C:775:ARG:HH11	1.82	0.45
1:E:513:ASP:O	1:E:517:THR:HG22	2.17	0.45
1:B:212:PRO:O	1:B:213:PRO:C	2.54	0.45
1:E:1068:LEU:HD12	1:E:1069:VAL:N	2.31	0.45
1:E:901:TRP:CE3	1:E:1060:GLY:HA2	2.52	0.45
4:X:16:DA:C2'	4:X:17:DG:H8	2.30	0.45
1:B:527:ARG:HD2	1:B:527:ARG:C	2.36	0.45
2:F:117:ASP:O	2:F:118:ASP:HB3	2.17	0.45
1:B:954:PHE:CZ	1:B:977:LEU:HD23	2.52	0.45
3:D:343:THR:OG1	3:D:344:GLU:N	2.49	0.45
1:B:225:ILE:HG23	1:B:321:LEU:HD23	1.97	0.45
1:E:1018:GLN:NE2	2:F:30:PHE:O	2.49	0.45
2:F:30:PHE:O	2:F:32:PRO:HD3	2.17	0.45
3:D:80:ASN:O	3:D:83:GLU:N	2.49	0.45
2:C:208:PRO:O	2:C:234:ILE:HG13	2.16	0.45
1:B:1108:ASP:O	1:B:1111:TYR:HB2	2.16	0.45
2:C:548:LEU:HD22	2:C:549:PRO:HD2	1.98	0.45
2:F:304:GLY:O	2:F:307:GLY:N	2.49	0.45
3:G:1:MET:HB3	3:G:2:LYS:H	1.65	0.45
1:B:1002:LEU:HD22	1:B:1007:VAL:HG12	1.97	0.45
3:D:582:ASP:HB2	3:D:585:ILE:HG12	1.98	0.45
1:E:1027:ILE:HA	1:E:1172:PHE:HD1	1.82	0.45
1:B:709:ARG:O	1:B:713:GLN:NE2	2.50	0.45
2:F:848:PHE:O	2:F:852:ARG:HB3	2.17	0.45
2:C:531:MET:HE3	2:C:561:VAL:HG22	1.99	0.45
1:E:73:ARG:HH11	1:E:73:ARG:HB3	1.81	0.45
3:D:126:VAL:HG13	3:D:166:ILE:H	1.82	0.45
3:D:126:VAL:HG13	3:D:166:ILE:CD1	2.46	0.45
1:E:252:ILE:HG12	1:E:254:ARG:H	1.81	0.45
3:G:261:LEU:CB	3:G:287:PRO:HD3	2.47	0.45
2:F:878:TYR:CG	4:Y:9:5IU:H4'	2.51	0.45
1:B:947:ARG:HD2	1:B:1086:LEU:HD21	1.99	0.45
1:E:812:HIS:CG	1:E:813:CYS:N	2.85	0.45
1:B:988:PRO:O	1:B:991:THR:HG22	2.16	0.45
1:B:924:LEU:O	1:B:926:VAL:N	2.48	0.45
1:B:252:ILE:CG2	1:B:254:ARG:HB2	2.46	0.45
3:D:224:PRO:O	3:D:225:LEU:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:TYR:O	1:B:100:LEU:HB2	2.17	0.45
2:C:831:THR:HG22	2:C:951:GLN:HB2	1.98	0.45
1:E:24:SER:HB2	1:E:27:THR:HG21	1.97	0.45
3:G:441:LEU:HA	3:G:536:MET:O	2.16	0.45
2:F:947:CYS:SG	2:F:1021:SER:OG	2.68	0.45
3:D:427:GLU:N	3:D:428:PRO:CD	2.80	0.45
3:D:31:GLU:OE2	3:D:88:SER:HB2	2.16	0.45
1:B:568:ARG:HG3	1:B:568:ARG:HH11	1.80	0.45
1:E:901:TRP:CH2	1:E:1060:GLY:HA2	2.52	0.45
1:E:146:MET:CE	1:E:150:GLN:HG3	2.46	0.45
1:B:106:ASP:OD2	1:B:109:GLN:HB2	2.16	0.45
1:B:1170:GLU:O	1:B:1174:GLY:N	2.48	0.45
3:D:161:ALA:HB3	3:D:184:LEU:HD21	1.97	0.45
4:Y:22:DG:C3'	4:Y:23:DC:C5'	2.92	0.45
4:Y:45:DT:C2'	4:Y:46:5IU:H5'	2.46	0.45
3:D:79:GLN:HG3	3:D:80:ASN:N	2.32	0.45
2:C:207:LEU:HB2	2:C:234:ILE:HD11	1.98	0.45
1:B:1062:LEU:CD2	1:B:1113:LEU:HD22	2.46	0.45
1:B:427:ILE:O	1:B:430:TYR:HB3	2.17	0.45
1:E:1040:ILE:HD11	1:E:1168:MET:HE1	1.98	0.45
3:D:525:SER:O	3:D:527:LEU:N	2.49	0.45
3:G:301:LEU:O	3:G:305:GLU:HG2	2.16	0.45
3:G:375:ASN:ND2	3:G:567:TYR:CE1	2.85	0.45
3:G:412:LEU:HD22	3:G:462:MET:CG	2.47	0.45
3:G:455:ASN:ND2	3:G:533:THR:O	2.49	0.45
3:D:405:ILE:O	3:D:409:GLU:HG3	2.16	0.45
2:C:445:ARG:HH11	2:C:452:GLU:CD	2.20	0.45
1:B:169:ARG:O	1:B:173:TYR:HB2	2.17	0.45
3:G:322:THR:HG23	3:G:350:ASP:OD1	2.16	0.45
3:D:192:ALA:O	3:D:193:ASP:C	2.55	0.45
2:F:535:TYR:HD1	2:F:558:ALA:HB1	1.81	0.45
2:C:333:ASN:HD22	2:C:336:HIS:CD2	2.35	0.45
2:C:240:PHE:HE2	2:C:242:ASN:ND2	2.15	0.45
3:G:192:ALA:O	3:G:193:ASP:C	2.55	0.45
3:G:184:LEU:C	3:G:184:LEU:HD13	2.36	0.45
3:G:223:LEU:HD23	3:G:223:LEU:N	2.30	0.45
1:B:860:LEU:HG	1:B:860:LEU:O	2.17	0.45
2:C:955:TRP:CD1	3:D:262:HIS:NE2	2.85	0.45
3:D:73:SER:O	3:D:75:ILE:HG13	2.17	0.45
3:D:80:ASN:HB3	3:D:83:GLU:CB	2.39	0.45
1:B:1061:MET:HE1	2:C:52:GLN:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:142:ARG:NH2	2:C:705:ASP:OD1	2.49	0.45
2:F:273:GLU:OE2	2:F:273:GLU:CA	2.64	0.45
1:B:892:THR:HG22	2:C:804:ARG:CZ	2.46	0.45
3:D:302:ALA:HA	3:D:305:GLU:HG2	1.99	0.45
1:B:514:TYR:CD1	1:B:514:TYR:O	2.70	0.45
1:B:513:ASP:O	1:B:517:THR:CG2	2.65	0.45
2:F:1100:GLU:N	2:F:1100:GLU:OE1	2.50	0.45
2:F:450:VAL:O	2:F:453:ALA:HB3	2.16	0.45
2:C:392:ARG:O	2:C:396:MET:HG2	2.16	0.45
1:B:434:ARG:CG	1:B:434:ARG:HH11	2.30	0.45
2:F:244:CYS:SG	2:F:345:LEU:HB2	2.57	0.45
1:B:784:PRO:O	1:B:788:ASP:OD1	2.35	0.45
3:D:247:GLN:O	3:D:251:GLN:HA	2.17	0.45
3:G:126:VAL:HG13	3:G:166:ILE:CD1	2.47	0.45
4:X:45:DT:C2'	4:X:46:5IU:H5'	2.45	0.45
3:D:455:ASN:ND2	3:D:533:THR:O	2.49	0.45
1:B:595:GLU:HA	1:B:598:TRP:HE3	1.82	0.45
1:B:900:ASN:O	1:B:900:ASN:CG	2.54	0.45
1:B:860:LEU:HD23	1:B:860:LEU:H	1.82	0.45
1:E:557:LEU:HB2	1:E:754:LEU:HD12	1.99	0.45
3:G:307:GLY:CA	3:G:597:ARG:HH21	2.30	0.45
2:C:440:SER:O	2:C:441:ASP:CB	2.65	0.45
1:B:1082:LYS:O	1:B:1142:PHE:HA	2.16	0.45
2:C:277:PHE:CD1	2:C:278:ARG:N	2.84	0.45
1:E:681:GLU:O	1:E:685:THR:HG23	2.17	0.45
2:F:377:HIS:NE2	2:F:728:TYR:CE1	2.84	0.45
1:E:83:LEU:O	1:E:83:LEU:HD22	2.16	0.45
1:B:345:ARG:NH1	1:B:346:ARG:HG2	2.32	0.45
2:F:841:TRP:O	2:F:842:ALA:HB3	2.16	0.45
4:X:34:DC:H1'	4:X:35:DA:H5'	1.98	0.45
1:E:919:ASP:OD2	2:F:653:ARG:NH1	2.50	0.45
1:E:427:ILE:O	1:E:430:TYR:HB3	2.17	0.45
1:B:586:SER:O	1:B:589:GLU:OE1	2.35	0.45
2:F:220:PRO:HD2	2:F:223:TYR:CD1	2.51	0.45
3:D:131:GLU:O	3:D:131:GLU:HG2	2.17	0.45
3:D:126:VAL:HA	3:D:166:ILE:HD13	1.98	0.45
1:B:741:ILE:HG21	1:B:801:LEU:HD22	1.99	0.45
1:E:527:ARG:C	1:E:527:ARG:HD2	2.38	0.45
2:C:104:GLU:N	2:C:112:ARG:HG3	2.13	0.45
1:B:252:ILE:HG23	1:B:254:ARG:H	1.82	0.45
1:E:689:HIS:HE1	1:E:725:GLN:O	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:79:GLN:HG3	3:G:80:ASN:N	2.32	0.45
2:C:272:ARG:O	2:C:273:GLU:HB2	2.17	0.45
3:G:526:ARG:HH12	3:G:536:MET:HE2	1.81	0.45
3:D:301:LEU:HD22	3:D:565:LEU:HA	1.99	0.45
3:D:116:GLU:HG2	3:D:603:LEU:HD12	1.99	0.45
1:B:154:GLU:HG2	1:B:155:ASP:N	2.32	0.45
4:Y:34:DC:H2''	4:Y:35:DA:H5'	1.99	0.45
1:B:728:ARG:CB	1:B:728:ARG:HH21	2.30	0.45
1:E:12:ARG:HG3	1:E:12:ARG:O	2.17	0.45
1:B:193:LEU:O	1:B:193:LEU:HD23	2.17	0.45
1:E:262:GLN:C	1:E:265:TRP:HB3	2.37	0.45
1:B:561:ARG:HH12	1:B:584:ARG:HB2	1.81	0.45
2:C:138:TYR:HE1	2:C:165:GLN:HE22	1.64	0.45
1:E:831:THR:C	1:E:833:VAL:N	2.70	0.45
1:E:988:PRO:O	1:E:991:THR:HG22	2.16	0.45
2:C:1030:GLY:HA2	2:C:1035:LEU:HB2	1.98	0.45
3:D:597:ARG:CD	3:D:597:ARG:C	2.85	0.45
2:C:538:GLU:HB3	3:D:111:ARG:NH1	2.32	0.45
1:E:504:MET:HE3	1:E:514:TYR:HD2	1.81	0.45
1:E:513:ASP:O	1:E:517:THR:CG2	2.65	0.45
1:B:648:TYR:CE2	1:B:664:LEU:HD13	2.51	0.45
1:E:709:ARG:O	1:E:713:GLN:NE2	2.50	0.45
3:D:427:GLU:N	3:D:428:PRO:HD2	2.32	0.45
3:D:330:SER:HA	3:D:335:THR:O	2.17	0.45
2:C:821:VAL:O	2:C:821:VAL:HG22	2.15	0.45
1:B:871:GLN:OE1	1:B:871:GLN:HA	2.16	0.45
3:G:282:LEU:HD23	3:G:286:LEU:HG	1.99	0.44
4:X:12:DT:C2'	4:X:13:DG:H5'	2.35	0.44
1:E:752:VAL:CG1	1:E:809:SER:HB3	2.33	0.44
2:F:951:GLN:O	2:F:952:ILE:CG2	2.64	0.44
1:B:812:HIS:CG	1:B:813:CYS:N	2.84	0.44
1:E:1137:GLY:O	1:E:1158:THR:O	2.35	0.44
2:F:403:LEU:HD22	2:F:404:THR:O	2.17	0.44
2:F:261:LEU:HD11	2:F:281:GLU:OE1	2.17	0.44
1:B:1061:MET:HG3	2:C:48:MET:HE3	1.99	0.44
3:G:385:VAL:HG21	3:G:396:ARG:NH1	2.32	0.44
2:F:273:GLU:HA	2:F:273:GLU:OE2	2.17	0.44
1:E:1036:LEU:O	1:E:1040:ILE:HG12	2.17	0.44
2:C:278:ARG:O	2:C:279:ASP:C	2.56	0.44
2:C:358:PHE:CZ	2:C:768:ASN:OD1	2.70	0.44
1:E:52:ARG:HG2	1:E:52:ARG:HH21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:LEU:HD21	2:C:703:ARG:HB3	1.99	0.44
2:C:185:HIS:HB2	2:C:186:ARG:H	1.30	0.44
1:B:854:ARG:NH1	1:B:854:ARG:HG2	2.32	0.44
2:C:245:ARG:HA	2:C:326:PHE:CZ	2.53	0.44
2:F:915:ILE:O	2:F:919:THR:CG2	2.65	0.44
1:B:89:ARG:C	1:B:91:THR:N	2.70	0.44
3:D:317:ALA:C	3:D:319:ALA:H	2.20	0.44
3:D:547:ASP:HA	3:D:574:ARG:HB2	1.99	0.44
2:C:177:HIS:O	2:C:180:GLY:N	2.47	0.44
1:B:73:ARG:HB3	1:B:73:ARG:HH11	1.82	0.44
3:D:118:THR:O	3:D:283:ILE:CD1	2.65	0.44
1:E:252:ILE:CG2	1:E:254:ARG:HB2	2.46	0.44
3:G:241:HIS:CB	4:Y:3:5IU:H4'	2.46	0.44
1:B:600:LEU:HD12	1:B:711:LEU:HD12	1.99	0.44
2:C:656:ALA:O	2:C:658:PRO:CD	2.59	0.44
1:E:950:SER:N	1:E:951:PRO:HD2	2.32	0.44
3:D:15:GLN:O	3:D:16:LEU:CB	2.64	0.44
2:F:374:ILE:HG12	2:F:727:LEU:HB3	2.00	0.44
3:G:425:ARG:O	3:G:425:ARG:HG3	2.16	0.44
1:E:595:GLU:HA	1:E:598:TRP:HE3	1.82	0.44
2:F:582:ARG:HD3	2:F:587:TRP:CZ2	2.52	0.44
1:B:328:ILE:O	1:B:331:ALA:N	2.50	0.44
2:F:641:LEU:HD22	2:F:645:LEU:HD22	1.99	0.44
1:E:328:ILE:O	1:E:331:ALA:N	2.50	0.44
1:E:431:MET:O	1:E:434:ARG:HB3	2.17	0.44
3:D:303:SER:O	3:D:311:GLY:HA3	2.16	0.44
1:B:386:PHE:C	1:B:388:ASP:H	2.21	0.44
1:E:573:LEU:HD23	1:E:573:LEU:O	2.17	0.44
3:D:261:LEU:HD12	3:D:286:LEU:HA	1.99	0.44
4:Y:8:DC:H2''	4:Y:9:5IU:O5'	2.17	0.44
4:Y:12:DT:C2'	4:Y:13:DG:H5'	2.35	0.44
3:D:201:LEU:HG	3:D:233:ILE:HG22	1.97	0.44
2:C:161:ALA:O	2:C:165:GLN:HG3	2.18	0.44
1:B:267:ASP:C	1:B:269:ILE:N	2.69	0.44
1:E:1158:THR:HG22	1:E:1159:ARG:N	2.32	0.44
1:E:467:ALA:C	1:E:469:MET:H	2.20	0.44
1:E:194:LEU:HD22	1:E:198:ASN:HB2	2.00	0.44
2:C:872:LEU:HD22	2:C:880:ILE:HD12	1.99	0.44
1:E:416:LYS:HE2	1:E:803:TYR:CZ	2.52	0.44
2:C:172:LEU:HD23	2:C:172:LEU:O	2.17	0.44
3:D:425:ARG:O	3:D:425:ARG:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:LEU:HD12	3:D:106:ARG:O	2.18	0.44
3:D:333:THR:C	3:D:335:THR:H	2.21	0.44
1:E:83:LEU:CD1	1:E:114:LEU:HD11	2.47	0.44
1:E:39:ARG:HD2	1:E:44:LEU:HB3	1.98	0.44
1:E:154:GLU:HG2	1:E:155:ASP:H	1.82	0.44
1:E:170:ARG:HA	2:F:517:PRO:CG	2.47	0.44
1:E:586:SER:HB2	1:E:724:SER:O	2.17	0.44
2:F:333:ASN:O	2:F:337:ASN:ND2	2.50	0.44
2:F:190:TYR:CD1	2:F:190:TYR:C	2.91	0.44
2:C:125:PHE:HB2	2:C:636:LEU:HD21	1.98	0.44
2:F:112:ARG:HH11	2:F:112:ARG:CG	2.26	0.44
1:E:900:ASN:O	1:E:900:ASN:CG	2.55	0.44
1:E:581:LEU:HD21	1:E:728:ARG:HH12	1.82	0.44
1:E:809:SER:HG	1:E:813:CYS:HB2	1.80	0.44
1:E:222:HIS:CE1	1:E:226:VAL:CG2	3.01	0.44
3:G:80:ASN:HB3	3:G:83:GLU:CB	2.41	0.44
3:G:359:TYR:CD1	3:G:360:ARG:N	2.85	0.44
2:C:749:GLN:HA	2:C:752:ILE:HD11	1.99	0.44
2:F:139:LEU:HD23	2:F:146:LEU:HD12	1.99	0.44
3:G:15:GLN:O	3:G:16:LEU:CB	2.64	0.44
1:E:937:GLU:HA	1:E:938:PRO:HD2	1.68	0.44
3:D:551:LEU:N	3:D:578:SER:O	2.43	0.44
2:F:374:ILE:HA	2:F:727:LEU:O	2.17	0.44
2:F:1019:TYR:C	2:F:1021:SER:N	2.71	0.44
3:G:333:THR:C	3:G:335:THR:H	2.20	0.44
2:F:388:VAL:HG22	2:F:799:ARG:HH12	1.82	0.44
4:X:34:DC:H2''	4:X:35:DA:H5'	1.99	0.44
2:C:311:ILE:O	2:C:311:ILE:HD13	2.18	0.44
1:E:63:THR:HG22	1:E:384:ASP:OD1	2.17	0.44
3:D:199:ILE:HG23	3:D:265:VAL:HG22	1.98	0.44
1:E:236:TRP:CZ3	1:E:240:VAL:HG21	2.53	0.44
1:B:876:GLN:N	1:B:877:PRO:CD	2.81	0.44
4:Y:16:DA:H2'	4:Y:17:DG:C8	2.52	0.44
3:D:132:VAL:CG1	3:D:134:GLU:HG2	2.47	0.44
3:D:133:ASP:O	3:D:135:ALA:N	2.50	0.44
1:B:1118:LEU:HD22	1:B:1122:LEU:HG	1.99	0.44
2:C:951:GLN:O	2:C:952:ILE:CG2	2.62	0.44
1:B:233:LYS:O	1:B:237:ARG:CG	2.66	0.44
2:F:172:LEU:O	2:F:172:LEU:HD23	2.18	0.44
1:E:518:MET:CE	1:E:816:GLY:HA3	2.48	0.44
2:C:377:HIS:CD2	2:C:728:TYR:CE1	3.06	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:562:THR:CG2	3:G:594:THR:HG23	2.48	0.44
2:C:312:TYR:CD1	2:C:313:LEU:HD23	2.52	0.44
1:E:154:GLU:HG2	1:E:155:ASP:N	2.32	0.44
2:C:582:ARG:HD3	2:C:587:TRP:CE2	2.53	0.44
1:B:402:HIS:NE2	1:B:403:HIS:CD2	2.86	0.44
2:F:964:LEU:HB2	2:F:996:SER:CB	2.47	0.44
2:F:457:LEU:HB3	2:F:594:MET:CE	2.47	0.44
1:B:626:LEU:O	1:B:630:THR:HG23	2.18	0.44
1:E:268:LYS:C	1:E:268:LYS:HE3	2.38	0.44
1:B:486:ALA:HB3	1:B:542:ASN:OD1	2.17	0.44
3:D:255:HIS:HA	3:D:260:PRO:HD2	2.00	0.44
1:B:286:LEU:CD1	1:B:306:ARG:HD3	2.29	0.44
2:C:117:ASP:O	2:C:118:ASP:HB3	2.18	0.44
1:B:362:LEU:HD11	1:B:396:ILE:HG23	1.98	0.44
1:E:168:TRP:O	1:E:172:CYS:HB2	2.18	0.44
1:E:225:ILE:HG23	1:E:321:LEU:HD23	1.99	0.44
1:B:672:GLU:O	2:C:814:GLY:HA3	2.17	0.44
3:D:53:LEU:CD1	3:D:58:LEU:HD12	2.47	0.44
1:E:669:ASN:HB3	1:E:672:GLU:OE2	2.16	0.44
2:C:75:ARG:NH1	2:C:208:PRO:HD3	2.33	0.44
1:E:1082:LYS:O	1:E:1142:PHE:HA	2.18	0.44
1:B:763:GLN:HE21	1:B:764:GLU:H	1.65	0.44
2:F:530:ARG:HG2	2:F:547:VAL:CG1	2.48	0.44
3:G:551:LEU:N	3:G:578:SER:O	2.44	0.44
1:E:550:ARG:O	1:E:553:ASP:N	2.40	0.44
2:C:478:VAL:HG13	2:C:600:LEU:O	2.17	0.44
1:B:5:ALA:HB1	1:B:441:TYR:HA	1.99	0.44
2:F:24:GLU:O	2:F:210:ARG:NH2	2.50	0.44
2:F:540:ALA:O	2:F:541:GLN:HB2	2.18	0.44
1:E:1027:ILE:HG13	1:E:1027:ILE:O	2.17	0.44
1:E:854:ARG:NH1	1:E:854:ARG:HG2	2.33	0.44
3:G:137:LEU:HD22	3:G:141:LEU:HD11	2.00	0.44
2:F:45:TRP:HB2	2:F:670:ILE:HD13	1.99	0.44
2:C:287:PHE:HB2	2:C:293:GLN:HB3	2.00	0.44
2:C:91:MET:HB2	2:C:132:ALA:HB1	2.00	0.44
2:F:845:VAL:HG13	2:F:1093:LEU:HD11	1.99	0.44
1:E:120:GLN:HA	1:E:120:GLN:OE1	2.18	0.44
4:Y:23:DC:H2"	4:Y:24:DT:C6	2.52	0.44
1:E:1051:PRO:O	1:E:1052:PRO:O	2.35	0.44
1:B:761:ARG:CG	1:B:822:ARG:HH22	2.26	0.44
3:G:133:ASP:OD2	3:G:136:LEU:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1050:TYR:OH	2:F:1118:ARG:HA	2.18	0.44
1:B:1158:THR:HG22	1:B:1159:ARG:N	2.33	0.44
1:B:236:TRP:CZ3	1:B:240:VAL:HG21	2.53	0.44
2:C:207:LEU:CB	2:C:208:PRO:CD	2.92	0.44
3:D:154:GLN:HA	3:D:355:LEU:HD22	2.00	0.44
1:B:416:LYS:HD2	1:B:468:PHE:CZ	2.53	0.44
1:E:1036:LEU:HA	1:E:1039:LEU:HD21	2.00	0.44
1:E:771:ARG:CG	1:E:771:ARG:HH11	2.28	0.44
2:C:352:GLY:HA3	2:C:358:PHE:HB2	1.99	0.44
2:F:392:ARG:HD3	2:F:392:ARG:HA	1.86	0.44
1:E:514:TYR:CD1	1:E:514:TYR:O	2.70	0.44
1:B:906:TYR:O	1:B:906:TYR:CG	2.69	0.44
2:F:985:LEU:HB2	2:F:1020:LEU:HD13	2.00	0.44
2:F:177:HIS:O	2:F:180:GLY:N	2.45	0.44
1:E:62:VAL:HG23	1:E:62:VAL:O	2.17	0.44
2:C:14:GLU:HG3	2:C:49:THR:HG21	1.98	0.44
1:B:934:VAL:O	1:B:934:VAL:HG12	2.17	0.44
1:E:252:ILE:HG23	1:E:254:ARG:H	1.82	0.44
3:G:252:ARG:O	3:G:253:LEU:HG	2.17	0.44
1:E:563:GLU:O	1:E:567:VAL:HG23	2.17	0.44
1:B:283:PRO:CD	1:B:314:ASP:HB2	2.42	0.44
3:G:200:ARG:CB	3:G:263:LEU:HD23	2.32	0.44
2:F:104:GLU:H	2:F:112:ARG:HH11	1.65	0.44
2:C:117:ASP:OD2	2:C:117:ASP:N	2.51	0.44
1:B:823:ARG:NH2	1:B:828:LYS:NZ	2.65	0.44
1:B:182:VAL:HG21	1:B:272:TRP:CH2	2.53	0.44
2:C:415:ILE:H	2:C:663:THR:CG2	2.31	0.44
1:E:613:ARG:HD2	2:F:854:GLN:O	2.18	0.44
1:B:610:ASN:ND2	1:B:613:ARG:NH1	2.64	0.44
2:C:534:GLY:O	2:C:536:ALA:O	2.36	0.44
2:C:173:VAL:O	2:C:176:THR:HG23	2.18	0.44
1:E:514:TYR:CE2	1:E:518:MET:HG3	2.53	0.44
3:G:330:SER:HA	3:G:335:THR:O	2.18	0.44
2:C:1100:GLU:N	2:C:1100:GLU:OE1	2.51	0.44
3:D:405:ILE:HA	3:D:408:LEU:HD12	1.99	0.44
1:B:1148:LYS:CD	1:B:1148:LYS:H	2.31	0.44
1:E:490:VAL:CG1	1:E:495:THR:HG22	2.48	0.44
1:B:15:LEU:HD13	1:B:40:LEU:HD23	2.00	0.44
1:E:402:HIS:NE2	1:E:403:HIS:CD2	2.86	0.44
2:C:333:ASN:O	2:C:337:ASN:ND2	2.51	0.44
1:B:728:ARG:HG3	1:B:728:ARG:H	1.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:SER:HB3	1:E:733:LYS:O	2.18	0.44
1:B:62:VAL:HA	1:B:127:PHE:O	2.18	0.44
1:E:1038:THR:O	1:E:1041:ARG:HB3	2.18	0.44
1:E:193:LEU:O	1:E:193:LEU:HD23	2.17	0.44
3:D:126:VAL:CG2	3:D:166:ILE:HD13	2.40	0.44
4:X:23:DC:H2''	4:X:24:DT:C6	2.53	0.44
2:C:885:LEU:HD12	2:C:969:PRO:CG	2.34	0.44
3:G:266:LEU:HD23	3:G:286:LEU:HD21	1.99	0.44
3:G:275:ASP:OD1	4:Y:2:5IU:O4	2.35	0.44
1:B:563:GLU:O	1:B:567:VAL:HG23	2.17	0.44
2:F:363:ASN:ND2	2:F:363:ASN:N	2.30	0.44
3:G:213:THR:CG2	3:G:235:GLU:CA	2.92	0.44
3:G:541:SER:O	3:G:544:SER:HB2	2.18	0.44
2:F:103:LEU:HD11	2:F:115:LEU:HD13	1.98	0.44
1:B:222:HIS:CG	1:B:272:TRP:HH2	2.36	0.44
1:E:837:ALA:O	1:E:841:LEU:HG	2.18	0.44
2:C:1038:LEU:HD22	2:C:1090:TYR:CE1	2.53	0.44
1:E:200:TYR:O	1:E:201:LEU:CB	2.54	0.44
2:F:709:ARG:NH2	2:F:709:ARG:CG	2.80	0.44
3:G:389:ASP:C	3:G:391:THR:N	2.52	0.44
3:D:385:VAL:HG21	3:D:396:ARG:NH1	2.33	0.44
2:F:537:MET:CA	3:G:110:ASN:HB3	2.47	0.44
3:G:531:GLU:O	3:G:531:GLU:HG3	2.18	0.44
2:F:1042:GLY:O	2:F:1046:LEU:HB2	2.18	0.44
1:B:513:ASP:O	1:B:517:THR:HG22	2.17	0.44
1:E:447:TRP:O	1:E:448:ARG:HB2	2.17	0.44
3:G:397:LEU:HB2	3:G:580:TYR:CD2	2.53	0.44
1:E:153:ILE:HG13	1:E:154:GLU:N	2.31	0.44
1:E:375:ARG:HD2	1:E:404:GLN:NE2	2.33	0.44
3:D:170:SER:HA	3:D:296:GLY:O	2.17	0.44
2:F:716:PHE:CG	2:F:747:LEU:HD13	2.53	0.44
3:D:137:LEU:HD22	3:D:141:LEU:HD11	1.99	0.44
2:F:333:ASN:HB2	2:F:336:HIS:H	1.83	0.44
2:C:194:ILE:HG23	2:C:229:ALA:HB2	1.99	0.44
1:E:934:VAL:HG12	1:E:934:VAL:O	2.18	0.44
3:D:244:LEU:HB3	3:D:255:HIS:NE2	2.32	0.43
3:D:278:MET:HE3	4:X:2:5IU:I5	2.88	0.43
2:F:1080:MET:HG3	4:Y:11:DA:N3	2.33	0.43
4:Y:46:5IU:C2'	4:Y:47:DA:C5'	2.77	0.43
1:E:584:ARG:NH1	1:E:584:ARG:HG2	2.33	0.43
3:G:212:LEU:HA	3:G:212:LEU:HD23	1.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:119:VAL:CG1	3:D:600:LEU:HD21	2.48	0.43
2:C:998:LEU:HD22	2:C:1000:LEU:HD21	2.00	0.43
3:G:33:PRO:HG3	3:G:73:SER:HB3	2.00	0.43
1:E:1108:ASP:O	1:E:1112:GLN:OE1	2.36	0.43
1:E:66:GLU:HA	1:E:66:GLU:OE1	2.18	0.43
3:G:565:LEU:C	3:G:565:LEU:HD23	2.39	0.43
2:C:1:MET:CG	2:C:3:ARG:HE	2.28	0.43
2:F:396:MET:HE1	2:F:674:VAL:HG13	1.99	0.43
2:F:37:VAL:HG21	2:F:42:MET:CB	2.47	0.43
1:B:447:TRP:O	1:B:448:ARG:CB	2.66	0.43
3:G:555:SER:O	3:G:556:GLN:HG2	2.18	0.43
1:B:268:LYS:HE3	1:B:268:LYS:C	2.38	0.43
3:D:376:ARG:HB3	3:D:377:GLY:H	1.63	0.43
2:C:388:VAL:HG22	2:C:799:ARG:HH12	1.83	0.43
2:C:760:TYR:HE1	2:C:765:GLU:HG3	1.82	0.43
1:B:766:ALA:HB2	1:B:787:VAL:HG22	1.99	0.43
2:F:531:MET:HE3	2:F:561:VAL:HG22	2.00	0.43
2:F:287:PHE:HB2	2:F:293:GLN:HB3	1.99	0.43
1:E:228:ARG:HD2	1:E:316:LEU:HD21	2.00	0.43
1:B:460:LEU:O	1:B:463:GLN:HG2	2.17	0.43
4:X:16:DA:H2'	4:X:17:DG:C8	2.53	0.43
3:D:213:THR:HG21	3:D:235:GLU:CA	2.48	0.43
3:G:212:LEU:O	3:G:216:LEU:HB2	2.18	0.43
3:G:263:LEU:HD12	3:G:263:LEU:O	2.19	0.43
2:F:1015:GLN:O	2:F:1018:HIS:HB3	2.18	0.43
2:C:104:GLU:H	2:C:112:ARG:HH11	1.64	0.43
1:B:600:LEU:HD22	1:B:652:TRP:CH2	2.53	0.43
3:G:225:LEU:CD2	3:G:229:GLN:HA	2.49	0.43
1:E:823:ARG:NH2	1:E:828:LYS:NZ	2.66	0.43
1:B:237:ARG:HE	1:B:266:ILE:HG21	1.83	0.43
2:F:404:THR:OG1	2:F:406:ARG:HG3	2.18	0.43
2:F:7:SER:HB3	2:F:13:LEU:CG	2.42	0.43
3:D:176:GLY:O	3:D:180:THR:HB	2.18	0.43
2:C:273:GLU:CA	2:C:273:GLU:OE2	2.65	0.43
1:E:1062:LEU:CD2	1:E:1113:LEU:HD22	2.46	0.43
1:B:729:LEU:N	1:B:729:LEU:HD22	2.26	0.43
2:C:3:ARG:HG3	2:C:3:ARG:HH21	1.82	0.43
1:B:984:SER:C	1:B:986:TRP:H	2.21	0.43
3:D:91:VAL:HG13	3:D:100:MET:CE	2.47	0.43
2:F:396:MET:HE2	2:F:674:VAL:HG22	2.00	0.43
3:D:538:VAL:HG21	3:D:565:LEU:CD2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:MET:HE3	1:B:514:TYR:HD2	1.83	0.43
1:E:646:ASP:O	1:E:649:ARG:HG3	2.17	0.43
2:F:1076:GLU:HG3	2:F:1076:GLU:O	2.17	0.43
2:F:634:LEU:O	2:F:635:SER:C	2.56	0.43
2:C:245:ARG:HA	2:C:326:PHE:CE1	2.53	0.43
1:E:62:VAL:HA	1:E:127:PHE:O	2.18	0.43
2:F:1063:THR:C	2:F:1065:GLN:N	2.71	0.43
2:F:445:ARG:NH1	2:F:452:GLU:OE1	2.51	0.43
2:F:525:ARG:HG2	2:F:525:ARG:HH11	1.83	0.43
1:B:875:ASN:C	1:B:877:PRO:CD	2.84	0.43
3:G:133:ASP:O	3:G:135:ALA:N	2.51	0.43
2:C:103:LEU:HD11	2:C:115:LEU:HD13	1.99	0.43
1:B:1137:GLY:O	1:B:1138:VAL:HB	2.18	0.43
1:B:100:LEU:O	1:B:104:ILE:HG13	2.19	0.43
1:B:1093:TYR:CZ	1:B:1144:ARG:HB2	2.53	0.43
2:F:278:ARG:O	2:F:279:ASP:C	2.56	0.43
2:F:545:GLN:C	2:F:547:VAL:N	2.70	0.43
1:E:13:LEU:HD11	1:E:441:TYR:CE2	2.53	0.43
3:G:28:ALA:HB1	3:G:35:VAL:HG23	2.00	0.43
2:F:367:LEU:O	2:F:368:ASP:HB3	2.18	0.43
2:C:392:ARG:NH1	2:C:392:ARG:HG2	2.33	0.43
2:F:334:LEU:O	2:F:338:ILE:HG12	2.17	0.43
1:B:1032:ILE:H	1:B:1032:ILE:HD12	1.82	0.43
1:E:1032:ILE:HD12	1:E:1032:ILE:H	1.84	0.43
2:F:522:HIS:HE1	2:F:905:GLY:O	2.00	0.43
1:B:638:TRP:O	1:B:642:VAL:HG23	2.17	0.43
3:D:340:GLY:O	3:D:341:THR:OG1	2.32	0.43
3:D:11:VAL:HG21	3:D:21:VAL:HG11	2.01	0.43
1:B:120:GLN:HA	1:B:120:GLN:OE1	2.17	0.43
3:D:122:PHE:CE1	3:D:166:ILE:HG12	2.54	0.43
4:X:23:DC:C2'	4:X:24:DT:C6	3.01	0.43
1:E:611:THR:HG22	2:F:858:ARG:NH2	2.33	0.43
3:G:220:LEU:HA	3:G:223:LEU:CD2	2.48	0.43
1:E:860:LEU:O	1:E:860:LEU:HG	2.19	0.43
2:F:884:LEU:HG	2:F:917:TRP:CZ2	2.53	0.43
2:F:440:SER:O	2:F:441:ASP:CB	2.65	0.43
2:C:5:TYR:CD2	2:C:323:LEU:HD11	2.53	0.43
3:D:527:LEU:HA	3:D:528:PRO:HD3	1.73	0.43
2:C:544:TRP:CE2	2:C:545:GLN:HG2	2.54	0.43
2:F:943:ILE:CG2	2:F:986:VAL:HG13	2.49	0.43
1:B:54:LEU:HD13	1:B:380:VAL:CG1	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:991:GLY:O	2:F:992:GLY:C	2.55	0.43
1:B:939:THR:O	1:B:941:THR:HG23	2.18	0.43
2:C:435:LEU:HA	2:C:436:PRO:HD3	1.87	0.43
1:B:52:ARG:HH21	1:B:52:ARG:HG2	1.84	0.43
2:C:25:ARG:C	2:C:26:LEU:O	2.55	0.43
1:E:50:PHE:CE2	1:E:52:ARG:HD3	2.52	0.43
3:G:556:GLN:HA	3:G:585:ILE:CD1	2.48	0.43
2:C:245:ARG:HD3	2:C:344:GLU:OE2	2.18	0.43
2:C:915:ILE:O	2:C:919:THR:HG22	2.18	0.43
2:C:36:LEU:HD13	2:C:65:PRO:HA	2.00	0.43
3:G:221:ARG:O	3:G:221:ARG:HG2	2.19	0.43
1:E:835:GLN:HB3	1:E:835:GLN:HE21	1.70	0.43
2:C:878:TYR:CG	4:X:9:5IU:H4'	2.53	0.43
1:B:761:ARG:HD2	4:X:45:DT:OP1	2.18	0.43
1:B:584:ARG:NH1	1:B:584:ARG:HG2	2.33	0.43
3:D:212:LEU:O	3:D:216:LEU:HB2	2.17	0.43
1:E:282:LEU:C	1:E:284:GLU:H	2.22	0.43
1:E:947:ARG:HD2	1:E:1086:LEU:HD21	2.01	0.43
1:B:1085:TRP:O	1:B:1086:LEU:HD23	2.19	0.43
2:C:77:LEU:HB3	2:C:78:PRO:HD2	2.00	0.43
1:E:267:ASP:C	1:E:269:ILE:N	2.71	0.43
1:E:471:ARG:HD2	1:E:472:GLU:OE1	2.17	0.43
1:B:490:VAL:CG1	1:B:495:THR:HG22	2.48	0.43
1:B:1108:ASP:O	1:B:1112:GLN:OE1	2.36	0.43
2:C:142:ARG:HH21	2:C:705:ASP:CG	2.20	0.43
2:C:273:GLU:OE2	2:C:273:GLU:HA	2.19	0.43
1:E:1112:GLN:HB3	1:E:1168:MET:SD	2.59	0.43
3:D:370:LEU:HD23	3:D:577:LEU:HD23	2.00	0.43
2:C:70:TRP:CZ3	2:C:84:SER:HB2	2.53	0.43
2:F:286:LEU:HA	2:F:291:GLY:O	2.19	0.43
1:E:518:MET:HE2	1:E:816:GLY:HA3	2.00	0.43
3:G:423:GLN:C	3:G:425:ARG:N	2.69	0.43
2:C:602:ASP:HB3	2:C:605:THR:OG1	2.19	0.43
1:B:1127:ALA:O	1:B:1128:ASP:HB3	2.18	0.43
1:E:732:ASP:HA	1:E:735:LEU:HD12	2.00	0.43
3:G:405:ILE:HA	3:G:408:LEU:HD12	1.99	0.43
2:C:540:ALA:O	2:C:541:GLN:HB2	2.18	0.43
1:B:1120:ARG:HB2	2:C:56:ILE:HD12	2.00	0.43
2:C:388:VAL:HG13	2:C:799:ARG:HH11	1.82	0.43
2:F:311:ILE:HD13	2:F:311:ILE:O	2.18	0.43
3:G:317:ALA:C	3:G:319:ALA:N	2.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1170:GLU:O	1:E:1174:GLY:N	2.50	0.43
2:C:1048:THR:OG1	2:C:1070:LYS:HG3	2.19	0.43
2:F:1106:VAL:O	2:F:1107:GLU:C	2.57	0.43
2:C:175:TYR:CZ	2:C:179:LEU:HD11	2.53	0.43
2:C:1097:LEU:HA	2:C:1097:LEU:HD23	1.81	0.43
1:E:234:GLN:C	1:E:236:TRP:N	2.72	0.43
4:X:8:DC:H2''	4:X:9:5IU:O5'	2.19	0.43
3:G:242:ARG:O	3:G:243:LEU:C	2.56	0.43
3:G:275:ASP:OD1	4:Y:2:5IU:C4	2.67	0.43
1:B:567:VAL:HB	1:B:738:ILE:HD12	2.00	0.43
1:B:283:PRO:HB3	1:B:314:ASP:CG	2.39	0.43
1:E:1085:TRP:O	1:E:1086:LEU:HD23	2.19	0.43
3:G:132:VAL:CG1	3:G:134:GLU:HG2	2.48	0.43
2:C:106:GLU:HA	2:C:109:THR:OG1	2.19	0.43
1:E:269:ILE:HG22	1:E:270:SER:H	1.83	0.43
1:E:466:ASP:OD2	1:E:471:ARG:HA	2.19	0.43
2:C:701:PRO:HA	2:C:705:ASP:OD1	2.18	0.43
3:D:234:PRO:HB2	3:D:236:ASP:HB2	2.00	0.43
3:D:120:ALA:CB	3:D:603:LEU:HB3	2.49	0.43
2:F:367:LEU:CB	2:F:761:LEU:HD23	2.48	0.43
2:C:574:TRP:HE3	2:C:578:LEU:CD1	2.32	0.43
2:F:333:ASN:H	2:F:336:HIS:HB2	1.83	0.43
1:B:62:VAL:O	1:B:62:VAL:HG23	2.18	0.43
1:B:451:PRO:HG2	1:B:452:GLY:H	1.84	0.43
2:C:695:ASP:O	2:C:696:LEU:C	2.56	0.43
2:F:695:ASP:O	2:F:696:LEU:C	2.57	0.43
1:E:446:ASN:OD1	1:E:446:ASN:O	2.37	0.43
2:F:878:TYR:CD1	4:Y:9:5IU:H4'	2.53	0.43
1:E:875:ASN:C	1:E:877:PRO:CD	2.85	0.43
2:C:828:LEU:HB2	2:C:1028:ARG:HD2	2.01	0.43
1:E:1061:MET:HG3	2:F:48:MET:CE	2.49	0.43
4:X:36:DG:N9	4:X:37:DT:H72	2.34	0.43
2:F:441:ASP:OD2	2:F:662:CYS:HB2	2.19	0.43
3:G:387:GLN:C	3:G:389:ASP:H	2.22	0.43
2:C:141:TYR:O	2:C:142:ARG:CG	2.67	0.43
1:E:1107:TYR:O	1:E:1110:GLN:N	2.52	0.43
2:C:1046:LEU:CD2	2:C:1110:GLN:HG3	2.44	0.43
2:C:536:ALA:O	2:C:537:MET:O	2.37	0.43
2:F:986:VAL:HG12	2:F:987:TYR:N	2.34	0.43
2:F:70:TRP:CZ3	2:F:84:SER:HB2	2.54	0.43
3:D:565:LEU:C	3:D:565:LEU:HD23	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:504:MET:CE	1:E:518:MET:HG2	2.49	0.43
3:G:427:GLU:N	3:G:428:PRO:CD	2.81	0.43
3:G:427:GLU:N	3:G:428:PRO:HD2	2.34	0.43
2:F:845:VAL:CG1	2:F:1093:LEU:HD11	2.49	0.43
2:C:475:ASP:O	2:C:477:PRO:HD3	2.18	0.43
1:E:89:ARG:C	1:E:91:THR:H	2.22	0.43
1:B:961:ASP:CG	1:B:961:ASP:O	2.57	0.43
4:Y:23:DC:C2'	4:Y:24:DT:C6	3.02	0.43
2:F:882:GLN:HA	2:F:969:PRO:HG2	2.00	0.43
3:D:213:THR:CG2	3:D:235:GLU:CA	2.92	0.43
3:G:213:THR:HG21	3:G:235:GLU:CA	2.48	0.43
1:E:283:PRO:HB3	1:E:314:ASP:CG	2.39	0.43
2:C:363:ASN:ND2	2:C:363:ASN:N	2.32	0.43
3:D:526:ARG:HH22	3:D:533:THR:HG21	1.81	0.43
2:C:228:GLN:HE21	2:C:319:SER:H	1.66	0.43
1:B:555:SER:HA	1:B:737:GLN:O	2.19	0.43
2:C:50:LEU:O	2:C:54:PHE:HB2	2.19	0.43
2:C:966:ARG:NH1	2:C:983:GLU:OE1	2.44	0.43
3:D:387:GLN:C	3:D:389:ASP:H	2.21	0.43
3:G:175:THR:CG2	3:G:176:GLY:N	2.80	0.43
1:B:1112:GLN:HB3	1:B:1168:MET:SD	2.59	0.43
2:F:272:ARG:O	2:F:273:GLU:HB2	2.19	0.43
1:E:939:THR:O	1:E:941:THR:HG23	2.19	0.43
1:E:218:LEU:HD21	1:E:323:ILE:HG12	2.01	0.43
1:B:937:GLU:O	1:B:939:THR:N	2.46	0.43
2:F:290:ASP:HB2	2:F:291:GLY:H	1.51	0.43
3:G:561:VAL:CG1	3:G:589:ALA:HB2	2.48	0.43
1:B:534:GLN:OE1	1:B:880:VAL:HG23	2.18	0.43
3:D:423:GLN:C	3:D:425:ARG:N	2.70	0.43
1:B:150:GLN:HE21	1:B:150:GLN:CA	2.31	0.43
2:C:837:LEU:HD23	2:C:837:LEU:HA	1.89	0.43
2:F:388:VAL:HG13	2:F:799:ARG:HH11	1.84	0.43
1:E:170:ARG:HA	2:F:517:PRO:HG2	2.00	0.43
1:E:345:ARG:HH12	1:E:346:ARG:HG2	1.83	0.43
2:F:190:TYR:CE1	2:F:191:GLN:HG3	2.54	0.43
1:E:89:ARG:C	1:E:91:THR:N	2.70	0.43
2:F:248:TRP:N	2:F:248:TRP:CD1	2.87	0.43
3:G:356:GLN:HB2	3:G:356:GLN:HE21	1.62	0.43
2:C:858:ARG:HG3	2:C:858:ARG:HH11	1.84	0.43
1:E:860:LEU:H	1:E:860:LEU:HD23	1.83	0.43
1:B:591:LEU:HB3	2:C:1095:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1125:ARG:HB3	2:C:28:ASP:CB	2.49	0.43
3:D:229:GLN:O	3:D:232:ARG:CG	2.67	0.43
3:G:154:GLN:HA	3:G:355:LEU:HD22	2.00	0.43
2:C:544:TRP:CD2	2:C:545:GLN:HG2	2.54	0.43
2:F:3:ARG:HG3	2:F:3:ARG:HH21	1.83	0.43
2:F:392:ARG:HG2	2:F:392:ARG:NH1	2.33	0.43
3:G:98:THR:HG23	3:G:99:PRO:HD2	2.01	0.43
2:F:75:ARG:NH1	2:F:208:PRO:HD3	2.34	0.43
1:B:1021:MET:HE2	1:B:1069:VAL:HG21	1.98	0.43
3:G:582:ASP:C	3:G:584:ARG:N	2.70	0.43
2:F:377:HIS:CD2	2:F:728:TYR:CE1	3.06	0.43
2:C:868:GLU:HB2	2:C:869:PRO:HD2	2.01	0.43
1:E:434:ARG:HH11	1:E:434:ARG:CG	2.31	0.43
1:B:452:GLY:HA2	1:B:864:ASP:OD1	2.19	0.43
1:B:12:ARG:O	1:B:12:ARG:HG3	2.18	0.43
3:G:379:LYS:HG3	3:G:379:LYS:H	1.60	0.43
1:B:1025:LEU:HD11	1:B:1117:ALA:HA	2.00	0.43
4:X:4:5IU:H6	4:X:4:5IU:H2'	1.72	0.43
3:G:208:ALA:O	3:G:209:ALA:C	2.57	0.43
4:Y:3:5IU:H2''	4:Y:4:5IU:C5'	2.32	0.43
1:B:824:ARG:CB	4:X:16:DA:OP2	2.54	0.43
2:C:1012:ALA:H	2:C:1015:GLN:NE2	1.93	0.43
2:C:1015:GLN:O	2:C:1018:HIS:HB3	2.18	0.43
1:E:555:SER:HA	1:E:737:GLN:O	2.19	0.43
1:E:924:LEU:HD22	1:E:949:ALA:HB1	2.00	0.43
1:E:597:LEU:O	1:E:597:LEU:HD23	2.19	0.43
3:G:597:ARG:CD	3:G:597:ARG:C	2.86	0.43
2:F:50:LEU:O	2:F:54:PHE:HB2	2.19	0.43
3:D:53:LEU:HD11	3:D:58:LEU:CD1	2.49	0.43
1:B:587:VAL:CG1	1:B:690:ILE:HG13	2.48	0.43
3:G:376:ARG:HB3	3:G:377:GLY:H	1.64	0.43
3:G:537:THR:OG1	3:G:540:LYS:HG3	2.18	0.43
2:C:530:ARG:HG2	2:C:547:VAL:CG1	2.49	0.43
1:B:218:LEU:HD21	1:B:323:ILE:HG12	2.01	0.43
1:E:984:SER:C	1:E:986:TRP:H	2.22	0.43
1:B:39:ARG:HG3	1:B:39:ARG:NH1	2.33	0.43
2:F:764:ASP:HB3	2:F:767:LEU:CD1	2.49	0.43
1:B:390:ASP:OD2	1:B:392:GLN:HB2	2.19	0.43
1:E:550:ARG:O	1:E:551:ALA:C	2.57	0.43
2:F:72:MET:HE1	2:F:208:PRO:HD2	1.99	0.43
3:G:326:ALA:HB1	3:G:338:PRO:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ALA:HB1	1:B:441:TYR:CA	2.48	0.43
2:C:819:GLU:OE1	2:C:820:PHE:N	2.52	0.43
2:C:367:LEU:O	2:C:368:ASP:HB3	2.19	0.43
1:E:1101:ALA:O	1:E:1104:ALA:HB3	2.19	0.43
1:E:638:TRP:O	1:E:642:VAL:HG23	2.19	0.43
1:E:12:ARG:CG	1:E:12:ARG:O	2.67	0.43
3:D:317:ALA:C	3:D:319:ALA:N	2.73	0.43
2:F:445:ARG:HD3	2:F:455:ILE:HD12	2.01	0.43
2:C:845:VAL:CG1	2:C:1093:LEU:HD11	2.48	0.43
1:B:912:ARG:HA	1:B:912:ARG:HD3	1.71	0.43
3:D:208:ALA:O	3:D:209:ALA:C	2.57	0.42
4:X:2:5IU:H2''	4:X:3:5IU:C5'	2.49	0.42
1:E:1051:PRO:CD	1:E:1052:PRO:HD2	2.41	0.42
1:B:932:ALA:HB2	1:B:947:ARG:CG	2.49	0.42
1:B:947:ARG:N	1:B:947:ARG:HD3	2.27	0.42
1:B:600:LEU:HD11	1:B:694:LEU:HD21	2.01	0.42
1:E:868:GLN:HB3	1:E:868:GLN:HE21	1.62	0.42
2:F:1038:LEU:HD22	2:F:1090:TYR:CE1	2.54	0.42
3:D:344:GLU:C	3:D:349:ARG:HD2	2.39	0.42
1:E:222:HIS:NE2	1:E:272:TRP:HH2	2.17	0.42
2:F:998:LEU:HD22	2:F:1000:LEU:HD21	2.01	0.42
2:C:272:ARG:O	2:C:273:GLU:CB	2.67	0.42
1:E:1102:MET:CA	1:E:1102:MET:HE3	2.49	0.42
1:E:380:VAL:HG13	1:E:380:VAL:O	2.19	0.42
1:B:39:ARG:HD2	1:B:44:LEU:HB3	2.00	0.42
2:F:475:ASP:O	2:F:477:PRO:HD3	2.18	0.42
1:B:1127:ALA:O	1:B:1128:ASP:CB	2.67	0.42
3:D:52:CYS:SG	3:D:106:ARG:CG	3.07	0.42
2:F:246:TYR:CD2	2:F:275:PRO:HD3	2.54	0.42
2:C:240:PHE:CE2	2:C:242:ASN:ND2	2.87	0.42
1:B:12:ARG:O	1:B:12:ARG:CG	2.67	0.42
1:B:1029:GLU:HA	1:B:1030:PRO:HD2	1.86	0.42
2:C:120:ASP:O	2:C:121:LYS:HB2	2.19	0.42
1:E:998:LEU:C	1:E:1000:ALA:H	2.22	0.42
3:G:369:GLN:HB3	3:G:384:THR:HG21	2.01	0.42
3:D:244:LEU:HD22	3:D:255:HIS:CB	2.48	0.42
3:D:266:LEU:HD23	3:D:286:LEU:HD21	2.01	0.42
2:F:341:ASP:OD2	2:F:365:ARG:NH1	2.52	0.42
1:B:1075:ARG:NH1	1:B:1132:GLU:O	2.53	0.42
3:D:225:LEU:CD2	3:D:229:GLN:HA	2.49	0.42
1:E:831:THR:O	1:E:833:VAL:N	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ARG:NH1	1:E:221:ARG:HG2	2.33	0.42
1:E:1135:PHE:CG	1:E:1136:GLY:N	2.87	0.42
1:B:669:ASN:O	1:B:673:ASN:ND2	2.52	0.42
2:C:411:MET:HA	2:C:662:CYS:O	2.19	0.42
2:F:807:LEU:N	2:F:808:PRO:HD2	2.34	0.42
2:F:141:TYR:O	2:F:142:ARG:CG	2.67	0.42
1:B:1107:TYR:O	1:B:1111:TYR:HD1	2.02	0.42
1:B:1082:LYS:HD2	1:B:1140:TYR:CE1	2.54	0.42
2:F:266:ARG:HH21	2:F:272:ARG:HE	1.68	0.42
2:F:5:TYR:CE2	2:F:323:LEU:HD11	2.54	0.42
2:C:374:ILE:HA	2:C:727:LEU:O	2.19	0.42
1:B:893:LEU:HD11	2:C:432:ASP:HB2	2.01	0.42
3:D:300:GLN:HA	3:D:568:THR:CG2	2.48	0.42
1:B:637:ALA:HA	1:B:640:VAL:CG2	2.49	0.42
2:F:1022:GLN:O	2:F:1025:GLU:HB3	2.19	0.42
1:E:730:GLU:HA	1:E:730:GLU:OE1	2.19	0.42
2:F:574:TRP:HE3	2:F:578:LEU:CD1	2.32	0.42
1:B:154:GLU:HG2	1:B:155:ASP:H	1.84	0.42
2:C:634:LEU:O	2:C:635:SER:C	2.56	0.42
3:G:557:ARG:HB3	3:G:558:THR:H	1.27	0.42
2:F:595:LEU:HD23	2:F:609:MET:HE3	2.00	0.42
2:F:240:PHE:HE2	2:F:242:ASN:ND2	2.17	0.42
1:E:352:ASP:O	1:E:356:SER:HB2	2.19	0.42
3:G:233:ILE:N	3:G:233:ILE:CD1	2.83	0.42
3:D:455:ASN:HD21	3:D:532:THR:C	2.22	0.42
1:B:807:THR:HG22	1:B:807:THR:O	2.19	0.42
1:E:233:LYS:O	1:E:237:ARG:CG	2.68	0.42
1:B:899:ASP:HB3	1:B:1059:ARG:NH1	2.20	0.42
1:B:168:TRP:O	1:B:172:CYS:HB2	2.18	0.42
1:B:658:MET:HB3	1:B:659:PRO:CD	2.39	0.42
3:G:102:LEU:HD12	3:G:106:ARG:O	2.19	0.42
2:C:448:HIS:HA	2:C:449:PRO:HD3	1.89	0.42
2:C:699:GLN:H	2:C:699:GLN:HG2	1.63	0.42
2:C:767:LEU:H	2:C:767:LEU:HD23	1.83	0.42
1:B:426:ASP:O	1:B:429:THR:CG2	2.63	0.42
1:E:426:ASP:O	1:E:429:THR:CG2	2.64	0.42
2:F:25:ARG:C	2:F:26:LEU:O	2.55	0.42
2:C:368:ASP:OD1	2:C:370:LEU:HB2	2.19	0.42
1:E:1169:ASP:O	1:E:1172:PHE:HB3	2.19	0.42
1:E:703:SER:O	1:E:706:ALA:HB3	2.19	0.42
2:C:625:GLY:C	2:C:627:GLN:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:835:GLN:HE21	1:B:835:GLN:HB3	1.72	0.42
3:D:254:ARG:O	3:D:255:HIS:CB	2.66	0.42
3:D:240:LEU:CD2	3:D:274:ILE:HD12	2.49	0.42
1:B:531:GLN:O	1:B:535:ARG:HD3	2.19	0.42
4:X:10:DA:H4'	4:X:11:DA:OP1	2.19	0.42
3:D:130:ILE:O	3:D:132:VAL:HG23	2.20	0.42
1:B:711:LEU:HD22	1:B:715:ILE:HD11	2.01	0.42
2:C:160:GLU:O	2:C:161:ALA:HB3	2.19	0.42
1:E:97:TYR:O	1:E:100:LEU:HB2	2.19	0.42
3:G:229:GLN:O	3:G:230:LYS:HD2	2.19	0.42
3:G:229:GLN:O	3:G:232:ARG:CG	2.67	0.42
2:F:1036:LEU:O	2:F:1037:VAL:CB	2.62	0.42
2:F:1038:LEU:HA	2:F:1039:PRO:HD2	1.81	0.42
1:B:735:LEU:O	1:B:736:VAL:C	2.55	0.42
2:F:253:ASP:O	2:F:255:ALA:N	2.52	0.42
2:F:1:MET:CG	2:F:3:ARG:HE	2.28	0.42
2:C:775:ARG:HB3	2:C:775:ARG:NH1	2.34	0.42
3:D:300:GLN:OE1	3:D:567:TYR:HE2	2.01	0.42
1:E:504:MET:SD	1:E:517:THR:HG21	2.59	0.42
2:F:449:PRO:HB2	2:F:450:VAL:H	1.70	0.42
1:B:345:ARG:HH12	1:B:346:ARG:HG2	1.84	0.42
2:C:190:TYR:C	2:C:190:TYR:CD1	2.92	0.42
2:C:333:ASN:HB2	2:C:336:HIS:H	1.84	0.42
1:E:386:PHE:C	1:E:388:ASP:H	2.21	0.42
2:C:595:LEU:HD23	2:C:609:MET:HE3	2.01	0.42
3:G:253:LEU:HD13	3:G:255:HIS:NE2	2.34	0.42
3:G:278:MET:HE3	4:Y:2:5IU:I5	2.89	0.42
1:E:567:VAL:HB	1:E:738:ILE:HD12	2.01	0.42
1:B:924:LEU:HD22	1:B:949:ALA:HB1	2.00	0.42
3:G:228:GLU:O	3:G:230:LYS:N	2.50	0.42
1:E:827:LYS:HE2	1:E:831:THR:HG22	2.00	0.42
2:C:664:LEU:HD22	2:C:685:TYR:CZ	2.52	0.42
2:C:521:GLN:HG2	2:C:526:PHE:CE1	2.54	0.42
2:C:699:GLN:HE21	2:C:699:GLN:HB3	1.59	0.42
2:C:290:ASP:HB2	2:C:291:GLY:H	1.51	0.42
1:B:380:VAL:O	1:B:380:VAL:HG13	2.19	0.42
1:E:940:LEU:HD22	1:E:986:TRP:CH2	2.54	0.42
2:F:767:LEU:CD2	2:F:767:LEU:N	2.82	0.42
2:F:775:ARG:HB3	2:F:775:ARG:HH11	1.83	0.42
3:D:301:LEU:N	3:D:568:THR:CG2	2.80	0.42
1:B:1002:LEU:HD13	1:B:1008:SER:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:ARG:CG	1:E:52:ARG:NH2	2.80	0.42
1:B:606:PRO:HB2	1:B:642:VAL:HG13	2.01	0.42
1:E:1025:LEU:HD11	1:E:1117:ALA:HA	2.01	0.42
1:E:455:ASN:N	1:E:455:ASN:HD22	2.16	0.42
1:E:912:ARG:HD3	1:E:912:ARG:HA	1.70	0.42
1:E:785:GLU:N	1:E:785:GLU:OE1	2.47	0.42
1:B:1049:GLY:O	1:B:1051:PRO:CD	2.68	0.42
2:C:552:GLU:HA	2:C:552:GLU:OE1	2.20	0.42
3:G:287:PRO:C	3:G:289:HIS:N	2.73	0.42
2:C:1050:TYR:OH	2:C:1118:ARG:HA	2.19	0.42
2:C:27:ASP:HB3	2:C:29:PRO:HD2	2.01	0.42
3:G:370:LEU:HD23	3:G:577:LEU:HD23	2.00	0.42
3:D:307:GLY:N	3:D:597:ARG:HH21	2.17	0.42
1:E:468:PHE:CE1	1:E:475:PHE:HB2	2.54	0.42
2:F:943:ILE:O	2:F:953:THR:HA	2.19	0.42
1:E:763:GLN:HE21	1:E:764:GLU:H	1.66	0.42
2:F:394:LEU:HA	2:F:394:LEU:HD12	1.89	0.42
2:C:62:PHE:N	2:C:63:PRO:CD	2.82	0.42
2:F:582:ARG:HD3	2:F:587:TRP:CE2	2.55	0.42
2:F:701:PRO:HA	2:F:705:ASP:OD1	2.19	0.42
4:Y:34:DC:H1'	4:Y:35:DA:H5''	2.02	0.42
1:B:703:SER:O	1:B:706:ALA:HB3	2.19	0.42
2:F:936:GLN:O	2:F:960:GLN:HG2	2.18	0.42
3:D:198:ARG:HB2	3:D:263:LEU:HA	2.01	0.42
2:C:78:PRO:CD	2:C:192:ARG:NH1	2.77	0.42
3:D:79:GLN:C	3:D:81:TRP:N	2.72	0.42
2:F:901:PHE:HD1	2:F:917:TRP:CZ3	2.36	0.42
2:C:441:ASP:O	2:C:649:ARG:HD3	2.19	0.42
2:C:689:LEU:CD2	2:C:708:ARG:HD2	2.49	0.42
1:E:628:ILE:O	1:E:632:ASN:ND2	2.52	0.42
3:G:344:GLU:C	3:G:349:ARG:HD2	2.40	0.42
1:E:414:ASP:OD1	1:E:416:LYS:N	2.48	0.42
1:B:414:ASP:HA	1:B:415:PRO:HD2	1.96	0.42
1:E:707:LEU:O	1:E:710:TRP:HB3	2.19	0.42
3:G:459:GLU:O	3:G:463:GLN:HG3	2.20	0.42
2:F:173:VAL:O	2:F:176:THR:HG23	2.19	0.42
2:F:396:MET:HE2	2:F:674:VAL:HG21	2.01	0.42
2:C:1019:TYR:C	2:C:1021:SER:N	2.70	0.42
1:B:63:THR:HG22	1:B:384:ASP:OD1	2.19	0.42
2:F:199:SER:C	2:F:201:THR:N	2.73	0.42
3:G:555:SER:O	3:G:585:ILE:HG13	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:81:PRO:HG3	2:F:182:PRO:HB2	2.01	0.42
2:C:333:ASN:H	2:C:336:HIS:HB2	1.84	0.42
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.67	0.42
1:E:843:GLN:OE1	1:E:853:LEU:HG	2.20	0.42
2:C:43:ALA:O	2:C:47:GLN:HG3	2.19	0.42
1:B:911:GLN:HA	1:B:911:GLN:NE2	2.35	0.42
4:Y:4:5IU:H6	4:Y:4:5IU:H2'	1.66	0.42
1:E:237:ARG:HE	1:E:266:ILE:HG21	1.84	0.42
2:C:943:ILE:CD1	2:C:943:ILE:N	2.82	0.42
1:B:672:GLU:HG3	1:B:672:GLU:H	1.61	0.42
2:F:405:PRO:CG	2:F:658:PRO:HB2	2.49	0.42
1:B:1061:MET:HG3	2:C:48:MET:HE2	2.00	0.42
2:C:401:PRO:O	2:C:403:LEU:N	2.52	0.42
3:D:177:LYS:HA	3:D:180:THR:HG22	2.01	0.42
1:B:610:ASN:O	1:B:612:LEU:N	2.53	0.42
1:B:355:LEU:HD11	1:B:392:GLN:HE21	1.83	0.42
1:E:637:ALA:HA	1:E:640:VAL:CG2	2.49	0.42
1:E:212:PRO:O	1:E:213:PRO:C	2.57	0.42
1:B:699:THR:CG2	2:C:423:GLN:HE22	2.33	0.42
1:B:431:MET:O	1:B:434:ARG:HB3	2.19	0.42
1:B:89:ARG:C	1:B:91:THR:H	2.22	0.42
1:B:134:GLN:HB3	1:B:354:MET:SD	2.59	0.42
2:F:896:ARG:HH11	2:F:896:ARG:HG2	1.85	0.42
1:B:443:LEU:N	1:B:443:LEU:HD23	2.33	0.42
4:X:5:5IU:H6	4:X:5:5IU:H2'	1.80	0.42
3:G:244:LEU:HD13	3:G:255:HIS:CD2	2.54	0.42
3:G:255:HIS:HA	3:G:259:ASN:HB3	2.00	0.42
1:E:907:SER:C	1:E:909:LEU:H	2.22	0.42
1:E:423:ARG:HD3	1:E:423:ARG:HA	1.83	0.42
2:F:117:ASP:N	2:F:117:ASP:OD2	2.52	0.42
3:D:228:GLU:O	3:D:230:LYS:N	2.49	0.42
1:B:861:CYS:SG	1:B:866:ALA:CA	3.04	0.42
3:G:549:ALA:HB3	3:G:573:ALA:HB2	2.02	0.42
1:E:1039:LEU:H	1:E:1039:LEU:CD2	2.28	0.42
3:G:442:CYS:O	3:G:537:THR:HA	2.20	0.42
2:F:544:TRP:CE2	2:F:545:GLN:HG2	2.55	0.42
4:Y:39:DC:C2'	4:Y:40:DT:OP2	2.64	0.42
3:G:527:LEU:HA	3:G:528:PRO:HD3	1.78	0.42
3:D:538:VAL:HG21	3:D:565:LEU:HD21	2.01	0.42
2:F:997:ARG:CG	2:F:1007:ARG:HG3	2.48	0.42
2:F:602:ASP:HB3	2:F:605:THR:OG1	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1022:GLN:O	2:C:1025:GLU:HB3	2.19	0.42
1:E:1127:ALA:O	1:E:1128:ASP:HB3	2.20	0.42
2:C:37:VAL:HG21	2:C:42:MET:CB	2.48	0.42
2:C:396:MET:HE3	2:C:726:LYS:HG3	2.01	0.42
2:C:367:LEU:CB	2:C:761:LEU:HD23	2.49	0.42
2:C:398:GLU:O	2:C:399:GLU:C	2.58	0.42
1:B:843:GLN:OE1	1:B:853:LEU:HG	2.19	0.42
2:C:300:LEU:O	2:C:300:LEU:HG	2.20	0.42
2:C:1068:ARG:HG2	2:C:1068:ARG:HH21	1.85	0.42
3:G:4:GLN:HE21	3:G:4:GLN:HB2	1.61	0.42
3:G:269:ASP:O	3:G:270:GLU:HB2	2.20	0.42
1:E:156:GLU:HA	1:E:159:LEU:HB3	2.01	0.42
3:G:198:ARG:HB2	3:G:263:LEU:HA	2.01	0.42
1:B:597:LEU:HD12	1:B:715:ILE:CD1	2.35	0.42
1:B:710:TRP:O	1:B:714:HIS:HD2	2.02	0.42
1:B:831:THR:O	1:B:833:VAL:N	2.50	0.42
1:B:471:ARG:HD2	1:B:472:GLU:OE1	2.19	0.42
1:E:955:LEU:N	1:E:955:LEU:HD23	2.35	0.42
4:X:37:DT:C2'	4:X:38:DG:C5'	2.96	0.42
3:D:169:ILE:HB	3:D:295:LEU:CD2	2.43	0.42
1:B:468:PHE:CE1	1:B:475:PHE:HB2	2.55	0.42
1:B:142:PHE:CB	2:C:110:LEU:HD22	2.44	0.42
1:B:248:GLU:HB3	1:B:249:SER:H	1.69	0.42
1:B:685:THR:HG22	2:C:787:MET:HE2	2.01	0.42
3:G:234:PRO:HB2	3:G:236:ASP:HB2	2.00	0.42
2:F:775:ARG:HB3	2:F:775:ARG:NH1	2.35	0.42
3:G:330:SER:HB2	3:G:336:HIS:HA	2.01	0.42
2:C:392:ARG:HA	2:C:392:ARG:HD3	1.84	0.42
1:E:491:PHE:HE1	1:E:532:ALA:HB3	1.85	0.42
1:B:398:ARG:NH2	1:B:402:HIS:CE1	2.87	0.42
1:B:152:LEU:HD11	1:B:351:PHE:CE1	2.55	0.42
2:F:474:LEU:HD21	2:F:485:ILE:HD12	2.01	0.42
1:B:3:ASP:OD2	1:B:3:ASP:N	2.53	0.42
3:G:247:GLN:HE21	3:G:247:GLN:HB2	1.60	0.41
2:F:839:ARG:CB	4:Y:7:5IU:I5	3.38	0.41
4:Y:16:DA:H2''	4:Y:17:DG:C8	2.55	0.41
1:B:282:LEU:HA	1:B:285:SER:OG	2.21	0.41
1:E:222:HIS:CD2	1:E:272:TRP:CH2	3.06	0.41
2:C:829:PRO:O	2:C:830:GLU:HG3	2.20	0.41
2:F:77:LEU:CD1	2:F:189:LEU:HG	2.50	0.41
2:C:405:PRO:HG2	2:C:658:PRO:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:ARG:N	2:F:143:PRO:CD	2.83	0.41
1:E:416:LYS:HD2	1:E:468:PHE:CE1	2.55	0.41
3:D:175:THR:CG2	3:D:176:GLY:N	2.83	0.41
3:G:302:ALA:HA	3:G:305:GLU:HG2	2.00	0.41
3:G:526:ARG:HH12	3:G:536:MET:HE3	1.85	0.41
3:D:123:PHE:O	3:D:124:ASN:OD1	2.38	0.41
1:B:518:MET:CE	1:B:816:GLY:HA3	2.50	0.41
3:G:27:VAL:HG12	3:G:90:ALA:HB1	2.02	0.41
2:F:72:MET:HE3	2:F:230:LEU:HD11	2.02	0.41
3:D:326:ALA:HB1	3:D:338:PRO:O	2.19	0.41
1:B:779:ASP:O	1:B:781:ASN:N	2.53	0.41
2:F:479:LEU:HA	2:F:598:PHE:O	2.20	0.41
1:E:150:GLN:CA	1:E:150:GLN:HE21	2.30	0.41
3:G:170:SER:O	3:G:354:LEU:HA	2.20	0.41
2:C:843:HIS:HE1	2:C:1087:ASP:OD2	2.03	0.41
2:F:102:LEU:HD13	2:F:108:PHE:CZ	2.55	0.41
2:F:378:VAL:HG22	2:F:731:TYR:CZ	2.54	0.41
2:F:670:ILE:HG23	2:F:671:PRO:HD2	2.02	0.41
2:F:333:ASN:HD22	2:F:336:HIS:CD2	2.37	0.41
2:C:407:ASP:HB3	2:C:673:LYS:HB2	2.02	0.41
2:C:936:GLN:O	2:C:960:GLN:HG2	2.20	0.41
2:F:111:LEU:HD13	2:F:127:LEU:HD21	2.01	0.41
3:D:322:THR:HG23	3:D:350:ASP:OD1	2.19	0.41
3:G:254:ARG:O	3:G:260:PRO:CG	2.68	0.41
1:E:823:ARG:NE	1:E:825:GLY:HA3	2.35	0.41
1:B:749:TYR:HB2	1:B:752:VAL:HG12	2.03	0.41
1:E:222:HIS:CG	1:E:272:TRP:HH2	2.38	0.41
1:B:1124:HIS:HE1	2:C:54:PHE:CD1	2.38	0.41
1:B:920:LEU:HD23	2:C:650:ILE:CG1	2.50	0.41
2:F:411:MET:HA	2:F:662:CYS:O	2.20	0.41
3:G:345:ALA:HB3	3:G:349:ARG:CG	2.41	0.41
1:B:1036:LEU:HA	1:B:1039:LEU:HD21	2.03	0.41
3:D:570:VAL:HG13	3:D:577:LEU:CD2	2.50	0.41
3:G:600:LEU:HD22	3:G:604:PHE:CE1	2.55	0.41
3:G:301:LEU:N	3:G:568:THR:CG2	2.76	0.41
2:C:536:ALA:O	3:D:111:ARG:NE	2.53	0.41
1:E:1130:ASP:N	1:E:1134:HIS:HD2	2.13	0.41
1:B:390:ASP:OD1	1:B:393:GLN:HG3	2.20	0.41
1:E:211:PRO:HA	1:E:212:PRO:HD3	1.95	0.41
3:G:405:ILE:O	3:G:409:GLU:HG3	2.20	0.41
1:B:194:LEU:C	1:B:196:ASP:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:716:PHE:CG	2:C:747:LEU:HD13	2.55	0.41
2:C:1063:THR:C	2:C:1065:GLN:H	2.24	0.41
2:C:282:ASN:O	2:C:283:ALA:C	2.58	0.41
2:C:760:TYR:CE1	2:C:765:GLU:HG3	2.54	0.41
2:F:525:ARG:HG2	2:F:525:ARG:NH1	2.35	0.41
2:F:240:PHE:CE2	2:F:242:ASN:ND2	2.88	0.41
2:C:39:SER:OG	2:C:668:ARG:HB2	2.19	0.41
2:C:391:ASP:OD2	2:C:801:SER:HA	2.19	0.41
2:F:625:GLY:C	2:F:627:GLN:H	2.23	0.41
2:F:398:GLU:O	2:F:399:GLU:C	2.58	0.41
1:B:1094:THR:O	1:B:1096:GLN:N	2.53	0.41
2:C:902:ARG:HB2	2:C:907:LEU:HD12	2.02	0.41
1:B:998:LEU:C	1:B:1000:ALA:H	2.23	0.41
3:G:274:ILE:CG2	3:G:278:MET:HG2	2.46	0.41
1:B:527:ARG:HG2	1:B:527:ARG:NH1	2.34	0.41
2:F:106:GLU:HA	2:F:109:THR:OG1	2.20	0.41
1:B:1137:GLY:O	1:B:1158:THR:O	2.38	0.41
1:E:924:LEU:CD1	2:F:607:ALA:HA	2.51	0.41
1:E:827:LYS:NZ	1:E:829:GLY:HA2	2.36	0.41
1:B:557:LEU:HB2	1:B:754:LEU:HD12	2.01	0.41
3:D:73:SER:O	3:D:75:ILE:N	2.53	0.41
3:D:388:GLN:O	3:D:389:ASP:O	2.38	0.41
2:C:234:ILE:HG22	2:C:236:ILE:HG13	2.02	0.41
1:E:416:LYS:O	1:E:800:ARG:HG2	2.20	0.41
1:B:1102:MET:CA	1:B:1102:MET:HE3	2.49	0.41
2:C:87:ASN:HD22	2:C:89:GLN:N	2.18	0.41
1:E:763:GLN:NE2	1:E:764:GLU:H	2.18	0.41
2:C:997:ARG:CG	2:C:1007:ARG:HG3	2.49	0.41
3:D:35:VAL:CG2	3:D:36:THR:N	2.83	0.41
2:C:819:GLU:OE2	2:C:821:VAL:HG13	2.20	0.41
2:C:479:LEU:HA	2:C:598:PHE:O	2.19	0.41
3:D:170:SER:O	3:D:354:LEU:HA	2.19	0.41
1:B:1129:TYR:C	1:B:1129:TYR:CD1	2.93	0.41
1:B:386:PHE:CE1	1:B:389:THR:HG21	2.55	0.41
2:C:287:PHE:O	2:C:288:ASN:C	2.58	0.41
2:C:845:VAL:HG13	2:C:1093:LEU:HD11	2.01	0.41
2:F:760:TYR:CE1	2:F:765:GLU:HG3	2.56	0.41
3:G:436:ASN:CG	3:G:436:ASN:O	2.58	0.41
3:G:244:LEU:CD2	3:G:255:HIS:CB	2.91	0.41
3:G:264:ASP:OD1	3:G:289:HIS:NE2	2.51	0.41
2:C:1118:ARG:CG	2:C:1118:ARG:NH2	2.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:740:THR:O	1:B:741:ILE:C	2.59	0.41
1:E:527:ARG:NH1	1:E:527:ARG:HG2	2.35	0.41
1:B:652:TRP:HE1	1:B:657:VAL:HG22	1.82	0.41
1:B:711:LEU:HD22	1:B:715:ILE:CD1	2.51	0.41
2:F:557:ILE:C	2:F:559:GLU:N	2.73	0.41
1:B:823:ARG:NE	1:B:825:GLY:HA3	2.35	0.41
1:E:920:LEU:CD1	2:F:608:ALA:HB2	2.51	0.41
2:C:1037:VAL:HA	2:C:1109:SER:CB	2.40	0.41
1:E:725:GLN:HE21	1:E:725:GLN:HB3	1.62	0.41
2:C:708:ARG:O	2:C:709:ARG:C	2.58	0.41
2:C:13:LEU:O	2:C:239:LEU:HD23	2.20	0.41
1:E:1093:TYR:CZ	1:E:1144:ARG:HB2	2.56	0.41
1:E:1155:ILE:HG13	1:E:1156:TYR:N	2.35	0.41
1:B:579:VAL:HG11	1:B:732:ASP:HB3	2.00	0.41
1:B:730:GLU:OE1	1:B:730:GLU:HA	2.21	0.41
2:F:552:GLU:HA	2:F:552:GLU:OE1	2.20	0.41
1:E:17:GLY:HA2	1:E:408:ALA:HA	2.02	0.41
1:B:771:ARG:HH21	1:B:793:GLU:CG	2.32	0.41
1:E:390:ASP:OD2	1:E:392:GLN:HB2	2.20	0.41
1:B:446:ASN:C	1:B:447:TRP:O	2.58	0.41
1:E:57:GLU:HG3	1:E:57:GLU:H	1.35	0.41
2:F:336:HIS:HE1	2:F:724:GLN:O	2.03	0.41
2:F:287:PHE:O	2:F:288:ASN:C	2.59	0.41
2:F:760:TYR:HE1	2:F:765:GLU:HG3	1.84	0.41
3:D:539:HIS:ND1	3:D:539:HIS:C	2.74	0.41
3:D:287:PRO:C	3:D:289:HIS:N	2.71	0.41
2:F:858:ARG:HH11	2:F:858:ARG:HG3	1.84	0.41
3:D:220:LEU:HD11	3:D:233:ILE:HD11	2.02	0.41
3:D:115:ASN:HB3	3:D:276:LEU:CD2	2.35	0.41
2:C:404:THR:HB	2:C:405:PRO:HD2	2.02	0.41
1:E:658:MET:HB3	1:E:659:PRO:CD	2.43	0.41
2:F:966:ARG:NH1	2:F:983:GLU:OE1	2.45	0.41
2:F:708:ARG:O	2:F:709:ARG:C	2.59	0.41
1:B:1040:ILE:CD1	1:B:1168:MET:HE1	2.50	0.41
1:E:761:ARG:CG	1:E:822:ARG:HH22	2.28	0.41
1:E:8:LEU:HD13	1:E:10:PRO:CD	2.47	0.41
1:B:514:TYR:O	1:B:515:GLN:HG2	2.19	0.41
3:D:363:SER:HB3	3:D:365:SER:H	1.86	0.41
1:E:779:ASP:C	1:E:781:ASN:N	2.73	0.41
1:B:1027:ILE:HA	1:B:1172:PHE:HD1	1.85	0.41
3:D:27:VAL:HG12	3:D:90:ALA:HB1	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:34:DC:H1'	4:Y:35:DA:H5'	2.02	0.41
1:E:316:LEU:HD23	1:E:316:LEU:HA	1.69	0.41
1:B:228:ARG:HD2	1:B:316:LEU:HD21	2.02	0.41
1:E:911:GLN:NE2	1:E:911:GLN:HA	2.34	0.41
3:D:410:GLU:HG2	3:D:410:GLU:H	1.69	0.41
1:B:721:ASN:N	1:B:721:ASN:HD22	2.17	0.41
2:F:856:ASN:O	2:F:858:ARG:HG3	2.21	0.41
1:E:1049:GLY:O	1:E:1051:PRO:CD	2.69	0.41
1:E:909:LEU:HD21	1:E:1106:ARG:CB	2.51	0.41
3:D:229:GLN:O	3:D:230:LYS:HD2	2.19	0.41
1:B:950:SER:N	1:B:951:PRO:HD2	2.36	0.41
1:E:1118:LEU:HD22	1:E:1122:LEU:HG	2.02	0.41
2:F:405:PRO:HG2	2:F:658:PRO:CG	2.51	0.41
1:E:1124:HIS:CE1	2:F:54:PHE:CD1	3.09	0.41
2:C:998:LEU:CD2	2:C:1000:LEU:HD21	2.51	0.41
3:G:79:GLN:C	3:G:81:TRP:N	2.73	0.41
2:F:272:ARG:O	2:F:273:GLU:CB	2.68	0.41
3:G:455:ASN:O	3:G:459:GLU:HG3	2.20	0.41
3:G:463:GLN:C	3:G:465:LYS:N	2.74	0.41
1:B:39:ARG:HD2	1:B:44:LEU:CB	2.50	0.41
2:F:285:GLN:O	2:F:286:LEU:HB2	2.21	0.41
1:B:377:ARG:HG3	1:B:377:ARG:NH1	2.35	0.41
2:F:795:GLN:O	2:F:800:GLN:HG2	2.20	0.41
1:B:121:MET:C	1:B:123:GLU:N	2.74	0.41
1:E:1129:TYR:CD1	1:E:1129:TYR:C	2.93	0.41
1:E:895:ARG:HG2	1:E:896:LEU:N	2.35	0.41
3:G:137:LEU:O	3:G:141:LEU:HG	2.20	0.41
2:F:407:ASP:HB3	2:F:673:LYS:HB2	2.02	0.41
1:E:721:ASN:N	1:E:721:ASN:HD22	2.19	0.41
2:C:896:ARG:HG2	2:C:896:ARG:HH11	1.86	0.41
3:G:255:HIS:CE1	3:G:281:ARG:HB3	2.55	0.41
1:E:932:ALA:CB	1:E:947:ARG:NE	2.84	0.41
1:E:728:ARG:HG3	1:E:728:ARG:H	1.56	0.41
1:E:924:LEU:O	1:E:926:VAL:N	2.49	0.41
1:E:263:ALA:O	1:E:266:ILE:HG12	2.21	0.41
1:E:469:MET:SD	1:E:795:LEU:HD11	2.60	0.41
1:B:1040:ILE:HD12	1:B:1112:GLN:NE2	2.34	0.41
2:F:415:ILE:CB	2:F:663:THR:HG23	2.44	0.41
3:D:370:LEU:HD22	3:D:394:GLU:OE2	2.21	0.41
3:G:538:VAL:HG21	3:G:565:LEU:CD2	2.51	0.41
1:E:771:ARG:HH21	1:E:793:GLU:CG	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:PHE:CE2	1:B:52:ARG:HD3	2.55	0.41
3:D:556:GLN:O	3:D:557:ARG:HB2	2.20	0.41
3:G:31:GLU:OE2	3:G:88:SER:HB2	2.21	0.41
1:E:1148:LYS:H	1:E:1148:LYS:CD	2.32	0.41
2:F:699:GLN:HG2	2:F:699:GLN:H	1.64	0.41
2:C:532:LEU:O	2:C:535:TYR:HB3	2.20	0.41
1:E:896:LEU:HD12	1:E:898:GLY:N	2.36	0.41
1:B:728:ARG:HE	2:C:739:ASN:HB2	1.86	0.41
2:C:293:GLN:HG3	2:C:293:GLN:O	2.20	0.41
1:E:617:ALA:O	2:F:1092:ARG:HD2	2.21	0.41
1:E:432:LYS:HB2	1:E:774:PHE:HD1	1.86	0.41
1:E:784:PRO:O	1:E:788:ASP:OD1	2.37	0.41
2:C:653:ARG:HH11	2:C:653:ARG:HG2	1.86	0.41
1:E:961:ASP:O	1:E:961:ASP:CG	2.58	0.41
3:D:248:PRO:HD3	4:X:4:5IU:O2	2.21	0.41
3:D:165:ARG:HH21	3:D:288:ASP:HA	1.82	0.41
3:D:133:ASP:OD2	3:D:136:LEU:HB3	2.21	0.41
1:B:652:TRP:CE2	1:B:657:VAL:HG22	2.56	0.41
3:D:115:ASN:HD22	3:D:115:ASN:HA	1.66	0.41
1:B:262:GLN:CA	1:B:265:TRP:HB3	2.50	0.41
3:D:17:ARG:NH1	3:D:20:ASP:OD1	2.53	0.41
2:F:405:PRO:HG2	2:F:658:PRO:HG2	2.02	0.41
2:C:403:LEU:HD22	2:C:404:THR:O	2.20	0.41
2:C:425:VAL:C	2:C:427:GLY:H	2.24	0.41
3:G:73:SER:O	3:G:75:ILE:N	2.53	0.41
1:B:1082:LYS:HE2	1:B:1107:TYR:CE1	2.56	0.41
2:C:5:TYR:CE2	2:C:323:LEU:HD11	2.55	0.41
2:F:321:GLN:O	2:F:323:LEU:CD2	2.63	0.41
3:D:549:ALA:HB3	3:D:573:ALA:HB2	2.03	0.41
3:D:570:VAL:HG22	3:D:577:LEU:HD21	2.02	0.41
3:G:412:LEU:CD1	3:G:461:PHE:HD2	2.34	0.41
3:G:526:ARG:C	3:G:526:ARG:HE	2.24	0.41
3:G:533:THR:OG1	3:G:534:TRP:N	2.53	0.41
3:G:533:THR:C	3:G:535:ALA:N	2.73	0.41
3:D:300:GLN:O	3:D:302:ALA:N	2.54	0.41
1:B:346:ARG:NE	1:B:348:GLU:OE1	2.52	0.41
1:B:199:ARG:H	1:B:199:ARG:HG3	1.73	0.41
1:B:1063:LYS:HE2	1:B:1063:LYS:HB3	1.89	0.41
2:C:670:ILE:HG23	2:C:671:PRO:HD2	2.02	0.41
2:C:129:SER:C	2:C:131:ALA:N	2.74	0.41
2:F:221:PRO:O	2:F:225:GLN:HG3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:255:HIS:HD1	3:D:256:HIS:N	2.18	0.41
3:D:282:LEU:HD23	3:D:286:LEU:HG	2.02	0.41
2:F:1081:VAL:O	2:F:1082:ARG:HG3	2.21	0.41
2:F:347:ASN:HD21	2:F:349:ALA:N	2.14	0.41
2:F:104:GLU:CG	2:F:104:GLU:O	2.58	0.41
2:C:105:ARG:O	2:C:106:GLU:CB	2.49	0.41
1:B:234:GLN:C	1:B:236:TRP:N	2.73	0.41
1:B:827:LYS:HE2	1:B:831:THR:HG22	2.02	0.41
1:E:226:VAL:HG13	1:E:269:ILE:HD13	2.03	0.41
1:B:222:HIS:NE2	1:B:272:TRP:HH2	2.19	0.41
3:G:597:ARG:HH11	3:G:598:SER:CB	2.31	0.41
1:B:466:ASP:OD2	1:B:471:ARG:HA	2.21	0.41
2:C:884:LEU:HG	2:C:917:TRP:CZ2	2.56	0.41
1:E:945:PHE:HA	1:E:946:PRO:HD2	1.84	0.41
2:C:709:ARG:NH2	2:C:709:ARG:CG	2.82	0.41
1:E:672:GLU:H	1:E:672:GLU:HG3	1.64	0.41
2:C:749:GLN:O	2:C:752:ILE:HD12	2.20	0.41
2:C:266:ARG:HH21	2:C:272:ARG:HE	1.68	0.41
1:E:1107:TYR:O	1:E:1111:TYR:HD1	2.03	0.41
2:C:374:ILE:HG12	2:C:727:LEU:HB3	2.01	0.41
3:G:300:GLN:OE1	3:G:567:TYR:HE2	2.04	0.41
3:G:526:ARG:NH1	3:G:536:MET:CE	2.82	0.41
2:C:139:LEU:HD23	2:C:146:LEU:HD12	2.03	0.41
1:B:771:ARG:NH1	1:B:771:ARG:CG	2.84	0.41
2:F:372:SER:OG	2:F:726:LYS:HE2	2.20	0.41
2:F:373:SER:O	2:F:374:ILE:HB	2.21	0.41
1:B:514:TYR:CE2	1:B:518:MET:HG3	2.56	0.41
3:G:337:VAL:HA	3:G:338:PRO:HD2	1.94	0.41
2:C:59:ASN:N	2:C:60:ILE:HD12	2.36	0.41
2:F:24:GLU:O	2:F:26:LEU:N	2.53	0.41
3:D:330:SER:HB2	3:D:336:HIS:HA	2.02	0.41
1:E:39:ARG:HD2	1:E:44:LEU:CB	2.51	0.41
2:F:1008:PHE:HA	2:F:1009:PRO:HD3	1.70	0.41
2:C:396:MET:HE2	2:C:674:VAL:HG21	2.03	0.41
1:E:1172:PHE:CE2	1:E:1173:ALA:HB2	2.55	0.41
2:F:1071:PHE:HD2	2:F:1072:LEU:HD23	1.86	0.41
2:F:175:TYR:CE2	2:F:179:LEU:HD11	2.56	0.41
1:B:194:LEU:C	1:B:196:ASP:H	2.23	0.41
3:D:101:ILE:HD11	3:D:110:ASN:OD1	2.21	0.41
2:F:837:LEU:O	2:F:841:TRP:HD1	2.03	0.41
2:C:841:TRP:O	2:C:842:ALA:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:915:ILE:O	2:F:919:THR:HG22	2.20	0.41
2:C:191:GLN:HB2	2:C:191:GLN:HE21	1.52	0.41
1:B:895:ARG:HG2	1:B:896:LEU:N	2.35	0.41
2:C:1068:ARG:HG2	2:C:1068:ARG:NH2	2.34	0.41
1:B:849:ASP:HB3	1:B:852:GLY:H	1.85	0.41
1:E:1067:ASP:HB2	1:E:1080:ASP:HA	2.02	0.41
1:E:460:LEU:O	1:E:463:GLN:HG2	2.20	0.41
2:F:282:ASN:O	2:F:283:ALA:C	2.59	0.41
1:B:1067:ASP:HB2	1:B:1080:ASP:HA	2.02	0.41
3:D:436:ASN:CG	3:D:436:ASN:O	2.58	0.41
2:C:1106:VAL:O	2:C:1107:GLU:C	2.59	0.41
3:D:62:GLU:H	3:D:62:GLU:CD	2.24	0.41
2:F:1001:ARG:NH2	4:Y:10:DA:OP1	2.54	0.41
2:C:1001:ARG:NH2	4:X:10:DA:OP1	2.54	0.41
1:B:739:VAL:CG2	1:B:743:LYS:HB2	2.51	0.41
1:B:311:GLU:O	1:B:314:ASP:HB3	2.21	0.41
2:F:105:ARG:O	2:F:106:GLU:CB	2.50	0.41
1:E:749:TYR:HB2	1:E:752:VAL:HG12	2.03	0.41
1:B:253:ASP:C	1:B:255:ARG:N	2.71	0.41
2:C:832:VAL:HG22	2:C:952:ILE:HG22	2.03	0.41
2:C:945:LEU:HD11	2:C:989:ALA:C	2.41	0.41
2:F:27:ASP:HB3	2:F:29:PRO:HD2	2.02	0.41
1:B:672:GLU:OE1	2:C:808:PRO:HG3	2.21	0.41
2:C:557:ILE:C	2:C:559:GLU:N	2.74	0.41
2:C:557:ILE:CD1	2:C:557:ILE:H	2.14	0.41
2:C:1038:LEU:HA	2:C:1039:PRO:HD2	1.82	0.41
1:E:194:LEU:C	1:E:196:ASP:N	2.74	0.41
1:B:1061:MET:HE3	2:C:48:MET:CA	2.49	0.41
2:C:142:ARG:CZ	2:C:697:MET:HG3	2.51	0.41
2:F:834:LEU:HD22	2:F:834:LEU:HA	1.95	0.41
2:F:834:LEU:O	2:F:838:GLN:HG3	2.21	0.41
2:F:392:ARG:O	2:F:396:MET:HG2	2.21	0.41
3:G:151:ILE:HA	3:G:335:THR:HG21	2.02	0.41
1:B:8:LEU:HD13	1:B:10:PRO:CD	2.49	0.41
2:C:837:LEU:O	2:C:841:TRP:HD1	2.03	0.41
1:E:199:ARG:HG3	1:E:199:ARG:H	1.76	0.41
1:B:455:ASN:N	1:B:455:ASN:ND2	2.69	0.41
2:F:1069:THR:O	2:F:1073:GLN:HB2	2.21	0.41
3:G:204:PRO:CG	3:G:274:ILE:HD13	2.41	0.40
3:G:282:LEU:HD23	3:G:282:LEU:O	2.21	0.40
2:C:159:GLY:C	2:C:160:GLU:O	2.59	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:GLN:HB2	1:B:262:GLN:HE21	1.53	0.40
4:X:49:DA:C2	4:X:50:5IU:C4	3.04	0.40
3:G:80:ASN:O	3:G:83:GLU:N	2.54	0.40
3:G:358:SER:HB2	3:G:359:TYR:H	1.75	0.40
1:B:732:ASP:C	1:B:734:HIS:N	2.74	0.40
2:C:285:GLN:O	2:C:286:LEU:HB2	2.21	0.40
1:B:34:ALA:CB	1:B:79:ASN:ND2	2.82	0.40
2:C:146:LEU:HD13	2:C:169:TRP:CZ2	2.56	0.40
2:C:767:LEU:CD2	2:C:767:LEU:N	2.84	0.40
1:E:571:LEU:HD12	1:E:571:LEU:HA	1.94	0.40
1:E:713:GLN:HB2	1:E:713:GLN:HE21	1.56	0.40
2:C:59:ASN:C	2:C:60:ILE:HD12	2.41	0.40
3:D:557:ARG:HB3	3:D:558:THR:H	1.27	0.40
3:G:397:LEU:HD13	3:G:410:GLU:OE1	2.21	0.40
2:C:574:TRP:HE3	2:C:578:LEU:HD13	1.86	0.40
2:C:333:ASN:ND2	2:C:336:HIS:CD2	2.89	0.40
1:E:719:ASP:O	1:E:720:SER:O	2.39	0.40
1:E:1094:THR:O	1:E:1096:GLN:N	2.55	0.40
1:E:849:ASP:HB3	1:E:852:GLY:H	1.86	0.40
2:F:1082:ARG:HH11	2:F:1082:ARG:CB	2.34	0.40
2:F:1081:VAL:HG12	4:Y:10:DA:H2"	2.03	0.40
1:B:1102:MET:CE	1:B:1111:TYR:OH	2.70	0.40
1:B:1107:TYR:O	1:B:1110:GLN:N	2.54	0.40
2:C:141:TYR:O	2:C:142:ARG:CB	2.68	0.40
2:C:142:ARG:N	2:C:143:PRO:CD	2.84	0.40
3:G:300:GLN:O	3:G:302:ALA:N	2.55	0.40
2:C:286:LEU:HA	2:C:291:GLY:O	2.22	0.40
1:B:940:LEU:HD22	1:B:986:TRP:CH2	2.56	0.40
3:G:561:VAL:HG12	3:G:561:VAL:O	2.21	0.40
1:B:901:TRP:CD1	1:B:901:TRP:C	2.94	0.40
1:B:550:ARG:O	1:B:553:ASP:N	2.42	0.40
2:F:819:GLU:OE1	2:F:820:PHE:N	2.54	0.40
1:E:901:TRP:C	1:E:901:TRP:CD1	2.93	0.40
2:C:532:LEU:HD13	3:D:23:PHE:HA	2.02	0.40
4:Y:33:DG:H2"	4:Y:34:DC:OP2	2.21	0.40
2:F:14:GLU:OE2	2:F:14:GLU:C	2.59	0.40
3:G:317:ALA:O	3:G:319:ALA:N	2.53	0.40
2:F:848:PHE:CE1	2:F:1033:ALA:HA	2.56	0.40
1:B:1028:SER:O	1:B:1029:GLU:O	2.39	0.40
1:B:843:GLN:O	1:B:845:GLY:N	2.53	0.40
3:G:340:GLY:O	3:G:341:THR:OG1	2.33	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1008:SER:O	1:E:1009:LEU:C	2.60	0.40
2:C:248:TRP:CD1	2:C:248:TRP:N	2.89	0.40
3:D:244:LEU:HD13	3:D:255:HIS:CE1	2.56	0.40
3:D:270:GLU:HB3	3:D:273:MET:HE2	2.03	0.40
3:D:271:ALA:HA	3:D:274:ILE:HG12	2.03	0.40
1:B:1052:PRO:O	1:B:1053:LEU:HD23	2.21	0.40
3:G:62:GLU:H	3:G:62:GLU:CD	2.22	0.40
1:B:879:GLN:CB	1:E:883:VAL:HG11	2.49	0.40
1:E:876:GLN:N	1:E:877:PRO:CD	2.84	0.40
3:D:207:LYS:HZ1	3:D:544:SER:HA	1.85	0.40
3:D:533:THR:C	3:D:535:ALA:N	2.74	0.40
1:B:11:LEU:HD21	1:B:100:LEU:HD23	2.03	0.40
1:E:1061:MET:HE3	2:F:48:MET:HA	2.03	0.40
2:F:141:TYR:O	2:F:142:ARG:CB	2.69	0.40
2:F:536:ALA:O	2:F:537:MET:O	2.39	0.40
3:D:450:GLY:O	3:D:454:LEU:HB2	2.22	0.40
3:D:555:SER:O	3:D:556:GLN:HG2	2.21	0.40
3:D:561:VAL:HG12	3:D:561:VAL:O	2.21	0.40
2:F:868:GLU:HB2	2:F:869:PRO:HD2	2.04	0.40
1:B:268:LYS:HE3	1:B:268:LYS:HA	2.03	0.40
2:C:388:VAL:HG11	2:C:784:HIS:NE2	2.36	0.40
1:B:195:ARG:O	1:B:195:ARG:HG2	2.21	0.40
3:G:199:ILE:HG12	3:G:265:VAL:HG13	2.03	0.40
2:F:297:ASN:HD22	2:F:341:ASP:HB3	1.86	0.40
2:C:78:PRO:HD2	2:C:192:ARG:HH12	1.85	0.40
1:B:694:LEU:HA	1:B:694:LEU:HD12	1.84	0.40
1:B:595:GLU:HA	1:B:598:TRP:CE3	2.57	0.40
1:B:231:THR:O	1:B:234:GLN:HB2	2.22	0.40
2:F:604:GLU:O	2:F:607:ALA:HB3	2.20	0.40
2:C:943:ILE:HG22	2:C:945:LEU:HD23	2.03	0.40
3:G:53:LEU:CD1	3:G:58:LEU:HD12	2.51	0.40
2:F:749:GLN:O	2:F:752:ILE:HD12	2.22	0.40
2:C:266:ARG:HD2	2:C:269:PHE:CG	2.56	0.40
3:G:373:ALA:CB	3:G:380:THR:HB	2.46	0.40
2:C:253:ASP:O	2:C:255:ALA:N	2.53	0.40
2:F:394:LEU:HD23	2:F:802:TYR:HB2	2.03	0.40
3:G:90:ALA:O	3:G:100:MET:HE2	2.21	0.40
2:F:234:ILE:HG22	2:F:236:ILE:HG13	2.02	0.40
1:B:446:ASN:O	1:B:446:ASN:OD1	2.40	0.40
2:C:199:SER:C	2:C:201:THR:N	2.74	0.40
2:C:964:LEU:HB2	2:C:996:SER:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:524:TRP:HE3	2:F:528:LEU:HD21	1.87	0.40
1:B:688:LEU:O	1:B:691:SER:HB2	2.20	0.40
3:G:586:LEU:O	3:G:586:LEU:HD23	2.22	0.40
3:D:239:THR:CG2	4:X:4:5IU:OP1	2.53	0.40
1:E:262:GLN:CA	1:E:265:TRP:HB3	2.51	0.40
1:E:282:LEU:C	1:E:282:LEU:HD13	2.42	0.40
1:E:311:GLU:O	1:E:314:ASP:HB3	2.22	0.40
1:E:1084:ASN:HB3	1:E:1085:TRP:H	1.60	0.40
1:B:932:ALA:HB2	1:B:947:ARG:HG2	2.04	0.40
2:F:557:ILE:C	2:F:559:GLU:H	2.25	0.40
1:B:990:LEU:O	1:B:994:ILE:HG13	2.20	0.40
1:B:868:GLN:HB3	1:B:868:GLN:HE21	1.61	0.40
1:B:226:VAL:HG13	1:B:269:ILE:CD1	2.51	0.40
1:E:807:THR:O	1:E:807:THR:HG22	2.21	0.40
3:D:33:PRO:HG3	3:D:73:SER:HB3	2.04	0.40
2:C:506:ILE:HG13	2:C:568:LEU:HD12	2.03	0.40
2:F:425:VAL:C	2:F:427:GLY:H	2.25	0.40
1:B:919:ASP:HA	2:C:652:GLN:HG3	2.02	0.40
3:G:425:ARG:HD3	3:G:425:ARG:HA	1.91	0.40
2:C:24:GLU:O	2:C:26:LEU:N	2.54	0.40
2:C:1082:ARG:HH11	2:C:1082:ARG:CB	2.32	0.40
2:F:611:LEU:HD23	2:F:611:LEU:C	2.42	0.40
2:F:1077:GLY:H	2:F:1083:GLY:HA3	1.84	0.40
2:F:1075:TYR:CZ	2:F:1097:LEU:HG	2.57	0.40
1:E:623:LEU:HA	1:E:623:LEU:HD23	1.93	0.40
1:E:3:ASP:N	1:E:3:ASP:OD2	2.54	0.40
2:C:1053:GLN:N	2:C:1053:GLN:OE1	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1149/1180 (97%)	883 (77%)	173 (15%)	93 (8%)	1	15
1	E	1149/1180 (97%)	885 (77%)	173 (15%)	91 (8%)	1	16
2	C	1119/1122 (100%)	870 (78%)	164 (15%)	85 (8%)	1	17
2	F	1119/1122 (100%)	870 (78%)	162 (14%)	87 (8%)	1	16
3	D	541/608 (89%)	374 (69%)	97 (18%)	70 (13%)	0	7
3	G	541/608 (89%)	375 (69%)	95 (18%)	71 (13%)	0	7
All	All	5618/5820 (96%)	4257 (76%)	864 (15%)	497 (9%)	1	14

All (497) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	GLY
1	B	18	GLU
1	B	95	PRO
1	B	96	LEU
1	B	155	ASP
1	B	214	ASP
1	B	244	ASP
1	B	259	ARG
1	B	276	GLU
1	B	282	LEU
1	B	307	HIS
1	B	308	PRO
1	B	320	PRO
1	B	463	GLN
1	B	492	LYS
1	B	514	TYR
1	B	678	ALA
1	B	720	SER
1	B	782	ALA
1	B	844	LYS
1	B	870	ALA
1	B	875	ASN
1	B	879	GLN
1	B	912	ARG
1	B	916	ILE
1	B	938	PRO
1	B	1002	LEU
1	B	1007	VAL
1	B	1050	CYS
1	B	1052	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1085	TRP
1	B	1090	SER
1	B	1143	LEU
2	C	23	ARG
2	C	28	ASP
2	C	60	ILE
2	C	117	ASP
2	C	119	SER
2	C	160	GLU
2	C	271	ASP
2	C	279	ASP
2	C	282	ASN
2	C	290	ASP
2	C	368	ASP
2	C	399	GLU
2	C	658	PRO
2	C	689	LEU
2	C	736	ILE
2	C	829	PRO
2	C	843	HIS
2	C	862	SER
2	C	948	ASN
2	C	958	GLN
2	C	992	GLY
2	C	1013	ALA
2	C	1036	LEU
2	C	1083	GLY
3	D	16	LEU
3	D	65	HIS
3	D	78	LEU
3	D	79	GLN
3	D	95	ASP
3	D	131	GLU
3	D	132	VAL
3	D	151	ILE
3	D	193	ASP
3	D	222	GLN
3	D	227	ASP
3	D	237	ALA
3	D	256	HIS
3	D	259	ASN
3	D	260	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	279	MET
3	D	280	SER
3	D	345	ALA
3	D	346	ALA
3	D	365	SER
3	D	388	GLN
3	D	391	THR
3	D	529	GLU
3	D	557	ARG
3	D	558	THR
1	E	17	GLY
1	E	18	GLU
1	E	95	PRO
1	E	96	LEU
1	E	155	ASP
1	E	214	ASP
1	E	244	ASP
1	E	259	ARG
1	E	276	GLU
1	E	282	LEU
1	E	307	HIS
1	E	308	PRO
1	E	463	GLN
1	E	492	LYS
1	E	514	TYR
1	E	678	ALA
1	E	720	SER
1	E	782	ALA
1	E	844	LYS
1	E	875	ASN
1	E	879	GLN
1	E	912	ARG
1	E	916	ILE
1	E	938	PRO
1	E	1002	LEU
1	E	1007	VAL
1	E	1050	CYS
1	E	1052	PRO
1	E	1085	TRP
1	E	1090	SER
1	E	1143	LEU
2	F	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	28	ASP
2	F	60	ILE
2	F	117	ASP
2	F	119	SER
2	F	160	GLU
2	F	271	ASP
2	F	279	ASP
2	F	282	ASN
2	F	290	ASP
2	F	368	ASP
2	F	399	GLU
2	F	658	PRO
2	F	689	LEU
2	F	829	PRO
2	F	843	HIS
2	F	862	SER
2	F	948	ASN
2	F	958	GLN
2	F	992	GLY
2	F	1013	ALA
2	F	1036	LEU
2	F	1083	GLY
3	G	16	LEU
3	G	65	HIS
3	G	79	GLN
3	G	95	ASP
3	G	131	GLU
3	G	132	VAL
3	G	151	ILE
3	G	193	ASP
3	G	222	GLN
3	G	227	ASP
3	G	237	ALA
3	G	245	GLY
3	G	256	HIS
3	G	259	ASN
3	G	260	PRO
3	G	280	SER
3	G	345	ALA
3	G	346	ALA
3	G	365	SER
3	G	388	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	391	THR
3	G	451	VAL
3	G	526	ARG
3	G	529	GLU
3	G	557	ARG
3	G	558	THR
1	B	24	SER
1	B	239	ALA
1	B	250	SER
1	B	252	ILE
1	B	261	ASN
1	B	470	PHE
1	B	471	ARG
1	B	731	SER
1	B	827	LYS
1	B	861	CYS
1	B	1073	GLU
1	B	1088	GLU
2	C	25	ARG
2	C	27	ASP
2	C	53	LYS
2	C	56	ILE
2	C	106	GLU
2	C	120	ASP
2	C	200	ALA
2	C	288	ASN
2	C	304	GLY
2	C	432	ASP
2	C	449	PRO
2	C	503	ARG
2	C	537	MET
2	C	540	ALA
2	C	630	ASP
2	C	692	LEU
2	C	861	ASP
2	C	910	GLY
2	C	990	SER
2	C	1078	ASN
3	D	2	LYS
3	D	3	LEU
3	D	14	LYS
3	D	29	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	67	LEU
3	D	74	GLU
3	D	80	ASN
3	D	225	LEU
3	D	229	GLN
3	D	232	ARG
3	D	245	GLY
3	D	255	HIS
3	D	261	LEU
3	D	338	PRO
3	D	340	GLY
3	D	376	ARG
3	D	390	PHE
3	D	426	ALA
3	D	450	GLY
3	D	451	VAL
3	D	526	ARG
3	D	530	HIS
3	D	533	THR
3	D	583	GLU
3	D	594	THR
1	E	24	SER
1	E	239	ALA
1	E	250	SER
1	E	252	ILE
1	E	261	ASN
1	E	320	PRO
1	E	364	SER
1	E	470	PHE
1	E	471	ARG
1	E	731	SER
1	E	827	LYS
1	E	861	CYS
1	E	870	ALA
1	E	1073	GLU
1	E	1088	GLU
2	F	25	ARG
2	F	27	ASP
2	F	53	LYS
2	F	200	ALA
2	F	262	THR
2	F	288	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	304	GLY
2	F	432	ASP
2	F	449	PRO
2	F	537	MET
2	F	540	ALA
2	F	630	ASP
2	F	692	LEU
2	F	736	ILE
2	F	861	ASP
2	F	910	GLY
2	F	990	SER
2	F	1078	ASN
3	G	2	LYS
3	G	3	LEU
3	G	14	LYS
3	G	29	GLY
3	G	67	LEU
3	G	74	GLU
3	G	78	LEU
3	G	80	ASN
3	G	229	GLN
3	G	232	ARG
3	G	255	HIS
3	G	261	LEU
3	G	279	MET
3	G	338	PRO
3	G	340	GLY
3	G	376	ARG
3	G	390	PHE
3	G	426	ALA
3	G	450	GLY
3	G	530	HIS
3	G	533	THR
3	G	583	GLU
3	G	594	THR
1	B	44	LEU
1	B	107	LYS
1	B	235	GLN
1	B	260	SER
1	B	324	ARG
1	B	331	ALA
1	B	364	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	515	GLN
1	B	609	GLU
1	B	611	THR
1	B	629	GLU
1	B	718	PRO
1	B	761	ARG
1	B	780	LEU
1	B	826	ASP
1	B	937	GLU
1	B	985	GLN
1	B	1057	GLN
1	B	1087	GLY
1	B	1095	GLN
2	C	142	ARG
2	C	262	THR
2	C	273	GLU
2	C	283	ALA
2	C	602	ASP
2	C	705	ASP
2	C	795	GLN
2	C	831	THR
2	C	854	GLN
2	C	866	ASP
3	D	134	GLU
3	D	234	PRO
3	D	235	GLU
3	D	272	SER
3	D	301	LEU
3	D	598	SER
1	E	44	LEU
1	E	107	LYS
1	E	220	SER
1	E	235	GLN
1	E	260	SER
1	E	310	PHE
1	E	324	ARG
1	E	331	ALA
1	E	515	GLN
1	E	609	GLU
1	E	629	GLU
1	E	761	ARG
1	E	780	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	826	ASP
1	E	832	ASP
1	E	937	GLU
1	E	985	GLN
1	E	1057	GLN
1	E	1087	GLY
1	E	1095	GLN
2	F	56	ILE
2	F	106	GLU
2	F	120	ASP
2	F	142	ARG
2	F	273	GLU
2	F	283	ALA
2	F	433	ARG
2	F	446	GLN
2	F	503	ARG
2	F	602	ASP
2	F	705	ASP
2	F	795	GLN
2	F	831	THR
2	F	854	GLN
3	G	60	ASN
3	G	134	GLU
3	G	225	LEU
3	G	234	PRO
3	G	235	GLU
3	G	272	SER
3	G	301	LEU
3	G	452	ALA
3	G	598	SER
1	B	220	SER
1	B	269	ILE
1	B	310	PHE
1	B	366	SER
1	B	469	MET
1	B	712	SER
1	B	830	ASP
1	B	832	ASP
1	B	905	SER
1	B	1111	TYR
1	B	1128	ASP
1	B	1161	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	54	PHE
2	C	182	PRO
2	C	261	LEU
2	C	429	ALA
2	C	433	ARG
2	C	446	GLN
2	C	451	LEU
2	C	686	PRO
2	C	937	PRO
3	D	60	ASN
3	D	126	VAL
3	D	339	ALA
3	D	425	ARG
3	D	428	PRO
3	D	452	ALA
1	E	269	ILE
1	E	366	SER
1	E	469	MET
1	E	718	PRO
1	E	759	ASN
1	E	766	ALA
1	E	830	ASP
1	E	905	SER
1	E	1005	THR
1	E	1009	LEU
1	E	1030	PRO
1	E	1111	TYR
1	E	1128	ASP
1	E	1161	ASN
2	F	54	PHE
2	F	83	GLU
2	F	201	THR
2	F	429	ALA
2	F	431	ALA
2	F	451	LEU
2	F	686	PRO
2	F	866	ASP
2	F	933	ALA
2	F	937	PRO
3	G	339	ALA
3	G	425	ARG
3	G	428	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4	VAL
1	B	249	SER
1	B	934	VAL
1	B	1005	THR
1	B	1029	GLU
1	B	1127	ALA
1	B	1138	VAL
2	C	76	VAL
2	C	83	GLU
2	C	201	THR
2	C	252	LYS
2	C	401	PRO
2	C	467	SER
2	C	544	TRP
2	C	659	VAL
2	C	1037	VAL
3	D	146	PRO
3	D	147	VAL
3	D	221	ARG
3	D	223	LEU
3	D	427	GLU
1	E	4	VAL
1	E	249	SER
1	E	712	SER
1	E	1029	GLU
1	E	1127	ALA
1	E	1138	VAL
2	F	76	VAL
2	F	182	PRO
2	F	252	LYS
2	F	261	LEU
2	F	367	LEU
2	F	401	PRO
2	F	467	SER
2	F	477	PRO
2	F	659	VAL
2	F	734	ARG
2	F	1037	VAL
3	G	146	PRO
3	G	223	LEU
3	G	278	MET
3	G	427	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	51	PRO
1	B	156	GLU
1	B	699	THR
1	B	1030	PRO
1	B	1126	ILE
2	C	286	LEU
2	C	374	ILE
2	C	477	PRO
2	C	933	ALA
3	D	393	ILE
1	E	934	VAL
1	E	1126	ILE
2	F	286	LEU
2	F	374	ILE
3	G	147	VAL
3	G	309	VAL
3	G	318	ASN
3	G	393	ILE
1	B	605	THR
2	C	206	GLY
2	C	295	VAL
2	C	430	PRO
3	D	309	VAL
1	E	51	PRO
2	F	206	GLY
2	F	295	VAL
2	F	296	GLY
2	F	430	PRO
3	G	126	VAL
3	G	528	PRO
1	B	477	PRO
2	C	207	LEU
2	C	296	GLY
2	C	450	VAL
3	D	528	PRO
2	F	207	LEU
2	F	450	VAL
2	C	461	PRO
2	C	796	PRO
1	E	605	THR
1	B	328	ILE
1	B	946	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	685	TYR
2	F	461	PRO
2	F	796	PRO
1	E	876	GLN
2	F	844	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	978/999 (98%)	848 (87%)	130 (13%)	5	30
1	E	978/999 (98%)	848 (87%)	130 (13%)	5	30
2	C	976/977 (100%)	838 (86%)	138 (14%)	4	28
2	F	976/977 (100%)	835 (86%)	141 (14%)	4	26
3	D	443/492 (90%)	374 (84%)	69 (16%)	3	23
3	G	443/492 (90%)	378 (85%)	65 (15%)	4	25
All	All	4794/4936 (97%)	4121 (86%)	673 (14%)	4	28

All (673) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	18	GLU
1	B	30	THR
1	B	52	ARG
1	B	57	GLU
1	B	60	LEU
1	B	63	THR
1	B	72	LEU
1	B	73	ARG
1	B	77	ARG
1	B	83	LEU
1	B	87	CYS
1	B	94	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	95	PRO
1	B	96	LEU
1	B	103	GLU
1	B	105	ASP
1	B	107	LYS
1	B	135	ARG
1	B	150	GLN
1	B	151	GLN
1	B	152	LEU
1	B	168	TRP
1	B	187	TRP
1	B	194	LEU
1	B	196	ASP
1	B	214	ASP
1	B	215	ASP
1	B	218	LEU
1	B	234	GLN
1	B	242	GLU
1	B	244	ASP
1	B	249	SER
1	B	262	GLN
1	B	265	TRP
1	B	268	LYS
1	B	272	TRP
1	B	274	GLU
1	B	275	GLU
1	B	278	ASN
1	B	284	GLU
1	B	310	PHE
1	B	316	LEU
1	B	330	ARG
1	B	332	LEU
1	B	354	MET
1	B	358	LEU
1	B	363	ARG
1	B	365	GLU
1	B	368	GLU
1	B	377	ARG
1	B	423	ARG
1	B	432	LYS
1	B	434	ARG
1	B	436	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	445	THR
1	B	448	ARG
1	B	470	PHE
1	B	471	ARG
1	B	494	GLU
1	B	496	GLN
1	B	501	MET
1	B	517	THR
1	B	527	ARG
1	B	558	VAL
1	B	559	ARG
1	B	566	GLN
1	B	572	THR
1	B	591	LEU
1	B	605	THR
1	B	610	ASN
1	B	633	ASN
1	B	643	GLU
1	B	649	ARG
1	B	688	LEU
1	B	694	LEU
1	B	704	GLU
1	B	707	LEU
1	B	711	LEU
1	B	713	GLN
1	B	728	ARG
1	B	729	LEU
1	B	736	VAL
1	B	743	LYS
1	B	752	VAL
1	B	753	TRP
1	B	754	LEU
1	B	763	GLN
1	B	765	GLN
1	B	771	ARG
1	B	786	SER
1	B	802	LEU
1	B	806	LEU
1	B	815	LEU
1	B	826	ASP
1	B	830	ASP
1	B	831	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	832	ASP
1	B	838	LEU
1	B	853	LEU
1	B	878	TRP
1	B	885	THR
1	B	889	ASN
1	B	891	LYS
1	B	893	LEU
1	B	904	THR
1	B	919	ASP
1	B	924	LEU
1	B	936	GLU
1	B	939	THR
1	B	947	ARG
1	B	962	LEU
1	B	963	ASP
1	B	964	PHE
1	B	974	ARG
1	B	976	LYS
1	B	987	GLU
1	B	1007	VAL
1	B	1008	SER
1	B	1021	MET
1	B	1037	ASP
1	B	1046	LEU
1	B	1059	ARG
1	B	1086	LEU
1	B	1109	LEU
1	B	1116	LEU
1	B	1118	LEU
1	B	1129	TYR
1	B	1155	ILE
1	B	1172	PHE
2	C	2	LEU
2	C	9	ARG
2	C	25	ARG
2	C	27	ASP
2	C	37	VAL
2	C	53	LYS
2	C	59	ASN
2	C	60	ILE
2	C	83	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	87	ASN
2	C	97	THR
2	C	105	ARG
2	C	106	GLU
2	C	107	ASP
2	C	108	PHE
2	C	110	LEU
2	C	119	SER
2	C	144	ASP
2	C	168	LEU
2	C	176	THR
2	C	182	PRO
2	C	185	HIS
2	C	190	TYR
2	C	191	GLN
2	C	196	THR
2	C	207	LEU
2	C	210	ARG
2	C	230	LEU
2	C	241	THR
2	C	251	ILE
2	C	253	ASP
2	C	264	GLN
2	C	269	PHE
2	C	273	GLU
2	C	274	LEU
2	C	276	LEU
2	C	277	PHE
2	C	287	PHE
2	C	290	ASP
2	C	311	ILE
2	C	316	ASP
2	C	323	LEU
2	C	332	ASP
2	C	335	LEU
2	C	343	LEU
2	C	344	GLU
2	C	347	ASN
2	C	353	VAL
2	C	355	ILE
2	C	356	GLU
2	C	363	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	367	LEU
2	C	370	LEU
2	C	383	GLN
2	C	384	ARG
2	C	400	ASP
2	C	403	LEU
2	C	432	ASP
2	C	442	ARG
2	C	445	ARG
2	C	456	SER
2	C	458	LEU
2	C	482	ARG
2	C	487	GLU
2	C	488	GLU
2	C	490	LEU
2	C	504	TRP
2	C	533	LEU
2	C	551	ASP
2	C	552	GLU
2	C	557	ILE
2	C	572	ASN
2	C	575	ARG
2	C	582	ARG
2	C	584	LEU
2	C	592	ARG
2	C	627	GLN
2	C	634	LEU
2	C	635	SER
2	C	636	LEU
2	C	641	LEU
2	C	645	LEU
2	C	646	ASP
2	C	658	PRO
2	C	660	ASN
2	C	688	GLN
2	C	696	LEU
2	C	699	GLN
2	C	709	ARG
2	C	717	LEU
2	C	734	ARG
2	C	736	ILE
2	C	746	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	764	ASP
2	C	765	GLU
2	C	767	LEU
2	C	780	LEU
2	C	807	LEU
2	C	821	VAL
2	C	827	THR
2	C	834	LEU
2	C	853	LEU
2	C	856	ASN
2	C	859	THR
2	C	867	THR
2	C	868	GLU
2	C	871	ILE
2	C	872	LEU
2	C	877	ARG
2	C	883	GLN
2	C	884	LEU
2	C	885	LEU
2	C	896	ARG
2	C	897	LEU
2	C	901	PHE
2	C	919	THR
2	C	927	LEU
2	C	943	ILE
2	C	948	ASN
2	C	952	ILE
2	C	955	TRP
2	C	962	ASP
2	C	966	ARG
2	C	968	ARG
2	C	986	VAL
2	C	997	ARG
2	C	998	LEU
2	C	1035	LEU
2	C	1046	LEU
2	C	1053	GLN
2	C	1055	ASP
2	C	1057	MET
2	C	1087	ASP
2	C	1092	ARG
2	C	1096	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	1097	LEU
2	C	1098	THR
2	C	1121	GLN
3	D	3	LEU
3	D	4	GLN
3	D	6	GLN
3	D	21	VAL
3	D	37	LEU
3	D	53	LEU
3	D	71	CYS
3	D	77	GLU
3	D	91	VAL
3	D	96	GLU
3	D	105	ASP
3	D	115	ASN
3	D	121	ARG
3	D	125	GLU
3	D	128	HIS
3	D	130	ILE
3	D	134	GLU
3	D	137	LEU
3	D	142	ASP
3	D	149	ASP
3	D	150	GLU
3	D	188	LEU
3	D	195	GLU
3	D	212	LEU
3	D	220	LEU
3	D	223	LEU
3	D	228	GLU
3	D	229	GLN
3	D	233	ILE
3	D	239	THR
3	D	240	LEU
3	D	241	HIS
3	D	242	ARG
3	D	243	LEU
3	D	244	LEU
3	D	251	GLN
3	D	263	LEU
3	D	264	ASP
3	D	265	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	276	LEU
3	D	278	MET
3	D	281	ARG
3	D	284	ASP
3	D	300	GLN
3	D	304	VAL
3	D	325	ARG
3	D	348	LEU
3	D	349	ARG
3	D	354	LEU
3	D	356	GLN
3	D	369	GLN
3	D	378	ASP
3	D	380	THR
3	D	384	THR
3	D	392	ASP
3	D	397	LEU
3	D	398	LEU
3	D	436	ASN
3	D	457	ARG
3	D	526	ARG
3	D	529	GLU
3	D	532	THR
3	D	534	TRP
3	D	579	LEU
3	D	586	LEU
3	D	590	ILE
3	D	594	THR
3	D	595	GLU
3	D	598	SER
1	E	16	GLN
1	E	18	GLU
1	E	30	THR
1	E	52	ARG
1	E	57	GLU
1	E	60	LEU
1	E	63	THR
1	E	72	LEU
1	E	73	ARG
1	E	77	ARG
1	E	83	LEU
1	E	87	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	94	ASN
1	E	95	PRO
1	E	96	LEU
1	E	103	GLU
1	E	105	ASP
1	E	107	LYS
1	E	135	ARG
1	E	150	GLN
1	E	151	GLN
1	E	152	LEU
1	E	168	TRP
1	E	187	TRP
1	E	194	LEU
1	E	196	ASP
1	E	214	ASP
1	E	215	ASP
1	E	218	LEU
1	E	234	GLN
1	E	242	GLU
1	E	244	ASP
1	E	249	SER
1	E	262	GLN
1	E	265	TRP
1	E	268	LYS
1	E	272	TRP
1	E	274	GLU
1	E	275	GLU
1	E	278	ASN
1	E	284	GLU
1	E	310	PHE
1	E	316	LEU
1	E	330	ARG
1	E	332	LEU
1	E	354	MET
1	E	358	LEU
1	E	363	ARG
1	E	365	GLU
1	E	368	GLU
1	E	377	ARG
1	E	423	ARG
1	E	432	LYS
1	E	434	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	436	GLU
1	E	445	THR
1	E	448	ARG
1	E	470	PHE
1	E	471	ARG
1	E	494	GLU
1	E	496	GLN
1	E	501	MET
1	E	517	THR
1	E	527	ARG
1	E	558	VAL
1	E	559	ARG
1	E	566	GLN
1	E	572	THR
1	E	591	LEU
1	E	605	THR
1	E	610	ASN
1	E	633	ASN
1	E	643	GLU
1	E	649	ARG
1	E	688	LEU
1	E	694	LEU
1	E	704	GLU
1	E	707	LEU
1	E	711	LEU
1	E	713	GLN
1	E	728	ARG
1	E	729	LEU
1	E	736	VAL
1	E	743	LYS
1	E	752	VAL
1	E	753	TRP
1	E	754	LEU
1	E	763	GLN
1	E	765	GLN
1	E	771	ARG
1	E	786	SER
1	E	802	LEU
1	E	806	LEU
1	E	815	LEU
1	E	826	ASP
1	E	830	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	831	THR
1	E	832	ASP
1	E	838	LEU
1	E	853	LEU
1	E	878	TRP
1	E	885	THR
1	E	889	ASN
1	E	891	LYS
1	E	893	LEU
1	E	904	THR
1	E	919	ASP
1	E	924	LEU
1	E	936	GLU
1	E	939	THR
1	E	947	ARG
1	E	962	LEU
1	E	963	ASP
1	E	964	PHE
1	E	974	ARG
1	E	976	LYS
1	E	987	GLU
1	E	1007	VAL
1	E	1008	SER
1	E	1021	MET
1	E	1037	ASP
1	E	1046	LEU
1	E	1059	ARG
1	E	1086	LEU
1	E	1109	LEU
1	E	1116	LEU
1	E	1118	LEU
1	E	1129	TYR
1	E	1155	ILE
1	E	1172	PHE
2	F	2	LEU
2	F	9	ARG
2	F	25	ARG
2	F	27	ASP
2	F	37	VAL
2	F	53	LYS
2	F	59	ASN
2	F	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	83	GLU
2	F	87	ASN
2	F	97	THR
2	F	105	ARG
2	F	107	ASP
2	F	108	PHE
2	F	110	LEU
2	F	119	SER
2	F	144	ASP
2	F	168	LEU
2	F	176	THR
2	F	182	PRO
2	F	183	ARG
2	F	185	HIS
2	F	190	TYR
2	F	191	GLN
2	F	196	THR
2	F	207	LEU
2	F	210	ARG
2	F	230	LEU
2	F	241	THR
2	F	251	ILE
2	F	253	ASP
2	F	264	GLN
2	F	269	PHE
2	F	273	GLU
2	F	274	LEU
2	F	276	LEU
2	F	277	PHE
2	F	282	ASN
2	F	287	PHE
2	F	290	ASP
2	F	311	ILE
2	F	316	ASP
2	F	323	LEU
2	F	332	ASP
2	F	335	LEU
2	F	343	LEU
2	F	344	GLU
2	F	347	ASN
2	F	353	VAL
2	F	355	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	356	GLU
2	F	363	ASN
2	F	367	LEU
2	F	370	LEU
2	F	383	GLN
2	F	384	ARG
2	F	400	ASP
2	F	403	LEU
2	F	432	ASP
2	F	442	ARG
2	F	445	ARG
2	F	456	SER
2	F	458	LEU
2	F	467	SER
2	F	482	ARG
2	F	487	GLU
2	F	488	GLU
2	F	490	LEU
2	F	494	ARG
2	F	504	TRP
2	F	533	LEU
2	F	551	ASP
2	F	552	GLU
2	F	557	ILE
2	F	572	ASN
2	F	575	ARG
2	F	582	ARG
2	F	584	LEU
2	F	592	ARG
2	F	627	GLN
2	F	634	LEU
2	F	635	SER
2	F	636	LEU
2	F	641	LEU
2	F	645	LEU
2	F	646	ASP
2	F	658	PRO
2	F	660	ASN
2	F	688	GLN
2	F	696	LEU
2	F	699	GLN
2	F	709	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	717	LEU
2	F	734	ARG
2	F	736	ILE
2	F	746	VAL
2	F	764	ASP
2	F	765	GLU
2	F	767	LEU
2	F	780	LEU
2	F	807	LEU
2	F	821	VAL
2	F	827	THR
2	F	834	LEU
2	F	853	LEU
2	F	856	ASN
2	F	859	THR
2	F	867	THR
2	F	868	GLU
2	F	871	ILE
2	F	872	LEU
2	F	877	ARG
2	F	883	GLN
2	F	884	LEU
2	F	885	LEU
2	F	896	ARG
2	F	897	LEU
2	F	901	PHE
2	F	919	THR
2	F	927	LEU
2	F	943	ILE
2	F	948	ASN
2	F	952	ILE
2	F	955	TRP
2	F	962	ASP
2	F	966	ARG
2	F	968	ARG
2	F	986	VAL
2	F	997	ARG
2	F	998	LEU
2	F	1035	LEU
2	F	1046	LEU
2	F	1053	GLN
2	F	1055	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	1057	MET
2	F	1087	ASP
2	F	1092	ARG
2	F	1096	GLN
2	F	1097	LEU
2	F	1098	THR
2	F	1121	GLN
3	G	3	LEU
3	G	4	GLN
3	G	6	GLN
3	G	21	VAL
3	G	37	LEU
3	G	53	LEU
3	G	77	GLU
3	G	91	VAL
3	G	96	GLU
3	G	105	ASP
3	G	121	ARG
3	G	125	GLU
3	G	128	HIS
3	G	130	ILE
3	G	134	GLU
3	G	137	LEU
3	G	142	ASP
3	G	149	ASP
3	G	150	GLU
3	G	188	LEU
3	G	195	GLU
3	G	212	LEU
3	G	220	LEU
3	G	228	GLU
3	G	229	GLN
3	G	233	ILE
3	G	239	THR
3	G	240	LEU
3	G	241	HIS
3	G	242	ARG
3	G	243	LEU
3	G	263	LEU
3	G	264	ASP
3	G	265	VAL
3	G	276	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	278	MET
3	G	281	ARG
3	G	284	ASP
3	G	304	VAL
3	G	325	ARG
3	G	344	GLU
3	G	348	LEU
3	G	349	ARG
3	G	354	LEU
3	G	356	GLN
3	G	361	PHE
3	G	369	GLN
3	G	378	ASP
3	G	380	THR
3	G	384	THR
3	G	392	ASP
3	G	397	LEU
3	G	398	LEU
3	G	436	ASN
3	G	457	ARG
3	G	526	ARG
3	G	529	GLU
3	G	532	THR
3	G	534	TRP
3	G	579	LEU
3	G	586	LEU
3	G	590	ILE
3	G	594	THR
3	G	595	GLU
3	G	598	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (266) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	109	GLN
1	B	130	HIS
1	B	150	GLN
1	B	151	GLN
1	B	181	GLN
1	B	202	GLN
1	B	222	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	224	GLN
1	B	234	GLN
1	B	262	GLN
1	B	315	GLN
1	B	392	GLN
1	B	403	HIS
1	B	404	GLN
1	B	455	ASN
1	B	484	ASN
1	B	496	GLN
1	B	515	GLN
1	B	531	GLN
1	B	566	GLN
1	B	610	ASN
1	B	624	ASN
1	B	633	ASN
1	B	695	GLN
1	B	705	HIS
1	B	713	GLN
1	B	721	ASN
1	B	725	GLN
1	B	726	GLN
1	B	763	GLN
1	B	765	GLN
1	B	769	HIS
1	B	812	HIS
1	B	834	HIS
1	B	835	GLN
1	B	848	GLN
1	B	868	GLN
1	B	875	ASN
1	B	876	GLN
1	B	881	ASN
1	B	889	ASN
1	B	900	ASN
1	B	911	GLN
1	B	944	GLN
1	B	966	GLN
1	B	999	GLN
1	B	1011	GLN
1	B	1042	GLN
1	B	1057	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1072	HIS
1	B	1095	GLN
1	B	1103	GLN
1	B	1110	GLN
1	B	1124	HIS
1	B	1134	HIS
1	B	1152	GLN
2	C	6	HIS
2	C	8	ASN
2	C	38	GLN
2	C	52	GLN
2	C	87	ASN
2	C	126	GLN
2	C	162	GLN
2	C	165	GLN
2	C	177	HIS
2	C	178	GLN
2	C	188	ASN
2	C	191	GLN
2	C	228	GLN
2	C	264	GLN
2	C	267	HIS
2	C	285	GLN
2	C	333	ASN
2	C	336	HIS
2	C	347	ASN
2	C	354	ASN
2	C	363	ASN
2	C	383	GLN
2	C	423	GLN
2	C	446	GLN
2	C	510	ASN
2	C	521	GLN
2	C	522	HIS
2	C	563	HIS
2	C	572	ASN
2	C	580	GLN
2	C	617	GLN
2	C	647	GLN
2	C	681	ASN
2	C	699	GLN
2	C	737	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	768	ASN
2	C	792	GLN
2	C	793	ASN
2	C	795	GLN
2	C	800	GLN
2	C	812	GLN
2	C	822	GLN
2	C	843	HIS
2	C	850	GLN
2	C	879	GLN
2	C	936	GLN
2	C	939	GLN
2	C	948	ASN
2	C	976	GLN
2	C	979	GLN
2	C	984	HIS
2	C	1015	GLN
2	C	1022	GLN
2	C	1065	GLN
2	C	1078	ASN
2	C	1091	GLN
2	C	1110	GLN
3	D	4	GLN
3	D	6	GLN
3	D	15	GLN
3	D	79	GLN
3	D	115	ASN
3	D	139	GLN
3	D	247	GLN
3	D	251	GLN
3	D	256	HIS
3	D	328	GLN
3	D	356	GLN
3	D	369	GLN
3	D	388	GLN
3	D	423	GLN
3	D	433	GLN
3	D	460	GLN
3	D	464	GLN
3	D	530	HIS
3	D	542	GLN
1	E	16	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	109	GLN
1	E	150	GLN
1	E	151	GLN
1	E	181	GLN
1	E	202	GLN
1	E	222	HIS
1	E	224	GLN
1	E	234	GLN
1	E	262	GLN
1	E	315	GLN
1	E	392	GLN
1	E	403	HIS
1	E	404	GLN
1	E	455	ASN
1	E	484	ASN
1	E	496	GLN
1	E	515	GLN
1	E	531	GLN
1	E	566	GLN
1	E	610	ASN
1	E	633	ASN
1	E	695	GLN
1	E	705	HIS
1	E	713	GLN
1	E	721	ASN
1	E	725	GLN
1	E	726	GLN
1	E	763	GLN
1	E	765	GLN
1	E	769	HIS
1	E	812	HIS
1	E	834	HIS
1	E	835	GLN
1	E	848	GLN
1	E	868	GLN
1	E	875	ASN
1	E	876	GLN
1	E	879	GLN
1	E	889	ASN
1	E	900	ASN
1	E	911	GLN
1	E	944	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	966	GLN
1	E	999	GLN
1	E	1011	GLN
1	E	1042	GLN
1	E	1057	GLN
1	E	1072	HIS
1	E	1095	GLN
1	E	1103	GLN
1	E	1110	GLN
1	E	1124	HIS
1	E	1134	HIS
1	E	1152	GLN
2	F	8	ASN
2	F	38	GLN
2	F	52	GLN
2	F	87	ASN
2	F	126	GLN
2	F	162	GLN
2	F	165	GLN
2	F	177	HIS
2	F	178	GLN
2	F	188	ASN
2	F	191	GLN
2	F	228	GLN
2	F	264	GLN
2	F	267	HIS
2	F	285	GLN
2	F	333	ASN
2	F	336	HIS
2	F	347	ASN
2	F	354	ASN
2	F	363	ASN
2	F	423	GLN
2	F	446	GLN
2	F	510	ASN
2	F	521	GLN
2	F	522	HIS
2	F	563	HIS
2	F	572	ASN
2	F	580	GLN
2	F	617	GLN
2	F	643	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	647	GLN
2	F	681	ASN
2	F	699	GLN
2	F	737	GLN
2	F	768	ASN
2	F	792	GLN
2	F	793	ASN
2	F	795	GLN
2	F	800	GLN
2	F	812	GLN
2	F	822	GLN
2	F	843	HIS
2	F	850	GLN
2	F	879	GLN
2	F	882	GLN
2	F	936	GLN
2	F	939	GLN
2	F	948	ASN
2	F	958	GLN
2	F	976	GLN
2	F	979	GLN
2	F	984	HIS
2	F	1015	GLN
2	F	1022	GLN
2	F	1065	GLN
2	F	1078	ASN
2	F	1091	GLN
2	F	1110	GLN
3	G	4	GLN
3	G	6	GLN
3	G	15	GLN
3	G	60	ASN
3	G	79	GLN
3	G	115	ASN
3	G	139	GLN
3	G	247	GLN
3	G	259	ASN
3	G	328	GLN
3	G	356	GLN
3	G	369	GLN
3	G	388	GLN
3	G	423	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	433	GLN
3	G	439	GLN
3	G	460	GLN
3	G	464	GLN
3	G	530	HIS
3	G	542	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

18 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	5IU	X	1	4	13,18,22	1.38	3 (23%)	14,26,33	3.73	1 (7%)
4	5IU	X	2	4	12,21,22	1.48	3 (25%)	14,30,33	3.68	2 (14%)
4	5IU	X	3	4	12,21,22	1.42	3 (25%)	14,30,33	3.75	1 (7%)
4	5IU	X	4	4	12,21,22	1.43	4 (33%)	14,30,33	3.67	1 (7%)
4	5IU	X	46	4	12,21,22	1.46	3 (25%)	14,30,33	3.54	1 (7%)
4	5IU	X	5	4	12,21,22	2.11	3 (25%)	14,30,33	4.18	1 (7%)
4	5IU	X	50	4	12,21,22	1.33	3 (25%)	14,30,33	3.68	1 (7%)
4	5IU	X	7	4	12,21,22	1.45	3 (25%)	14,30,33	3.73	2 (14%)
4	5IU	X	9	4	12,21,22	1.49	3 (25%)	14,30,33	3.56	1 (7%)
4	5IU	Y	1	4	13,18,22	1.30	2 (15%)	14,26,33	3.65	1 (7%)
4	5IU	Y	2	4	12,21,22	1.47	3 (25%)	14,30,33	3.69	2 (14%)
4	5IU	Y	3	4	12,21,22	1.40	3 (25%)	14,30,33	3.72	2 (14%)
4	5IU	Y	4	4	12,21,22	1.41	3 (25%)	14,30,33	3.70	1 (7%)
4	5IU	Y	46	4	12,21,22	1.44	3 (25%)	14,30,33	3.60	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	5IU	Y	5	4	12,21,22	1.46	3 (25%)	14,30,33	3.61	2 (14%)
4	5IU	Y	50	4	12,21,22	1.34	3 (25%)	14,30,33	3.71	1 (7%)
4	5IU	Y	7	4	12,21,22	1.48	3 (25%)	14,30,33	3.70	2 (14%)
4	5IU	Y	9	4	12,21,22	1.48	3 (25%)	14,30,33	3.59	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	5IU	X	1	4	-	0/2/18/22	0/2/2/2
4	5IU	X	2	4	-	0/3/21/22	0/2/2/2
4	5IU	X	3	4	-	0/3/21/22	0/2/2/2
4	5IU	X	4	4	-	0/3/21/22	0/2/2/2
4	5IU	X	46	4	-	0/3/21/22	0/2/2/2
4	5IU	X	5	4	-	0/3/21/22	0/2/2/2
4	5IU	X	50	4	-	0/3/21/22	0/2/2/2
4	5IU	X	7	4	-	0/3/21/22	0/2/2/2
4	5IU	X	9	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	1	4	-	0/2/18/22	0/2/2/2
4	5IU	Y	2	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	3	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	4	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	46	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	5	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	50	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	7	4	-	0/3/21/22	0/2/2/2
4	5IU	Y	9	4	-	0/3/21/22	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	9	5IU	C5-I5	-3.71	2.02	2.10
4	Y	9	5IU	C5-I5	-3.60	2.02	2.10
4	X	1	5IU	C5-I5	-3.20	2.03	2.10
4	Y	1	5IU	C5-I5	-3.02	2.04	2.10
4	Y	5	5IU	C6-C5	-2.98	1.31	1.38
4	Y	2	5IU	C5-I5	-2.91	2.04	2.10
4	X	2	5IU	C5-I5	-2.89	2.04	2.10
4	Y	7	5IU	C5-I5	-2.82	2.04	2.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	46	5IU	C6-C5	-2.81	1.31	1.38
4	Y	2	5IU	C6-C5	-2.81	1.31	1.38
4	X	4	5IU	C5-I5	-2.73	2.04	2.10
4	Y	7	5IU	C6-C5	-2.58	1.32	1.38
4	X	7	5IU	C6-C5	-2.56	1.32	1.38
4	X	7	5IU	C5-I5	-2.56	2.05	2.10
4	X	3	5IU	C5-I5	-2.55	2.05	2.10
4	X	46	5IU	C5-I5	-2.53	2.05	2.10
4	X	50	5IU	C5-I5	-2.49	2.05	2.10
4	Y	46	5IU	C6-C5	-2.44	1.32	1.38
4	Y	3	5IU	C5-I5	-2.43	2.05	2.10
4	Y	5	5IU	C5-I5	-2.37	2.05	2.10
4	Y	50	5IU	C5-I5	-2.37	2.05	2.10
4	Y	46	5IU	C5-I5	-2.32	2.05	2.10
4	X	9	5IU	C6-C5	-2.31	1.33	1.38
4	Y	4	5IU	C5-I5	-2.30	2.05	2.10
4	X	3	5IU	C6-C5	-2.28	1.33	1.38
4	Y	9	5IU	C6-C5	-2.22	1.33	1.38
4	Y	3	5IU	C6-C5	-2.20	1.33	1.38
4	X	5	5IU	C6-C5	-2.06	1.33	1.38
4	X	2	5IU	C6-C5	-2.05	1.33	1.38
4	X	4	5IU	C6-C5	-2.03	1.33	1.38
4	X	4	5IU	C6-N1	2.10	1.38	1.35
4	X	1	5IU	C6-N1	2.24	1.38	1.35
4	Y	50	5IU	C6-N1	2.26	1.38	1.35
4	X	50	5IU	C6-N1	2.29	1.38	1.35
4	Y	4	5IU	C6-N1	2.30	1.38	1.35
4	X	50	5IU	C4-N3	2.40	1.37	1.33
4	X	9	5IU	C4-N3	2.45	1.37	1.33
4	Y	1	5IU	C4-N3	2.49	1.37	1.33
4	Y	9	5IU	C4-N3	2.52	1.37	1.33
4	X	1	5IU	C4-N3	2.56	1.37	1.33
4	Y	50	5IU	C4-N3	2.61	1.37	1.33
4	Y	2	5IU	C4-N3	2.67	1.38	1.33
4	X	4	5IU	C4-N3	2.83	1.38	1.33
4	X	3	5IU	C4-N3	2.96	1.38	1.33
4	X	5	5IU	C4-N3	3.00	1.38	1.33
4	Y	4	5IU	C4-N3	3.01	1.38	1.33
4	X	2	5IU	C4-N3	3.04	1.38	1.33
4	Y	3	5IU	C4-N3	3.06	1.38	1.33
4	X	7	5IU	C4-N3	3.08	1.38	1.33
4	Y	7	5IU	C4-N3	3.11	1.38	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	46	5IU	C4-N3	3.14	1.38	1.33
4	Y	5	5IU	C4-N3	3.15	1.38	1.33
4	Y	46	5IU	C4-N3	3.21	1.39	1.33
4	X	5	5IU	C6-N1	6.17	1.44	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	7	5IU	C2'-C1'-N1	-3.12	106.57	114.16
4	Y	5	5IU	C2'-C1'-N1	-3.08	106.67	114.16
4	X	7	5IU	C2'-C1'-N1	-3.03	106.80	114.16
4	Y	2	5IU	C2'-C1'-N1	-2.42	108.27	114.16
4	X	2	5IU	C2'-C1'-N1	-2.41	108.30	114.16
4	Y	3	5IU	C2'-C1'-N1	-2.01	109.27	114.16
4	Y	5	5IU	C4-N3-C2	13.02	126.50	115.25
4	X	46	5IU	C4-N3-C2	13.11	126.58	115.25
4	Y	7	5IU	C4-N3-C2	13.26	126.71	115.25
4	X	9	5IU	C4-N3-C2	13.29	126.74	115.25
4	Y	46	5IU	C4-N3-C2	13.33	126.77	115.25
4	Y	9	5IU	C4-N3-C2	13.38	126.81	115.25
4	X	7	5IU	C4-N3-C2	13.40	126.83	115.25
4	X	2	5IU	C4-N3-C2	13.46	126.88	115.25
4	Y	2	5IU	C4-N3-C2	13.51	126.92	115.25
4	Y	3	5IU	C4-N3-C2	13.51	126.93	115.25
4	X	4	5IU	C4-N3-C2	13.62	127.02	115.25
4	Y	1	5IU	C4-N3-C2	13.63	127.03	115.25
4	X	3	5IU	C4-N3-C2	13.64	127.04	115.25
4	X	50	5IU	C4-N3-C2	13.68	127.07	115.25
4	Y	4	5IU	C4-N3-C2	13.74	127.12	115.25
4	Y	50	5IU	C4-N3-C2	13.77	127.15	115.25
4	X	1	5IU	C4-N3-C2	13.90	127.26	115.25
4	X	5	5IU	C4-N3-C2	15.57	128.71	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 104 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	1	5IU	1	0
4	X	2	5IU	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	3	5IU	12	0
4	X	4	5IU	6	0
4	X	46	5IU	11	0
4	X	5	5IU	3	0
4	X	50	5IU	1	0
4	X	7	5IU	6	0
4	X	9	5IU	6	0
4	Y	1	5IU	3	0
4	Y	2	5IU	14	0
4	Y	3	5IU	13	0
4	Y	4	5IU	4	0
4	Y	46	5IU	10	0
4	Y	5	5IU	1	0
4	Y	7	5IU	9	0
4	Y	9	5IU	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	1155/1180 (97%)	-0.19	27 (2%) 64 48	54, 111, 179, 259	0
1	E	1155/1180 (97%)	-0.12	33 (2%) 55 40	59, 121, 179, 215	0
2	C	1121/1122 (99%)	-0.36	6 (0%) 91 86	42, 90, 155, 226	0
2	F	1121/1122 (99%)	-0.23	14 (1%) 81 69	54, 107, 172, 222	0
3	D	547/608 (89%)	0.72	93 (17%) 2 2	71, 165, 222, 251	0
3	G	547/608 (89%)	-0.07	20 (3%) 45 32	55, 114, 188, 243	0
4	X	37/51 (72%)	0.68	5 (13%) 4 4	82, 168, 227, 236	0
4	Y	37/51 (72%)	0.90	3 (8%) 15 10	106, 168, 222, 247	0
All	All	5720/5922 (96%)	-0.10	201 (3%) 48 34	42, 112, 190, 259	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	464	GLN	13.8
3	D	465	LYS	10.0
3	D	463	GLN	8.1
1	E	305	PRO	7.1
3	D	72	VAL	6.9
1	B	876	GLN	6.7
3	D	76	GLY	6.5
3	D	446	GLU	5.8
3	D	77	GLU	5.8
3	D	398	LEU	5.7
3	D	67	LEU	5.5
1	E	935	VAL	5.4
1	E	306	ARG	5.0
3	D	388	GLN	4.9
3	D	442	CYS	4.9
3	D	361	PHE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	1149	GLU	4.7
2	F	280	SER	4.6
3	D	360	ARG	4.5
3	D	429	ASP	4.5
3	D	466	ARG	4.5
2	F	281	GLU	4.5
3	D	444	LEU	4.5
1	E	885	THR	4.5
1	B	913	GLY	4.5
1	B	912	ARG	4.4
1	E	920	LEU	4.3
3	D	71	CYS	4.2
3	D	247	GLN	4.2
2	C	280	SER	4.2
3	D	606	SER	4.2
3	D	526	ARG	4.1
3	D	427	GLU	4.0
1	B	934	VAL	4.0
3	D	399	GLN	4.0
1	E	824	ARG	4.0
3	G	247	GLN	3.9
3	D	319	ALA	3.9
1	E	934	VAL	3.9
1	B	305	PRO	3.9
3	G	257	ALA	3.8
1	B	932	ALA	3.8
3	G	340	GLY	3.7
2	F	860	GLU	3.7
3	G	76	GLY	3.7
2	C	281	GLU	3.7
3	D	428	PRO	3.7
1	B	884	SER	3.6
1	B	880	VAL	3.6
3	G	79	GLN	3.6
1	E	933	SER	3.6
3	D	362	GLY	3.6
3	D	70	THR	3.6
1	B	261	ASN	3.5
3	D	528	PRO	3.5
3	D	431	ILE	3.5
3	D	359	TYR	3.5
3	D	13	HIS	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	575	ARG	3.4
3	D	68	LEU	3.4
1	E	913	GLY	3.4
3	D	365	SER	3.4
3	D	432	ILE	3.4
3	D	194	GLY	3.4
3	D	525	SER	3.3
3	G	1	MET	3.3
3	D	61	ASN	3.3
1	E	827	LYS	3.3
3	D	402	GLU	3.3
3	D	79	GLN	3.3
3	D	364	ASP	3.3
1	E	876	GLN	3.3
1	B	933	SER	3.2
3	D	460	GLN	3.2
2	F	263	ARG	3.2
3	D	341	THR	3.2
3	G	253	LEU	3.1
1	B	827	LYS	3.1
3	D	196	ARG	3.1
1	B	241	GLY	3.0
1	B	915	GLY	3.0
1	B	1149	GLU	3.0
3	D	445	ARG	3.0
1	E	814	SER	3.0
2	F	156	GLU	3.0
3	D	383	LYS	3.0
3	D	64	SER	3.0
1	B	874	ASP	2.9
1	E	938	PRO	2.9
3	G	70	THR	2.9
3	D	535	ALA	2.9
2	F	260	LEU	2.8
3	G	391	THR	2.8
3	D	604	PHE	2.8
3	D	363	SER	2.8
3	D	73	SER	2.8
3	D	418	TYR	2.8
3	D	219	ALA	2.8
1	B	826	ASP	2.8
2	F	262	THR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	603	LEU	2.8
1	B	898	GLY	2.8
1	B	154	GLU	2.8
3	D	340	GLY	2.7
3	D	550	ALA	2.7
1	B	935	VAL	2.7
3	G	64	SER	2.7
3	D	384	THR	2.7
1	B	914	HIS	2.7
3	D	419	LEU	2.7
1	B	1073	GLU	2.7
3	D	248	PRO	2.7
4	X	31	DT	2.6
2	F	352	GLY	2.6
3	D	416	GLY	2.6
3	D	400	SER	2.6
3	D	387	GLN	2.6
3	D	193	ASP	2.6
1	E	887	GLU	2.6
3	D	218	LYS	2.6
3	G	71	CYS	2.6
1	B	654	LYS	2.6
3	D	224	PRO	2.6
1	E	825	GLY	2.6
3	D	578	SER	2.6
3	D	394	GLU	2.6
3	D	252	ARG	2.5
2	F	936	GLN	2.5
3	D	369	GLN	2.5
1	E	582	SER	2.5
3	D	401	GLY	2.5
1	E	813	CYS	2.5
3	D	65	HIS	2.5
3	D	131	GLU	2.5
1	E	3	ASP	2.5
1	E	912	ARG	2.4
3	G	361	PHE	2.4
1	E	321	LEU	2.4
2	C	279	ASP	2.4
3	D	403	ASP	2.4
3	D	78	LEU	2.4
3	D	246	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	921	MET	2.4
3	G	65	HIS	2.4
3	G	256	HIS	2.4
2	F	775	ARG	2.4
3	G	388	GLN	2.4
1	E	509	CYS	2.4
1	B	920	LEU	2.3
3	G	67	LEU	2.3
1	E	927	ASP	2.3
3	D	161	ALA	2.3
3	D	147	VAL	2.3
3	D	66	PRO	2.3
2	F	241	THR	2.3
3	D	214	GLU	2.3
3	D	439	GLN	2.3
3	D	426	ALA	2.3
2	C	276	LEU	2.3
2	F	283	ALA	2.3
3	G	73	SER	2.3
1	E	823	ARG	2.3
3	D	391	THR	2.3
2	C	285	GLN	2.3
1	E	936	GLU	2.2
1	E	152	LEU	2.2
3	D	462	MET	2.2
3	D	164	ARG	2.2
4	Y	51	DA	2.2
1	E	886	ALA	2.2
1	B	916	ILE	2.2
4	Y	32	DA	2.2
3	G	128	HIS	2.2
1	E	721	ASN	2.2
4	X	33	DG	2.2
2	F	953	THR	2.2
4	Y	31	DT	2.2
1	B	824	ARG	2.2
3	D	443	ALA	2.2
4	X	25	DA	2.1
4	X	32	DA	2.1
3	G	167	SER	2.1
3	G	196	ARG	2.1
1	B	877	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	1015	ARG	2.1
4	X	24	DT	2.1
2	F	285	GLN	2.1
3	D	450	GLY	2.1
1	E	937	GLU	2.1
3	D	386	PHE	2.1
1	E	830	ASP	2.1
2	C	278	ARG	2.1
1	E	877	PRO	2.1
3	D	461	PHE	2.1
3	D	128	HIS	2.1
3	D	167	SER	2.0
3	D	132	VAL	2.0
1	B	285	SER	2.0
3	D	195	GLU	2.0
3	D	356	GLN	2.0
3	D	580	TYR	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	5IU	X	50	20/21	0.85	0.28	-	108,155,260,260	0
4	5IU	Y	3	20/21	0.57	0.66	-	108,300,300,300	0
4	5IU	X	9	20/21	0.92	0.18	-	58,108,124,124	0
4	5IU	X	4	20/21	0.83	0.35	-	108,140,235,235	0
4	5IU	X	5	20/21	0.83	0.39	-	108,156,300,300	0
4	5IU	Y	9	20/21	0.93	0.16	-	102,108,148,148	0
4	5IU	X	7	20/21	0.82	0.21	-	108,158,216,216	0
4	5IU	Y	5	20/21	0.42	0.72	-	108,300,300,300	0
4	5IU	Y	4	20/21	0.48	0.47	-	108,300,300,300	0
4	5IU	X	3	20/21	0.82	0.31	-	108,179,254,254	0
4	5IU	Y	1	17/21	0.03	1.16	-	234,234,300,300	0
4	5IU	X	46	20/21	0.84	0.18	-	108,165,189,189	0
4	5IU	Y	50	20/21	0.84	0.25	-	108,170,300,300	0
4	5IU	X	2	20/21	0.61	0.34	-	108,164,275,275	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	5IU	Y	2	20/21	0.37	0.94	-	108,300,300,300	0
4	5IU	Y	46	20/21	0.84	0.18	-	108,158,252,252	0
4	5IU	X	1	17/21	0.76	0.51	-	200,200,300,300	0
4	5IU	Y	7	20/21	0.75	0.26	-	108,181,300,300	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	B	4000	1/1	0.95	0.58	2.17	108,108,108,108	0
5	CA	E	4000	1/1	0.91	0.37	-0.24	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.