



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:44 PM EDT

PDB ID : 2IJZ
Title : Crystal structure of aminopeptidase
Authors : Min, T.; Burley, S.K.; Shapiro, L.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2006-10-02
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

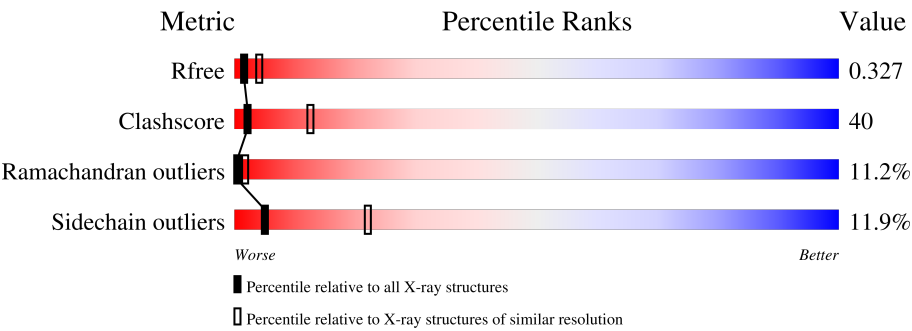
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	428	
1	B	428	
1	C	428	
1	D	428	
1	E	428	
1	F	428	
1	G	428	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	428	<div><div></div><div>39%39%10%•11%</div></div>
1	I	428	<div><div></div><div>39%36%12%•11%</div></div>
1	J	428	<div><div></div><div>42%36%10%•11%</div></div>
1	K	428	<div><div></div><div>36%41%10%•11%</div></div>
1	L	428	<div><div></div><div>39%38%10%•11%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37617 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 Probable M18-family aminopeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	B	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	C	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	D	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	E	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	F	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	G	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	H	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	I	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	J	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	K	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			
1	L	379	Total	C	N	O	S	0	0	0
			2870	1795	519	546	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
B	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
C	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
D	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
E	154	ASN	ALA	engineered mutation	UNP Q9HYZ3

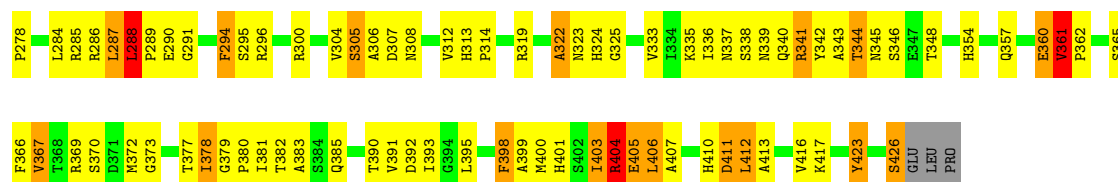
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
G	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
H	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
I	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
J	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
K	154	ASN	ALA	engineered mutation	UNP Q9HYZ3
L	154	ASN	ALA	engineered mutation	UNP Q9HYZ3

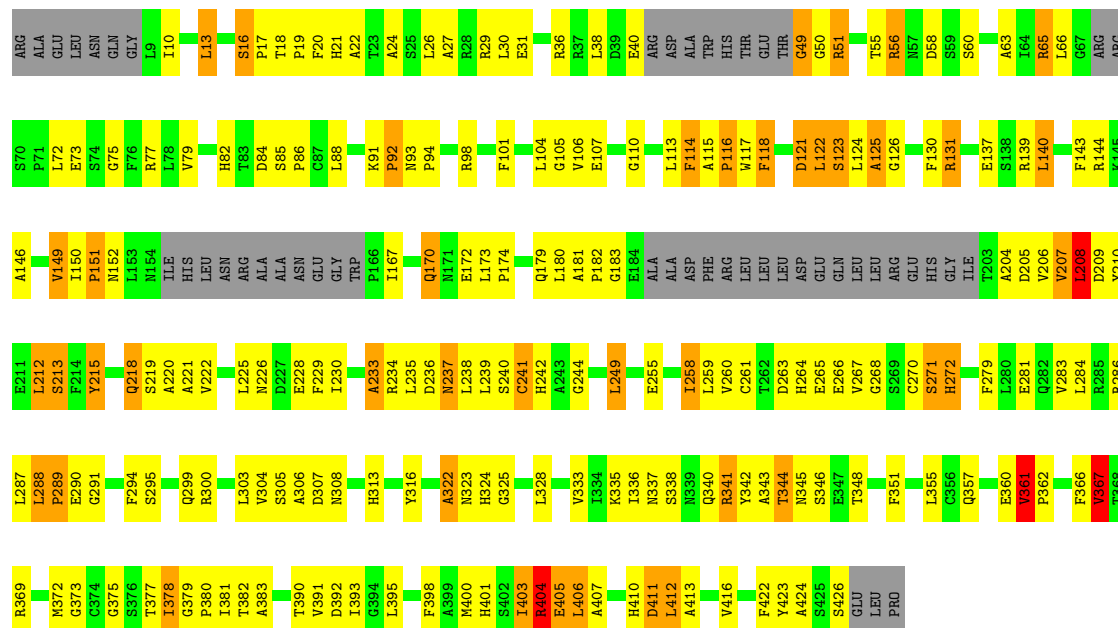
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	262	Total O 262 262	0	0
2	B	271	Total O 271 271	0	0
2	C	298	Total O 298 298	0	0
2	D	247	Total O 247 247	0	0
2	E	268	Total O 268 268	0	0
2	F	247	Total O 247 247	0	0
2	G	255	Total O 255 255	0	0
2	H	252	Total O 252 252	0	0
2	I	274	Total O 274 274	0	0
2	J	258	Total O 258 258	0	0
2	K	276	Total O 276 276	0	0
2	L	269	Total O 269 269	0	0



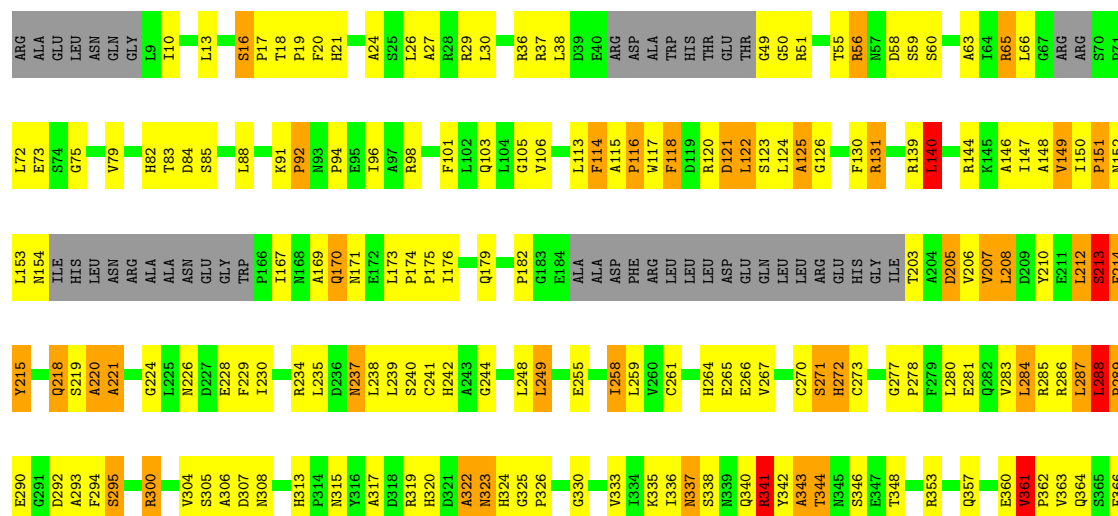
• Molecule 1: Probable M18-family aminopeptidase 2

Chain C: 39% 38% 10% • 11%



• Molecule 1: Probable M18-family aminopeptidase 2

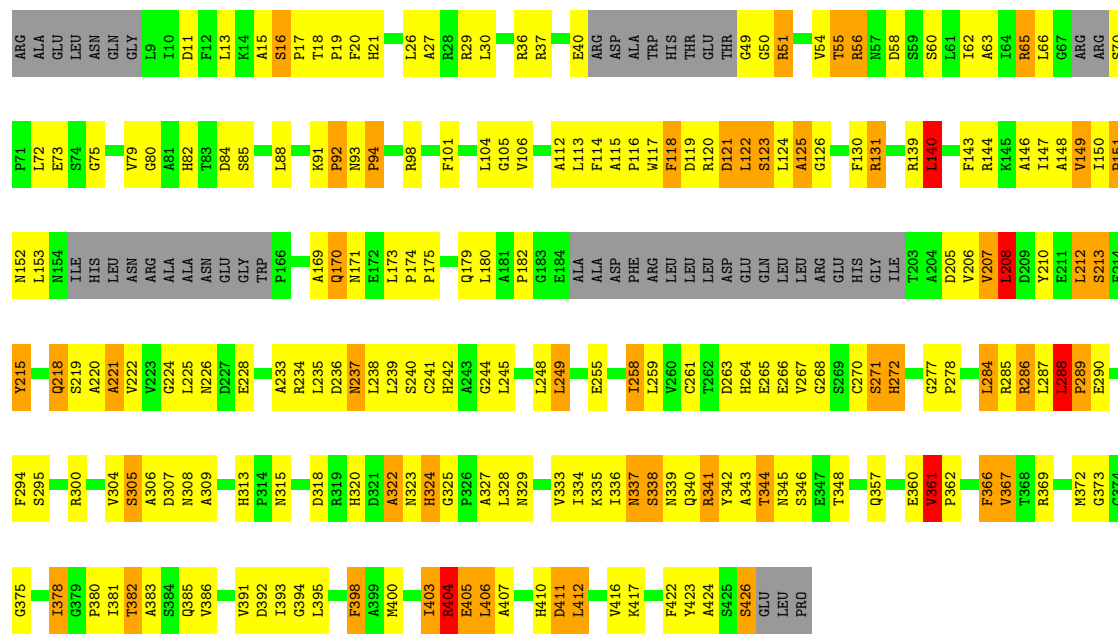
Chain D: 40% 37% 11% • 11%





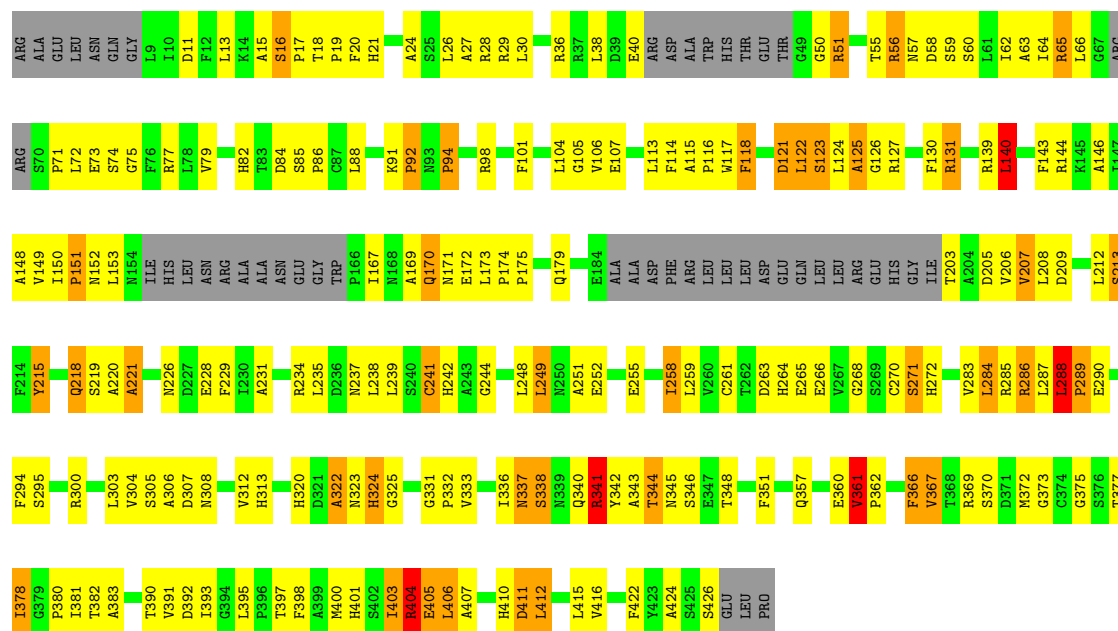
• Molecule 1: Probable M18-family aminopeptidase 2

Chain E: 39% 37% 11% • 11%



• Molecule 1: Probable M18-family aminopeptidase 2

Chain F: 40% 38% 9% • 11%

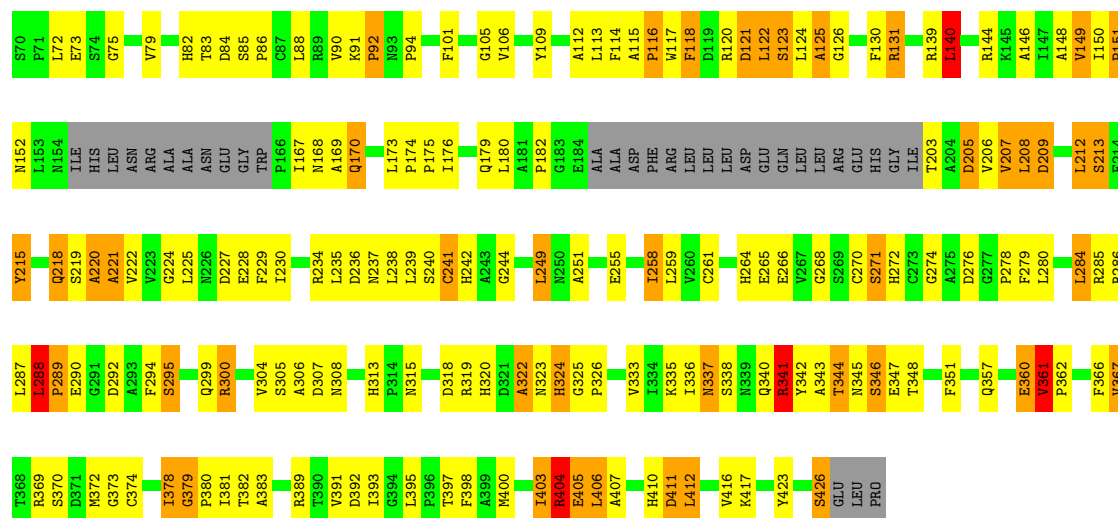


• Molecule 1: Probable M18-family aminopeptidase 2

T377	F294	Q218	P151	L72	ARG
T378	S219	S219	N152	E73	ALA
G379	S295	A220	L153		GLU
P380		A221	N154	R77	LEU
I381	R300	V222	I1E	L78	ASN
T382		V223	HIS	V79	GLN
A383	L303		LEU		GLY
S384	V304	N226	ASN	H82	L9
Q385	S305		ARG	T33	I10
	A306	F229	ALA	D84	D11
T390	D307	I230	ASN	S85	F12
V391	N308		ASN	P86	L13
D392		R234	GLU	C87	
I393	H313	L235	GLY		S16
G394		D236	TRP	R89	P17
L395	A317	N237	P166	V90	T18
	H320	L238		K91	P19
F398	D321	L239	Q170	P92	F20
A399	A322	S240	M171	N93	H21
M400	C322	C241	E172	P94	
	N323	H242	L173		A24
I403	H324	A243	T174	F101	S25
R404	R324	G244	G183		L26
E405	G325	L245	E184	L104	A27
L406	V333	E246	Q179	G105	R28
A407	L334	A247	L180	G106	R29
	K335	L248	A181	E107	L30
H410	L336	L249	G183		
D411	N337		E184	L113	R37
L412	S338	E255	ALA	F114	L38
A413	N340		ALA	D39	
H414	Q340	L258	ASP	A115	E40
L415	R341	L259	PHE	P116	ARG
V416	V342	V250	ARG	F117	ASP
	A343	C261	LEU	W118	ALA
F422	T344		LEU	D119	TRP
	N345	H264	LEU	R120	
S426	E346	E265	LEU	D121	HIS
GLU	E347	E266	ASP	L122	THR
LEU	T348	V267	GLU	S123	GLU
PRO		G268	GLN	L124	THR
	F351	S269	LEU	A125	G49
		C270	LEU	G126	G50
	Q357	S271	ARG	R127	R51
		H272	GLU		
	E360	D276	HIS	F130	T55
V363	P362	G277	GLY	R131	R56
		T278	I1E		N57
S365		F279	T203	E137	D58
F366	V367	L280	A204	S138	S59
T367	T368	E281	V206	R139	S60
R369		G282	V207	L140	
	S369	V283	L208	F143	A63
	S370	L284	D209	R144	R65
D371		R285		K145	L66
G372	S373	R286	L212	A146	
G373	G374	L287	S213	I147	ARG
			F214	L149	ARG
			Y215	V149	S70
				L150	R74

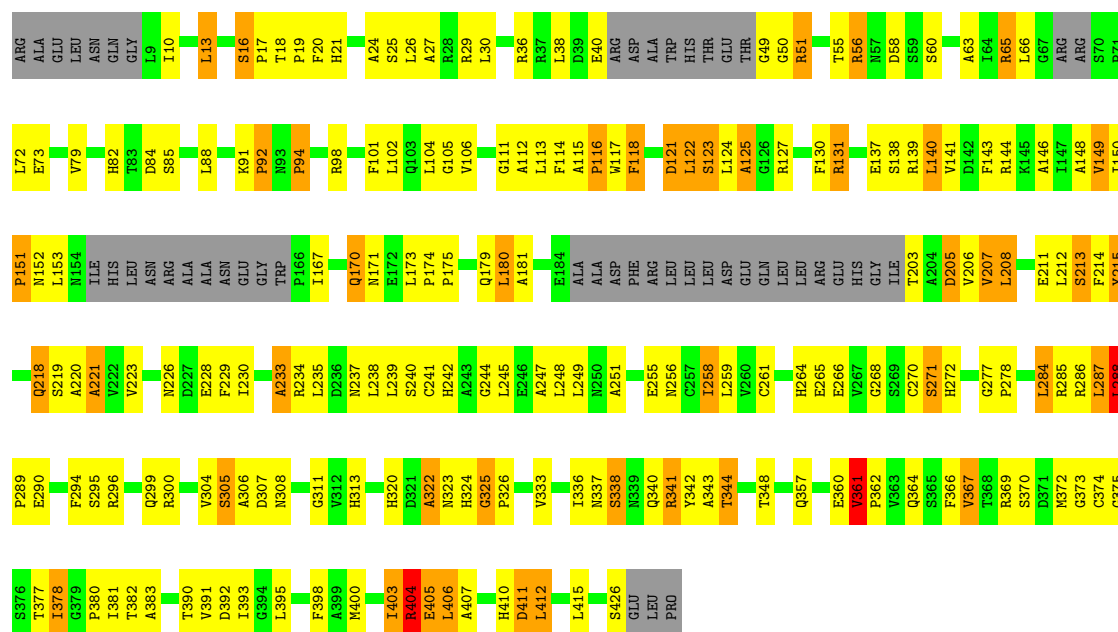
[illegible]

ARG	ALA	GLU	LEU	ASV	GLN	LY	L9	I10		L13	S16	P17	T18	P19	F20	H21	A24	S25	L26	A27	R28	R29	L30		R36	R37	L38	D39	E40	ARC	ASP	ALA	TRP	HIS	THR	GLU	THR	THR	G49	C50	R51	Y52	Y53	V54	T55	R56	L57	D58	S59	S60		A63	L64	R65	L66	G67	ARG	A68
-----	-----	-----	-----	-----	-----	----	----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	-----	-----



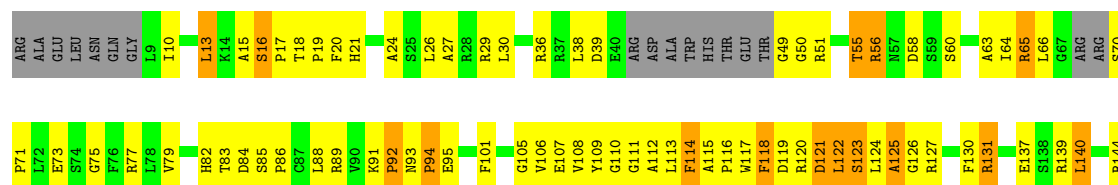
• Molecule 1: Probable M18-family aminopeptidase 2

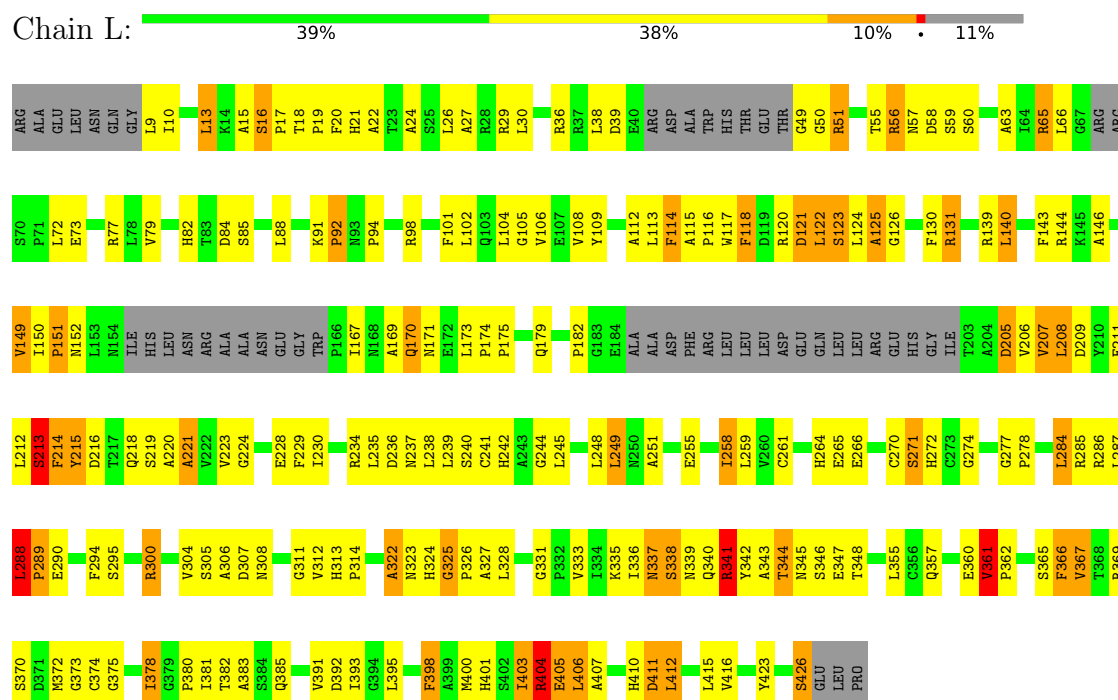
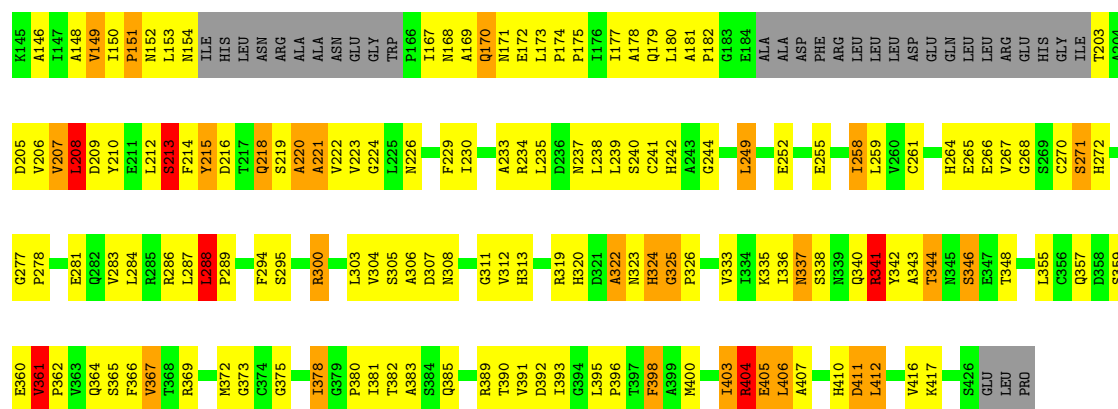
Chain J: 42% 36% 10% • 11%



• Molecule 1: Probable M18-family aminopeptidase 2

Chain K: 36% 41% 10% • 11%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	134.68Å 134.55Å 134.60Å 60.12° 60.10° 60.16°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	52.9 (20.00-3.00) 73.0 (20.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.291 0.317 , 0.327	Depositor DCC
R_{free} test set	9838 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage

Continued on next page...

¹Intensities estimated from amplitudes.

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

Continued from previous page...

Property	Value	Source
Estimated twinning fraction	0.033 for h-l,h,h-k 0.033 for k,k-l,-h+k 0.030 for l,-h+l,-k+l 0.030 for h-k,h-l,h 0.031 for -k+l,l,-h+l 0.031 for k-l,-h+k,k 0.408 for k,l,h 0.408 for l,h,k 0.417 for h-k,-k+l,-k 0.417 for h-l,-l,k-l 0.409 for -k,h-k,-k+l 0.409 for -h+k,-h,-h+l 0.407 for -h+l,-h+k,-h 0.407 for -l,k-l,h-l 0.032 for -h+k,k,k-l 0.033 for -h+l,-k+l,l 0.029 for h,h-k,h-l 0.032 for -h,-l,-k 0.033 for -k,-h,-l 0.033 for -l,-k,-h 0.427 for k-l,h-l,-l 0.427 for -k+l,-k,h-k 0.419 for -h,-h+l,-h+k	Xtriage
F_o, F_c correlation	0.63	EDS
Total number of atoms	37617	wwPDB-VP
Average B, all atoms (\AA^2)	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	2/2926 (0.1%)	0.57	0/3970
1	B	0.64	1/2926 (0.0%)	0.59	1/3970 (0.0%)
1	C	0.37	2/2926 (0.1%)	0.58	0/3970
1	D	0.35	0/2926	0.63	2/3970 (0.1%)
1	E	0.75	1/2926 (0.0%)	0.59	1/3970 (0.0%)
1	F	0.39	1/2926 (0.0%)	0.57	1/3970 (0.0%)
1	G	0.35	0/2926	0.58	0/3970
1	H	0.42	1/2926 (0.0%)	0.58	1/3970 (0.0%)
1	I	0.58	1/2926 (0.0%)	0.58	0/3970
1	J	0.44	1/2926 (0.0%)	0.59	1/3970 (0.0%)
1	K	0.37	1/2926 (0.0%)	0.57	0/3970
1	L	0.61	1/2926 (0.0%)	0.58	1/3970 (0.0%)
All	All	0.49	12/35112 (0.0%)	0.58	8/47640 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	2
1	E	0	1
1	G	0	1
1	I	0	1
1	L	0	1
All	All	0	7

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	426	SER	C-O	35.87	1.91	1.23
1	B	426	SER	C-O	29.30	1.79	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	426	SER	C-O	27.37	1.75	1.23
1	I	426	SER	C-O	25.28	1.71	1.23
1	J	426	SER	C-O	15.10	1.52	1.23
1	H	426	SER	C-O	13.75	1.49	1.23
1	F	426	SER	C-O	11.14	1.44	1.23
1	A	426	SER	C-O	10.94	1.44	1.23
1	K	213	SER	CB-OG	7.15	1.51	1.42
1	A	49	GLY	N-CA	6.13	1.55	1.46
1	C	49	GLY	N-CA	6.13	1.55	1.46
1	C	426	SER	C-O	-5.06	1.13	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	426	SER	CA-C-O	15.91	153.50	120.10
1	B	426	SER	CA-C-O	-8.93	101.35	120.10
1	J	426	SER	CA-C-O	-8.68	101.87	120.10
1	L	426	SER	CA-C-O	-7.23	104.91	120.10
1	E	426	SER	CA-C-O	-6.53	106.38	120.10
1	H	426	SER	CA-C-O	-6.11	107.27	120.10
1	F	426	SER	CA-C-O	-5.89	107.74	120.10
1	D	213	SER	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	212	LEU	Peptide
1	D	212	LEU	Peptide
1	D	213	SER	Peptide
1	E	212	LEU	Peptide
1	G	212	LEU	Peptide
1	I	212	LEU	Peptide
1	L	213	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2870	0	2800	237	0
1	B	2870	0	2800	242	0
1	C	2870	0	2800	225	0
1	D	2870	0	2800	228	0
1	E	2870	0	2800	240	0
1	F	2870	0	2800	225	0
1	G	2870	0	2800	206	0
1	H	2870	0	2800	232	0
1	I	2870	0	2800	259	0
1	J	2870	0	2800	227	0
1	K	2870	0	2800	236	0
1	L	2870	0	2800	235	0
2	A	262	0	0	132	0
2	B	271	0	0	117	0
2	C	298	0	0	136	0
2	D	247	0	0	105	0
2	E	268	0	0	124	0
2	F	247	0	0	111	0
2	G	255	0	0	93	0
2	H	252	0	0	117	0
2	I	274	0	0	152	0
2	J	258	0	0	129	0
2	K	276	0	0	123	0
2	L	269	0	0	118	0
All	All	37617	0	33600	2700	0

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

All (2700) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:230:ILE:CD1	2:L:582:HOH:O	1.71	1.33
1:L:230:ILE:HD13	2:L:582:HOH:O	1.23	1.33
1:F:13:LEU:HD22	2:F:655:HOH:O	1.29	1.32
1:I:361:VAL:HG23	2:I:581:HOH:O	1.26	1.32
1:K:181:ALA:HB3	2:K:550:HOH:O	1.13	1.30
1:K:378:ILE:HG22	2:K:691:HOH:O	1.15	1.28
1:I:426:SER:C	1:I:426:SER:O	1.71	1.28
1:J:38:LEU:HD13	2:J:506:HOH:O	1.22	1.28
1:L:55:THR:HG21	2:L:530:HOH:O	1.28	1.27
1:C:55:THR:HG21	2:C:490:HOH:O	1.31	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:426:SER:C	1:L:426:SER:O	1.75	1.25
1:H:55:THR:HG21	2:H:495:HOH:O	1.08	1.24
1:J:378:ILE:HG22	2:J:573:HOH:O	1.29	1.24
1:E:180:LEU:HD12	2:E:671:HOH:O	1.37	1.24
1:B:55:THR:HG21	2:B:443:HOH:O	1.07	1.23
1:J:180:LEU:HD12	2:J:654:HOH:O	1.30	1.23
1:D:230:ILE:CD1	2:D:646:HOH:O	1.88	1.22
1:F:55:THR:HG21	2:F:499:HOH:O	1.06	1.21
1:B:126:GLY:HA3	2:B:580:HOH:O	1.39	1.21
1:E:208:LEU:HD13	2:E:579:HOH:O	1.39	1.20
1:G:148:ALA:O	2:G:450:HOH:O	1.54	1.20
1:E:27:ALA:HB1	2:E:591:HOH:O	1.41	1.20
1:B:426:SER:O	1:B:426:SER:C	1.79	1.20
1:K:148:ALA:O	2:K:481:HOH:O	1.58	1.19
1:J:238:LEU:HD21	2:J:590:HOH:O	1.02	1.19
1:H:210:TYR:CE1	2:H:559:HOH:O	1.93	1.18
1:E:40:GLU:O	2:E:523:HOH:O	1.61	1.18
1:A:323:ASN:HB3	2:A:619:HOH:O	1.00	1.17
1:B:354:HIS:CD2	2:B:540:HOH:O	1.92	1.17
1:K:55:THR:HG21	2:K:551:HOH:O	1.00	1.17
1:L:115:ALA:HB3	2:L:557:HOH:O	1.44	1.17
1:E:288:LEU:HD23	2:E:626:HOH:O	0.99	1.17
1:J:55:THR:HG21	2:J:445:HOH:O	0.99	1.16
1:F:229:PHE:CE2	2:F:611:HOH:O	1.97	1.15
2:A:612:HOH:O	1:E:322:ALA:HB2	1.47	1.14
1:E:417:LYS:NZ	2:E:451:HOH:O	1.80	1.14
1:L:167:ILE:HD11	2:L:511:HOH:O	1.44	1.14
1:J:10:ILE:HG13	2:J:533:HOH:O	0.97	1.13
1:D:55:THR:HG21	2:D:449:HOH:O	0.98	1.13
1:F:148:ALA:O	2:F:453:HOH:O	1.63	1.13
1:C:107:GLU:HG2	2:D:480:HOH:O	1.49	1.12
2:G:591:HOH:O	1:J:167:ILE:HD11	1.50	1.12
1:A:55:THR:HG21	2:A:434:HOH:O	0.94	1.12
1:I:55:THR:HG21	2:I:511:HOH:O	0.97	1.12
1:B:212:LEU:HD11	2:B:510:HOH:O	1.50	1.11
1:L:324:HIS:CD2	2:L:612:HOH:O	2.00	1.11
1:J:285:ARG:O	2:J:568:HOH:O	1.69	1.11
1:K:212:LEU:HD11	2:K:681:HOH:O	1.50	1.11
1:B:212:LEU:HD21	2:B:645:HOH:O	1.51	1.10
1:E:308:ASN:OD1	2:E:664:HOH:O	1.70	1.10
1:H:339:ASN:HB3	2:H:497:HOH:O	1.49	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ALA:HB2	2:I:607:HOH:O	1.52	1.09
1:G:55:THR:HG21	2:G:494:HOH:O	0.92	1.09
1:E:212:LEU:HD11	2:E:666:HOH:O	1.50	1.09
1:B:131:ARG:HG2	2:B:552:HOH:O	1.50	1.08
1:J:82:HIS:O	2:J:510:HOH:O	1.70	1.08
1:E:55:THR:HG21	2:E:519:HOH:O	0.92	1.08
1:E:426:SER:O	1:E:426:SER:C	1.91	1.08
1:B:151:PRO:HB3	2:B:633:HOH:O	1.51	1.08
1:G:374:CYS:HB2	2:J:539:HOH:O	1.51	1.07
1:G:361:VAL:HB	1:G:362:PRO:HA	1.07	1.07
1:J:361:VAL:HB	1:J:362:PRO:HA	1.07	1.07
1:E:361:VAL:HB	1:E:362:PRO:HA	1.07	1.06
1:I:322:ALA:HB2	2:I:650:HOH:O	1.54	1.06
1:C:361:VAL:HB	1:C:362:PRO:HA	1.08	1.05
2:C:629:HOH:O	1:D:322:ALA:HB2	1.54	1.05
1:I:27:ALA:HB1	2:I:651:HOH:O	1.55	1.05
1:L:9:LEU:N	2:L:517:HOH:O	1.88	1.05
1:A:361:VAL:HB	1:A:362:PRO:HA	1.07	1.05
1:D:361:VAL:HB	1:D:362:PRO:HA	1.06	1.05
1:K:361:VAL:HB	1:K:362:PRO:HA	1.05	1.05
1:B:247:ALA:HB1	2:B:569:HOH:O	1.57	1.04
1:F:361:VAL:HB	1:F:362:PRO:HA	1.07	1.04
1:H:361:VAL:HB	1:H:362:PRO:HA	1.07	1.04
1:I:10:ILE:HA	2:I:585:HOH:O	1.54	1.04
1:K:212:LEU:HD21	2:K:591:HOH:O	0.88	1.04
1:B:361:VAL:HB	1:B:362:PRO:HA	1.06	1.04
1:E:126:GLY:HA3	2:E:595:HOH:O	1.57	1.04
1:F:212:LEU:HD11	2:F:446:HOH:O	1.57	1.04
1:I:361:VAL:HB	1:I:362:PRO:HA	1.06	1.04
1:E:212:LEU:HD21	2:E:528:HOH:O	1.54	1.04
1:A:171:ASN:O	2:A:657:HOH:O	1.73	1.03
1:G:93:ASN:ND2	2:G:667:HOH:O	1.90	1.03
1:H:167:ILE:CD1	2:H:509:HOH:O	2.04	1.03
1:L:361:VAL:HB	1:L:362:PRO:HA	1.06	1.03
2:B:543:HOH:O	1:K:208:LEU:HD13	1.56	1.03
1:C:126:GLY:HA3	2:C:639:HOH:O	1.56	1.03
1:E:218:GLN:HG3	2:E:631:HOH:O	1.58	1.03
1:J:151:PRO:HB3	2:J:484:HOH:O	1.58	1.03
1:J:141:VAL:HG13	2:J:441:HOH:O	1.59	1.02
1:K:361:VAL:HB	1:K:362:PRO:CA	1.89	1.02
1:L:361:VAL:HB	1:L:362:PRO:CA	1.90	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLN:HG3	2:B:564:HOH:O	1.60	1.01
1:C:208:LEU:HD13	2:F:530:HOH:O	1.59	1.01
1:J:322:ALA:HB2	2:L:486:HOH:O	1.59	1.01
1:G:131:ARG:HG2	2:G:466:HOH:O	1.59	1.01
1:J:148:ALA:O	2:J:432:HOH:O	1.75	1.01
1:C:218:GLN:HG3	2:C:511:HOH:O	1.60	1.01
1:C:361:VAL:HB	1:C:362:PRO:CA	1.91	1.01
1:J:305:SER:HB2	2:J:575:HOH:O	1.58	1.01
2:J:584:HOH:O	1:K:322:ALA:HB2	1.59	1.01
1:A:361:VAL:HB	1:A:362:PRO:CA	1.91	1.01
1:B:354:HIS:HD2	2:B:540:HOH:O	1.28	1.01
1:G:361:VAL:HB	1:G:362:PRO:CA	1.91	1.01
1:K:406:LEU:HD21	2:K:537:HOH:O	1.58	1.01
1:C:65:ARG:HG3	2:C:496:HOH:O	1.59	1.00
1:C:335:LYS:HB3	2:C:520:HOH:O	1.61	1.00
1:E:361:VAL:HB	1:E:362:PRO:CA	1.91	1.00
1:F:361:VAL:HB	1:F:362:PRO:CA	1.91	1.00
1:J:361:VAL:HB	1:J:362:PRO:CA	1.91	1.00
1:C:17:PRO:HB3	2:C:553:HOH:O	1.59	1.00
1:F:131:ARG:HG2	2:F:621:HOH:O	1.60	1.00
1:G:247:ALA:HB1	2:G:584:HOH:O	1.60	1.00
1:G:378:ILE:CG2	2:G:472:HOH:O	2.10	1.00
1:H:361:VAL:HB	1:H:362:PRO:CA	1.91	1.00
1:I:236:ASP:OD1	2:I:537:HOH:O	1.80	1.00
1:A:238:LEU:HD21	2:A:436:HOH:O	1.63	0.99
1:I:126:GLY:HA3	2:I:536:HOH:O	1.62	0.99
1:L:65:ARG:HG3	2:L:564:HOH:O	1.61	0.99
1:L:251:ALA:HB1	2:L:497:HOH:O	1.61	0.99
1:D:361:VAL:HB	1:D:362:PRO:CA	1.90	0.99
1:B:361:VAL:HB	1:B:362:PRO:CA	1.90	0.99
1:L:245:LEU:O	2:L:691:HOH:O	1.81	0.99
1:I:361:VAL:HB	1:I:362:PRO:CA	1.90	0.99
1:F:378:ILE:HG22	2:F:648:HOH:O	1.62	0.98
1:F:322:ALA:HB2	2:H:541:HOH:O	1.62	0.98
1:D:287:LEU:HD22	2:D:525:HOH:O	1.63	0.98
1:C:212:LEU:O	2:C:716:HOH:O	1.82	0.98
1:C:230:ILE:HD13	2:C:487:HOH:O	1.62	0.98
1:C:233:ALA:O	2:C:586:HOH:O	1.81	0.98
1:H:344:THR:HG22	2:H:617:HOH:O	1.61	0.98
1:L:17:PRO:HB3	2:L:438:HOH:O	1.62	0.98
1:F:248:LEU:HB3	2:F:502:HOH:O	1.63	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:ALA:HB1	2:H:587:HOH:O	1.62	0.97
1:K:216:ASP:O	2:K:600:HOH:O	1.82	0.97
1:A:319:ARG:HG3	2:A:602:HOH:O	1.64	0.97
1:C:230:ILE:CD1	2:C:487:HOH:O	2.11	0.97
2:B:573:HOH:O	1:C:322:ALA:HB2	1.65	0.96
1:C:40:GLU:C	2:C:661:HOH:O	2.04	0.96
1:C:220:ALA:HB2	2:C:680:HOH:O	1.65	0.96
1:K:218:GLN:HG3	2:K:544:HOH:O	1.66	0.96
2:C:532:HOH:O	1:F:151:PRO:HB3	1.65	0.95
1:G:40:GLU:O	2:G:615:HOH:O	1.84	0.95
1:E:122:LEU:HD12	2:E:533:HOH:O	1.66	0.95
1:C:258:ILE:HD13	1:C:258:ILE:H	1.30	0.95
1:D:83:THR:HA	2:D:516:HOH:O	1.65	0.95
1:F:57:ASN:HB3	2:F:650:HOH:O	1.66	0.95
1:A:258:ILE:HD13	1:A:258:ILE:H	1.31	0.95
1:G:406:LEU:HA	2:G:439:HOH:O	1.66	0.95
1:I:292:ASP:OD2	2:I:578:HOH:O	1.83	0.95
1:F:406:LEU:HD21	2:F:637:HOH:O	1.65	0.95
1:F:378:ILE:CG2	2:F:648:HOH:O	2.12	0.94
1:D:228:GLU:O	2:D:451:HOH:O	1.84	0.94
1:I:17:PRO:HB3	2:I:433:HOH:O	1.67	0.94
1:I:276:ASP:OD2	2:I:574:HOH:O	1.85	0.94
1:K:258:ILE:HD13	1:K:258:ILE:H	1.32	0.94
1:G:17:PRO:HG3	2:G:592:HOH:O	1.67	0.94
1:C:151:PRO:HB3	2:C:465:HOH:O	1.64	0.94
1:F:167:ILE:HD12	2:F:649:HOH:O	1.67	0.94
1:E:406:LEU:HA	2:E:505:HOH:O	1.66	0.94
1:K:126:GLY:HA3	2:K:598:HOH:O	1.67	0.94
1:E:147:ILE:HG21	2:H:473:HOH:O	1.68	0.94
1:F:411:ASP:O	2:F:673:HOH:O	1.86	0.94
1:J:206:VAL:HG23	2:J:502:HOH:O	1.68	0.94
1:E:258:ILE:H	1:E:258:ILE:HD13	1.33	0.93
1:D:406:LEU:HA	2:D:485:HOH:O	1.66	0.93
1:D:230:ILE:HD13	2:D:646:HOH:O	1.58	0.93
1:B:342:TYR:HD2	2:B:527:HOH:O	1.51	0.93
1:J:233:ALA:O	2:J:620:HOH:O	1.86	0.93
1:G:258:ILE:H	1:G:258:ILE:HD13	1.30	0.93
1:H:258:ILE:HD13	1:H:258:ILE:H	1.34	0.93
1:I:258:ILE:HD13	1:I:258:ILE:H	1.33	0.93
1:J:258:ILE:H	1:J:258:ILE:HD13	1.31	0.93
1:K:203:THR:HG22	2:K:543:HOH:O	1.68	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ALA:HB1	2:B:503:HOH:O	1.68	0.93
1:J:324:HIS:O	2:J:468:HOH:O	1.85	0.93
1:K:212:LEU:CD1	2:K:681:HOH:O	2.11	0.92
1:L:258:ILE:HD13	1:L:258:ILE:H	1.31	0.92
1:I:251:ALA:HB1	2:I:554:HOH:O	1.69	0.92
1:J:218:GLN:HG3	2:J:597:HOH:O	1.69	0.92
1:I:176:ILE:HD11	2:I:624:HOH:O	1.69	0.92
1:L:151:PRO:HB3	2:L:516:HOH:O	1.67	0.92
1:E:17:PRO:HB3	2:E:543:HOH:O	1.67	0.92
1:L:139:ARG:HD3	2:L:681:HOH:O	1.70	0.92
1:H:218:GLN:HG3	2:H:431:HOH:O	1.68	0.92
1:I:151:PRO:HA	2:I:656:HOH:O	1.68	0.92
1:F:167:ILE:CD1	2:F:649:HOH:O	2.17	0.92
1:D:258:ILE:HD13	1:D:258:ILE:H	1.33	0.91
1:G:317:ALA:HB2	2:J:549:HOH:O	1.70	0.91
1:A:403:ILE:HA	2:A:543:HOH:O	1.69	0.91
2:F:617:HOH:O	1:H:89:ARG:HG2	1.69	0.91
1:F:258:ILE:HD13	1:F:258:ILE:H	1.32	0.91
1:H:146:ALA:HB1	2:H:560:HOH:O	1.70	0.91
1:E:147:ILE:CG2	2:H:473:HOH:O	2.16	0.91
1:L:328:LEU:HD23	2:L:501:HOH:O	1.70	0.91
1:A:417:LYS:NZ	2:A:448:HOH:O	2.01	0.91
1:L:171:ASN:HB3	2:L:454:HOH:O	1.68	0.91
1:L:122:LEU:HD12	2:L:541:HOH:O	1.70	0.91
1:A:417:LYS:HB3	2:A:621:HOH:O	1.72	0.90
1:B:258:ILE:H	1:B:258:ILE:HD13	1.32	0.90
1:E:49:GLY:N	2:E:437:HOH:O	2.04	0.90
1:G:89:ARG:HB2	2:G:533:HOH:O	1.69	0.90
1:K:17:PRO:HB3	2:K:644:HOH:O	1.71	0.90
1:I:285:ARG:O	2:I:546:HOH:O	1.90	0.90
1:B:127:ARG:NH2	2:B:571:HOH:O	2.04	0.89
2:J:584:HOH:O	1:K:322:ALA:CB	2.16	0.89
1:G:9:LEU:N	2:G:474:HOH:O	2.05	0.89
1:A:126:GLY:HA3	2:A:449:HOH:O	1.71	0.89
1:E:169:ALA:HB2	2:I:535:HOH:O	1.71	0.89
1:G:245:LEU:HD21	2:G:592:HOH:O	1.70	0.89
1:C:27:ALA:HB1	2:C:516:HOH:O	1.71	0.89
1:A:108:VAL:HG13	2:A:655:HOH:O	1.69	0.89
1:E:56:ARG:HD2	2:I:479:HOH:O	1.73	0.89
1:F:206:VAL:HA	2:F:583:HOH:O	1.70	0.89
1:H:182:PRO:HG3	2:H:630:HOH:O	1.73	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ALA:O	2:C:538:HOH:O	1.89	0.89
1:G:144:ARG:NH2	2:G:577:HOH:O	2.04	0.89
2:A:539:HOH:O	1:D:98:ARG:HD2	1.71	0.88
1:E:139:ARG:NH2	2:E:480:HOH:O	2.03	0.88
1:K:15:ALA:HB1	2:K:593:HOH:O	1.73	0.88
1:I:218:GLN:HG3	2:I:456:HOH:O	1.71	0.88
1:L:115:ALA:HB1	2:L:532:HOH:O	1.72	0.88
1:A:284:LEU:HA	2:A:486:HOH:O	1.74	0.88
1:K:406:LEU:HA	2:K:511:HOH:O	1.72	0.88
1:H:247:ALA:HB1	2:H:568:HOH:O	1.72	0.88
1:I:322:ALA:CB	2:I:650:HOH:O	2.17	0.88
1:L:126:GLY:HA3	2:L:578:HOH:O	1.73	0.88
1:F:212:LEU:HD21	2:F:471:HOH:O	1.74	0.88
1:E:362:PRO:HG3	2:E:585:HOH:O	1.74	0.88
1:I:206:VAL:HA	2:I:570:HOH:O	1.74	0.87
1:L:228:GLU:O	2:L:505:HOH:O	1.90	0.87
1:B:208:LEU:HD13	2:K:588:HOH:O	1.75	0.87
1:D:206:VAL:HA	2:D:546:HOH:O	1.73	0.87
1:F:400:MET:SD	2:F:581:HOH:O	2.32	0.87
1:E:173:LEU:HD12	2:E:506:HOH:O	1.73	0.87
1:G:361:VAL:HG23	2:G:574:HOH:O	1.72	0.87
1:K:206:VAL:HA	2:K:563:HOH:O	1.74	0.87
1:K:230:ILE:CD1	2:K:533:HOH:O	2.21	0.87
1:K:300:ARG:CZ	2:K:532:HOH:O	2.23	0.87
2:A:538:HOH:O	1:I:169:ALA:HB2	1.75	0.87
2:F:555:HOH:O	1:G:322:ALA:HB2	1.74	0.87
1:H:212:LEU:HD11	2:H:472:HOH:O	1.74	0.87
1:B:146:ALA:HB1	2:K:507:HOH:O	1.73	0.86
1:D:323:ASN:HB3	2:D:602:HOH:O	1.73	0.86
1:H:220:ALA:HB2	2:H:646:HOH:O	1.75	0.86
1:L:108:VAL:HA	2:L:575:HOH:O	1.75	0.86
1:B:377:THR:HG22	2:D:536:HOH:O	1.74	0.86
1:G:406:LEU:HD21	2:G:601:HOH:O	1.74	0.86
1:I:324:HIS:CD2	2:I:560:HOH:O	2.28	0.86
1:K:83:THR:HA	2:K:602:HOH:O	1.74	0.86
1:J:247:ALA:HB1	2:J:454:HOH:O	1.73	0.86
1:H:267:VAL:HG13	2:H:484:HOH:O	1.74	0.86
1:J:144:ARG:HB2	2:J:530:HOH:O	1.74	0.86
1:C:357:GLN:OE1	2:C:565:HOH:O	1.93	0.86
2:C:629:HOH:O	1:D:322:ALA:CB	2.16	0.86
1:D:206:VAL:O	2:D:512:HOH:O	1.92	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:LEU:HD22	2:D:521:HOH:O	1.75	0.86
1:G:115:ALA:N	2:G:543:HOH:O	2.09	0.86
1:I:83:THR:HA	2:I:690:HOH:O	1.75	0.86
1:D:218:GLN:HG3	2:D:505:HOH:O	1.76	0.86
1:A:151:PRO:HB3	2:A:507:HOH:O	1.74	0.86
1:D:363:VAL:HG13	2:D:491:HOH:O	1.75	0.85
1:A:66:LEU:HD12	2:A:652:HOH:O	1.74	0.85
1:G:40:GLU:OE1	2:G:594:HOH:O	1.94	0.85
2:C:648:HOH:O	1:F:144:ARG:HB2	1.77	0.85
1:I:150:ILE:HD11	2:L:562:HOH:O	1.76	0.85
1:L:114:PHE:HB3	2:L:509:HOH:O	1.75	0.85
1:B:222:VAL:HG23	2:B:619:HOH:O	1.77	0.85
1:I:112:ALA:HB2	2:I:659:HOH:O	1.75	0.85
1:B:233:ALA:O	2:B:470:HOH:O	1.95	0.85
1:L:326:PRO:HB3	2:L:599:HOH:O	1.74	0.85
1:E:322:ALA:HA	2:E:441:HOH:O	1.77	0.85
1:C:228:GLU:O	2:C:438:HOH:O	1.95	0.84
1:C:236:ASP:OD1	2:C:558:HOH:O	1.94	0.84
1:G:281:GLU:OE2	2:G:683:HOH:O	1.94	0.84
1:B:37:ARG:HD2	2:B:567:HOH:O	1.78	0.84
1:H:374:CYS:HA	2:H:467:HOH:O	1.77	0.84
1:H:131:ARG:HG2	2:H:494:HOH:O	1.75	0.84
2:B:565:HOH:O	1:C:377:THR:HG22	1.77	0.84
2:G:553:HOH:O	1:H:322:ALA:HB2	1.75	0.84
1:E:378:ILE:HG21	2:E:504:HOH:O	1.77	0.84
1:E:386:VAL:HA	2:E:641:HOH:O	1.77	0.83
1:F:218:GLN:HG3	2:F:544:HOH:O	1.79	0.83
1:I:101:PHE:CD2	2:I:624:HOH:O	2.31	0.83
1:L:123:SER:HB3	1:L:215:TYR:HE2	1.42	0.83
1:C:98:ARG:HD2	2:F:565:HOH:O	1.79	0.83
1:H:276:ASP:OD2	2:H:637:HOH:O	1.96	0.83
1:I:39:ASP:OD1	2:I:542:HOH:O	1.96	0.83
1:J:38:LEU:CD1	2:J:506:HOH:O	1.94	0.83
1:L:328:LEU:CD2	2:L:501:HOH:O	2.25	0.83
1:I:289:PRO:HB2	2:I:599:HOH:O	1.77	0.83
1:J:127:ARG:HA	1:J:213:SER:HB3	1.60	0.83
1:C:260:VAL:HG11	2:C:555:HOH:O	1.76	0.83
1:B:167:ILE:HG13	2:B:566:HOH:O	1.79	0.83
1:K:324:HIS:CD2	2:K:503:HOH:O	2.31	0.83
2:A:522:HOH:O	1:D:171:ASN:HB2	1.79	0.83
1:K:230:ILE:HD13	2:K:701:HOH:O	1.76	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:GLY:N	2:C:567:HOH:O	2.13	0.82
1:K:416:VAL:HB	2:K:640:HOH:O	1.79	0.82
1:F:406:LEU:HA	2:F:481:HOH:O	1.78	0.82
1:J:229:PHE:CD1	2:J:630:HOH:O	2.31	0.82
1:L:211:GLU:OE2	2:L:476:HOH:O	1.97	0.82
1:H:323:ASN:HB3	2:H:513:HOH:O	1.80	0.82
1:I:139:ARG:HD3	2:I:564:HOH:O	1.79	0.82
2:A:612:HOH:O	1:E:322:ALA:CB	2.17	0.82
1:B:148:ALA:O	2:B:439:HOH:O	1.95	0.82
1:G:20:PHE:HD1	2:G:510:HOH:O	1.62	0.82
1:J:406:LEU:HA	2:J:515:HOH:O	1.80	0.82
1:I:176:ILE:CD1	2:I:624:HOH:O	2.24	0.82
1:J:49:GLY:N	2:J:442:HOH:O	2.13	0.82
1:L:339:ASN:HB3	2:L:521:HOH:O	1.78	0.82
1:E:26:LEU:HG	1:E:27:ALA:H	1.46	0.81
1:L:167:ILE:HD12	2:L:694:HOH:O	1.78	0.81
1:L:406:LEU:HD11	2:L:568:HOH:O	1.79	0.81
1:G:378:ILE:HG22	2:G:627:HOH:O	1.78	0.81
1:H:86:PRO:HD3	2:H:439:HOH:O	1.78	0.81
1:J:220:ALA:HB2	2:J:504:HOH:O	1.81	0.81
1:E:130:PHE:O	2:E:539:HOH:O	1.98	0.81
1:H:274:GLY:O	2:H:453:HOH:O	1.99	0.81
2:I:449:HOH:O	1:L:374:CYS:HB3	1.80	0.81
1:H:49:GLY:N	2:H:557:HOH:O	2.13	0.81
1:H:98:ARG:HD2	2:H:531:HOH:O	1.80	0.81
1:G:107:GLU:HG2	2:H:515:HOH:O	1.80	0.81
1:A:148:ALA:O	2:A:495:HOH:O	1.97	0.81
1:A:322:ALA:CB	2:I:607:HOH:O	2.18	0.81
2:F:555:HOH:O	1:G:322:ALA:CB	2.27	0.81
1:H:40:GLU:OE1	2:H:654:HOH:O	1.97	0.81
1:A:358:ASP:HA	2:A:639:HOH:O	1.78	0.81
1:C:139:ARG:HD3	2:C:517:HOH:O	1.79	0.81
1:F:13:LEU:HD13	2:F:655:HOH:O	1.81	0.80
1:G:220:ALA:HB2	2:G:578:HOH:O	1.81	0.80
1:F:322:ALA:CB	2:H:541:HOH:O	2.20	0.80
1:I:123:SER:HB3	1:I:215:TYR:HE2	1.45	0.80
1:A:218:GLN:HG3	2:A:442:HOH:O	1.82	0.80
1:C:290:GLU:HB3	2:C:493:HOH:O	1.81	0.80
1:F:415:LEU:HB2	2:F:673:HOH:O	1.80	0.80
1:G:208:LEU:HD13	2:J:555:HOH:O	1.81	0.80
1:H:167:ILE:HD13	2:H:509:HOH:O	1.74	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLY:N	2:A:446:HOH:O	2.14	0.80
1:B:361:VAL:CB	1:B:362:PRO:HA	2.02	0.80
1:F:212:LEU:O	2:F:476:HOH:O	1.99	0.80
1:J:378:ILE:CG2	2:J:573:HOH:O	2.04	0.80
1:C:210:TYR:CD1	2:C:668:HOH:O	2.34	0.80
1:I:361:VAL:CB	1:I:362:PRO:HA	2.02	0.80
1:L:13:LEU:HB3	2:L:626:HOH:O	1.81	0.80
1:A:225:LEU:HD22	2:A:640:HOH:O	1.82	0.80
1:B:123:SER:HB3	1:B:215:TYR:HE2	1.47	0.80
1:K:56:ARG:HD2	2:L:483:HOH:O	1.79	0.80
1:B:22:ALA:HB3	2:B:475:HOH:O	1.82	0.79
1:C:10:ILE:HG23	1:C:13:LEU:HD22	1.63	0.79
1:D:182:PRO:HB3	2:D:540:HOH:O	1.83	0.79
1:J:49:GLY:N	2:J:622:HOH:O	2.16	0.79
1:B:65:ARG:HG3	2:B:608:HOH:O	1.82	0.79
1:C:22:ALA:HB3	2:C:646:HOH:O	1.82	0.79
2:G:553:HOH:O	1:H:322:ALA:CB	2.29	0.79
1:E:148:ALA:O	2:E:440:HOH:O	2.00	0.79
1:J:51:ARG:HB3	2:J:493:HOH:O	1.83	0.79
1:B:212:LEU:O	2:B:658:HOH:O	1.99	0.79
1:D:182:PRO:CB	2:D:540:HOH:O	2.31	0.79
1:F:40:GLU:O	2:F:612:HOH:O	2.01	0.79
1:F:107:GLU:HG2	2:F:654:HOH:O	1.83	0.79
1:K:182:PRO:HB3	2:K:664:HOH:O	1.83	0.79
1:B:319:ARG:HG3	2:K:560:HOH:O	1.81	0.78
1:F:77:ARG:NH1	2:F:659:HOH:O	1.94	0.78
1:H:323:ASN:CA	2:H:513:HOH:O	2.31	0.78
1:L:167:ILE:CD1	2:L:511:HOH:O	2.09	0.78
1:B:182:PRO:HG3	2:B:558:HOH:O	1.82	0.78
1:H:139:ARG:NE	2:H:526:HOH:O	2.15	0.78
1:B:93:ASN:HB2	2:C:500:HOH:O	1.83	0.78
1:E:40:GLU:C	2:E:523:HOH:O	2.12	0.78
1:A:289:PRO:HB2	2:E:602:HOH:O	1.83	0.78
1:C:182:PRO:HG3	2:C:604:HOH:O	1.82	0.78
1:C:281:GLU:HG2	2:D:589:HOH:O	1.83	0.78
1:I:144:ARG:NH2	2:I:491:HOH:O	2.03	0.78
1:L:115:ALA:N	2:L:512:HOH:O	2.16	0.78
1:E:222:VAL:HG21	2:E:682:HOH:O	1.82	0.78
1:G:276:ASP:OD2	2:G:628:HOH:O	2.00	0.78
1:D:280:LEU:HD11	2:D:631:HOH:O	1.83	0.78
1:J:212:LEU:O	2:J:434:HOH:O	2.02	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ARG:HG2	2:E:645:HOH:O	1.83	0.78
1:B:229:PHE:CD1	2:K:642:HOH:O	2.36	0.78
1:E:115:ALA:HB1	2:E:586:HOH:O	1.83	0.78
1:H:323:ASN:CB	2:H:513:HOH:O	2.30	0.78
1:L:327:ALA:HB2	2:L:525:HOH:O	1.82	0.78
1:E:123:SER:HB3	1:E:215:TYR:HE2	1.47	0.78
1:H:144:ARG:NH2	2:H:626:HOH:O	2.14	0.78
1:A:287:LEU:HD22	2:A:679:HOH:O	1.83	0.78
1:E:144:ARG:NH2	2:E:524:HOH:O	2.17	0.77
1:I:115:ALA:N	2:I:590:HOH:O	2.17	0.77
1:I:342:TYR:CD2	2:I:530:HOH:O	2.37	0.77
1:I:406:LEU:HD21	2:I:544:HOH:O	1.82	0.77
1:B:151:PRO:CB	2:B:633:HOH:O	2.19	0.77
1:E:239:LEU:HG	2:E:664:HOH:O	1.82	0.77
1:H:167:ILE:HD12	2:H:509:HOH:O	1.76	0.77
2:C:543:HOH:O	1:D:377:THR:HG22	1.84	0.77
1:J:285:ARG:NE	2:J:595:HOH:O	2.15	0.77
1:B:126:GLY:O	1:B:213:SER:HB3	1.85	0.77
1:F:403:ILE:HG23	2:F:591:HOH:O	1.85	0.77
1:I:417:LYS:NZ	2:I:664:HOH:O	2.17	0.77
1:J:130:PHE:O	2:J:537:HOH:O	2.03	0.77
1:J:151:PRO:CA	2:J:484:HOH:O	2.33	0.77
1:H:54:VAL:HB	2:H:621:HOH:O	1.84	0.77
1:B:70:SER:N	2:B:444:HOH:O	2.16	0.77
1:C:229:PHE:CE2	2:C:727:HOH:O	2.36	0.77
1:K:361:VAL:CB	1:K:362:PRO:HA	2.01	0.77
1:A:374:CYS:HB3	2:D:654:HOH:O	1.83	0.77
1:B:65:ARG:NH2	2:B:531:HOH:O	2.17	0.77
1:C:40:GLU:OE1	2:C:616:HOH:O	2.03	0.77
1:I:94:PRO:HA	2:I:476:HOH:O	1.84	0.77
1:L:51:ARG:HB2	2:L:462:HOH:O	1.83	0.77
1:L:403:ILE:HA	2:L:545:HOH:O	1.82	0.77
1:I:238:LEU:HD21	2:I:670:HOH:O	1.84	0.77
1:K:209:ASP:HB2	2:K:680:HOH:O	1.84	0.77
2:C:600:HOH:O	1:F:231:ALA:HB2	1.83	0.77
1:G:378:ILE:HG21	2:G:472:HOH:O	1.80	0.77
1:H:406:LEU:HA	2:H:432:HOH:O	1.85	0.77
1:A:123:SER:HB3	1:A:215:TYR:HE2	1.49	0.76
1:E:272:HIS:HB3	2:E:563:HOH:O	1.84	0.76
2:J:583:HOH:O	1:K:341:ARG:HB2	1.83	0.76
1:F:397:THR:HG22	2:F:581:HOH:O	1.85	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:PRO:HB3	2:L:553:HOH:O	1.83	0.76
1:A:168:ASN:O	2:A:622:HOH:O	2.03	0.76
1:J:26:LEU:HG	1:J:27:ALA:H	1.49	0.76
1:J:251:ALA:HB1	2:J:604:HOH:O	1.86	0.76
1:K:398:PHE:HB3	2:K:507:HOH:O	1.84	0.76
2:G:534:HOH:O	1:J:140:LEU:HD11	1.86	0.76
1:I:228:GLU:O	2:I:513:HOH:O	2.02	0.76
1:J:151:PRO:CB	2:J:484:HOH:O	2.21	0.76
1:K:167:ILE:HA	2:K:516:HOH:O	1.85	0.76
1:L:65:ARG:CG	2:L:564:HOH:O	2.24	0.76
1:C:115:ALA:HB1	2:C:618:HOH:O	1.85	0.76
1:L:123:SER:HB3	1:L:215:TYR:CE2	2.20	0.76
2:C:486:HOH:O	1:F:229:PHE:CD1	2.38	0.76
1:D:319:ARG:NH2	2:D:487:HOH:O	2.17	0.76
1:E:322:ALA:N	2:E:441:HOH:O	2.18	0.76
1:L:285:ARG:NE	2:L:503:HOH:O	2.18	0.76
1:D:122:LEU:HD12	2:D:555:HOH:O	1.85	0.76
1:G:284:LEU:HD12	2:G:506:HOH:O	1.84	0.76
1:I:10:ILE:HG22	2:I:585:HOH:O	1.86	0.76
1:J:322:ALA:CB	2:L:486:HOH:O	2.23	0.76
1:H:246:GLU:OE1	2:H:664:HOH:O	2.02	0.76
1:D:169:ALA:HB2	2:D:527:HOH:O	1.85	0.76
1:G:77:ARG:HB3	2:G:640:HOH:O	1.86	0.76
1:G:126:GLY:HA3	2:G:581:HOH:O	1.85	0.76
1:G:320:HIS:ND1	2:G:496:HOH:O	2.18	0.75
1:C:26:LEU:HG	1:C:27:ALA:H	1.51	0.75
1:E:30:LEU:CD2	2:E:459:HOH:O	2.35	0.75
1:J:228:GLU:HB3	2:J:630:HOH:O	1.85	0.75
1:I:300:ARG:NH2	2:I:526:HOH:O	2.18	0.75
1:J:320:HIS:ND1	2:J:658:HOH:O	2.19	0.75
1:C:123:SER:HB3	1:C:215:TYR:HE2	1.50	0.75
1:E:15:ALA:HB1	2:E:552:HOH:O	1.85	0.75
1:I:285:ARG:HD3	2:I:591:HOH:O	1.86	0.75
1:K:324:HIS:HB3	2:K:531:HOH:O	1.86	0.75
1:A:374:CYS:CB	2:D:654:HOH:O	2.33	0.75
1:F:342:TYR:HD2	2:F:597:HOH:O	1.68	0.75
1:G:223:VAL:HG23	2:G:498:HOH:O	1.84	0.75
1:I:182:PRO:HB3	2:I:510:HOH:O	1.85	0.75
2:K:462:HOH:O	1:L:322:ALA:HB2	1.86	0.75
1:I:222:VAL:HG23	2:I:617:HOH:O	1.84	0.75
1:D:174:PRO:HB3	2:D:669:HOH:O	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:ALA:N	2:H:537:HOH:O	2.19	0.75
1:I:378:ILE:CG2	2:I:691:HOH:O	2.34	0.75
1:D:36:ARG:HG2	2:D:508:HOH:O	1.85	0.75
1:E:206:VAL:HG13	2:E:526:HOH:O	1.86	0.75
1:J:247:ALA:O	2:J:506:HOH:O	2.04	0.75
1:C:173:LEU:HD12	2:C:433:HOH:O	1.85	0.74
1:K:403:ILE:HA	2:K:541:HOH:O	1.87	0.74
1:A:342:TYR:HA	2:A:500:HOH:O	1.86	0.74
1:H:211:GLU:OE2	2:H:498:HOH:O	2.05	0.74
1:K:137:GLU:HA	2:K:585:HOH:O	1.86	0.74
1:L:115:ALA:HA	1:L:117:TRP:N	2.03	0.74
1:F:375:GLY:HA2	2:F:584:HOH:O	1.87	0.74
1:A:56:ARG:HD2	2:E:494:HOH:O	1.87	0.74
1:A:406:LEU:HD21	2:A:573:HOH:O	1.87	0.74
1:I:417:LYS:HB3	2:I:636:HOH:O	1.87	0.74
1:K:10:ILE:HG23	1:K:13:LEU:HD22	1.67	0.74
1:K:71:PRO:O	2:K:703:HOH:O	2.04	0.74
1:L:361:VAL:CB	1:L:362:PRO:HA	2.02	0.74
1:F:115:ALA:HB1	2:F:550:HOH:O	1.88	0.74
1:L:355:LEU:HD23	2:L:662:HOH:O	1.87	0.74
1:A:115:ALA:HA	1:A:117:TRP:N	2.03	0.74
1:A:182:PRO:HG3	2:A:598:HOH:O	1.86	0.74
1:I:326:PRO:HB3	2:L:677:HOH:O	1.87	0.74
1:J:296:ARG:NH2	2:J:479:HOH:O	2.20	0.74
1:D:205:ASP:HB3	2:D:497:HOH:O	1.87	0.74
1:E:245:LEU:HA	2:E:577:HOH:O	1.86	0.74
1:B:49:GLY:N	2:B:496:HOH:O	2.21	0.74
1:D:416:VAL:HB	2:D:643:HOH:O	1.87	0.74
1:E:36:ARG:HG2	2:E:471:HOH:O	1.87	0.74
1:F:337:ASN:OD1	2:F:617:HOH:O	2.05	0.74
1:G:361:VAL:CB	1:G:362:PRO:HA	2.03	0.74
1:J:211:GLU:OE2	2:J:594:HOH:O	2.04	0.74
1:J:228:GLU:O	2:J:433:HOH:O	2.06	0.74
1:A:168:ASN:HB2	2:A:622:HOH:O	1.88	0.73
1:A:205:ASP:HA	2:A:518:HOH:O	1.86	0.73
1:B:115:ALA:HA	1:B:117:TRP:N	2.02	0.73
1:F:115:ALA:HA	1:F:117:TRP:N	2.03	0.73
1:F:342:TYR:HA	2:F:597:HOH:O	1.88	0.73
1:A:131:ARG:HG2	2:A:578:HOH:O	1.87	0.73
1:K:169:ALA:HB2	2:K:685:HOH:O	1.88	0.73
1:B:342:TYR:CD2	2:B:527:HOH:O	2.33	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:117:TRP:HB2	2:I:448:HOH:O	1.89	0.73
1:D:330:GLY:O	2:D:556:HOH:O	2.07	0.73
1:J:123:SER:HB3	1:J:215:TYR:HE2	1.54	0.73
1:G:115:ALA:HA	1:G:117:TRP:N	2.03	0.73
2:I:472:HOH:O	1:L:98:ARG:HD2	1.88	0.73
1:D:361:VAL:CB	1:D:362:PRO:HA	2.02	0.73
1:H:358:ASP:HA	2:H:577:HOH:O	1.88	0.73
1:L:167:ILE:CD1	2:L:694:HOH:O	2.34	0.73
1:C:289:PRO:HB2	2:C:620:HOH:O	1.89	0.73
1:E:417:LYS:HE3	2:E:486:HOH:O	1.87	0.73
1:J:115:ALA:HB1	2:J:535:HOH:O	1.89	0.73
1:K:151:PRO:HB3	2:K:597:HOH:O	1.89	0.73
1:E:115:ALA:HA	1:E:117:TRP:N	2.04	0.73
1:E:285:ARG:NH2	2:E:566:HOH:O	2.20	0.72
1:F:336:ILE:HG23	2:F:627:HOH:O	1.89	0.72
1:J:268:GLY:HA3	2:J:554:HOH:O	1.88	0.72
1:E:115:ALA:N	2:E:559:HOH:O	2.20	0.72
1:H:115:ALA:HA	1:H:117:TRP:N	2.04	0.72
2:K:462:HOH:O	1:L:322:ALA:CB	2.37	0.72
1:L:322:ALA:N	2:L:602:HOH:O	2.21	0.72
1:L:403:ILE:O	1:L:404:ARG:HB2	1.89	0.72
1:D:114:PHE:HB3	2:D:442:HOH:O	1.88	0.72
1:G:212:LEU:O	2:G:545:HOH:O	2.07	0.72
1:C:115:ALA:HA	1:C:117:TRP:N	2.04	0.72
1:C:229:PHE:CD2	2:C:727:HOH:O	2.42	0.72
1:C:233:ALA:C	2:C:586:HOH:O	2.26	0.72
1:G:126:GLY:O	1:G:213:SER:HB3	1.90	0.72
1:D:281:GLU:OE2	2:D:476:HOH:O	2.08	0.72
1:E:126:GLY:O	1:E:213:SER:HB3	1.88	0.72
1:I:182:PRO:CB	2:I:510:HOH:O	2.37	0.72
1:I:403:ILE:HA	2:I:608:HOH:O	1.89	0.72
1:C:406:LEU:HA	2:C:451:HOH:O	1.90	0.72
1:E:284:LEU:HA	2:E:608:HOH:O	1.89	0.72
1:H:398:PHE:HE2	2:H:519:HOH:O	1.73	0.72
1:J:98:ARG:NH1	2:J:549:HOH:O	2.23	0.72
1:K:115:ALA:HA	1:K:117:TRP:N	2.05	0.72
1:L:26:LEU:HG	1:L:27:ALA:H	1.55	0.72
1:H:56:ARG:NH2	2:H:506:HOH:O	2.22	0.72
1:H:126:GLY:O	1:H:213:SER:HB3	1.90	0.72
1:H:234:ARG:HB3	1:H:237:ASN:ND2	2.04	0.72
1:I:320:HIS:ND1	2:I:492:HOH:O	2.21	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:56:ARG:NH2	2:L:536:HOH:O	2.23	0.72
1:F:226:ASN:ND2	2:F:537:HOH:O	2.22	0.72
1:A:123:SER:HB3	1:A:215:TYR:CE2	2.25	0.71
1:B:348:THR:HG23	1:B:391:VAL:HG22	1.72	0.71
1:I:51:ARG:NH2	2:I:621:HOH:O	2.23	0.71
1:A:151:PRO:CB	2:A:507:HOH:O	2.35	0.71
1:D:115:ALA:HB1	2:D:489:HOH:O	1.89	0.71
1:D:319:ARG:CZ	2:D:487:HOH:O	2.37	0.71
1:L:347:GLU:OE1	2:L:443:HOH:O	2.08	0.71
1:E:322:ALA:CA	2:E:441:HOH:O	2.37	0.71
1:E:361:VAL:CB	1:E:362:PRO:HA	2.03	0.71
1:H:123:SER:HB3	1:H:215:TYR:HE2	1.55	0.71
1:K:234:ARG:HB3	1:K:237:ASN:ND2	2.05	0.71
1:C:116:PRO:HD2	2:C:521:HOH:O	1.91	0.71
1:D:115:ALA:HA	1:D:117:TRP:N	2.04	0.71
1:D:272:HIS:HB3	2:D:510:HOH:O	1.90	0.71
1:G:218:GLN:HG3	2:G:563:HOH:O	1.90	0.71
1:D:230:ILE:HD11	2:D:646:HOH:O	1.67	0.71
1:E:226:ASN:ND2	2:E:590:HOH:O	2.21	0.71
1:H:148:ALA:O	2:H:586:HOH:O	2.07	0.71
1:B:229:PHE:CE1	2:K:642:HOH:O	2.42	0.71
1:I:26:LEU:HG	1:I:27:ALA:H	1.56	0.71
1:A:89:ARG:HB2	2:A:690:HOH:O	1.89	0.71
1:G:239:LEU:CD2	2:G:617:HOH:O	2.38	0.71
1:I:90:VAL:HG22	2:I:583:HOH:O	1.91	0.71
1:K:26:LEU:HG	1:K:27:ALA:H	1.54	0.71
1:B:154:ASN:HB3	2:B:596:HOH:O	1.90	0.71
1:D:385:GLN:HB2	2:D:432:HOH:O	1.89	0.71
1:E:398:PHE:HB3	2:H:560:HOH:O	1.91	0.71
1:H:95:GLU:HG3	2:H:559:HOH:O	1.90	0.71
1:I:115:ALA:HA	1:I:117:TRP:N	2.06	0.71
1:I:168:ASN:ND2	2:I:641:HOH:O	2.22	0.71
1:I:342:TYR:HD2	2:I:530:HOH:O	1.72	0.71
1:K:403:ILE:O	1:K:404:ARG:HB2	1.91	0.71
1:B:212:LEU:CD2	2:B:645:HOH:O	2.19	0.71
1:H:204:ALA:O	2:H:612:HOH:O	2.08	0.71
1:J:115:ALA:HA	1:J:117:TRP:N	2.05	0.71
2:J:485:HOH:O	1:L:169:ALA:HB2	1.91	0.71
1:A:151:PRO:CA	2:A:507:HOH:O	2.38	0.70
1:C:210:TYR:CE1	2:C:668:HOH:O	2.44	0.70
1:J:17:PRO:HB3	2:J:564:HOH:O	1.89	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:170:GLN:HA	2:F:468:HOH:O	1.90	0.70
1:K:89:ARG:HG2	2:L:633:HOH:O	1.91	0.70
1:G:258:ILE:H	1:G:258:ILE:CD1	2.04	0.70
1:J:256:ASN:HA	2:J:523:HOH:O	1.90	0.70
1:L:348:THR:HG23	1:L:391:VAL:HG22	1.72	0.70
1:B:370:SER:HB3	2:B:634:HOH:O	1.90	0.70
1:C:258:ILE:H	1:C:258:ILE:CD1	2.05	0.70
1:D:212:LEU:HD11	2:D:673:HOH:O	1.92	0.70
1:G:373:GLY:HA2	2:G:561:HOH:O	1.92	0.70
1:K:258:ILE:H	1:K:258:ILE:CD1	2.05	0.70
1:A:258:ILE:H	1:A:258:ILE:CD1	2.05	0.70
1:B:38:LEU:HB2	2:B:569:HOH:O	1.89	0.70
1:B:70:SER:C	2:B:444:HOH:O	2.30	0.70
1:I:389:ARG:NH2	2:I:517:HOH:O	2.25	0.70
1:L:234:ARG:HB3	1:L:237:ASN:ND2	2.06	0.70
1:B:290:GLU:HG3	2:C:493:HOH:O	1.92	0.70
1:F:98:ARG:HD2	2:F:442:HOH:O	1.91	0.70
1:F:268:GLY:HA3	2:F:516:HOH:O	1.92	0.70
1:G:234:ARG:HB3	1:G:237:ASN:ND2	2.07	0.70
1:G:337:ASN:OD1	2:G:459:HOH:O	2.09	0.70
1:I:360:GLU:OE1	2:I:637:HOH:O	2.09	0.70
1:E:82:HIS:CD2	1:E:239:LEU:HD22	2.26	0.70
1:F:234:ARG:HB3	1:F:237:ASN:ND2	2.07	0.70
1:I:374:CYS:HB3	2:L:655:HOH:O	1.91	0.70
1:J:25:SER:O	2:J:674:HOH:O	2.10	0.70
1:K:82:HIS:CD2	1:K:239:LEU:HD22	2.27	0.70
1:K:123:SER:HB3	1:K:215:TYR:HE2	1.56	0.70
1:L:274:GLY:O	2:L:585:HOH:O	2.10	0.70
1:C:130:PHE:O	2:C:512:HOH:O	2.10	0.70
1:E:21:HIS:HD2	2:E:679:HOH:O	1.74	0.70
1:E:93:ASN:OD1	2:E:535:HOH:O	2.10	0.69
1:I:299:GLN:HG2	2:I:565:HOH:O	1.91	0.69
1:K:65:ARG:HH21	1:K:255:GLU:HG3	1.57	0.69
1:C:82:HIS:CD2	1:C:239:LEU:HD22	2.27	0.69
1:B:169:ALA:HB2	2:C:653:HOH:O	1.91	0.69
2:F:595:HOH:O	1:G:377:THR:HG22	1.93	0.69
1:B:360:GLU:HG2	2:B:457:HOH:O	1.93	0.69
1:J:82:HIS:CD2	1:J:239:LEU:HD22	2.27	0.69
1:A:403:ILE:O	1:A:404:ARG:HB2	1.91	0.69
1:F:126:GLY:HA3	2:G:497:HOH:O	1.91	0.69
1:H:403:ILE:O	1:H:404:ARG:HB2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:403:ILE:O	1:J:404:ARG:HB2	1.89	0.69
2:A:494:HOH:O	1:D:151:PRO:HD3	1.93	0.69
1:B:123:SER:HB3	1:B:215:TYR:CE2	2.27	0.69
1:I:123:SER:HB3	1:I:215:TYR:CE2	2.27	0.69
1:I:209:ASP:OD1	2:I:466:HOH:O	2.10	0.69
1:J:234:ARG:HB3	1:J:237:ASN:ND2	2.06	0.69
1:J:258:ILE:H	1:J:258:ILE:CD1	2.05	0.69
1:A:131:ARG:NH2	2:A:475:HOH:O	1.96	0.69
1:E:412:LEU:H	1:E:412:LEU:HD13	1.57	0.69
1:H:169:ALA:HB2	2:H:596:HOH:O	1.93	0.69
1:K:115:ALA:N	2:K:519:HOH:O	2.25	0.69
1:L:403:ILE:HD11	2:L:463:HOH:O	1.92	0.69
1:A:285:ARG:CZ	2:A:508:HOH:O	2.41	0.69
1:A:412:LEU:HD13	1:A:412:LEU:H	1.58	0.69
1:B:70:SER:O	2:B:444:HOH:O	2.11	0.69
1:A:342:TYR:CD2	2:A:500:HOH:O	2.46	0.69
1:B:56:ARG:NH2	2:B:529:HOH:O	2.26	0.69
1:F:203:THR:HA	2:F:572:HOH:O	1.93	0.69
1:H:361:VAL:CB	1:H:362:PRO:HA	2.03	0.69
1:I:238:LEU:CD2	2:I:670:HOH:O	2.41	0.69
1:C:351:PHE:C	2:C:631:HOH:O	2.31	0.68
1:B:258:ILE:H	1:B:258:ILE:CD1	2.06	0.68
1:C:51:ARG:NH2	2:C:464:HOH:O	2.25	0.68
1:H:51:ARG:HB3	2:H:618:HOH:O	1.92	0.68
1:J:179:GLN:O	2:J:459:HOH:O	2.11	0.68
1:L:151:PRO:CB	2:L:516:HOH:O	2.34	0.68
1:A:82:HIS:CD2	1:A:239:LEU:HD22	2.28	0.68
1:A:151:PRO:HA	2:A:562:HOH:O	1.93	0.68
1:D:65:ARG:HH21	1:D:255:GLU:HG3	1.59	0.68
1:D:395:LEU:HD12	2:D:649:HOH:O	1.92	0.68
1:D:403:ILE:O	1:D:404:ARG:HB2	1.93	0.68
1:F:403:ILE:O	1:F:404:ARG:HB2	1.92	0.68
1:L:17:PRO:HA	1:L:20:PHE:HB3	1.76	0.68
1:C:93:ASN:O	2:C:485:HOH:O	2.11	0.68
1:K:230:ILE:HD11	2:K:533:HOH:O	1.86	0.68
1:L:122:LEU:CD1	2:L:541:HOH:O	2.32	0.68
1:D:300:ARG:NH2	2:D:499:HOH:O	2.11	0.68
1:E:234:ARG:HB3	1:E:237:ASN:ND2	2.08	0.68
1:H:206:VAL:HA	2:H:527:HOH:O	1.92	0.68
1:E:267:VAL:O	2:E:474:HOH:O	2.11	0.68
1:E:403:ILE:O	1:E:404:ARG:HB2	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:123:SER:HB3	1:G:215:TYR:HE2	1.59	0.68
1:G:371:ASP:OD2	2:G:638:HOH:O	2.12	0.68
1:J:220:ALA:CB	2:J:504:HOH:O	2.41	0.68
1:B:82:HIS:CD2	1:B:239:LEU:HD22	2.29	0.68
1:F:251:ALA:HB1	2:F:485:HOH:O	1.93	0.68
1:L:82:HIS:CD2	1:L:239:LEU:HD22	2.28	0.68
1:L:258:ILE:H	1:L:258:ILE:CD1	2.06	0.68
1:A:208:LEU:HD13	2:D:575:HOH:O	1.92	0.68
1:B:291:GLY:O	2:B:585:HOH:O	2.12	0.68
1:D:412:LEU:HD13	1:D:412:LEU:H	1.59	0.68
1:G:154:ASN:HB2	2:G:456:HOH:O	1.92	0.68
1:J:17:PRO:HG3	2:J:564:HOH:O	1.93	0.68
1:A:288:LEU:HB2	2:A:504:HOH:O	1.93	0.68
1:E:324:HIS:HB3	2:E:510:HOH:O	1.94	0.68
1:H:371:ASP:OD1	2:H:438:HOH:O	2.11	0.68
1:C:361:VAL:CB	1:C:362:PRO:HA	2.03	0.68
1:A:234:ARG:HB3	1:A:237:ASN:ND2	2.08	0.67
1:F:411:ASP:C	2:F:673:HOH:O	2.30	0.67
2:G:437:HOH:O	1:J:229:PHE:HD1	1.77	0.67
1:G:49:GLY:N	2:G:475:HOH:O	2.27	0.67
1:C:291:GLY:HA2	2:C:626:HOH:O	1.93	0.67
1:G:283:VAL:CG2	2:G:614:HOH:O	2.42	0.67
1:H:82:HIS:CD2	1:H:239:LEU:HD22	2.29	0.67
1:H:258:ILE:H	1:H:258:ILE:CD1	2.05	0.67
1:H:412:LEU:H	1:H:412:LEU:HD13	1.59	0.67
1:A:114:PHE:HB3	2:A:534:HOH:O	1.92	0.67
1:A:220:ALA:HB2	2:A:456:HOH:O	1.94	0.67
2:A:481:HOH:O	1:D:144:ARG:HB3	1.94	0.67
1:F:284:LEU:HD21	2:F:445:HOH:O	1.94	0.67
1:F:412:LEU:HD13	1:F:412:LEU:H	1.59	0.67
1:I:403:ILE:O	1:I:404:ARG:HB2	1.94	0.67
1:B:147:ILE:HG21	2:K:682:HOH:O	1.93	0.67
1:E:30:LEU:HD23	2:E:459:HOH:O	1.91	0.67
1:G:139:ARG:HD3	2:G:670:HOH:O	1.94	0.67
2:G:550:HOH:O	1:H:385:GLN:HG2	1.93	0.67
1:H:101:PHE:HD2	1:H:179:GLN:HG2	1.60	0.67
1:H:300:ARG:NH2	2:H:532:HOH:O	2.28	0.67
1:K:122:LEU:HD23	1:K:140:LEU:O	1.95	0.67
1:B:101:PHE:HD2	1:B:179:GLN:HG2	1.60	0.67
1:F:51:ARG:HB3	2:F:484:HOH:O	1.95	0.67
1:J:144:ARG:NH2	2:J:636:HOH:O	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:233:ALA:C	2:J:620:HOH:O	2.28	0.67
1:K:30:LEU:HD23	2:K:620:HOH:O	1.94	0.67
1:B:174:PRO:HB2	2:B:638:HOH:O	1.93	0.67
1:E:417:LYS:CE	2:E:486:HOH:O	2.41	0.67
1:G:82:HIS:CD2	1:G:239:LEU:HD22	2.29	0.67
2:G:437:HOH:O	1:J:229:PHE:CD1	2.47	0.67
1:I:65:ARG:HH21	1:I:255:GLU:HG3	1.59	0.67
1:I:412:LEU:HD13	1:I:412:LEU:H	1.59	0.67
1:A:251:ALA:HB1	2:A:568:HOH:O	1.95	0.67
1:C:234:ARG:HB3	1:C:237:ASN:ND2	2.09	0.67
1:F:101:PHE:HD2	1:F:179:GLN:HG2	1.59	0.67
1:F:369:ARG:HE	1:H:170:GLN:HE22	1.43	0.67
1:F:395:LEU:HD21	2:F:673:HOH:O	1.94	0.67
1:A:26:LEU:HG	1:A:27:ALA:H	1.59	0.67
1:B:234:ARG:HB3	1:B:237:ASN:ND2	2.10	0.67
1:C:316:TYR:CZ	2:C:595:HOH:O	2.46	0.67
1:A:235:LEU:HD12	1:A:404:ARG:HD2	1.77	0.66
1:F:13:LEU:CD2	2:F:655:HOH:O	2.06	0.66
1:H:123:SER:HB3	1:H:215:TYR:CE2	2.30	0.66
1:J:140:LEU:HA	2:J:623:HOH:O	1.95	0.66
1:D:101:PHE:HD2	1:D:179:GLN:HG2	1.60	0.66
1:E:212:LEU:HD23	2:E:676:HOH:O	1.94	0.66
1:E:268:GLY:HA3	2:E:542:HOH:O	1.96	0.66
1:I:234:ARG:HB3	1:I:237:ASN:ND2	2.10	0.66
1:I:239:LEU:HD12	2:I:559:HOH:O	1.95	0.66
1:B:312:VAL:HA	2:B:528:HOH:O	1.94	0.66
1:F:228:GLU:O	2:F:483:HOH:O	2.12	0.66
1:G:50:GLY:H	1:G:66:LEU:HB2	1.60	0.66
1:K:130:PHE:O	1:K:131:ARG:HB2	1.95	0.66
1:L:412:LEU:HD13	1:L:412:LEU:H	1.60	0.66
1:B:182:PRO:HB3	2:B:680:HOH:O	1.94	0.66
1:D:234:ARG:HB3	1:D:237:ASN:ND2	2.11	0.66
1:F:15:ALA:HB1	2:F:608:HOH:O	1.94	0.66
1:A:285:ARG:NH2	2:A:508:HOH:O	2.27	0.66
1:B:206:VAL:HA	2:B:489:HOH:O	1.96	0.66
1:C:239:LEU:HD21	2:C:450:HOH:O	1.95	0.66
1:I:101:PHE:HD2	1:I:179:GLN:HG2	1.61	0.66
1:L:65:ARG:HH21	1:L:255:GLU:HG3	1.59	0.66
1:C:401:HIS:HE1	2:C:439:HOH:O	1.77	0.66
1:D:50:GLY:H	1:D:66:LEU:HB2	1.60	0.66
1:G:101:PHE:HD2	1:G:179:GLN:HG2	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:153:LEU:HA	2:K:464:HOH:O	1.95	0.66
1:B:412:LEU:HD13	1:B:412:LEU:H	1.60	0.66
1:I:17:PRO:HA	1:I:20:PHE:HB3	1.77	0.66
1:A:13:LEU:HD22	2:A:544:HOH:O	1.95	0.66
1:A:122:LEU:HD12	2:A:632:HOH:O	1.94	0.66
1:A:357:GLN:OE1	2:A:452:HOH:O	2.13	0.66
1:C:123:SER:HB3	1:C:215:TYR:CE2	2.30	0.66
1:E:263:ASP:OD1	2:E:588:HOH:O	2.13	0.66
1:F:361:VAL:CB	1:F:362:PRO:HA	2.03	0.66
1:I:92:PRO:O	1:I:212:LEU:HB2	1.95	0.66
1:K:101:PHE:HD2	1:K:179:GLN:HG2	1.61	0.66
1:E:119:ASP:OD2	2:E:586:HOH:O	2.13	0.66
1:F:123:SER:HB3	1:F:215:TYR:HE2	1.61	0.66
1:G:26:LEU:HG	1:G:27:ALA:H	1.60	0.66
1:H:15:ALA:HB1	2:H:488:HOH:O	1.95	0.66
1:H:50:GLY:H	1:H:66:LEU:HB2	1.61	0.66
1:J:17:PRO:CG	2:J:564:HOH:O	2.42	0.66
1:J:65:ARG:HH21	1:J:255:GLU:HG3	1.61	0.66
1:J:412:LEU:HD13	1:J:412:LEU:H	1.59	0.66
1:C:116:PRO:CD	2:C:521:HOH:O	2.43	0.66
1:E:62:ILE:HD12	2:E:456:HOH:O	1.95	0.66
1:E:123:SER:HB3	1:E:215:TYR:CE2	2.31	0.66
1:H:222:VAL:HG23	2:H:520:HOH:O	1.94	0.66
1:I:50:GLY:H	1:I:66:LEU:HB2	1.60	0.66
1:I:167:ILE:HD11	2:I:507:HOH:O	1.94	0.66
1:K:171:ASN:HB2	2:K:663:HOH:O	1.96	0.66
1:K:233:ALA:O	2:K:610:HOH:O	2.13	0.66
1:L:101:PHE:HD2	1:L:179:GLN:HG2	1.60	0.66
1:A:285:ARG:HD3	2:A:577:HOH:O	1.95	0.65
1:G:422:PHE:O	2:G:640:HOH:O	2.14	0.65
1:L:378:ILE:HG22	2:L:658:HOH:O	1.94	0.65
1:B:50:GLY:H	1:B:66:LEU:HB2	1.61	0.65
1:F:252:GLU:OE2	2:F:458:HOH:O	2.13	0.65
1:L:50:GLY:H	1:L:66:LEU:HB2	1.61	0.65
1:B:171:ASN:ND2	2:B:482:HOH:O	2.30	0.65
1:G:65:ARG:HH21	1:G:255:GLU:HG3	1.59	0.65
1:H:378:ILE:CG2	2:H:673:HOH:O	2.44	0.65
1:D:82:HIS:CD2	1:D:239:LEU:HD22	2.31	0.65
1:F:50:GLY:H	1:F:66:LEU:HB2	1.61	0.65
1:G:226:ASN:ND2	2:G:528:HOH:O	2.30	0.65
1:G:412:LEU:HD13	1:G:412:LEU:H	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:180:LEU:CD1	2:J:654:HOH:O	2.05	0.65
1:K:114:PHE:HA	2:K:524:HOH:O	1.95	0.65
1:D:205:ASP:OD1	2:D:628:HOH:O	2.14	0.65
1:F:13:LEU:CD1	2:F:655:HOH:O	2.40	0.65
1:G:213:SER:O	2:G:593:HOH:O	2.15	0.65
1:H:65:ARG:HH21	1:H:255:GLU:HG3	1.61	0.65
1:I:36:ARG:HG2	2:I:647:HOH:O	1.95	0.65
1:I:106:VAL:HG12	2:I:583:HOH:O	1.96	0.65
1:L:216:ASP:O	2:L:576:HOH:O	2.14	0.65
1:C:151:PRO:CB	2:C:465:HOH:O	2.32	0.65
1:F:82:HIS:CD2	1:F:239:LEU:HD22	2.31	0.65
1:F:171:ASN:HB3	2:F:524:HOH:O	1.97	0.65
1:K:18:THR:HB	1:K:19:PRO:HD3	1.79	0.65
1:K:107:GLU:HG2	2:L:621:HOH:O	1.96	0.65
1:A:108:VAL:CG1	2:A:655:HOH:O	2.34	0.65
1:A:327:ALA:HB2	2:A:572:HOH:O	1.97	0.65
2:A:602:HOH:O	1:D:151:PRO:HG2	1.96	0.65
1:D:248:LEU:HB3	2:D:521:HOH:O	1.95	0.65
1:E:50:GLY:H	1:E:66:LEU:HB2	1.61	0.65
1:G:131:ARG:HG3	2:G:441:HOH:O	1.97	0.65
1:J:30:LEU:HD23	2:J:621:HOH:O	1.96	0.65
2:B:585:HOH:O	1:D:281:GLU:HG2	1.96	0.65
1:E:17:PRO:HA	1:E:20:PHE:HB3	1.79	0.65
1:L:108:VAL:HG13	2:L:575:HOH:O	1.97	0.65
1:A:127:ARG:NH2	2:A:684:HOH:O	2.29	0.65
1:B:403:ILE:O	1:B:404:ARG:HB2	1.97	0.65
1:H:417:LYS:HB3	2:H:658:HOH:O	1.97	0.65
1:E:329:ASN:OD1	2:E:452:HOH:O	2.15	0.65
1:E:337:ASN:OD1	2:E:645:HOH:O	2.14	0.65
1:H:210:TYR:CD1	2:H:559:HOH:O	2.35	0.65
1:H:366:PHE:HZ	2:H:515:HOH:O	1.80	0.65
1:I:82:HIS:CD2	1:I:239:LEU:HD22	2.32	0.65
1:J:17:PRO:HA	1:J:20:PHE:HB3	1.78	0.65
1:K:322:ALA:N	2:K:528:HOH:O	2.28	0.65
1:A:222:VAL:HG23	2:A:631:HOH:O	1.95	0.64
1:E:258:ILE:H	1:E:258:ILE:CD1	2.06	0.64
1:K:26:LEU:HB2	1:K:124:LEU:CD1	2.27	0.64
1:A:285:ARG:NE	2:A:508:HOH:O	2.29	0.64
1:D:30:LEU:CD1	2:D:516:HOH:O	2.44	0.64
1:G:403:ILE:O	1:G:404:ARG:HB2	1.95	0.64
1:J:171:ASN:ND2	2:J:586:HOH:O	2.16	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:HIS:O	2:A:521:HOH:O	2.15	0.64
1:C:222:VAL:HG23	2:C:614:HOH:O	1.98	0.64
1:E:222:VAL:HG23	2:E:661:HOH:O	1.96	0.64
1:J:170:GLN:HA	2:J:521:HOH:O	1.97	0.64
1:B:385:GLN:HB2	2:B:461:HOH:O	1.97	0.64
1:C:403:ILE:O	1:C:404:ARG:HB2	1.95	0.64
1:D:148:ALA:O	2:D:520:HOH:O	2.14	0.64
1:E:101:PHE:HD2	1:E:179:GLN:HG2	1.62	0.64
1:I:426:SER:HA	2:I:548:HOH:O	1.98	0.64
1:K:17:PRO:HA	1:K:20:PHE:HB3	1.80	0.64
1:B:14:LYS:HB3	2:B:593:HOH:O	1.98	0.64
1:I:18:THR:HB	1:I:19:PRO:HD3	1.79	0.64
1:G:10:ILE:HG23	1:G:13:LEU:HD22	1.80	0.64
1:G:150:ILE:HD11	2:J:461:HOH:O	1.97	0.64
1:L:27:ALA:HB1	2:L:542:HOH:O	1.97	0.64
1:A:85:SER:HB2	1:A:238:LEU:HD12	1.80	0.64
1:A:107:GLU:HG2	2:E:570:HOH:O	1.96	0.64
1:D:26:LEU:HB2	1:D:124:LEU:CD1	2.28	0.64
1:E:225:LEU:CD1	2:E:479:HOH:O	2.45	0.64
1:J:10:ILE:HG12	1:J:13:LEU:HD22	1.79	0.64
1:L:92:PRO:O	1:L:212:LEU:HB2	1.98	0.64
2:B:478:HOH:O	1:K:312:VAL:HG11	1.97	0.64
1:C:17:PRO:HA	1:C:20:PHE:HB3	1.79	0.64
1:C:131:ARG:HG3	2:C:483:HOH:O	1.98	0.64
1:H:288:LEU:HB2	2:H:501:HOH:O	1.98	0.64
1:J:85:SER:HB2	1:J:238:LEU:HD12	1.79	0.64
1:K:85:SER:HB2	1:K:238:LEU:HD12	1.80	0.64
1:A:17:PRO:HA	1:A:20:PHE:HB3	1.79	0.64
1:A:65:ARG:HH21	1:A:255:GLU:HG3	1.63	0.64
1:B:369:ARG:HE	1:D:170:GLN:HE22	1.45	0.64
1:C:151:PRO:CA	2:C:465:HOH:O	2.44	0.64
1:C:281:GLU:OE2	2:C:466:HOH:O	2.15	0.64
1:E:98:ARG:HD2	2:H:499:HOH:O	1.97	0.64
1:J:212:LEU:HB3	2:J:434:HOH:O	1.98	0.64
1:D:258:ILE:H	1:D:258:ILE:CD1	2.07	0.64
1:F:258:ILE:H	1:F:258:ILE:CD1	2.05	0.64
1:J:131:ARG:HG3	2:J:547:HOH:O	1.96	0.64
1:J:40:GLU:CD	2:J:663:HOH:O	2.37	0.63
1:K:222:VAL:HG12	2:K:631:HOH:O	1.99	0.63
1:B:65:ARG:CZ	2:B:531:HOH:O	2.44	0.63
1:K:108:VAL:HG11	2:L:661:HOH:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:267:VAL:HG13	2:K:454:HOH:O	1.98	0.63
1:A:101:PHE:HD2	1:A:179:GLN:HG2	1.62	0.63
1:D:283:VAL:HG21	2:D:570:HOH:O	1.98	0.63
1:E:18:THR:HB	1:E:19:PRO:HD3	1.81	0.63
1:I:347:GLU:OE2	2:I:483:HOH:O	2.15	0.63
1:D:283:VAL:CG2	2:D:570:HOH:O	2.46	0.63
1:F:18:THR:HB	1:F:19:PRO:HD3	1.81	0.63
1:H:55:THR:CG2	2:H:495:HOH:O	1.90	0.63
1:J:229:PHE:CE1	2:J:630:HOH:O	2.51	0.63
1:J:403:ILE:HA	2:J:639:HOH:O	1.98	0.63
1:A:206:VAL:HA	2:A:580:HOH:O	1.98	0.63
1:B:140:LEU:HD11	2:K:467:HOH:O	1.98	0.63
1:C:230:ILE:CG1	2:C:487:HOH:O	2.42	0.63
1:L:378:ILE:HG21	2:L:518:HOH:O	1.97	0.63
1:A:360:GLU:HA	2:A:441:HOH:O	1.99	0.63
1:A:361:VAL:CB	1:A:362:PRO:HA	2.03	0.63
1:B:17:PRO:HA	1:B:20:PHE:HB3	1.79	0.63
1:D:26:LEU:HG	1:D:27:ALA:H	1.62	0.63
1:D:284:LEU:HA	2:D:529:HOH:O	1.98	0.63
1:F:351:PHE:C	2:F:614:HOH:O	2.37	0.63
1:H:221:ALA:HB1	2:H:449:HOH:O	1.98	0.63
1:J:102:LEU:HD12	2:J:574:HOH:O	1.97	0.63
1:L:102:LEU:HD12	2:L:432:HOH:O	1.97	0.63
1:A:342:TYR:HD2	2:A:500:HOH:O	1.80	0.63
1:D:17:PRO:HA	1:D:20:PHE:HB3	1.81	0.63
1:F:412:LEU:HA	2:F:673:HOH:O	1.98	0.63
1:G:123:SER:HB3	1:G:215:TYR:CE2	2.33	0.63
1:J:235:LEU:HD12	1:J:404:ARG:HD2	1.80	0.63
1:K:82:HIS:O	2:K:602:HOH:O	2.16	0.63
1:L:10:ILE:HG23	1:L:13:LEU:HD22	1.79	0.63
2:A:450:HOH:O	1:D:229:PHE:HD1	1.80	0.63
1:C:144:ARG:NH2	2:C:720:HOH:O	1.84	0.63
1:F:26:LEU:HG	1:F:27:ALA:H	1.64	0.63
1:J:137:GLU:HG3	2:J:509:HOH:O	1.99	0.63
1:K:148:ALA:HB2	2:K:612:HOH:O	1.97	0.63
1:A:209:ASP:OD1	2:A:574:HOH:O	2.15	0.63
1:E:65:ARG:HH21	1:E:255:GLU:HG3	1.63	0.63
1:J:122:LEU:HD12	2:J:561:HOH:O	1.98	0.63
1:K:110:GLY:N	2:K:554:HOH:O	2.32	0.63
1:J:101:PHE:HD2	1:J:179:GLN:HG2	1.64	0.62
1:L:18:THR:HB	1:L:19:PRO:HD3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:PHE:HD2	1:C:179:GLN:HG2	1.63	0.62
1:J:123:SER:HB3	1:J:215:TYR:CE2	2.33	0.62
1:J:406:LEU:HD21	2:J:525:HOH:O	1.98	0.62
1:C:170:GLN:HA	2:C:433:HOH:O	1.99	0.62
1:D:60:SER:HB3	2:D:561:HOH:O	1.99	0.62
1:G:218:GLN:CG	2:G:563:HOH:O	2.47	0.62
1:G:322:ALA:N	2:G:571:HOH:O	2.28	0.62
1:K:336:ILE:HG21	1:K:340:GLN:HB2	1.81	0.62
2:B:651:HOH:O	1:D:273:CYS:HA	1.97	0.62
1:C:212:LEU:HD11	2:C:498:HOH:O	1.98	0.62
1:I:130:PHE:O	1:I:131:ARG:HB2	1.99	0.62
1:C:336:ILE:HG23	2:C:587:HOH:O	1.98	0.62
2:C:532:HOH:O	1:F:151:PRO:CB	2.35	0.62
1:E:406:LEU:HD21	2:E:654:HOH:O	1.99	0.62
1:J:285:ARG:CZ	2:J:595:HOH:O	2.45	0.62
1:A:170:GLN:HA	2:A:476:HOH:O	1.99	0.62
1:C:65:ARG:HH21	1:C:255:GLU:HG3	1.63	0.62
1:C:239:LEU:CD2	2:C:450:HOH:O	2.47	0.62
1:F:285:ARG:NE	2:F:451:HOH:O	2.32	0.62
1:K:412:LEU:H	1:K:412:LEU:HD13	1.64	0.62
1:A:13:LEU:HB3	2:A:544:HOH:O	2.00	0.62
1:C:56:ARG:NH2	2:C:453:HOH:O	2.33	0.62
1:F:85:SER:HB2	1:F:238:LEU:HD12	1.82	0.62
1:I:53:TYR:OH	2:I:582:HOH:O	1.96	0.62
1:C:406:LEU:HD21	2:C:667:HOH:O	2.00	0.62
1:E:249:LEU:HA	2:E:499:HOH:O	1.99	0.62
1:H:26:LEU:HG	1:H:27:ALA:H	1.63	0.62
1:I:228:GLU:HB3	2:L:657:HOH:O	1.98	0.62
1:I:258:ILE:H	1:I:258:ILE:CD1	2.05	0.62
1:E:85:SER:HB2	1:E:238:LEU:HD12	1.81	0.62
1:I:20:PHE:HD1	2:I:486:HOH:O	1.83	0.62
1:J:212:LEU:HD21	2:J:548:HOH:O	1.99	0.62
1:J:226:ASN:ND2	2:J:620:HOH:O	2.33	0.62
2:C:720:HOH:O	1:F:404:ARG:NH2	2.33	0.62
1:D:92:PRO:N	2:D:619:HOH:O	2.33	0.62
1:D:289:PRO:HB2	2:D:483:HOH:O	1.99	0.62
1:F:127:ARG:HA	1:F:213:SER:HB3	1.82	0.62
1:G:403:ILE:HA	2:G:624:HOH:O	1.99	0.62
1:K:77:ARG:HD2	2:K:579:HOH:O	1.99	0.62
1:L:85:SER:HB2	1:L:238:LEU:HD12	1.82	0.62
1:B:73:GLU:HB2	2:B:523:HOH:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:HIS:CE1	2:C:439:HOH:O	2.52	0.61
1:D:59:SER:HB3	2:D:498:HOH:O	2.00	0.61
1:E:225:LEU:HD13	2:E:479:HOH:O	2.00	0.61
1:I:85:SER:HB2	1:I:238:LEU:HD12	1.81	0.61
1:I:222:VAL:HG21	2:I:694:HOH:O	1.99	0.61
1:B:15:ALA:HB1	2:B:532:HOH:O	2.01	0.61
1:B:86:PRO:HD3	2:B:536:HOH:O	1.99	0.61
1:G:84:ASP:HB3	1:G:265:GLU:HG3	1.81	0.61
1:G:283:VAL:HG22	2:G:614:HOH:O	1.99	0.61
1:G:286:ARG:HB3	2:G:523:HOH:O	2.00	0.61
1:I:126:GLY:O	1:I:213:SER:HB3	2.00	0.61
1:B:115:ALA:N	2:B:539:HOH:O	2.32	0.61
1:F:17:PRO:HA	1:F:20:PHE:HB3	1.80	0.61
1:F:84:ASP:HB3	1:F:265:GLU:HG3	1.83	0.61
1:J:18:THR:HB	1:J:19:PRO:HD3	1.82	0.61
1:K:64:ILE:HG21	2:K:688:HOH:O	1.98	0.61
1:G:17:PRO:HA	1:G:20:PHE:HB3	1.82	0.61
1:G:149:VAL:HG12	1:J:113:LEU:HD11	1.83	0.61
1:I:26:LEU:HB2	1:I:124:LEU:CD1	2.31	0.61
1:I:222:VAL:CG2	2:I:617:HOH:O	2.43	0.61
1:J:50:GLY:H	1:J:66:LEU:HB2	1.66	0.61
1:D:85:SER:HB2	1:D:238:LEU:HD12	1.81	0.61
1:G:85:SER:HB2	1:G:238:LEU:HD12	1.83	0.61
1:G:284:LEU:HA	2:G:502:HOH:O	2.00	0.61
1:H:17:PRO:HA	1:H:20:PHE:HB3	1.82	0.61
1:I:406:LEU:HA	2:I:435:HOH:O	2.00	0.61
1:A:18:THR:HB	1:A:19:PRO:HD3	1.83	0.61
1:B:65:ARG:HH21	1:B:255:GLU:HG3	1.64	0.61
1:C:18:THR:HB	1:C:19:PRO:HD3	1.81	0.61
1:A:181:ALA:HB3	2:A:661:HOH:O	2.00	0.61
1:A:395:LEU:HD22	1:A:411:ASP:HB3	1.83	0.61
1:B:26:LEU:HB2	1:B:124:LEU:CD1	2.31	0.61
1:B:85:SER:HB2	1:B:238:LEU:HD12	1.83	0.61
1:C:264:HIS:CD2	2:C:551:HOH:O	2.54	0.61
1:D:18:THR:HB	1:D:19:PRO:HD3	1.82	0.61
1:E:170:GLN:HE22	1:I:369:ARG:HE	1.48	0.61
1:B:18:THR:HB	1:B:19:PRO:HD3	1.82	0.61
1:B:395:LEU:HD22	1:B:411:ASP:HB3	1.83	0.61
1:H:18:THR:HB	1:H:19:PRO:HD3	1.82	0.61
1:F:406:LEU:N	2:F:481:HOH:O	2.29	0.61
1:I:39:ASP:CG	2:I:542:HOH:O	2.39	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:395:LEU:HD22	1:I:411:ASP:HB3	1.83	0.61
1:L:242:HIS:HD2	1:L:306:ALA:HB1	1.65	0.61
1:B:65:ARG:CG	2:B:608:HOH:O	2.45	0.61
1:C:267:VAL:HG12	2:C:568:HOH:O	1.99	0.61
1:F:229:PHE:CD2	2:F:611:HOH:O	2.37	0.61
2:F:638:HOH:O	1:H:107:GLU:HG2	2.01	0.61
1:G:18:THR:HB	1:G:19:PRO:HD3	1.82	0.61
1:J:287:LEU:N	2:J:602:HOH:O	2.12	0.61
1:K:50:GLY:H	1:K:66:LEU:HB2	1.66	0.61
1:K:127:ARG:NH2	2:K:500:HOH:O	2.33	0.61
1:F:13:LEU:CG	2:F:655:HOH:O	2.45	0.60
1:G:180:LEU:N	2:G:454:HOH:O	2.33	0.60
1:B:314:PRO:HG3	2:K:499:HOH:O	2.02	0.60
1:C:167:ILE:HD11	2:C:662:HOH:O	2.01	0.60
1:C:406:LEU:N	2:C:451:HOH:O	2.30	0.60
1:D:326:PRO:HA	2:D:578:HOH:O	2.01	0.60
1:F:348:THR:HG23	1:F:391:VAL:HG22	1.84	0.60
1:H:88:LEU:HD23	1:H:106:VAL:HG21	1.83	0.60
1:I:150:ILE:C	1:I:152:ASN:H	2.04	0.60
1:K:403:ILE:HG23	2:K:541:HOH:O	2.00	0.60
1:A:323:ASN:CB	2:A:619:HOH:O	1.86	0.60
1:C:85:SER:HB2	1:C:238:LEU:HD12	1.83	0.60
1:C:150:ILE:C	1:C:152:ASN:H	2.04	0.60
2:C:532:HOH:O	1:F:151:PRO:CA	2.48	0.60
1:F:56:ARG:NH2	2:F:501:HOH:O	2.34	0.60
1:G:127:ARG:NH2	2:G:481:HOH:O	2.35	0.60
2:A:430:HOH:O	1:E:322:ALA:HB1	2.01	0.60
1:D:395:LEU:HD22	1:D:411:ASP:HB3	1.82	0.60
1:F:65:ARG:HH21	1:F:255:GLU:HG3	1.64	0.60
1:A:228:GLU:O	2:A:455:HOH:O	2.16	0.60
2:A:481:HOH:O	1:D:144:ARG:CB	2.50	0.60
1:B:26:LEU:HG	1:B:27:ALA:H	1.66	0.60
1:B:151:PRO:CA	2:B:633:HOH:O	2.48	0.60
1:C:222:VAL:CG2	2:C:614:HOH:O	2.49	0.60
1:F:26:LEU:HB2	1:F:124:LEU:CD1	2.32	0.60
1:H:111:GLY:HA2	2:H:458:HOH:O	2.00	0.60
1:H:360:GLU:HA	2:H:459:HOH:O	2.01	0.60
1:J:137:GLU:HB3	2:J:563:HOH:O	2.00	0.60
1:J:395:LEU:HD22	1:J:411:ASP:HB3	1.84	0.60
1:L:212:LEU:HD21	2:L:636:HOH:O	2.01	0.60
1:D:140:LEU:HD23	2:D:629:HOH:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ARG:HG2	2:E:587:HOH:O	2.02	0.60
1:G:229:PHE:HD1	2:J:443:HOH:O	1.83	0.60
1:A:225:LEU:CD2	2:A:640:HOH:O	2.43	0.60
1:D:389:ARG:NH1	2:D:651:HOH:O	2.34	0.60
1:E:150:ILE:C	1:E:152:ASN:H	2.04	0.60
1:F:286:ARG:HA	2:F:576:HOH:O	1.99	0.60
2:G:591:HOH:O	1:J:167:ILE:CD1	2.27	0.60
1:I:170:GLN:HA	2:I:458:HOH:O	2.02	0.60
1:H:85:SER:HB2	1:H:238:LEU:HD12	1.83	0.60
1:I:84:ASP:HB3	1:I:265:GLU:HG3	1.84	0.60
1:L:57:ASN:ND2	2:L:623:HOH:O	2.34	0.60
1:L:331:GLY:HA3	2:L:579:HOH:O	2.01	0.60
1:D:130:PHE:O	1:D:131:ARG:HB2	2.01	0.60
1:F:170:GLN:HE22	1:G:369:ARG:HE	1.48	0.60
1:G:16:SER:H	1:G:17:PRO:HD2	1.67	0.60
1:I:86:PRO:HD3	2:I:600:HOH:O	2.01	0.60
1:I:139:ARG:NH1	2:I:564:HOH:O	2.34	0.60
1:I:241:CYS:SG	2:I:573:HOH:O	2.56	0.60
1:L:284:LEU:HA	2:L:487:HOH:O	2.01	0.60
1:B:131:ARG:HG3	2:B:438:HOH:O	2.00	0.59
1:C:265:GLU:O	1:C:266:GLU:HB2	2.02	0.59
1:D:150:ILE:C	1:D:152:ASN:H	2.04	0.59
1:E:130:PHE:O	1:E:131:ARG:HB2	2.01	0.59
1:H:349:ALA:HB2	2:H:617:HOH:O	2.01	0.59
1:A:180:LEU:O	2:A:460:HOH:O	2.15	0.59
1:I:397:THR:OG1	2:I:432:HOH:O	2.16	0.59
1:L:235:LEU:HD12	1:L:404:ARG:HD2	1.84	0.59
1:C:92:PRO:O	1:C:212:LEU:HB2	2.03	0.59
1:D:84:ASP:HB3	1:D:265:GLU:HG3	1.83	0.59
1:E:84:ASP:HB3	1:E:265:GLU:HG3	1.83	0.59
1:I:122:LEU:HD23	1:I:140:LEU:O	2.01	0.59
1:J:370:SER:HB3	2:J:465:HOH:O	2.01	0.59
1:K:385:GLN:HB2	2:K:458:HOH:O	2.01	0.59
1:B:167:ILE:HA	2:B:551:HOH:O	2.01	0.59
1:C:126:GLY:O	1:C:213:SER:HB3	2.02	0.59
1:E:348:THR:HG23	1:E:391:VAL:HG22	1.83	0.59
1:F:91:LYS:HE2	2:F:519:HOH:O	2.02	0.59
1:F:123:SER:HB3	1:F:215:TYR:CE2	2.37	0.59
1:H:389:ARG:CZ	2:H:550:HOH:O	2.50	0.59
1:H:395:LEU:HD22	1:H:411:ASP:HB3	1.83	0.59
1:J:84:ASP:HB3	1:J:265:GLU:HG3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:LYS:NZ	2:B:533:HOH:O	2.27	0.59
1:C:230:ILE:HG12	2:C:487:HOH:O	2.01	0.59
1:H:77:ARG:NH1	2:H:558:HOH:O	2.08	0.59
1:I:10:ILE:CG2	2:I:585:HOH:O	2.45	0.59
1:J:180:LEU:HB2	2:J:654:HOH:O	2.01	0.59
1:B:149:VAL:HG12	1:K:113:LEU:HD11	1.83	0.59
1:G:171:ASN:ND2	2:G:660:HOH:O	1.95	0.59
1:I:264:HIS:HE1	2:I:596:HOH:O	1.84	0.59
1:A:171:ASN:ND2	2:A:585:HOH:O	2.35	0.59
2:A:450:HOH:O	1:D:229:PHE:CD1	2.51	0.59
1:D:66:LEU:HA	1:D:258:ILE:HG22	1.85	0.59
1:D:403:ILE:HG23	2:D:634:HOH:O	2.03	0.59
1:G:268:GLY:HA3	2:G:433:HOH:O	2.02	0.59
2:A:527:HOH:O	1:I:278:PRO:HG2	2.02	0.59
1:C:235:LEU:HD12	1:C:404:ARG:HD2	1.84	0.59
1:D:406:LEU:CA	2:D:485:HOH:O	2.37	0.59
1:F:342:TYR:CD2	2:F:597:HOH:O	2.48	0.59
1:L:324:HIS:NE2	2:L:612:HOH:O	2.19	0.59
1:F:150:ILE:C	1:F:152:ASN:H	2.05	0.59
1:G:300:ARG:HD3	2:G:659:HOH:O	2.01	0.59
1:H:323:ASN:N	2:H:513:HOH:O	2.35	0.59
1:J:181:ALA:HB3	2:J:612:HOH:O	2.03	0.59
1:J:212:LEU:HD11	2:J:488:HOH:O	2.02	0.59
1:A:171:ASN:HB2	2:A:657:HOH:O	2.02	0.59
1:C:86:PRO:HD3	2:C:566:HOH:O	2.02	0.59
1:G:395:LEU:HD22	1:G:411:ASP:HB3	1.84	0.59
1:K:150:ILE:C	1:K:152:ASN:H	2.07	0.59
1:B:66:LEU:HA	1:B:258:ILE:HG22	1.84	0.58
1:H:84:ASP:HB3	1:H:265:GLU:HG3	1.84	0.58
2:A:447:HOH:O	1:I:56:ARG:HD2	2.03	0.58
1:C:395:LEU:HD22	1:C:411:ASP:HB3	1.85	0.58
1:F:395:LEU:HD22	1:F:411:ASP:HB3	1.85	0.58
1:A:150:ILE:C	1:A:152:ASN:H	2.07	0.58
1:E:235:LEU:HD12	1:E:404:ARG:HD2	1.86	0.58
1:E:395:LEU:HD22	1:E:411:ASP:HB3	1.84	0.58
1:G:150:ILE:C	1:G:152:ASN:H	2.07	0.58
1:G:351:PHE:C	2:G:569:HOH:O	2.41	0.58
1:H:26:LEU:HB2	1:H:124:LEU:CD1	2.34	0.58
1:I:37:ARG:HG2	2:I:553:HOH:O	2.03	0.58
1:I:265:GLU:O	1:I:266:GLU:HB2	2.03	0.58
1:J:150:ILE:C	1:J:152:ASN:H	2.06	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:289:PRO:HB2	2:L:570:HOH:O	2.03	0.58
1:B:285:ARG:HD3	2:B:610:HOH:O	2.04	0.58
1:E:51:ARG:HB2	2:E:513:HOH:O	2.02	0.58
1:F:377:THR:HG22	2:F:567:HOH:O	2.02	0.58
1:G:218:GLN:HB2	2:G:679:HOH:O	2.02	0.58
1:I:212:LEU:N	2:I:601:HOH:O	2.34	0.58
1:J:265:GLU:O	1:J:266:GLU:HB2	2.03	0.58
1:L:385:GLN:HB2	2:L:489:HOH:O	2.02	0.58
1:E:265:GLU:O	1:E:266:GLU:HB2	2.02	0.58
1:G:38:LEU:HD21	1:G:63:ALA:HB2	1.85	0.58
1:G:66:LEU:HA	1:G:258:ILE:HG22	1.85	0.58
1:G:92:PRO:O	1:G:212:LEU:HB2	2.04	0.58
1:K:30:LEU:CD2	2:K:620:HOH:O	2.51	0.58
1:A:84:ASP:HB3	1:A:265:GLU:HG3	1.86	0.58
1:B:84:ASP:HB3	1:B:265:GLU:HG3	1.85	0.58
1:C:113:LEU:HD11	1:F:149:VAL:HG12	1.86	0.58
1:F:88:LEU:HD23	1:F:106:VAL:HG21	1.86	0.58
1:H:16:SER:H	1:H:17:PRO:HD2	1.69	0.58
2:I:480:HOH:O	1:L:314:PRO:HG3	2.04	0.58
1:K:39:ASP:HA	2:K:472:HOH:O	2.02	0.58
1:A:117:TRP:O	1:A:118:PHE:HB2	2.04	0.58
1:B:26:LEU:HB2	1:B:124:LEU:HD12	1.86	0.58
1:D:30:LEU:HD13	2:D:516:HOH:O	2.03	0.58
1:F:265:GLU:O	1:F:266:GLU:HB2	2.02	0.58
1:K:168:ASN:ND2	2:K:524:HOH:O	2.36	0.58
1:L:406:LEU:HA	2:L:446:HOH:O	2.04	0.58
2:B:573:HOH:O	1:C:322:ALA:CB	2.36	0.58
1:E:394:GLY:HA3	2:E:529:HOH:O	2.04	0.58
1:K:79:VAL:HG22	2:K:624:HOH:O	2.04	0.58
1:A:406:LEU:HA	2:A:565:HOH:O	2.03	0.58
1:C:122:LEU:HD11	1:C:139:ARG:H	1.69	0.58
1:F:171:ASN:CG	2:F:524:HOH:O	2.43	0.58
1:H:150:ILE:C	1:H:152:ASN:H	2.07	0.58
1:H:151:PRO:HD3	2:H:505:HOH:O	2.02	0.58
1:J:377:THR:HG22	2:J:591:HOH:O	2.02	0.58
1:G:150:ILE:O	1:G:152:ASN:N	2.33	0.57
1:G:230:ILE:CD1	2:G:662:HOH:O	2.51	0.57
1:J:322:ALA:HB1	2:L:480:HOH:O	2.04	0.57
1:B:16:SER:H	1:B:17:PRO:HD2	1.68	0.57
1:F:312:VAL:HA	2:F:503:HOH:O	2.03	0.57
1:F:366:PHE:HZ	2:F:638:HOH:O	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:LEU:HD11	2:G:645:HOH:O	2.03	0.57
1:J:374:CYS:HA	2:J:478:HOH:O	2.03	0.57
1:A:242:HIS:HD2	1:A:306:ALA:HB1	1.69	0.57
1:C:226:ASN:ND2	2:C:586:HOH:O	2.36	0.57
1:D:73:GLU:HB2	2:D:478:HOH:O	2.04	0.57
1:L:150:ILE:C	1:L:152:ASN:H	2.08	0.57
1:A:373:GLY:HA2	2:A:571:HOH:O	2.04	0.57
1:B:122:LEU:HD11	1:B:139:ARG:H	1.69	0.57
1:H:205:ASP:HB3	2:H:649:HOH:O	2.03	0.57
1:K:395:LEU:HD22	1:K:411:ASP:HB3	1.87	0.57
1:L:357:GLN:OE1	2:L:474:HOH:O	2.17	0.57
1:C:268:GLY:HA3	2:C:566:HOH:O	2.05	0.57
1:E:122:LEU:HD23	1:E:140:LEU:O	2.04	0.57
1:G:130:PHE:O	1:G:131:ARG:HB2	2.04	0.57
1:G:414:HIS:HB3	2:G:666:HOH:O	2.03	0.57
1:A:39:ASP:OD1	2:A:617:HOH:O	2.18	0.57
1:B:170:GLN:HA	2:B:506:HOH:O	2.04	0.57
1:C:65:ARG:CG	2:C:496:HOH:O	2.30	0.57
1:E:313:HIS:HD1	1:E:315:ASN:H	1.52	0.57
1:G:182:PRO:HB3	2:G:631:HOH:O	2.04	0.57
1:H:92:PRO:O	1:H:212:LEU:HB2	2.03	0.57
1:K:283:VAL:O	2:K:688:HOH:O	2.17	0.57
1:D:167:ILE:HG21	2:D:576:HOH:O	2.04	0.57
1:D:317:ALA:HB1	2:D:607:HOH:O	2.05	0.57
1:G:265:GLU:O	1:G:266:GLU:HB2	2.02	0.57
1:H:385:GLN:HB2	2:H:440:HOH:O	2.04	0.57
1:J:26:LEU:HB2	1:J:124:LEU:CD1	2.34	0.57
1:A:26:LEU:HB2	1:A:124:LEU:CD1	2.34	0.57
2:C:486:HOH:O	1:F:229:PHE:CE1	2.55	0.57
1:J:122:LEU:HD23	1:J:140:LEU:O	2.04	0.57
1:K:242:HIS:HD2	1:K:306:ALA:HB1	1.70	0.57
1:B:122:LEU:HD23	1:B:140:LEU:O	2.05	0.57
1:C:391:VAL:HA	2:C:612:HOH:O	2.03	0.57
1:F:395:LEU:HD12	2:F:554:HOH:O	2.04	0.57
1:I:122:LEU:HD12	2:I:609:HOH:O	2.05	0.57
1:K:288:LEU:HB2	2:K:564:HOH:O	2.04	0.57
1:C:16:SER:H	1:C:17:PRO:HD2	1.69	0.57
1:F:283:VAL:HG23	2:F:542:HOH:O	2.04	0.57
1:J:82:HIS:C	2:J:510:HOH:O	2.31	0.57
1:A:320:HIS:ND1	2:A:678:HOH:O	2.33	0.56
1:B:130:PHE:O	2:B:589:HOH:O	2.17	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:C	1:B:152:ASN:H	2.08	0.56
1:F:66:LEU:HA	1:F:258:ILE:HG22	1.87	0.56
1:G:113:LEU:HD11	1:J:149:VAL:HG12	1.87	0.56
1:I:16:SER:H	1:I:17:PRO:HD2	1.69	0.56
1:I:242:HIS:HD2	1:I:306:ALA:HB1	1.70	0.56
1:I:258:ILE:HD13	1:I:258:ILE:N	2.14	0.56
1:I:319:ARG:NH2	2:I:648:HOH:O	2.37	0.56
1:K:181:ALA:CB	2:K:550:HOH:O	1.96	0.56
1:L:395:LEU:HD22	1:L:411:ASP:HB3	1.87	0.56
1:L:398:PHE:HB2	2:L:697:HOH:O	2.05	0.56
1:C:290:GLU:HG3	2:C:615:HOH:O	2.04	0.56
1:H:150:ILE:O	1:H:152:ASN:N	2.35	0.56
1:L:151:PRO:CA	2:L:516:HOH:O	2.53	0.56
1:C:170:GLN:HE22	1:D:369:ARG:HE	1.53	0.56
1:C:242:HIS:HD2	1:C:306:ALA:HB1	1.70	0.56
1:D:265:GLU:HB2	2:D:498:HOH:O	2.04	0.56
1:E:66:LEU:HA	1:E:258:ILE:HG22	1.86	0.56
1:G:26:LEU:HB2	1:G:124:LEU:CD1	2.34	0.56
1:G:122:LEU:HD11	1:G:139:ARG:H	1.69	0.56
1:H:120:ARG:HD3	2:H:626:HOH:O	2.06	0.56
1:H:242:HIS:HD2	1:H:306:ALA:HB1	1.70	0.56
1:H:265:GLU:O	1:H:266:GLU:HB2	2.04	0.56
1:I:90:VAL:CG2	2:I:583:HOH:O	2.51	0.56
1:I:295:SER:HA	2:I:565:HOH:O	2.05	0.56
1:I:348:THR:HG23	1:I:391:VAL:HG22	1.87	0.56
1:J:16:SER:H	1:J:17:PRO:HD2	1.71	0.56
1:J:117:TRP:O	1:J:118:PHE:HB2	2.06	0.56
1:J:122:LEU:HD11	1:J:139:ARG:H	1.70	0.56
1:K:268:GLY:HA3	2:K:455:HOH:O	2.04	0.56
1:L:38:LEU:HD21	1:L:63:ALA:HB2	1.88	0.56
1:L:84:ASP:HB3	1:L:265:GLU:HG3	1.87	0.56
1:D:38:LEU:HD21	1:D:63:ALA:HB2	1.86	0.56
1:E:16:SER:H	1:E:17:PRO:HD2	1.69	0.56
1:J:40:GLU:OE1	2:J:663:HOH:O	2.18	0.56
1:B:77:ARG:HG2	2:B:611:HOH:O	2.05	0.56
1:B:249:LEU:HB3	1:B:423:TYR:HE2	1.70	0.56
1:D:265:GLU:O	1:D:266:GLU:HB2	2.04	0.56
1:F:16:SER:H	1:F:17:PRO:HD2	1.70	0.56
1:I:378:ILE:HG22	2:I:691:HOH:O	2.02	0.56
1:J:26:LEU:H	1:J:29:ARG:HB2	1.70	0.56
1:L:26:LEU:HB2	1:L:124:LEU:CD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:213:SER:O	1:L:214:PHE:HB2	2.04	0.56
1:A:16:SER:H	1:A:17:PRO:HD2	1.71	0.56
1:A:66:LEU:HA	1:A:258:ILE:HG22	1.86	0.56
1:B:115:ALA:O	2:B:539:HOH:O	2.18	0.56
1:C:167:ILE:HD13	2:C:634:HOH:O	2.06	0.56
1:D:30:LEU:HD11	2:D:516:HOH:O	2.04	0.56
1:I:66:LEU:HA	1:I:258:ILE:HG22	1.88	0.56
1:A:113:LEU:HD11	1:D:149:VAL:HG12	1.88	0.56
1:A:265:GLU:O	1:A:266:GLU:HB2	2.06	0.56
1:B:251:ALA:HB1	2:B:494:HOH:O	2.05	0.56
1:C:50:GLY:H	1:C:66:LEU:HB2	1.70	0.56
1:D:406:LEU:N	2:D:485:HOH:O	2.34	0.56
1:E:113:LEU:HD11	1:H:149:VAL:HG12	1.88	0.56
1:E:327:ALA:HB2	2:E:463:HOH:O	2.05	0.56
2:F:670:HOH:O	1:G:336:ILE:HG23	2.04	0.56
1:B:369:ARG:HE	1:D:170:GLN:NE2	2.04	0.56
1:B:413:ALA:HB1	2:B:465:HOH:O	2.05	0.56
1:C:56:ARG:HD2	2:D:523:HOH:O	2.05	0.56
1:C:412:LEU:H	1:C:412:LEU:HD13	1.71	0.56
2:C:485:HOH:O	1:D:322:ALA:HB1	2.05	0.56
1:E:88:LEU:HD23	1:E:106:VAL:HG21	1.87	0.56
1:E:171:ASN:HB2	2:E:647:HOH:O	2.06	0.56
1:E:385:GLN:HB2	2:E:516:HOH:O	2.05	0.56
1:F:92:PRO:O	1:F:212:LEU:HB2	2.05	0.56
1:G:317:ALA:CB	2:J:549:HOH:O	2.41	0.56
1:I:124:LEU:O	1:I:125:ALA:CB	2.54	0.56
1:J:369:ARG:HE	1:L:170:GLN:HE22	1.52	0.56
1:A:66:LEU:CD1	2:A:652:HOH:O	2.43	0.56
1:A:92:PRO:O	1:A:212:LEU:HB2	2.06	0.56
1:C:66:LEU:HA	1:C:258:ILE:HG22	1.87	0.56
1:C:149:VAL:HG12	1:F:113:LEU:HD11	1.88	0.56
1:D:124:LEU:O	1:D:125:ALA:CB	2.54	0.56
1:D:154:ASN:HB3	2:D:611:HOH:O	2.04	0.56
1:E:26:LEU:H	1:E:29:ARG:HB2	1.69	0.56
1:I:313:HIS:HD1	1:I:315:ASN:H	1.53	0.56
1:K:178:ALA:HA	2:K:642:HOH:O	2.06	0.56
1:K:265:GLU:O	1:K:266:GLU:HB2	2.05	0.56
1:B:113:LEU:HD11	1:K:149:VAL:HG12	1.87	0.55
1:C:26:LEU:H	1:C:29:ARG:HB2	1.71	0.55
1:D:16:SER:H	1:D:17:PRO:HD2	1.71	0.55
1:D:126:GLY:HA3	2:D:552:HOH:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:112:ALA:HB1	2:K:465:HOH:O	2.05	0.55
1:B:140:LEU:CD1	2:K:467:HOH:O	2.51	0.55
1:C:122:LEU:HD23	1:C:140:LEU:O	2.05	0.55
1:D:336:ILE:HD12	1:D:342:TYR:CZ	2.42	0.55
1:E:242:HIS:HD2	1:E:306:ALA:HB1	1.72	0.55
1:F:307:ASP:CG	1:F:308:ASN:H	2.10	0.55
1:G:56:ARG:HA	2:H:583:HOH:O	2.05	0.55
1:G:94:PRO:HA	2:G:509:HOH:O	2.05	0.55
1:H:122:LEU:HD23	1:H:140:LEU:O	2.05	0.55
1:I:379:GLY:HA3	2:I:596:HOH:O	2.06	0.55
1:J:26:LEU:HB2	1:J:124:LEU:HD12	1.87	0.55
1:L:16:SER:H	1:L:17:PRO:HD2	1.71	0.55
1:B:342:TYR:HA	2:B:527:HOH:O	2.05	0.55
1:C:124:LEU:O	1:C:125:ALA:CB	2.54	0.55
1:C:351:PHE:HA	2:C:631:HOH:O	2.07	0.55
1:G:21:HIS:HE1	1:G:234:ARG:HH11	1.54	0.55
1:I:318:ASP:OD1	2:I:454:HOH:O	2.18	0.55
1:L:26:LEU:H	1:L:29:ARG:HB2	1.72	0.55
1:A:122:LEU:HD23	1:A:140:LEU:O	2.06	0.55
1:A:348:THR:HG23	1:A:391:VAL:HG22	1.89	0.55
1:B:228:GLU:O	2:B:431:HOH:O	2.18	0.55
1:E:320:HIS:HB3	2:E:510:HOH:O	2.05	0.55
1:G:137:GLU:HB3	2:G:539:HOH:O	2.05	0.55
1:I:116:PRO:HD2	2:I:687:HOH:O	2.05	0.55
1:K:38:LEU:HD21	1:K:63:ALA:HB2	1.88	0.55
1:K:88:LEU:HD23	1:K:106:VAL:HG21	1.88	0.55
1:K:124:LEU:O	1:K:125:ALA:HB3	2.06	0.55
1:L:124:LEU:O	1:L:125:ALA:CB	2.54	0.55
1:A:378:ILE:HG22	2:A:614:HOH:O	2.06	0.55
1:B:242:HIS:HD2	1:B:306:ALA:HB1	1.70	0.55
1:C:92:PRO:N	2:C:572:HOH:O	2.38	0.55
1:C:150:ILE:O	1:C:152:ASN:N	2.37	0.55
1:C:336:ILE:HD12	1:C:342:TYR:CZ	2.42	0.55
1:E:140:LEU:HD23	2:E:659:HOH:O	2.06	0.55
1:E:212:LEU:CD2	2:E:528:HOH:O	2.28	0.55
1:H:307:ASP:CG	1:H:308:ASN:H	2.09	0.55
1:I:38:LEU:HD21	1:I:63:ALA:HB2	1.87	0.55
1:J:205:ASP:HA	2:J:610:HOH:O	2.07	0.55
1:J:206:VAL:HA	2:J:641:HOH:O	2.06	0.55
1:L:66:LEU:HA	1:L:258:ILE:HG22	1.88	0.55
1:L:88:LEU:HD23	1:L:106:VAL:HG21	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:PHE:O	1:A:131:ARG:HB2	2.06	0.55
1:H:38:LEU:HD21	1:H:63:ALA:HB2	1.89	0.55
1:I:274:GLY:O	2:I:436:HOH:O	2.18	0.55
1:J:242:HIS:HD2	1:J:306:ALA:HB1	1.72	0.55
1:A:374:CYS:HA	2:A:472:HOH:O	2.06	0.55
1:A:374:CYS:HB2	2:D:654:HOH:O	2.03	0.55
1:B:336:ILE:HD12	1:B:342:TYR:CE1	2.42	0.55
1:C:117:TRP:O	1:C:118:PHE:HB2	2.06	0.55
1:C:348:THR:HG23	1:C:391:VAL:HG22	1.88	0.55
1:D:179:GLN:N	2:D:440:HOH:O	2.38	0.55
1:D:295:SER:HB3	2:D:501:HOH:O	2.07	0.55
1:D:348:THR:HG23	1:D:391:VAL:HG22	1.88	0.55
1:E:122:LEU:HD11	1:E:139:ARG:H	1.72	0.55
1:E:131:ARG:HB2	2:E:539:HOH:O	2.05	0.55
1:G:124:LEU:O	1:G:125:ALA:CB	2.54	0.55
1:H:117:TRP:O	1:H:118:PHE:HB2	2.06	0.55
1:H:170:GLN:HA	2:H:483:HOH:O	2.07	0.55
1:H:258:ILE:HD13	1:H:258:ILE:N	2.14	0.55
1:H:378:ILE:HG22	2:H:546:HOH:O	2.06	0.55
1:I:26:LEU:H	1:I:29:ARG:HB2	1.72	0.55
1:J:284:LEU:HD11	2:J:638:HOH:O	2.07	0.55
1:B:92:PRO:O	1:B:212:LEU:HB2	2.07	0.55
1:B:180:LEU:O	2:B:459:HOH:O	2.18	0.55
1:E:124:LEU:O	1:E:125:ALA:CB	2.54	0.55
1:F:322:ALA:N	2:F:568:HOH:O	2.39	0.55
1:H:235:LEU:HD12	1:H:404:ARG:HD2	1.89	0.55
1:K:336:ILE:HD12	1:K:342:TYR:CE1	2.42	0.55
1:B:344:THR:HA	1:B:348:THR:HG21	1.89	0.55
1:D:122:LEU:HD11	1:D:139:ARG:H	1.72	0.55
1:D:364:GLN:HB2	2:D:556:HOH:O	2.06	0.55
1:E:169:ALA:CB	2:I:535:HOH:O	2.42	0.55
1:F:124:LEU:O	1:F:125:ALA:CB	2.54	0.55
1:L:265:GLU:O	1:L:266:GLU:HB2	2.06	0.55
1:A:171:ASN:HB2	2:A:585:HOH:O	2.06	0.55
1:D:123:SER:HB3	1:D:215:TYR:HE2	1.72	0.55
1:D:210:TYR:HA	1:D:212:LEU:HD12	1.88	0.55
1:E:336:ILE:HD12	1:E:342:TYR:CZ	2.42	0.55
1:G:229:PHE:CD1	2:J:443:HOH:O	2.53	0.55
1:G:307:ASP:CG	1:G:308:ASN:H	2.10	0.55
1:K:66:LEU:HA	1:K:258:ILE:HG22	1.89	0.55
2:B:663:HOH:O	1:K:150:ILE:HD11	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HB2	1:C:124:LEU:CD1	2.37	0.54
1:D:122:LEU:HD23	1:D:140:LEU:O	2.05	0.54
1:F:122:LEU:HD11	1:F:139:ARG:H	1.72	0.54
1:H:66:LEU:HA	1:H:258:ILE:HG22	1.88	0.54
1:H:336:ILE:HD12	1:H:342:TYR:CZ	2.42	0.54
1:B:131:ARG:NH2	2:B:546:HOH:O	2.40	0.54
1:E:346:SER:CB	2:E:569:HOH:O	2.54	0.54
1:G:26:LEU:H	1:G:29:ARG:HB2	1.73	0.54
1:G:170:GLN:HE22	1:H:369:ARG:HE	1.55	0.54
1:J:124:LEU:O	1:J:125:ALA:CB	2.55	0.54
1:K:16:SER:H	1:K:17:PRO:HD2	1.71	0.54
1:L:144:ARG:NH2	2:L:451:HOH:O	2.28	0.54
1:A:50:GLY:H	1:A:66:LEU:HB2	1.71	0.54
1:B:88:LEU:HD23	1:B:106:VAL:HG21	1.88	0.54
1:F:336:ILE:HD12	1:F:342:TYR:CZ	2.42	0.54
1:K:230:ILE:HD13	2:K:533:HOH:O	1.96	0.54
1:L:336:ILE:HD12	1:L:342:TYR:CZ	2.43	0.54
1:C:260:VAL:CG1	2:C:555:HOH:O	2.45	0.54
1:E:150:ILE:O	1:E:152:ASN:N	2.39	0.54
1:H:346:SER:CB	2:H:485:HOH:O	2.49	0.54
1:J:336:ILE:HD12	1:J:342:TYR:CZ	2.42	0.54
1:K:117:TRP:O	1:K:118:PHE:HB2	2.07	0.54
1:L:344:THR:HA	1:L:348:THR:HG21	1.88	0.54
1:A:26:LEU:H	1:A:29:ARG:HB2	1.72	0.54
1:A:124:LEU:O	1:A:125:ALA:CB	2.55	0.54
1:A:369:ARG:HE	1:I:170:GLN:HE22	1.54	0.54
1:B:76:PHE:CA	2:B:611:HOH:O	2.55	0.54
1:B:336:ILE:HG21	1:B:340:GLN:HB2	1.88	0.54
1:D:37:ARG:HD2	2:D:588:HOH:O	2.07	0.54
1:H:124:LEU:O	1:H:125:ALA:CB	2.55	0.54
1:J:324:HIS:C	2:J:468:HOH:O	2.39	0.54
1:L:122:LEU:HD11	1:L:139:ARG:H	1.72	0.54
1:A:336:ILE:HD12	1:A:342:TYR:CZ	2.43	0.54
1:B:124:LEU:O	1:B:125:ALA:CB	2.55	0.54
1:F:117:TRP:O	1:F:118:PHE:HB2	2.07	0.54
1:I:29:ARG:NH2	2:I:682:HOH:O	2.40	0.54
1:I:322:ALA:CA	2:I:650:HOH:O	2.52	0.54
1:I:373:GLY:HA2	2:I:518:HOH:O	2.08	0.54
1:K:110:GLY:HA3	2:K:636:HOH:O	2.07	0.54
1:K:144:ARG:NH2	2:K:582:HOH:O	2.17	0.54
1:L:15:ALA:HB1	2:L:577:HOH:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:288:LEU:HD11	2:L:672:HOH:O	2.08	0.54
1:L:307:ASP:CG	1:L:308:ASN:H	2.10	0.54
1:A:170:GLN:HE22	1:E:369:ARG:HE	1.56	0.54
1:B:21:HIS:HE1	1:B:234:ARG:HH11	1.56	0.54
1:G:63:ALA:HB3	1:G:261:CYS:HB3	1.89	0.54
1:H:285:ARG:NE	2:H:448:HOH:O	2.30	0.54
1:I:305:SER:OG	1:I:392:ASP:HA	2.08	0.54
1:J:92:PRO:O	1:J:212:LEU:HB2	2.07	0.54
1:J:150:ILE:O	1:J:152:ASN:N	2.37	0.54
1:L:150:ILE:HD13	2:L:610:HOH:O	2.08	0.54
1:B:307:ASP:CG	1:B:308:ASN:H	2.10	0.54
1:B:336:ILE:HD12	1:B:342:TYR:CZ	2.42	0.54
1:C:139:ARG:NH1	2:C:517:HOH:O	2.41	0.54
1:J:66:LEU:HA	1:J:258:ILE:HG22	1.89	0.54
1:J:130:PHE:O	1:J:131:ARG:HB2	2.06	0.54
1:K:26:LEU:HD22	1:K:125:ALA:HB2	1.89	0.54
1:L:175:PRO:HD2	2:L:583:HOH:O	2.08	0.54
1:A:91:LYS:HB3	1:A:92:PRO:HD2	1.89	0.54
1:B:36:ARG:HB3	2:B:526:HOH:O	2.06	0.54
1:B:137:GLU:HB3	2:B:548:HOH:O	2.07	0.54
1:G:336:ILE:HD12	1:G:342:TYR:CZ	2.42	0.54
1:I:295:SER:HB3	2:I:602:HOH:O	2.07	0.54
1:J:170:GLN:HE22	1:K:369:ARG:HE	1.56	0.54
1:K:70:SER:HB3	2:K:666:HOH:O	2.06	0.54
1:L:130:PHE:O	1:L:131:ARG:HB2	2.08	0.54
1:B:170:GLN:HE22	1:C:369:ARG:HE	1.56	0.54
1:C:63:ALA:HB3	1:C:261:CYS:HB3	1.90	0.54
1:G:88:LEU:HD23	1:G:106:VAL:HG21	1.91	0.54
1:H:324:HIS:CD2	2:H:451:HOH:O	2.61	0.54
1:J:290:GLU:HB3	2:J:644:HOH:O	2.08	0.54
1:K:170:GLN:HE22	1:L:369:ARG:HE	1.54	0.54
1:L:49:GLY:N	2:L:434:HOH:O	2.40	0.54
1:A:38:LEU:HD21	1:A:63:ALA:HB2	1.88	0.53
1:B:76:PHE:C	2:B:611:HOH:O	2.46	0.53
1:E:80:GLY:HA2	2:E:588:HOH:O	2.07	0.53
1:E:112:ALA:O	1:E:113:LEU:HB2	2.08	0.53
1:E:117:TRP:O	1:E:118:PHE:HB2	2.08	0.53
1:F:171:ASN:CB	2:F:524:HOH:O	2.55	0.53
1:G:94:PRO:HB2	1:G:105:GLY:H	1.73	0.53
1:H:167:ILE:HG21	2:H:528:HOH:O	2.08	0.53
1:J:88:LEU:HD23	1:J:106:VAL:HG21	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:348:THR:HG23	1:J:391:VAL:HG22	1.88	0.53
1:J:361:VAL:CB	1:J:362:PRO:HA	2.03	0.53
1:L:21:HIS:HE1	1:L:234:ARG:HH11	1.54	0.53
1:L:238:LEU:HB3	2:L:598:HOH:O	2.08	0.53
1:A:117:TRP:HB2	2:A:557:HOH:O	2.08	0.53
1:D:55:THR:HG22	1:D:58:ASP:HA	1.91	0.53
1:E:36:ARG:HD3	2:E:457:HOH:O	2.07	0.53
1:G:120:ARG:HG2	2:J:498:HOH:O	2.07	0.53
1:I:117:TRP:O	1:I:118:PHE:HB2	2.08	0.53
1:I:380:PRO:HA	1:I:383:ALA:HB3	1.90	0.53
1:J:203:THR:HG22	2:J:578:HOH:O	2.08	0.53
1:J:307:ASP:CG	1:J:308:ASN:H	2.11	0.53
2:J:644:HOH:O	1:L:290:GLU:HG3	2.07	0.53
1:A:13:LEU:HD13	2:A:544:HOH:O	2.08	0.53
1:C:26:LEU:O	1:C:30:LEU:HB2	2.07	0.53
1:G:117:TRP:O	1:G:118:PHE:HB2	2.09	0.53
1:G:137:GLU:HG3	2:G:598:HOH:O	2.08	0.53
1:I:60:SER:HB3	2:I:431:HOH:O	2.08	0.53
1:A:307:ASP:CG	1:A:308:ASN:H	2.12	0.53
1:D:238:LEU:HD22	1:D:400:MET:HG3	1.91	0.53
1:E:56:ARG:NH2	2:E:508:HOH:O	2.40	0.53
1:G:278:PRO:HG2	2:H:538:HOH:O	2.08	0.53
1:I:307:ASP:CG	1:I:308:ASN:H	2.12	0.53
1:K:234:ARG:HB2	2:K:610:HOH:O	2.09	0.53
1:C:264:HIS:CE1	2:C:551:HOH:O	2.61	0.53
1:D:150:ILE:O	1:D:152:ASN:N	2.38	0.53
1:D:305:SER:OG	1:D:392:ASP:HA	2.08	0.53
1:F:63:ALA:HB3	1:F:261:CYS:HB3	1.90	0.53
1:H:26:LEU:H	1:H:29:ARG:HB2	1.73	0.53
1:I:21:HIS:HE1	1:I:234:ARG:HH11	1.56	0.53
1:I:150:ILE:O	1:I:152:ASN:N	2.39	0.53
1:J:21:HIS:HE1	1:J:234:ARG:HH11	1.57	0.53
1:K:380:PRO:HA	1:K:383:ALA:HB3	1.91	0.53
1:B:265:GLU:O	1:B:266:GLU:HB2	2.07	0.53
1:D:37:ARG:HG3	2:D:588:HOH:O	2.09	0.53
1:K:93:ASN:HB2	2:L:504:HOH:O	2.09	0.53
1:K:252:GLU:HB3	2:K:449:HOH:O	2.08	0.53
1:L:117:TRP:O	1:L:118:PHE:HB2	2.08	0.53
1:A:115:ALA:N	2:A:677:HOH:O	2.42	0.53
1:A:406:LEU:HD11	2:A:666:HOH:O	2.07	0.53
1:B:112:ALA:HB1	2:B:639:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:HIS:HB3	2:C:676:HOH:O	2.08	0.53
1:F:26:LEU:H	1:F:29:ARG:HB2	1.74	0.53
1:I:63:ALA:HB3	1:I:261:CYS:HB3	1.90	0.53
1:I:227:ASP:CG	2:I:520:HOH:O	2.46	0.53
2:B:492:HOH:O	1:K:229:PHE:HD1	1.89	0.53
1:E:21:HIS:HE1	1:E:234:ARG:HH11	1.57	0.53
1:E:92:PRO:O	1:E:212:LEU:HB2	2.09	0.53
1:E:131:ARG:NH1	2:E:496:HOH:O	2.41	0.53
1:F:57:ASN:O	2:F:463:HOH:O	2.19	0.53
1:G:305:SER:OG	1:G:392:ASP:HA	2.09	0.53
1:H:374:CYS:HB3	2:H:597:HOH:O	2.09	0.53
1:I:336:ILE:HD12	1:I:342:TYR:CZ	2.43	0.53
1:K:17:PRO:CB	2:K:644:HOH:O	2.44	0.53
1:K:389:ARG:NH2	2:K:583:HOH:O	2.41	0.53
1:L:122:LEU:HD23	1:L:140:LEU:O	2.08	0.53
1:L:205:ASP:HB3	2:L:608:HOH:O	2.08	0.53
1:B:63:ALA:HB3	1:B:261:CYS:HB3	1.91	0.53
1:C:88:LEU:HD23	1:C:106:VAL:HG21	1.91	0.53
1:H:94:PRO:HB2	1:H:105:GLY:H	1.73	0.53
1:J:320:HIS:CE1	2:J:658:HOH:O	2.62	0.53
1:A:21:HIS:HE1	1:A:234:ARG:HH11	1.57	0.53
1:A:59:SER:HB3	2:A:606:HOH:O	2.09	0.53
1:C:55:THR:CG2	2:C:490:HOH:O	2.14	0.53
1:C:406:LEU:CA	2:C:451:HOH:O	2.50	0.53
1:E:170:GLN:NE2	1:I:369:ARG:HE	2.07	0.53
1:F:38:LEU:HD21	1:F:63:ALA:HB2	1.91	0.53
1:G:55:THR:HG22	1:G:58:ASP:HA	1.91	0.53
1:H:63:ALA:HB3	1:H:261:CYS:HB3	1.90	0.53
1:I:264:HIS:HD2	2:I:436:HOH:O	1.91	0.53
1:J:116:PRO:HG3	2:J:562:HOH:O	2.09	0.53
1:K:21:HIS:HE1	1:K:234:ARG:HH11	1.57	0.53
1:K:170:GLN:HA	2:K:493:HOH:O	2.08	0.53
1:L:36:ARG:NH1	2:L:607:HOH:O	2.43	0.53
1:B:26:LEU:H	1:B:29:ARG:HB2	1.74	0.52
1:B:91:LYS:HB3	1:B:92:PRO:HD2	1.91	0.52
1:C:31:GLU:HA	2:C:530:HOH:O	2.09	0.52
1:K:26:LEU:HB2	1:K:124:LEU:HD11	1.91	0.52
1:K:264:HIS:HD2	2:K:536:HOH:O	1.90	0.52
1:B:52:TYR:HB3	2:B:636:HOH:O	2.08	0.52
1:C:110:GLY:N	2:C:583:HOH:O	2.42	0.52
1:E:233:ALA:O	2:E:590:HOH:O	2.19	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:585:HOH:O	1:H:93:ASN:HB2	2.09	0.52
1:G:242:HIS:HD2	1:G:306:ALA:HB1	1.75	0.52
1:K:26:LEU:H	1:K:29:ARG:HB2	1.74	0.52
1:K:336:ILE:HD12	1:K:342:TYR:CZ	2.45	0.52
1:L:285:ARG:CZ	2:L:503:HOH:O	2.57	0.52
1:B:426:SER:O	1:B:426:SER:CA	2.57	0.52
1:D:288:LEU:HD22	1:D:289:PRO:HD2	1.90	0.52
1:D:313:HIS:HD1	1:D:315:ASN:H	1.56	0.52
1:D:320:HIS:HD2	2:D:569:HOH:O	1.93	0.52
1:E:228:GLU:HB3	2:E:689:HOH:O	2.08	0.52
1:E:334:ILE:HD11	2:E:529:HOH:O	2.09	0.52
1:F:242:HIS:HD2	1:F:306:ALA:HB1	1.74	0.52
1:G:340:GLN:HA	2:G:678:HOH:O	2.08	0.52
1:H:234:ARG:HB3	1:H:237:ASN:HD21	1.73	0.52
1:H:336:ILE:HD12	1:H:342:TYR:CE1	2.44	0.52
1:J:270:CYS:O	1:J:271:SER:HB2	2.09	0.52
1:L:94:PRO:HB2	1:L:105:GLY:H	1.75	0.52
1:B:290:GLU:HB2	2:C:602:HOH:O	2.10	0.52
1:C:378:ILE:HG22	2:C:529:HOH:O	2.09	0.52
1:G:37:ARG:HG3	2:G:616:HOH:O	2.09	0.52
1:H:167:ILE:HG13	2:H:518:HOH:O	2.08	0.52
1:K:320:HIS:HD2	2:K:558:HOH:O	1.92	0.52
1:B:267:VAL:HG13	2:B:476:HOH:O	2.09	0.52
1:C:367:VAL:HA	2:C:658:HOH:O	2.09	0.52
1:D:125:ALA:HB3	1:D:215:TYR:HA	1.91	0.52
1:E:149:VAL:HG12	1:H:113:LEU:HD11	1.91	0.52
1:F:59:SER:HB2	2:F:650:HOH:O	2.10	0.52
1:F:92:PRO:N	2:F:543:HOH:O	2.43	0.52
1:G:55:THR:CG2	2:G:494:HOH:O	1.79	0.52
1:I:66:LEU:HD13	2:I:561:HOH:O	2.09	0.52
1:J:29:ARG:NH2	2:J:650:HOH:O	2.42	0.52
1:B:38:LEU:HD13	2:B:569:HOH:O	2.08	0.52
1:B:226:ASN:ND2	2:B:470:HOH:O	2.42	0.52
1:C:144:ARG:HB2	2:F:662:HOH:O	2.09	0.52
1:D:63:ALA:HB3	1:D:261:CYS:HB3	1.90	0.52
1:D:88:LEU:HD23	1:D:106:VAL:HG21	1.90	0.52
1:D:307:ASP:CG	1:D:308:ASN:H	2.11	0.52
1:D:380:PRO:HA	1:D:383:ALA:HB3	1.91	0.52
1:E:395:LEU:HD12	2:E:442:HOH:O	2.08	0.52
1:F:152:ASN:OD1	2:F:652:HOH:O	2.19	0.52
1:K:63:ALA:HB3	1:K:261:CYS:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ALA:CB	2:A:456:HOH:O	2.55	0.52
1:B:285:ARG:CD	2:B:610:HOH:O	2.58	0.52
1:C:21:HIS:HE1	1:C:234:ARG:HH11	1.57	0.52
1:F:150:ILE:O	1:F:152:ASN:N	2.37	0.52
1:K:150:ILE:O	1:K:152:ASN:N	2.38	0.52
1:B:51:ARG:HB2	2:B:464:HOH:O	2.09	0.52
1:C:234:ARG:HH21	1:C:412:LEU:HD12	1.75	0.52
1:C:328:LEU:HD22	2:F:633:HOH:O	2.09	0.52
1:D:94:PRO:HB2	1:D:105:GLY:H	1.74	0.52
1:F:94:PRO:HB2	1:F:105:GLY:H	1.75	0.52
1:I:122:LEU:HD11	1:I:139:ARG:H	1.75	0.52
1:L:300:ARG:NH2	2:L:519:HOH:O	2.42	0.52
1:A:14:LYS:HB3	2:A:515:HOH:O	2.10	0.52
1:A:115:ALA:HB1	2:A:594:HOH:O	2.10	0.52
1:A:151:PRO:HA	2:A:507:HOH:O	2.04	0.52
1:I:26:LEU:HB2	1:I:124:LEU:HD12	1.90	0.52
2:I:527:HOH:O	1:L:328:LEU:HD22	2.10	0.52
1:J:92:PRO:N	2:J:514:HOH:O	2.43	0.52
1:K:26:LEU:O	1:K:30:LEU:HB2	2.10	0.52
1:L:63:ALA:HB3	1:L:261:CYS:HB3	1.91	0.52
1:A:270:CYS:O	1:A:271:SER:HB2	2.10	0.52
1:D:26:LEU:O	1:D:30:LEU:HB2	2.10	0.52
2:E:511:HOH:O	1:I:322:ALA:HB1	2.09	0.52
1:I:55:THR:HG22	1:I:58:ASP:HA	1.91	0.52
1:I:149:VAL:HG12	1:L:113:LEU:HD11	1.90	0.52
1:I:336:ILE:HG21	1:I:340:GLN:HB2	1.92	0.52
1:L:49:GLY:N	2:L:477:HOH:O	2.42	0.52
1:A:55:THR:HG22	1:A:58:ASP:HA	1.92	0.51
1:A:226:ASN:ND2	2:A:601:HOH:O	2.42	0.51
1:A:238:LEU:HD22	1:A:400:MET:HG3	1.91	0.51
1:C:40:GLU:CD	2:C:616:HOH:O	2.46	0.51
1:D:26:LEU:H	1:D:29:ARG:HB2	1.75	0.51
1:D:117:TRP:O	1:D:118:PHE:HB2	2.10	0.51
1:D:212:LEU:CD1	2:D:673:HOH:O	2.54	0.51
1:D:280:LEU:CD1	2:D:631:HOH:O	2.47	0.51
1:E:26:LEU:HB2	1:E:124:LEU:CD1	2.40	0.51
1:E:26:LEU:O	1:E:30:LEU:HB2	2.09	0.51
1:E:336:ILE:HD12	1:E:342:TYR:CE1	2.45	0.51
1:F:51:ARG:NH2	2:F:556:HOH:O	2.43	0.51
1:F:380:PRO:HA	1:F:383:ALA:HB3	1.92	0.51
1:G:26:LEU:O	1:G:30:LEU:HB2	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:THR:HA	2:I:649:HOH:O	2.09	0.51
1:A:150:ILE:O	1:A:152:ASN:N	2.39	0.51
1:A:357:GLN:HA	1:A:361:VAL:HG13	1.93	0.51
1:E:346:SER:HB2	2:E:569:HOH:O	2.11	0.51
1:I:238:LEU:HD22	1:I:400:MET:HG3	1.91	0.51
1:J:17:PRO:CB	2:J:564:HOH:O	2.50	0.51
1:J:26:LEU:O	1:J:30:LEU:HB2	2.10	0.51
1:L:120:ARG:HD3	2:L:451:HOH:O	2.09	0.51
1:A:36:ARG:NH1	2:A:435:HOH:O	2.43	0.51
1:A:126:GLY:O	1:A:213:SER:HB3	2.10	0.51
1:G:258:ILE:HD13	1:G:258:ILE:N	2.13	0.51
1:I:9:LEU:O	2:I:503:HOH:O	2.19	0.51
1:J:94:PRO:HB2	1:J:105:GLY:H	1.74	0.51
2:J:465:HOH:O	1:L:170:GLN:HA	2.11	0.51
1:K:123:SER:HA	2:K:600:HOH:O	2.10	0.51
1:K:305:SER:OG	1:K:392:ASP:HA	2.10	0.51
1:L:171:ASN:CB	2:L:454:HOH:O	2.41	0.51
1:A:258:ILE:HD13	2:A:651:HOH:O	2.09	0.51
1:B:38:LEU:HD21	1:B:63:ALA:HB2	1.93	0.51
1:B:345:ASN:H	1:B:348:THR:HB	1.76	0.51
1:C:94:PRO:HB2	1:C:105:GLY:H	1.75	0.51
1:E:146:ALA:C	1:H:313:HIS:HE2	2.14	0.51
1:F:336:ILE:HD12	1:F:342:TYR:CE1	2.46	0.51
1:I:10:ILE:H	1:I:10:ILE:HD13	1.75	0.51
1:K:307:ASP:CG	1:K:308:ASN:H	2.12	0.51
1:A:26:LEU:HB2	1:A:124:LEU:HD12	1.93	0.51
1:B:94:PRO:HB2	1:B:105:GLY:H	1.76	0.51
1:E:307:ASP:CG	1:E:308:ASN:H	2.14	0.51
1:F:21:HIS:HE1	1:F:234:ARG:HH11	1.57	0.51
1:I:336:ILE:HD12	1:I:342:TYR:CE1	2.46	0.51
1:K:235:LEU:HD12	1:K:404:ARG:HD2	1.92	0.51
1:L:230:ILE:CG1	2:L:582:HOH:O	2.28	0.51
1:D:21:HIS:HE1	1:D:234:ARG:HH11	1.57	0.51
1:D:37:ARG:CD	2:D:588:HOH:O	2.58	0.51
1:D:213:SER:HA	1:D:215:TYR:HB2	1.91	0.51
1:E:380:PRO:HA	1:E:383:ALA:HB3	1.92	0.51
1:H:122:LEU:HD11	1:H:139:ARG:H	1.75	0.51
1:J:63:ALA:HB3	1:J:261:CYS:HB3	1.92	0.51
1:K:238:LEU:HD22	1:K:400:MET:HG3	1.93	0.51
1:K:348:THR:HG23	1:K:391:VAL:HG22	1.92	0.51
1:L:305:SER:OG	1:L:392:ASP:HA	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:357:GLN:HA	1:L:361:VAL:HG13	1.93	0.51
1:B:305:SER:OG	1:B:392:ASP:HA	2.11	0.51
1:F:290:GLU:HG3	2:F:495:HOH:O	2.09	0.51
1:G:56:ARG:HD2	2:H:490:HOH:O	2.10	0.51
1:I:91:LYS:HB3	1:I:92:PRO:HD2	1.93	0.51
1:K:95:GLU:HG2	2:K:592:HOH:O	2.10	0.51
1:D:336:ILE:HG21	1:D:340:GLN:HB2	1.93	0.51
1:G:55:THR:CB	2:G:494:HOH:O	2.37	0.51
1:H:49:GLY:N	2:H:475:HOH:O	2.43	0.51
1:I:264:HIS:CD2	2:I:436:HOH:O	2.63	0.51
1:I:357:GLN:HA	1:I:361:VAL:HG13	1.93	0.51
1:A:88:LEU:HD23	1:A:106:VAL:HG21	1.91	0.51
1:C:283:VAL:HG21	2:C:561:HOH:O	2.11	0.51
1:C:307:ASP:CG	1:C:308:ASN:H	2.13	0.51
1:D:242:HIS:HD2	1:D:306:ALA:HB1	1.74	0.51
1:D:284:LEU:HD11	1:D:293:ALA:HB1	1.92	0.51
1:F:55:THR:HG22	1:F:58:ASP:HA	1.93	0.51
1:G:336:ILE:HD12	1:G:342:TYR:CE1	2.46	0.51
1:H:21:HIS:HE1	1:H:234:ARG:HH11	1.57	0.51
1:H:26:LEU:HB2	1:H:124:LEU:HD12	1.93	0.51
1:H:26:LEU:O	1:H:30:LEU:HB2	2.10	0.51
1:I:113:LEU:HD11	1:L:149:VAL:HG12	1.93	0.51
1:J:91:LYS:HB3	1:J:92:PRO:HD2	1.93	0.51
1:K:94:PRO:HB2	1:K:105:GLY:H	1.76	0.51
1:L:238:LEU:HD22	1:L:400:MET:HG3	1.93	0.51
1:B:117:TRP:O	1:B:118:PHE:HB2	2.10	0.51
1:B:270:CYS:O	1:B:271:SER:HB2	2.10	0.51
1:C:357:GLN:HA	1:C:361:VAL:HG13	1.93	0.51
1:F:122:LEU:HD23	1:F:140:LEU:O	2.10	0.51
1:F:270:CYS:O	1:F:271:SER:HB2	2.11	0.51
1:G:122:LEU:HD23	1:G:140:LEU:O	2.11	0.51
1:J:336:ILE:HD12	1:J:342:TYR:CE1	2.46	0.51
1:E:270:CYS:O	1:E:271:SER:HB2	2.10	0.50
1:H:336:ILE:HG21	1:H:340:GLN:HB2	1.92	0.50
1:I:173:LEU:HD12	2:I:458:HOH:O	2.11	0.50
1:J:258:ILE:HD13	1:J:258:ILE:N	2.14	0.50
1:L:55:THR:HG22	1:L:58:ASP:HA	1.93	0.50
1:L:212:LEU:HD11	2:L:449:HOH:O	2.11	0.50
1:A:26:LEU:O	1:A:30:LEU:HB2	2.12	0.50
1:D:26:LEU:HB2	1:D:124:LEU:HD11	1.91	0.50
1:D:267:VAL:HG13	2:D:548:HOH:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:LEU:HD22	1:E:400:MET:HG3	1.93	0.50
1:H:55:THR:HG22	1:H:58:ASP:HA	1.92	0.50
1:I:229:PHE:HD1	2:L:491:HOH:O	1.93	0.50
1:I:270:CYS:O	1:I:271:SER:HB2	2.11	0.50
1:K:26:LEU:HB2	1:K:124:LEU:HD12	1.93	0.50
1:K:258:ILE:HD13	1:K:258:ILE:N	2.14	0.50
1:L:380:PRO:HA	1:L:383:ALA:HB3	1.93	0.50
1:B:212:LEU:HD23	2:B:676:HOH:O	2.10	0.50
1:E:26:LEU:HB2	1:E:124:LEU:HD12	1.94	0.50
1:E:305:SER:OG	1:E:392:ASP:HA	2.12	0.50
1:F:26:LEU:O	1:F:30:LEU:HB2	2.11	0.50
1:F:320:HIS:HA	2:F:547:HOH:O	2.11	0.50
1:J:380:PRO:HA	1:J:383:ALA:HB3	1.93	0.50
1:K:170:GLN:NE2	1:L:369:ARG:HE	2.10	0.50
1:L:150:ILE:O	1:L:152:ASN:N	2.37	0.50
1:A:49:GLY:N	2:A:438:HOH:O	2.44	0.50
1:I:94:PRO:HB2	1:I:105:GLY:H	1.77	0.50
1:K:84:ASP:HB3	1:K:265:GLU:HG3	1.94	0.50
1:A:63:ALA:HB3	1:A:261:CYS:HB3	1.93	0.50
1:D:258:ILE:HD13	1:D:258:ILE:N	2.15	0.50
1:E:383:ALA:HA	2:E:516:HOH:O	2.10	0.50
1:F:305:SER:OG	1:F:392:ASP:HA	2.12	0.50
1:H:305:SER:OG	1:H:392:ASP:HA	2.12	0.50
1:H:389:ARG:NH1	2:H:456:HOH:O	2.44	0.50
1:I:49:GLY:N	2:I:508:HOH:O	2.44	0.50
1:A:149:VAL:HG12	1:D:113:LEU:HD11	1.94	0.50
1:B:150:ILE:O	1:B:152:ASN:N	2.38	0.50
1:C:378:ILE:CG2	2:C:529:HOH:O	2.60	0.50
1:D:290:GLU:HB2	2:D:483:HOH:O	2.11	0.50
1:D:323:ASN:CB	2:D:602:HOH:O	2.43	0.50
1:E:248:LEU:HB2	2:E:577:HOH:O	2.10	0.50
1:G:173:LEU:N	1:G:174:PRO:CD	2.75	0.50
1:G:380:PRO:HA	1:G:383:ALA:HB3	1.94	0.50
1:H:79:VAL:HA	1:H:304:VAL:O	2.12	0.50
1:H:115:ALA:HB1	2:H:561:HOH:O	2.11	0.50
1:I:65:ARG:HG3	2:I:643:HOH:O	2.12	0.50
1:I:150:ILE:HD13	2:I:500:HOH:O	2.10	0.50
1:J:238:LEU:HD22	1:J:400:MET:HG3	1.94	0.50
1:L:278:PRO:HA	2:L:637:HOH:O	2.11	0.50
2:A:668:HOH:O	1:D:228:GLU:HB3	2.12	0.50
1:D:49:GLY:N	2:D:475:HOH:O	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:ARG:HD2	2:E:628:HOH:O	2.12	0.50
1:F:264:HIS:CD2	2:F:582:HOH:O	2.65	0.50
1:F:285:ARG:CZ	2:F:451:HOH:O	2.59	0.50
1:I:148:ALA:O	2:I:498:HOH:O	2.19	0.50
1:K:223:VAL:HG12	2:K:645:HOH:O	2.12	0.50
1:L:355:LEU:HG	2:L:632:HOH:O	2.12	0.50
1:C:55:THR:HG22	1:C:58:ASP:HA	1.94	0.50
1:C:380:PRO:HA	1:C:383:ALA:HB3	1.92	0.50
1:G:119:ASP:HA	2:G:440:HOH:O	2.11	0.50
1:I:26:LEU:O	1:I:30:LEU:HB2	2.12	0.50
1:L:126:GLY:O	1:L:213:SER:HB3	2.11	0.50
1:A:313:HIS:HE2	1:D:146:ALA:C	2.15	0.50
1:B:249:LEU:HD11	1:B:416:VAL:HA	1.94	0.50
1:C:84:ASP:HB3	1:C:265:GLU:HG3	1.94	0.50
1:E:173:LEU:N	1:E:174:PRO:CD	2.75	0.50
1:E:426:SER:HA	2:E:493:HOH:O	2.11	0.50
1:F:139:ARG:HD2	2:F:528:HOH:O	2.12	0.50
1:K:55:THR:HG22	1:K:58:ASP:HA	1.93	0.50
1:K:212:LEU:O	1:K:213:SER:CB	2.59	0.50
1:K:234:ARG:HB3	1:K:237:ASN:HD21	1.76	0.50
1:B:231:ALA:HB3	2:B:511:HOH:O	2.10	0.49
1:F:130:PHE:O	1:F:131:ARG:HB2	2.12	0.49
1:A:29:ARG:NH1	2:A:511:HOH:O	2.28	0.49
1:A:258:ILE:HD13	1:A:258:ILE:N	2.14	0.49
1:B:135:LYS:HD3	2:B:629:HOH:O	2.13	0.49
1:C:130:PHE:O	1:C:131:ARG:HB2	2.11	0.49
1:C:313:HIS:HE2	1:F:146:ALA:C	2.15	0.49
1:E:94:PRO:HB2	1:E:105:GLY:H	1.77	0.49
1:H:249:LEU:HD11	1:H:416:VAL:HA	1.94	0.49
1:A:336:ILE:HD12	1:A:342:TYR:CE1	2.46	0.49
1:C:170:GLN:NE2	1:D:369:ARG:HE	2.10	0.49
1:D:230:ILE:HD13	2:D:462:HOH:O	2.12	0.49
1:D:288:LEU:CD1	2:D:625:HOH:O	2.61	0.49
1:E:212:LEU:CG	2:E:528:HOH:O	2.57	0.49
1:I:79:VAL:HA	1:I:304:VAL:O	2.13	0.49
1:K:60:SER:HB3	2:K:529:HOH:O	2.11	0.49
1:K:179:GLN:N	2:K:432:HOH:O	2.34	0.49
1:L:312:VAL:HG23	2:L:599:HOH:O	2.13	0.49
1:A:39:ASP:HB2	2:A:454:HOH:O	2.11	0.49
1:D:336:ILE:HD12	1:D:342:TYR:CE1	2.47	0.49
1:D:378:ILE:O	1:D:378:ILE:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:210:TYR:HB3	2:E:535:HOH:O	2.11	0.49
1:E:366:PHE:HZ	2:E:570:HOH:O	1.95	0.49
1:H:357:GLN:HA	1:H:361:VAL:HG13	1.94	0.49
1:I:66:LEU:HB3	2:I:598:HOH:O	2.11	0.49
1:J:38:LEU:HD21	1:J:63:ALA:HB2	1.95	0.49
1:K:26:LEU:CD2	1:K:125:ALA:HB2	2.43	0.49
1:B:406:LEU:HA	2:B:513:HOH:O	2.12	0.49
1:C:270:CYS:O	1:C:271:SER:HB2	2.12	0.49
1:D:235:LEU:HD12	1:D:404:ARG:HH11	1.77	0.49
1:E:55:THR:HG22	1:E:58:ASP:HA	1.93	0.49
1:H:131:ARG:HG3	2:H:437:HOH:O	2.13	0.49
1:H:173:LEU:N	1:H:174:PRO:CD	2.75	0.49
1:H:306:ALA:HB3	2:H:664:HOH:O	2.11	0.49
1:I:417:LYS:HD2	2:I:636:HOH:O	2.11	0.49
1:K:357:GLN:HA	1:K:361:VAL:HG13	1.95	0.49
1:L:336:ILE:HD12	1:L:342:TYR:CE1	2.47	0.49
1:A:122:LEU:CD1	2:A:632:HOH:O	2.58	0.49
1:A:380:PRO:HA	1:A:383:ALA:HB3	1.94	0.49
2:A:646:HOH:O	1:D:150:ILE:CD1	2.58	0.49
1:B:55:THR:HG22	1:B:58:ASP:HA	1.93	0.49
1:C:167:ILE:HG21	2:C:634:HOH:O	2.13	0.49
1:C:173:LEU:N	1:C:174:PRO:CD	2.75	0.49
1:D:353:ARG:HD2	2:D:445:HOH:O	2.13	0.49
1:D:357:GLN:HA	1:D:361:VAL:HG13	1.94	0.49
1:F:91:LYS:HB3	1:F:92:PRO:HD2	1.95	0.49
1:G:91:LYS:HB3	1:G:92:PRO:HD2	1.94	0.49
1:H:167:ILE:CD1	2:H:518:HOH:O	2.61	0.49
1:K:270:CYS:O	1:K:271:SER:HB2	2.13	0.49
1:L:245:LEU:CA	2:L:691:HOH:O	2.60	0.49
1:A:203:THR:HA	2:A:509:HOH:O	2.12	0.49
1:B:94:PRO:HA	2:B:442:HOH:O	2.11	0.49
1:D:115:ALA:N	2:D:538:HOH:O	2.44	0.49
1:F:173:LEU:N	1:F:174:PRO:CD	2.75	0.49
1:F:369:ARG:HE	1:H:170:GLN:NE2	2.10	0.49
1:F:406:LEU:CA	2:F:481:HOH:O	2.46	0.49
1:G:65:ARG:NH2	2:G:504:HOH:O	2.45	0.49
1:H:348:THR:HG23	1:H:391:VAL:HG22	1.95	0.49
1:K:124:LEU:O	1:K:125:ALA:CB	2.60	0.49
1:K:283:VAL:HG21	2:K:545:HOH:O	2.12	0.49
1:A:336:ILE:HG21	1:A:340:GLN:HB2	1.94	0.49
1:B:380:PRO:HA	1:B:383:ALA:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ARG:NH2	2:D:591:HOH:O	2.40	0.49
1:D:124:LEU:O	1:D:125:ALA:HB3	2.13	0.49
1:D:173:LEU:N	1:D:174:PRO:CD	2.76	0.49
1:G:235:LEU:HA	1:G:404:ARG:HA	1.95	0.49
1:G:378:ILE:O	1:G:378:ILE:HG12	2.12	0.49
1:K:173:LEU:N	1:K:174:PRO:CD	2.76	0.49
1:L:345:ASN:H	1:L:348:THR:HB	1.78	0.49
1:A:94:PRO:HB2	1:A:105:GLY:H	1.77	0.49
1:E:357:GLN:HA	1:E:361:VAL:HG13	1.95	0.49
1:F:378:ILE:O	1:F:378:ILE:HG12	2.13	0.49
1:K:111:GLY:HA2	2:K:473:HOH:O	2.11	0.49
1:B:20:PHE:O	1:B:24:ALA:N	2.39	0.49
1:B:233:ALA:C	2:B:470:HOH:O	2.45	0.49
1:C:91:LYS:HB3	1:C:92:PRO:HD2	1.94	0.49
1:F:77:ARG:HD2	2:F:659:HOH:O	2.13	0.49
1:G:270:CYS:O	1:G:271:SER:HB2	2.13	0.49
1:H:139:ARG:HD3	2:H:670:HOH:O	2.11	0.49
1:J:235:LEU:HA	1:J:404:ARG:HA	1.95	0.49
1:K:92:PRO:HA	1:K:213:SER:OG	2.13	0.49
1:A:173:LEU:HD12	2:A:476:HOH:O	2.12	0.48
1:B:89:ARG:HG2	2:C:698:HOH:O	2.13	0.48
1:B:218:GLN:CG	2:B:564:HOH:O	2.35	0.48
1:B:357:GLN:HA	1:B:361:VAL:HG13	1.95	0.48
1:C:305:SER:OG	1:C:392:ASP:HA	2.12	0.48
1:C:336:ILE:HD12	1:C:342:TYR:CE1	2.47	0.48
1:C:351:PHE:CA	2:C:631:HOH:O	2.61	0.48
1:D:249:LEU:HB3	1:D:423:TYR:HE2	1.77	0.48
1:F:79:VAL:HA	1:F:304:VAL:O	2.13	0.48
1:F:235:LEU:HA	1:F:404:ARG:HA	1.95	0.48
1:G:300:ARG:NH1	2:G:507:HOH:O	2.46	0.48
1:I:66:LEU:CD1	2:I:561:HOH:O	2.59	0.48
1:K:86:PRO:HD3	2:K:455:HOH:O	2.11	0.48
1:A:122:LEU:HD11	1:A:139:ARG:H	1.77	0.48
1:D:27:ALA:HB1	2:D:498:HOH:O	2.12	0.48
1:E:51:ARG:HB3	2:E:574:HOH:O	2.13	0.48
1:H:235:LEU:HD12	1:H:404:ARG:HH11	1.78	0.48
1:H:380:PRO:HA	1:H:383:ALA:HB3	1.95	0.48
1:J:285:ARG:CD	2:J:629:HOH:O	2.60	0.48
2:J:560:HOH:O	1:K:322:ALA:HB1	2.12	0.48
1:L:122:LEU:HD22	1:L:123:SER:N	2.27	0.48
1:C:125:ALA:HB3	1:C:215:TYR:HA	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ALA:C	2:C:617:HOH:O	2.52	0.48
1:D:235:LEU:HA	1:D:404:ARG:HA	1.95	0.48
1:E:58:ASP:HB2	2:E:635:HOH:O	2.11	0.48
1:G:313:HIS:HE2	1:J:146:ALA:C	2.16	0.48
1:K:359:SER:HB3	2:K:695:HOH:O	2.13	0.48
1:C:92:PRO:CD	2:C:572:HOH:O	2.61	0.48
1:E:120:ARG:HD3	2:E:524:HOH:O	2.12	0.48
1:F:264:HIS:CE1	2:F:582:HOH:O	2.66	0.48
1:G:125:ALA:HB3	1:G:215:TYR:HA	1.95	0.48
1:H:238:LEU:HD22	1:H:400:MET:HG3	1.95	0.48
1:I:346:SER:CB	2:I:646:HOH:O	2.48	0.48
1:I:406:LEU:CD2	2:I:544:HOH:O	2.50	0.48
1:J:173:LEU:N	1:J:174:PRO:CD	2.75	0.48
1:L:290:GLU:HB2	2:L:570:HOH:O	2.13	0.48
1:A:27:ALA:HB1	2:A:606:HOH:O	2.14	0.48
1:B:115:ALA:HB1	2:B:570:HOH:O	2.13	0.48
1:D:10:ILE:HG23	1:D:13:LEU:HD22	1.94	0.48
1:D:79:VAL:HA	1:D:304:VAL:O	2.14	0.48
1:D:270:CYS:O	1:D:271:SER:HB2	2.13	0.48
1:D:372:MET:HG2	1:D:373:GLY:H	1.79	0.48
1:E:122:LEU:HD22	1:E:123:SER:N	2.29	0.48
1:H:235:LEU:HA	1:H:404:ARG:HA	1.96	0.48
1:I:285:ARG:CD	2:I:591:HOH:O	2.53	0.48
1:I:300:ARG:NH1	2:I:627:HOH:O	2.46	0.48
1:I:351:PHE:HA	2:I:668:HOH:O	2.12	0.48
1:L:26:LEU:O	1:L:30:LEU:HB2	2.13	0.48
1:L:91:LYS:HB3	1:L:92:PRO:HD2	1.95	0.48
2:A:657:HOH:O	1:D:315:ASN:HB3	2.13	0.48
1:C:238:LEU:HD22	1:C:400:MET:HG3	1.96	0.48
1:I:125:ALA:HB3	1:I:215:TYR:HA	1.95	0.48
1:J:122:LEU:HD22	1:J:123:SER:N	2.29	0.48
1:K:226:ASN:ND2	2:K:570:HOH:O	2.46	0.48
1:L:173:LEU:N	1:L:174:PRO:CD	2.76	0.48
1:B:17:PRO:HB3	2:B:497:HOH:O	2.12	0.48
1:B:259:LEU:HD11	2:B:698:HOH:O	2.12	0.48
1:C:77:ARG:HG2	2:C:692:HOH:O	2.13	0.48
1:C:79:VAL:HA	1:C:304:VAL:O	2.13	0.48
1:C:146:ALA:HA	1:F:405:GLU:HG2	1.96	0.48
1:C:150:ILE:N	1:C:151:PRO:CD	2.77	0.48
1:C:183:GLY:HA2	2:C:714:HOH:O	2.14	0.48
1:D:292:ASP:N	2:D:625:HOH:O	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:LEU:HD22	1:F:400:MET:HG3	1.96	0.48
1:K:242:HIS:HE1	2:K:616:HOH:O	1.96	0.48
1:L:270:CYS:O	1:L:271:SER:HB2	2.13	0.48
1:B:57:ASN:CB	2:B:595:HOH:O	2.62	0.48
1:C:264:HIS:HD2	2:C:446:HOH:O	1.96	0.48
1:C:299:GLN:HG2	2:C:508:HOH:O	2.13	0.48
1:D:218:GLN:CG	2:D:505:HOH:O	2.47	0.48
1:F:122:LEU:HD22	1:F:123:SER:N	2.29	0.48
1:F:235:LEU:HD12	1:F:404:ARG:HD2	1.95	0.48
2:F:461:HOH:O	1:G:322:ALA:HB1	2.13	0.48
1:G:357:GLN:HA	1:G:361:VAL:HG13	1.96	0.48
1:H:169:ALA:HA	2:H:452:HOH:O	2.14	0.48
1:H:255:GLU:CG	2:H:491:HOH:O	2.60	0.48
1:H:329:ASN:HB3	2:H:650:HOH:O	2.13	0.48
1:I:146:ALA:C	1:L:313:HIS:HE2	2.16	0.48
1:K:122:LEU:HD11	1:K:139:ARG:H	1.79	0.48
1:L:26:LEU:HB2	1:L:124:LEU:HD12	1.96	0.48
1:L:336:ILE:HG21	1:L:340:GLN:HB2	1.94	0.48
1:A:323:ASN:CA	2:A:619:HOH:O	2.40	0.48
1:B:122:LEU:HD22	1:B:123:SER:N	2.28	0.48
1:B:227:ASP:HB3	2:B:511:HOH:O	2.13	0.48
2:C:532:HOH:O	1:F:151:PRO:HA	2.13	0.48
1:E:63:ALA:HB3	1:E:261:CYS:HB3	1.94	0.48
1:H:113:LEU:HD13	2:H:473:HOH:O	2.13	0.48
2:I:527:HOH:O	1:L:328:LEU:CD2	2.60	0.48
1:J:55:THR:HG22	1:J:58:ASP:HA	1.95	0.48
1:K:49:GLY:N	2:K:518:HOH:O	2.46	0.48
1:L:125:ALA:HB3	1:L:215:TYR:HA	1.95	0.48
1:B:173:LEU:N	1:B:174:PRO:CD	2.77	0.48
1:C:139:ARG:CD	2:C:517:HOH:O	2.49	0.48
1:E:91:LYS:HB3	1:E:92:PRO:HD2	1.96	0.48
1:H:65:ARG:HG3	2:H:618:HOH:O	2.13	0.48
1:I:88:LEU:HD23	1:I:106:VAL:HG21	1.94	0.48
1:J:333:VAL:HA	1:J:393:ILE:HG22	1.95	0.48
1:J:369:ARG:HE	1:L:170:GLN:NE2	2.12	0.48
1:K:127:ARG:CZ	2:K:500:HOH:O	2.62	0.48
1:L:258:ILE:HD13	1:L:258:ILE:N	2.14	0.48
1:A:235:LEU:HA	1:A:404:ARG:HA	1.96	0.47
1:C:336:ILE:HG21	1:C:340:GLN:HB2	1.95	0.47
1:D:117:TRP:HB2	2:D:457:HOH:O	2.12	0.47
1:F:26:LEU:HB2	1:F:124:LEU:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:ILE:HG21	1:F:340:GLN:HB2	1.96	0.47
1:J:336:ILE:HG21	1:J:340:GLN:HB2	1.95	0.47
1:L:230:ILE:HG12	2:L:582:HOH:O	2.04	0.47
1:L:235:LEU:HA	1:L:404:ARG:HA	1.96	0.47
1:A:115:ALA:CB	2:A:524:HOH:O	2.61	0.47
1:D:96:ILE:HD12	2:D:669:HOH:O	2.13	0.47
1:F:170:GLN:NE2	1:G:369:ARG:HE	2.09	0.47
1:G:235:LEU:HD12	1:G:404:ARG:HH11	1.80	0.47
1:I:150:ILE:N	1:I:151:PRO:CD	2.77	0.47
1:I:271:SER:OG	2:I:465:HOH:O	2.05	0.47
1:J:285:ARG:HD3	2:J:629:HOH:O	2.14	0.47
1:K:123:SER:HB3	1:K:215:TYR:CE2	2.43	0.47
1:K:180:LEU:O	2:K:483:HOH:O	2.20	0.47
1:B:26:LEU:O	1:B:30:LEU:HB2	2.14	0.47
1:B:37:ARG:HG2	2:B:454:HOH:O	2.12	0.47
1:C:38:LEU:HD21	1:C:63:ALA:HB2	1.95	0.47
1:C:146:ALA:C	1:F:313:HIS:HE2	2.17	0.47
1:D:335:LYS:HZ2	1:D:335:LYS:HB2	1.79	0.47
1:E:170:GLN:HG3	1:I:370:SER:HB2	1.97	0.47
1:H:206:VAL:O	1:H:207:VAL:C	2.53	0.47
1:H:270:CYS:O	1:H:271:SER:HB2	2.14	0.47
1:J:151:PRO:HA	2:J:484:HOH:O	2.09	0.47
1:K:79:VAL:HA	1:K:304:VAL:O	2.14	0.47
1:L:248:LEU:HB2	2:L:691:HOH:O	2.15	0.47
1:L:372:MET:HG2	1:L:373:GLY:H	1.79	0.47
1:A:173:LEU:N	1:A:174:PRO:CD	2.77	0.47
1:C:344:THR:HA	1:C:348:THR:HG21	1.96	0.47
1:G:79:VAL:HA	1:G:304:VAL:O	2.13	0.47
1:G:343:ALA:C	2:G:512:HOH:O	2.51	0.47
1:G:385:GLN:HB2	2:G:451:HOH:O	2.13	0.47
1:H:259:LEU:HD11	2:H:680:HOH:O	2.13	0.47
1:I:173:LEU:N	1:I:174:PRO:CD	2.77	0.47
1:K:150:ILE:N	1:K:151:PRO:CD	2.78	0.47
1:K:212:LEU:O	1:K:213:SER:HB2	2.14	0.47
1:L:77:ARG:HD2	2:L:665:HOH:O	2.15	0.47
1:L:79:VAL:HA	1:L:304:VAL:O	2.15	0.47
1:C:40:GLU:O	2:C:449:HOH:O	2.19	0.47
1:D:248:LEU:CD2	2:D:521:HOH:O	2.48	0.47
1:E:235:LEU:HA	1:E:404:ARG:HA	1.95	0.47
1:F:344:THR:HG23	2:F:506:HOH:O	2.15	0.47
1:H:150:ILE:N	1:H:151:PRO:CD	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:GLY:HA2	2:H:522:HOH:O	2.13	0.47
1:J:305:SER:OG	1:J:392:ASP:HA	2.14	0.47
1:K:20:PHE:O	1:K:24:ALA:N	2.40	0.47
1:C:151:PRO:HA	2:C:465:HOH:O	2.10	0.47
1:D:91:LYS:HB3	1:D:92:PRO:HD2	1.97	0.47
1:D:333:VAL:HA	1:D:393:ILE:HG22	1.95	0.47
1:F:357:GLN:HA	1:F:361:VAL:HG13	1.95	0.47
1:G:37:ARG:CG	2:G:616:HOH:O	2.62	0.47
1:H:113:LEU:CD1	2:H:473:HOH:O	2.62	0.47
1:K:319:ARG:CZ	2:K:676:HOH:O	2.62	0.47
1:L:235:LEU:HD12	1:L:404:ARG:HH11	1.80	0.47
1:A:144:ARG:HE	1:D:226:ASN:ND2	2.13	0.47
1:A:305:SER:OG	1:A:392:ASP:HA	2.14	0.47
2:E:642:HOH:O	1:H:328:LEU:HD22	2.14	0.47
1:F:28:ARG:HD2	1:F:126:GLY:H	1.80	0.47
1:G:122:LEU:HD22	1:G:123:SER:N	2.30	0.47
1:H:77:ARG:HD2	2:H:558:HOH:O	2.14	0.47
1:H:336:ILE:HG23	2:H:592:HOH:O	2.15	0.47
1:I:288:LEU:HD22	1:I:289:PRO:HD2	1.96	0.47
1:J:234:ARG:HB3	1:J:237:ASN:HD21	1.79	0.47
1:J:322:ALA:N	2:J:464:HOH:O	2.37	0.47
1:K:91:LYS:HB3	1:K:92:PRO:HD2	1.97	0.47
1:K:306:ALA:HB2	2:K:624:HOH:O	2.13	0.47
1:K:322:ALA:HA	2:K:528:HOH:O	2.15	0.47
1:K:403:ILE:CG2	2:K:541:HOH:O	2.59	0.47
1:A:264:HIS:HD2	2:A:484:HOH:O	1.96	0.47
1:F:62:ILE:HD13	2:F:542:HOH:O	2.14	0.47
1:F:391:VAL:HA	2:F:506:HOH:O	2.13	0.47
1:G:51:ARG:HB2	2:G:565:HOH:O	2.13	0.47
1:H:356:CYS:HB2	2:H:591:HOH:O	2.15	0.47
1:L:245:LEU:HA	2:L:691:HOH:O	2.14	0.47
1:A:206:VAL:O	1:A:207:VAL:C	2.53	0.47
1:B:258:ILE:HD13	1:B:258:ILE:N	2.15	0.47
1:D:150:ILE:N	1:D:151:PRO:CD	2.77	0.47
1:F:263:ASP:HA	2:F:582:HOH:O	2.15	0.47
1:G:404:ARG:HG2	1:J:144:ARG:NH2	2.30	0.47
1:H:378:ILE:O	1:H:378:ILE:HG12	2.15	0.47
1:I:122:LEU:CD1	2:I:609:HOH:O	2.62	0.47
1:I:284:LEU:HD12	2:I:634:HOH:O	2.13	0.47
1:J:150:ILE:N	1:J:151:PRO:CD	2.78	0.47
1:D:20:PHE:O	1:D:24:ALA:N	2.38	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ASP:H	1:D:219:SER:HA	1.80	0.47
1:D:369:ARG:C	2:D:544:HOH:O	2.53	0.47
1:E:150:ILE:N	1:E:151:PRO:CD	2.78	0.47
1:E:290:GLU:HB2	2:I:702:HOH:O	2.14	0.47
1:E:339:ASN:HB3	2:E:446:HOH:O	2.13	0.47
1:E:344:THR:HA	1:E:348:THR:HG21	1.96	0.47
1:E:372:MET:HG2	1:E:373:GLY:H	1.80	0.47
1:F:30:LEU:CD2	2:F:521:HOH:O	2.62	0.47
1:I:115:ALA:CB	2:I:533:HOH:O	2.63	0.47
1:I:280:LEU:HD23	2:I:478:HOH:O	2.14	0.47
1:L:206:VAL:O	1:L:207:VAL:C	2.54	0.47
1:L:234:ARG:HB3	1:L:237:ASN:HD21	1.78	0.47
1:A:100:GLY:HA2	2:A:513:HOH:O	2.14	0.46
1:B:313:HIS:HE2	1:K:146:ALA:C	2.19	0.46
1:B:322:ALA:HB1	2:D:526:HOH:O	2.14	0.46
1:E:125:ALA:HB3	1:E:215:TYR:HA	1.96	0.46
1:E:206:VAL:O	1:E:207:VAL:C	2.53	0.46
1:H:65:ARG:NH1	1:H:259:LEU:HD12	2.30	0.46
1:J:357:GLN:HA	1:J:361:VAL:HG13	1.95	0.46
1:C:206:VAL:O	1:C:207:VAL:C	2.53	0.46
1:D:26:LEU:HB2	1:D:124:LEU:HD12	1.97	0.46
1:E:336:ILE:HG21	1:E:340:GLN:HB2	1.97	0.46
1:F:258:ILE:HD13	1:F:258:ILE:N	2.14	0.46
1:H:71:PRO:HD2	1:H:74:SER:HB3	1.98	0.46
1:H:91:LYS:HB3	1:H:92:PRO:HD2	1.97	0.46
1:I:206:VAL:O	1:I:207:VAL:C	2.54	0.46
1:I:342:TYR:HA	2:I:530:HOH:O	2.15	0.46
1:J:206:VAL:O	1:J:207:VAL:C	2.54	0.46
1:L:378:ILE:O	1:L:378:ILE:HG12	2.14	0.46
1:B:76:PHE:HA	2:B:611:HOH:O	2.13	0.46
1:E:139:ARG:HD3	2:E:657:HOH:O	2.14	0.46
1:F:150:ILE:N	1:F:151:PRO:CD	2.78	0.46
1:G:56:ARG:NH2	2:G:476:HOH:O	2.41	0.46
1:I:10:ILE:CA	2:I:585:HOH:O	2.33	0.46
1:I:205:ASP:HA	2:I:593:HOH:O	2.14	0.46
1:K:320:HIS:CD2	2:K:558:HOH:O	2.68	0.46
1:A:335:LYS:HB3	2:A:691:HOH:O	2.16	0.46
1:B:65:ARG:NH1	1:B:259:LEU:HD12	2.30	0.46
1:C:115:ALA:CB	2:C:618:HOH:O	2.54	0.46
1:E:335:LYS:HB2	1:E:335:LYS:HZ2	1.80	0.46
1:F:344:THR:HA	1:F:348:THR:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:348:THR:HG23	1:G:391:VAL:HG22	1.98	0.46
1:H:51:ARG:NH2	2:H:455:HOH:O	2.48	0.46
1:I:335:LYS:HB2	1:I:335:LYS:HZ2	1.81	0.46
1:J:79:VAL:HA	1:J:304:VAL:O	2.15	0.46
1:K:235:LEU:HA	1:K:404:ARG:HA	1.97	0.46
1:K:378:ILE:O	1:K:378:ILE:HG12	2.16	0.46
1:L:249:LEU:HD11	1:L:416:VAL:HA	1.96	0.46
1:B:79:VAL:HA	1:B:304:VAL:O	2.14	0.46
1:B:238:LEU:HD22	1:B:400:MET:HG3	1.97	0.46
1:C:279:PHE:HD2	2:C:561:HOH:O	1.97	0.46
1:E:79:VAL:HA	1:E:304:VAL:O	2.15	0.46
1:I:65:ARG:NH1	1:I:259:LEU:HD12	2.31	0.46
1:J:65:ARG:NH1	1:J:259:LEU:HD12	2.31	0.46
1:K:125:ALA:HB3	1:K:215:TYR:HA	1.98	0.46
1:K:131:ARG:HG3	2:K:438:HOH:O	2.15	0.46
1:L:150:ILE:N	1:L:151:PRO:CD	2.79	0.46
1:B:206:VAL:O	1:B:207:VAL:C	2.53	0.46
1:C:60:SER:HA	1:C:264:HIS:HA	1.98	0.46
1:G:86:PRO:HD3	2:G:433:HOH:O	2.15	0.46
1:G:170:GLN:NE2	1:H:369:ARG:HE	2.14	0.46
1:G:206:VAL:O	1:G:207:VAL:C	2.54	0.46
1:G:335:LYS:HZ3	1:G:365:SER:HB2	1.81	0.46
1:H:347:GLU:OE1	2:H:504:HOH:O	2.21	0.46
1:L:426:SER:O	1:L:426:SER:CA	2.60	0.46
1:C:249:LEU:HB3	1:C:423:TYR:HE2	1.80	0.46
1:E:66:LEU:HD11	2:E:587:HOH:O	2.16	0.46
1:G:120:ARG:HA	2:G:577:HOH:O	2.14	0.46
1:I:322:ALA:HA	2:I:650:HOH:O	2.14	0.46
1:K:206:VAL:O	1:K:207:VAL:C	2.54	0.46
1:L:59:SER:HB3	2:L:542:HOH:O	2.15	0.46
1:L:112:ALA:O	1:L:113:LEU:HB2	2.16	0.46
1:A:140:LEU:HD23	2:A:547:HOH:O	2.16	0.46
1:A:345:ASN:H	1:A:348:THR:HB	1.81	0.46
1:B:73:GLU:HG2	2:B:520:HOH:O	2.16	0.46
1:B:150:ILE:N	1:B:151:PRO:CD	2.78	0.46
1:F:206:VAL:O	1:F:207:VAL:C	2.54	0.46
1:G:230:ILE:HD13	2:G:662:HOH:O	2.16	0.46
1:I:235:LEU:HD12	1:I:404:ARG:HH11	1.81	0.46
1:J:403:ILE:HD11	2:J:562:HOH:O	2.16	0.46
1:A:150:ILE:N	1:A:151:PRO:CD	2.78	0.46
1:A:369:ARG:HE	1:I:170:GLN:NE2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LEU:HB2	1:C:124:LEU:HD12	1.96	0.46
1:G:65:ARG:NH1	1:G:259:LEU:HD12	2.31	0.46
1:I:146:ALA:HA	1:L:405:GLU:HG2	1.97	0.46
1:L:339:ASN:CB	2:L:521:HOH:O	2.52	0.46
1:A:60:SER:HB2	2:A:487:HOH:O	2.15	0.46
1:C:36:ARG:NH1	2:C:459:HOH:O	2.40	0.46
1:H:122:LEU:HD22	1:H:123:SER:N	2.31	0.46
1:H:380:PRO:HB2	1:H:390:THR:HG21	1.98	0.46
1:I:218:GLN:CG	2:I:456:HOH:O	2.45	0.46
1:A:122:LEU:HD22	1:A:123:SER:N	2.31	0.45
1:A:227:ASP:HB3	2:A:588:HOH:O	2.16	0.45
1:B:131:ARG:HB2	2:B:589:HOH:O	2.16	0.45
1:B:360:GLU:HA	2:B:457:HOH:O	2.15	0.45
1:B:405:GLU:HG2	1:K:146:ALA:HA	1.97	0.45
1:C:225:LEU:HD22	2:C:574:HOH:O	2.15	0.45
1:C:344:THR:HG23	2:C:612:HOH:O	2.15	0.45
1:F:60:SER:N	2:F:650:HOH:O	2.47	0.45
1:G:150:ILE:N	1:G:151:PRO:CD	2.78	0.45
1:I:288:LEU:HB2	2:I:489:HOH:O	2.16	0.45
1:J:40:GLU:HG3	2:J:663:HOH:O	2.16	0.45
1:A:79:VAL:HA	1:A:304:VAL:O	2.16	0.45
1:A:344:THR:HA	1:A:348:THR:HG21	1.97	0.45
1:B:372:MET:HG2	1:B:373:GLY:H	1.80	0.45
1:D:37:ARG:HG2	2:D:443:HOH:O	2.15	0.45
1:D:277:GLY:HA2	1:D:278:PRO:HA	1.76	0.45
1:E:328:LEU:HD22	2:E:553:HOH:O	2.16	0.45
1:E:333:VAL:HA	1:E:393:ILE:HG22	1.98	0.45
1:I:122:LEU:HD22	1:I:123:SER:N	2.31	0.45
1:I:168:ASN:CG	2:I:641:HOH:O	2.53	0.45
1:L:333:VAL:HA	1:L:393:ILE:HG22	1.99	0.45
1:L:401:HIS:CE1	2:L:567:HOH:O	2.70	0.45
1:A:300:ARG:NH2	2:A:499:HOH:O	2.49	0.45
1:B:130:PHE:O	1:B:131:ARG:HB2	2.16	0.45
1:E:144:ARG:NH2	1:H:404:ARG:HG2	2.31	0.45
1:H:220:ALA:O	1:H:221:ALA:C	2.55	0.45
1:J:170:GLN:NE2	1:K:369:ARG:HE	2.14	0.45
1:K:372:MET:HG2	1:K:373:GLY:H	1.79	0.45
1:C:20:PHE:O	1:C:24:ALA:N	2.39	0.45
1:C:235:LEU:HA	1:C:404:ARG:HA	1.97	0.45
1:C:263:ASP:HA	2:C:551:HOH:O	2.15	0.45
1:C:316:TYR:OH	2:C:595:HOH:O	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:HD13	2:E:621:HOH:O	2.16	0.45
1:G:238:LEU:HD22	1:G:400:MET:HG3	1.97	0.45
1:G:333:VAL:HA	1:G:393:ILE:HG22	1.98	0.45
1:H:94:PRO:HB2	1:H:105:GLY:N	2.31	0.45
1:I:344:THR:HA	1:I:348:THR:HG21	1.97	0.45
1:I:345:ASN:H	1:I:348:THR:HB	1.82	0.45
1:J:372:MET:HG2	1:J:373:GLY:H	1.82	0.45
2:J:489:HOH:O	1:L:126:GLY:HA3	2.15	0.45
1:K:346:SER:CB	2:K:509:HOH:O	2.65	0.45
1:L:13:LEU:HD11	1:L:416:VAL:HG21	1.98	0.45
1:L:65:ARG:NH1	1:L:259:LEU:HD12	2.31	0.45
1:A:144:ARG:NH2	1:D:404:ARG:HG2	2.32	0.45
1:B:147:ILE:HD13	2:K:682:HOH:O	2.16	0.45
1:B:151:PRO:HD3	2:K:513:HOH:O	2.17	0.45
1:B:370:SER:HB2	1:D:170:GLN:HG3	1.98	0.45
1:C:137:GLU:HG3	2:C:578:HOH:O	2.16	0.45
1:E:26:LEU:HG	1:E:27:ALA:N	2.24	0.45
1:E:65:ARG:NH1	1:E:259:LEU:HD12	2.32	0.45
1:I:224:GLY:HA3	1:L:120:ARG:HH22	1.81	0.45
1:K:119:ASP:HA	2:K:671:HOH:O	2.14	0.45
1:K:322:ALA:CA	2:K:528:HOH:O	2.64	0.45
1:K:344:THR:HA	1:K:348:THR:HG21	1.98	0.45
1:A:112:ALA:O	1:A:113:LEU:HB2	2.17	0.45
1:A:257:CYS:HB2	2:A:651:HOH:O	2.16	0.45
1:A:372:MET:HG2	1:A:373:GLY:H	1.81	0.45
1:B:212:LEU:CG	2:B:645:HOH:O	2.60	0.45
1:B:378:ILE:HG12	1:B:378:ILE:O	2.16	0.45
1:F:30:LEU:HD23	2:F:521:HOH:O	2.15	0.45
1:F:345:ASN:H	1:F:348:THR:HB	1.81	0.45
1:I:290:GLU:HB2	2:I:599:HOH:O	2.16	0.45
1:K:152:ASN:HB3	1:K:153:LEU:H	1.65	0.45
1:L:117:TRP:HB2	2:L:475:HOH:O	2.17	0.45
1:D:123:SER:HB3	1:D:215:TYR:CE2	2.50	0.45
1:D:206:VAL:O	1:D:207:VAL:C	2.54	0.45
1:G:336:ILE:HG21	1:G:340:GLN:HB2	1.99	0.45
1:G:405:GLU:HG2	1:J:146:ALA:HA	1.99	0.45
1:I:279:PHE:HD2	2:I:667:HOH:O	1.98	0.45
1:I:372:MET:HG2	1:I:373:GLY:H	1.81	0.45
1:K:281:GLU:HG2	2:L:524:HOH:O	2.16	0.45
1:C:116:PRO:HG3	2:C:542:HOH:O	2.16	0.45
1:C:405:GLU:HG2	1:F:146:ALA:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:LEU:C	1:D:240:SER:H	2.20	0.45
1:F:173:LEU:HD12	2:F:468:HOH:O	2.15	0.45
1:F:333:VAL:HA	1:F:393:ILE:HG22	1.98	0.45
1:K:121:ASP:H	1:K:219:SER:HA	1.81	0.45
1:B:91:LYS:HE2	2:C:494:HOH:O	2.17	0.45
1:C:413:ALA:CB	2:C:617:HOH:O	2.65	0.45
1:D:285:ARG:NH1	2:D:458:HOH:O	2.50	0.45
1:H:130:PHE:O	1:H:131:ARG:HB2	2.17	0.45
1:H:167:ILE:HD11	2:H:518:HOH:O	2.17	0.45
1:I:20:PHE:O	1:I:24:ALA:N	2.41	0.45
1:J:25:SER:C	2:J:674:HOH:O	2.51	0.45
1:A:86:PRO:HD3	2:A:470:HOH:O	2.16	0.45
1:A:335:LYS:HZ2	1:A:335:LYS:HB2	1.82	0.45
1:B:238:LEU:C	1:B:240:SER:H	2.20	0.45
1:C:122:LEU:HD22	1:C:123:SER:N	2.32	0.45
1:G:220:ALA:O	1:G:221:ALA:C	2.56	0.45
1:I:174:PRO:HA	1:I:175:PRO:HD3	1.79	0.45
1:I:333:VAL:HA	1:I:393:ILE:HG22	1.98	0.45
1:L:220:ALA:O	1:L:221:ALA:C	2.56	0.45
2:A:539:HOH:O	1:D:98:ARG:CD	2.48	0.44
1:B:66:LEU:HD12	2:B:578:HOH:O	2.16	0.44
1:B:339:ASN:HB3	2:B:542:HOH:O	2.16	0.44
1:B:373:GLY:HA2	2:B:437:HOH:O	2.16	0.44
1:E:146:ALA:HA	1:H:405:GLU:HG2	1.99	0.44
1:E:224:GLY:HA2	2:E:648:HOH:O	2.16	0.44
1:F:235:LEU:HD12	1:F:404:ARG:HH11	1.82	0.44
1:H:372:MET:HG2	1:H:373:GLY:H	1.81	0.44
1:J:36:ARG:HB3	2:J:436:HOH:O	2.17	0.44
1:J:131:ARG:HB2	2:J:537:HOH:O	2.16	0.44
1:K:264:HIS:CD2	2:K:536:HOH:O	2.68	0.44
2:K:462:HOH:O	1:L:322:ALA:HB1	2.13	0.44
1:L:39:ASP:HA	2:L:609:HOH:O	2.16	0.44
1:B:288:LEU:N	2:B:624:HOH:O	2.49	0.44
1:C:65:ARG:NH1	1:C:259:LEU:HD12	2.33	0.44
1:C:182:PRO:HD3	2:C:538:HOH:O	2.16	0.44
1:C:335:LYS:HB2	1:C:335:LYS:HZ2	1.82	0.44
1:D:65:ARG:NH1	1:D:259:LEU:HD12	2.32	0.44
1:F:127:ARG:HA	1:F:213:SER:CB	2.47	0.44
1:G:20:PHE:O	1:G:24:ALA:N	2.40	0.44
1:H:98:ARG:CD	2:H:531:HOH:O	2.53	0.44
1:H:389:ARG:NH1	2:H:550:HOH:O	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:ARG:NH1	2:I:442:HOH:O	2.26	0.44
1:J:140:LEU:CA	2:J:623:HOH:O	2.59	0.44
1:A:125:ALA:HB3	1:A:215:TYR:HA	1.98	0.44
1:A:404:ARG:HG2	1:D:144:ARG:NH2	2.33	0.44
1:E:218:GLN:CG	2:E:631:HOH:O	2.38	0.44
1:F:220:ALA:O	1:F:221:ALA:C	2.55	0.44
1:I:405:GLU:HG2	1:L:146:ALA:HA	2.00	0.44
1:L:335:LYS:HZ2	1:L:335:LYS:HB2	1.82	0.44
2:A:481:HOH:O	1:D:176:ILE:CG2	2.66	0.44
1:B:146:ALA:HA	1:K:405:GLU:HG2	1.99	0.44
1:D:249:LEU:HD11	1:D:416:VAL:HA	2.00	0.44
1:F:62:ILE:HG13	2:F:482:HOH:O	2.17	0.44
2:F:519:HOH:O	1:G:366:PHE:HE1	2.01	0.44
1:H:238:LEU:HD21	2:H:611:HOH:O	2.17	0.44
1:K:300:ARG:NE	2:K:532:HOH:O	2.45	0.44
1:A:405:GLU:HG2	1:D:146:ALA:HA	1.99	0.44
1:C:204:ALA:HB3	2:C:664:HOH:O	2.17	0.44
1:E:378:ILE:HG22	2:E:554:HOH:O	2.17	0.44
2:G:550:HOH:O	1:H:385:GLN:CG	2.59	0.44
1:H:380:PRO:CB	1:H:390:THR:HG21	2.47	0.44
1:I:121:ASP:H	1:I:219:SER:HA	1.83	0.44
1:K:212:LEU:HD13	2:K:681:HOH:O	2.01	0.44
1:L:361:VAL:CB	1:L:362:PRO:CA	2.77	0.44
1:A:249:LEU:HD11	1:A:416:VAL:HA	1.98	0.44
1:A:378:ILE:O	1:A:378:ILE:HG12	2.18	0.44
1:D:122:LEU:HD22	1:D:123:SER:N	2.33	0.44
1:E:75:GLY:O	1:E:258:ILE:HD11	2.17	0.44
1:E:121:ASP:H	1:E:219:SER:HA	1.83	0.44
1:I:51:ARG:HB3	2:I:643:HOH:O	2.18	0.44
1:I:65:ARG:CG	2:I:643:HOH:O	2.64	0.44
1:I:404:ARG:HG2	1:L:144:ARG:NH2	2.32	0.44
1:J:357:GLN:NE2	2:J:458:HOH:O	2.50	0.44
1:K:65:ARG:NH1	1:K:259:LEU:HD12	2.32	0.44
1:A:65:ARG:NH1	1:A:259:LEU:HD12	2.32	0.44
1:E:405:GLU:HG2	1:H:146:ALA:HA	1.99	0.44
1:F:60:SER:HA	1:F:264:HIS:HA	1.98	0.44
1:F:370:SER:HB2	1:H:170:GLN:HG3	1.98	0.44
1:H:353:ARG:NH1	2:H:564:HOH:O	2.50	0.44
1:I:268:GLY:HA3	2:I:600:HOH:O	2.18	0.44
1:J:40:GLU:CG	2:J:663:HOH:O	2.66	0.44
1:J:60:SER:HA	1:J:264:HIS:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:288:LEU:HD11	2:J:661:HOH:O	2.18	0.44
1:C:104:LEU:HD12	1:C:143:PHE:HE2	1.83	0.44
1:D:320:HIS:CD2	2:D:569:HOH:O	2.70	0.44
1:E:30:LEU:HD22	2:E:459:HOH:O	2.09	0.44
1:E:60:SER:HA	1:E:264:HIS:HA	1.99	0.44
1:G:121:ASP:H	1:G:219:SER:HA	1.83	0.44
1:H:237:ASN:HA	1:H:240:SER:HB3	2.00	0.44
1:H:346:SER:HB2	2:H:485:HOH:O	2.13	0.44
1:I:120:ARG:HH22	1:L:224:GLY:HA3	1.81	0.44
1:J:344:THR:HA	1:J:348:THR:HG21	1.98	0.44
1:A:121:ASP:H	1:A:219:SER:HA	1.83	0.44
1:A:405:GLU:CG	1:D:146:ALA:HA	2.48	0.44
1:D:120:ARG:HD3	2:D:494:HOH:O	2.17	0.44
1:E:124:LEU:O	1:E:125:ALA:HB3	2.18	0.44
1:E:220:ALA:O	1:E:221:ALA:C	2.56	0.44
1:H:86:PRO:HG2	1:H:401:HIS:CG	2.53	0.44
1:I:378:ILE:O	1:I:378:ILE:HG12	2.18	0.44
1:J:111:GLY:HA2	2:J:579:HOH:O	2.17	0.44
1:K:346:SER:HB2	2:K:509:HOH:O	2.18	0.44
1:C:333:VAL:HA	1:C:393:ILE:HG22	1.99	0.43
1:D:26:LEU:CD2	1:D:125:ALA:HB2	2.48	0.43
1:D:212:LEU:O	1:D:213:SER:HB2	2.18	0.43
1:E:126:GLY:CA	2:E:595:HOH:O	2.39	0.43
1:E:309:ALA:N	2:E:529:HOH:O	2.50	0.43
1:F:121:ASP:H	1:F:219:SER:HA	1.83	0.43
1:H:125:ALA:HB3	1:H:215:TYR:HA	1.99	0.43
1:I:235:LEU:HA	1:I:404:ARG:HA	1.99	0.43
1:A:20:PHE:O	1:A:24:ALA:N	2.41	0.43
1:A:239:LEU:CD2	2:A:600:HOH:O	2.66	0.43
1:B:26:LEU:HD22	1:B:124:LEU:HG	2.00	0.43
1:B:55:THR:CG2	2:B:443:HOH:O	1.96	0.43
1:F:344:THR:CG2	2:F:506:HOH:O	2.66	0.43
1:F:415:LEU:CB	2:F:673:HOH:O	2.54	0.43
1:H:121:ASP:H	1:H:219:SER:HA	1.83	0.43
1:J:380:PRO:CB	1:J:390:THR:HG21	2.48	0.43
1:K:148:ALA:CB	2:K:612:HOH:O	2.60	0.43
1:B:60:SER:HA	1:B:264:HIS:HA	2.00	0.43
1:C:238:LEU:C	1:C:240:SER:H	2.22	0.43
1:E:235:LEU:HD12	1:E:404:ARG:HH11	1.83	0.43
1:F:21:HIS:NE2	1:F:241:CYS:HB3	2.33	0.43
1:F:86:PRO:HG2	1:F:401:HIS:CG	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:LEU:HD22	1:F:289:PRO:HD2	2.00	0.43
1:G:146:ALA:HA	1:J:405:GLU:HG2	2.00	0.43
1:I:144:ARG:NH2	1:L:404:ARG:HG2	2.34	0.43
1:I:322:ALA:N	2:I:512:HOH:O	2.27	0.43
1:J:122:LEU:HD11	1:J:138:SER:HB2	2.00	0.43
1:K:333:VAL:HA	1:K:393:ILE:HG22	1.99	0.43
1:K:335:LYS:HB2	1:K:335:LYS:HZ2	1.82	0.43
1:L:20:PHE:O	1:L:24:ALA:N	2.40	0.43
1:B:249:LEU:HD11	1:B:416:VAL:CA	2.49	0.43
1:C:249:LEU:HD11	1:C:416:VAL:HA	2.01	0.43
1:D:407:ALA:HB1	2:D:515:HOH:O	2.17	0.43
1:G:170:GLN:HA	2:G:514:HOH:O	2.17	0.43
1:G:218:GLN:CB	2:G:679:HOH:O	2.65	0.43
1:G:234:ARG:HB3	1:G:237:ASN:HD21	1.80	0.43
1:H:174:PRO:HA	1:H:175:PRO:HD3	1.79	0.43
1:J:174:PRO:HA	1:J:175:PRO:HD3	1.80	0.43
1:A:170:GLN:NE2	1:E:369:ARG:HE	2.15	0.43
1:B:333:VAL:HA	1:B:393:ILE:HG22	2.00	0.43
1:F:395:LEU:CD2	2:F:673:HOH:O	2.61	0.43
1:G:26:LEU:HB2	1:G:124:LEU:HD12	1.99	0.43
1:H:406:LEU:CA	2:H:432:HOH:O	2.55	0.43
1:J:56:ARG:NH2	2:J:577:HOH:O	2.49	0.43
1:K:277:GLY:HA2	1:K:278:PRO:HA	1.76	0.43
1:B:235:LEU:HD12	1:B:404:ARG:HH11	1.82	0.43
1:C:372:MET:HG2	1:C:373:GLY:H	1.84	0.43
1:E:26:LEU:HD22	1:E:125:ALA:HB2	2.00	0.43
1:H:287:LEU:HD12	2:H:584:HOH:O	2.19	0.43
1:J:220:ALA:O	1:J:221:ALA:C	2.57	0.43
1:K:335:LYS:HZ3	1:K:365:SER:HB2	1.83	0.43
1:A:333:VAL:HA	1:A:393:ILE:HG22	2.00	0.43
1:A:406:LEU:O	1:A:407:ALA:HB2	2.18	0.43
1:B:89:ARG:HA	1:B:216:ASP:HA	2.00	0.43
1:B:235:LEU:HD21	1:B:403:ILE:HG22	2.01	0.43
1:D:152:ASN:HB3	1:D:153:LEU:H	1.66	0.43
1:E:115:ALA:HB2	2:H:539:HOH:O	2.19	0.43
1:E:122:LEU:CD1	2:E:533:HOH:O	2.45	0.43
1:G:303:LEU:O	1:G:390:THR:HA	2.19	0.43
2:G:667:HOH:O	1:H:353:ARG:NH2	2.51	0.43
1:H:255:GLU:HG2	2:H:491:HOH:O	2.19	0.43
1:H:344:THR:HA	1:H:348:THR:HG21	2.01	0.43
1:A:235:LEU:HD12	1:A:404:ARG:HH11	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:THR:CB	2:B:443:HOH:O	2.54	0.43
1:B:120:ARG:HH22	1:K:224:GLY:HA3	1.82	0.43
1:B:137:GLU:HG3	2:B:456:HOH:O	2.19	0.43
1:B:379:GLY:HA3	1:B:380:PRO:HD3	1.91	0.43
1:F:20:PHE:O	1:F:24:ALA:N	2.40	0.43
1:F:131:ARG:HG3	2:F:492:HOH:O	2.18	0.43
1:I:225:LEU:HD11	2:I:504:HOH:O	2.18	0.43
1:J:143:PHE:HD2	2:J:558:HOH:O	2.00	0.43
1:J:378:ILE:HG12	1:J:378:ILE:O	2.18	0.43
1:L:277:GLY:HA2	1:L:278:PRO:HA	1.79	0.43
1:A:89:ARG:HA	1:A:216:ASP:HA	2.00	0.43
1:A:234:ARG:HB3	1:A:237:ASN:HD21	1.84	0.43
1:B:9:LEU:N	2:B:465:HOH:O	2.52	0.43
1:B:86:PRO:HG2	1:B:401:HIS:CG	2.54	0.43
1:B:235:LEU:HA	1:B:404:ARG:HA	2.00	0.43
1:B:404:ARG:HG2	1:K:144:ARG:NH2	2.34	0.43
1:C:92:PRO:CA	2:C:572:HOH:O	2.67	0.43
1:E:54:VAL:HB	2:E:691:HOH:O	2.19	0.43
1:E:378:ILE:O	1:E:378:ILE:HG12	2.19	0.43
1:F:169:ALA:HA	2:G:638:HOH:O	2.18	0.43
1:I:337:ASN:HA	1:I:341:ARG:HG2	2.01	0.43
1:L:229:PHE:HB2	1:L:230:ILE:H	1.69	0.43
1:L:238:LEU:C	1:L:240:SER:H	2.22	0.43
1:L:322:ALA:O	2:L:612:HOH:O	2.22	0.43
1:B:340:GLN:HA	2:B:468:HOH:O	2.19	0.43
1:D:103:GLN:HB3	2:D:669:HOH:O	2.17	0.43
1:D:213:SER:HB3	1:D:214:PHE:H	1.52	0.43
1:F:98:ARG:CD	2:F:442:HOH:O	2.59	0.43
1:F:249:LEU:HD11	1:F:416:VAL:HA	2.01	0.43
1:G:94:PRO:HB2	1:G:105:GLY:N	2.34	0.43
1:G:146:ALA:C	1:J:313:HIS:HE2	2.22	0.43
1:H:171:ASN:ND2	2:H:622:HOH:O	2.52	0.43
1:I:146:ALA:HA	1:L:405:GLU:CG	2.49	0.43
1:I:236:ASP:HA	2:I:608:HOH:O	2.18	0.43
1:J:26:LEU:HG	1:J:27:ALA:N	2.26	0.43
1:J:235:LEU:HD12	1:J:404:ARG:HH11	1.84	0.43
1:C:378:ILE:O	1:C:378:ILE:HG12	2.19	0.42
1:E:238:LEU:C	1:E:240:SER:H	2.22	0.42
1:I:151:PRO:CA	2:I:656:HOH:O	2.45	0.42
1:I:237:ASN:HA	1:I:240:SER:HB3	2.01	0.42
1:I:295:SER:CB	2:I:602:HOH:O	2.65	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:20:PHE:O	1:J:24:ALA:N	2.41	0.42
1:J:94:PRO:HB2	1:J:105:GLY:N	2.34	0.42
1:J:338:SER:HA	1:L:109:TYR:HA	2.00	0.42
1:K:182:PRO:CB	2:K:664:HOH:O	2.56	0.42
1:L:223:VAL:HG22	1:L:235:LEU:HB3	2.01	0.42
1:A:277:GLY:HA2	1:A:278:PRO:HA	1.78	0.42
1:B:70:SER:HA	1:B:71:PRO:HD3	1.94	0.42
1:B:146:ALA:C	1:K:313:HIS:HE2	2.21	0.42
1:B:220:ALA:O	1:B:221:ALA:C	2.56	0.42
1:H:20:PHE:O	1:H:24:ALA:N	2.39	0.42
1:I:238:LEU:C	1:I:240:SER:H	2.22	0.42
1:K:174:PRO:HA	1:K:175:PRO:HD3	1.78	0.42
1:K:220:ALA:O	1:K:221:ALA:C	2.57	0.42
1:L:150:ILE:CD1	2:L:610:HOH:O	2.67	0.42
1:L:378:ILE:CG2	2:L:518:HOH:O	2.59	0.42
1:A:120:ARG:HH22	1:D:224:GLY:HA3	1.84	0.42
1:A:182:PRO:CB	2:A:570:HOH:O	2.67	0.42
1:A:285:ARG:CD	2:A:577:HOH:O	2.62	0.42
1:D:288:LEU:HB2	2:D:522:HOH:O	2.18	0.42
1:E:104:LEU:HD12	1:E:143:PHE:HE2	1.84	0.42
1:F:65:ARG:NH1	1:F:259:LEU:HD12	2.33	0.42
1:F:91:LYS:HB2	1:F:94:PRO:HB3	2.00	0.42
1:G:60:SER:HA	1:G:264:HIS:HA	2.01	0.42
1:G:249:LEU:HD11	1:G:416:VAL:HA	2.01	0.42
1:A:60:SER:HA	1:A:264:HIS:HA	2.01	0.42
1:A:137:GLU:HB3	2:A:545:HOH:O	2.20	0.42
1:A:170:GLN:HE22	1:E:369:ARG:HB3	1.85	0.42
1:C:75:GLY:O	1:C:258:ILE:HD11	2.19	0.42
1:F:94:PRO:HB2	1:F:105:GLY:N	2.33	0.42
1:F:234:ARG:HB3	1:F:237:ASN:HD21	1.79	0.42
1:I:26:LEU:HD12	2:I:572:HOH:O	2.19	0.42
1:I:389:ARG:HG3	2:I:563:HOH:O	2.19	0.42
1:J:121:ASP:H	1:J:219:SER:HA	1.84	0.42
1:J:237:ASN:HA	1:J:240:SER:HB3	2.00	0.42
1:K:120:ARG:HD3	2:K:582:HOH:O	2.19	0.42
1:L:121:ASP:H	1:L:219:SER:HA	1.83	0.42
1:L:415:LEU:HD12	2:L:579:HOH:O	2.19	0.42
1:A:264:HIS:CD2	2:A:484:HOH:O	2.70	0.42
1:B:174:PRO:HA	1:B:175:PRO:HD3	1.80	0.42
1:B:294:PHE:O	1:B:296:ARG:N	2.53	0.42
1:C:114:PHE:HB2	1:C:115:ALA:H	1.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:LEU:HG	2:C:683:HOH:O	2.18	0.42
1:D:220:ALA:O	1:D:221:ALA:C	2.57	0.42
1:E:182:PRO:HB3	2:E:606:HOH:O	2.18	0.42
1:F:150:ILE:C	1:F:152:ASN:N	2.73	0.42
1:H:311:GLY:CA	2:H:589:HOH:O	2.67	0.42
1:I:60:SER:HA	1:I:264:HIS:HA	2.00	0.42
1:I:124:LEU:O	1:I:125:ALA:HB3	2.19	0.42
1:K:235:LEU:HD12	1:K:404:ARG:HH11	1.85	0.42
1:K:242:HIS:CE1	2:K:616:HOH:O	2.72	0.42
1:L:94:PRO:HB2	1:L:105:GLY:N	2.33	0.42
1:A:220:ALA:O	1:A:221:ALA:C	2.57	0.42
1:B:71:PRO:HD2	1:B:74:SER:HB3	2.00	0.42
1:B:235:LEU:HD12	1:B:404:ARG:NH1	2.34	0.42
1:B:380:PRO:HB2	1:B:390:THR:HG21	2.01	0.42
1:D:229:PHE:HB2	1:D:230:ILE:H	1.69	0.42
1:D:343:ALA:CB	1:D:390:THR:HB	2.49	0.42
1:D:344:THR:HA	1:D:348:THR:HG21	2.02	0.42
1:F:36:ARG:NH1	2:F:674:HOH:O	2.53	0.42
1:F:337:ASN:HA	1:F:341:ARG:HG2	2.02	0.42
1:G:372:MET:HG2	1:G:373:GLY:H	1.84	0.42
1:H:311:GLY:HA3	1:H:325:GLY:O	2.20	0.42
1:I:229:PHE:HB2	1:I:230:ILE:H	1.69	0.42
1:I:235:LEU:HD12	1:I:404:ARG:NH1	2.34	0.42
1:K:249:LEU:HD11	1:K:416:VAL:HA	2.00	0.42
1:A:104:LEU:HD12	1:A:143:PHE:HE2	1.85	0.42
1:A:234:ARG:HB2	1:A:407:ALA:HB3	2.02	0.42
1:C:86:PRO:HG2	1:C:401:HIS:CG	2.54	0.42
1:C:345:ASN:H	1:C:348:THR:HB	1.84	0.42
1:D:414:HIS:HD2	2:D:541:HOH:O	2.03	0.42
1:E:318:ASP:HB3	2:E:665:HOH:O	2.19	0.42
1:H:137:GLU:HB3	2:H:566:HOH:O	2.19	0.42
1:H:213:SER:HB2	1:H:214:PHE:H	1.43	0.42
1:J:112:ALA:O	1:J:113:LEU:HB2	2.20	0.42
1:K:337:ASN:HA	1:K:341:ARG:HG2	2.02	0.42
1:A:17:PRO:HB3	2:A:536:HOH:O	2.19	0.42
1:A:150:ILE:HD13	2:A:512:HOH:O	2.19	0.42
1:E:264:HIS:HD2	2:E:447:HOH:O	2.01	0.42
1:E:289:PRO:HB2	2:I:702:HOH:O	2.19	0.42
1:F:331:GLY:HA2	1:F:332:PRO:HD3	1.93	0.42
1:H:235:LEU:HD23	1:H:236:ASP:N	2.35	0.42
1:H:249:LEU:HD11	1:H:416:VAL:CA	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:152:ASN:HB3	1:J:153:LEU:H	1.68	0.42
1:J:395:LEU:HD21	1:J:415:LEU:HB2	2.02	0.42
1:A:370:SER:HB2	1:I:170:GLN:HG3	2.01	0.42
1:B:426:SER:O	1:B:426:SER:CB	2.68	0.42
1:D:75:GLY:O	1:D:258:ILE:HD11	2.20	0.42
1:D:206:VAL:HG23	2:D:658:HOH:O	2.20	0.42
1:D:273:CYS:HB2	2:D:510:HOH:O	2.20	0.42
1:E:150:ILE:C	1:E:152:ASN:N	2.72	0.42
1:E:404:ARG:HG2	1:H:144:ARG:NH2	2.34	0.42
2:I:449:HOH:O	1:L:374:CYS:CB	2.55	0.42
1:K:170:GLN:HG3	1:L:370:SER:HB2	2.01	0.42
1:L:337:ASN:HA	1:L:341:ARG:HG2	2.02	0.42
1:L:405:GLU:OE1	2:L:669:HOH:O	2.21	0.42
1:B:229:PHE:HB2	1:B:230:ILE:H	1.69	0.42
1:C:303:LEU:O	1:C:390:THR:HA	2.20	0.42
1:E:339:ASN:CB	2:E:446:HOH:O	2.67	0.42
1:H:303:LEU:O	1:H:390:THR:HA	2.19	0.42
1:J:311:GLY:HA3	1:J:325:GLY:O	2.20	0.42
1:K:154:ASN:HB2	2:K:482:HOH:O	2.20	0.42
1:B:94:PRO:HB2	1:B:105:GLY:N	2.35	0.41
1:B:104:LEU:HD12	1:B:143:PHE:HE2	1.84	0.41
1:B:230:ILE:HD13	2:B:602:HOH:O	2.20	0.41
1:C:344:THR:CG2	2:C:612:HOH:O	2.69	0.41
1:C:362:PRO:HG3	2:C:550:HOH:O	2.20	0.41
1:D:60:SER:HA	1:D:264:HIS:HA	2.01	0.41
1:D:94:PRO:HB2	1:D:105:GLY:N	2.34	0.41
1:D:337:ASN:HA	1:D:341:ARG:HG2	2.02	0.41
1:E:94:PRO:HB2	1:E:105:GLY:N	2.34	0.41
1:E:152:ASN:HB3	1:E:153:LEU:H	1.70	0.41
1:F:152:ASN:HB3	1:F:153:LEU:H	1.69	0.41
1:G:152:ASN:HB3	1:G:153:LEU:H	1.68	0.41
1:I:249:LEU:HD11	1:I:416:VAL:HA	2.00	0.41
1:J:277:GLY:HA3	2:J:624:HOH:O	2.20	0.41
1:K:303:LEU:O	1:K:390:THR:HA	2.20	0.41
1:L:60:SER:HA	1:L:264:HIS:HA	2.02	0.41
1:A:65:ARG:NH2	1:A:255:GLU:HG3	2.33	0.41
1:A:323:ASN:HA	2:A:619:HOH:O	2.13	0.41
1:B:287:LEU:C	2:B:624:HOH:O	2.59	0.41
1:C:413:ALA:HB1	2:C:617:HOH:O	2.20	0.41
1:D:116:PRO:HG3	2:D:461:HOH:O	2.20	0.41
1:E:115:ALA:CB	2:E:501:HOH:O	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:ILE:HD13	1:E:258:ILE:N	2.15	0.41
1:G:239:LEU:HD11	1:G:307:ASP:OD1	2.20	0.41
1:G:344:THR:HA	1:G:348:THR:HG21	2.00	0.41
1:H:60:SER:HA	1:H:264:HIS:HA	2.01	0.41
1:I:75:GLY:O	1:I:258:ILE:HD11	2.20	0.41
1:I:94:PRO:HB2	1:I:105:GLY:N	2.35	0.41
1:I:299:GLN:HB3	2:I:631:HOH:O	2.19	0.41
1:J:264:HIS:HD2	2:J:542:HOH:O	2.02	0.41
1:J:326:PRO:HD2	1:J:364:GLN:HE22	1.85	0.41
1:K:60:SER:HA	1:K:264:HIS:HA	2.01	0.41
1:E:70:SER:N	2:E:481:HOH:O	2.52	0.41
1:E:174:PRO:HA	1:E:175:PRO:HD3	1.79	0.41
1:F:126:GLY:O	1:F:213:SER:HB2	2.20	0.41
1:G:237:ASN:HA	1:G:240:SER:HB3	2.02	0.41
1:G:277:GLY:HA2	1:G:278:PRO:HA	1.77	0.41
1:G:305:SER:HB3	1:G:380:PRO:HG2	2.02	0.41
1:I:220:ALA:O	1:I:221:ALA:C	2.58	0.41
1:K:396:PRO:HA	2:K:686:HOH:O	2.20	0.41
1:L:22:ALA:HB3	2:L:573:HOH:O	2.20	0.41
1:L:312:VAL:CG2	2:L:599:HOH:O	2.67	0.41
1:A:238:LEU:C	1:A:240:SER:H	2.24	0.41
1:A:311:GLY:HA3	1:A:325:GLY:O	2.19	0.41
1:C:391:VAL:HG13	2:C:612:HOH:O	2.19	0.41
1:E:91:LYS:HB2	1:E:94:PRO:HB3	2.02	0.41
1:G:235:LEU:HD12	1:G:404:ARG:NH1	2.35	0.41
1:J:124:LEU:O	1:J:125:ALA:HB3	2.20	0.41
1:A:399:ALA:HB2	1:D:147:ILE:H	1.85	0.41
1:A:417:LYS:HE2	2:A:473:HOH:O	2.20	0.41
1:B:426:SER:O	1:B:426:SER:HB3	2.20	0.41
1:D:182:PRO:HB2	2:D:540:HOH:O	2.11	0.41
1:E:382:THR:HG21	2:E:548:HOH:O	2.20	0.41
1:F:104:LEU:HD12	1:F:143:PHE:HE2	1.85	0.41
1:F:174:PRO:HA	1:F:175:PRO:HD3	1.79	0.41
1:F:324:HIS:N	2:F:441:HOH:O	2.32	0.41
1:H:91:LYS:HB2	1:H:94:PRO:HB3	2.01	0.41
1:I:405:GLU:CG	1:L:146:ALA:HA	2.50	0.41
1:K:311:GLY:HA3	1:K:325:GLY:O	2.21	0.41
1:L:221:ALA:N	2:L:560:HOH:O	2.53	0.41
1:L:235:LEU:HD23	1:L:236:ASP:N	2.36	0.41
1:A:114:PHE:HB2	1:A:115:ALA:H	1.73	0.41
1:A:174:PRO:HA	1:A:175:PRO:HD3	1.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:SER:HA	1:I:109:TYR:HA	2.02	0.41
1:B:57:ASN:HB3	2:B:595:HOH:O	2.20	0.41
1:B:277:GLY:HA2	1:B:278:PRO:HA	1.78	0.41
1:C:121:ASP:H	1:C:219:SER:HA	1.85	0.41
1:C:403:ILE:HD11	2:C:542:HOH:O	2.20	0.41
1:E:131:ARG:NE	2:E:539:HOH:O	2.53	0.41
1:E:285:ARG:NH1	2:E:566:HOH:O	2.53	0.41
1:E:405:GLU:CG	1:H:146:ALA:HA	2.50	0.41
1:F:26:LEU:HD22	1:F:124:LEU:HG	2.02	0.41
1:F:380:PRO:HB2	1:F:390:THR:HG21	2.03	0.41
1:H:59:SER:HB3	2:H:587:HOH:O	2.20	0.41
1:J:245:LEU:HD21	2:J:564:HOH:O	2.20	0.41
1:K:150:ILE:C	1:K:152:ASN:N	2.74	0.41
1:K:239:LEU:HD11	1:K:307:ASP:OD1	2.21	0.41
1:K:305:SER:HB3	1:K:380:PRO:HG2	2.02	0.41
1:L:328:LEU:HD21	2:L:501:HOH:O	2.04	0.41
1:B:224:GLY:HA3	1:K:120:ARG:HH22	1.85	0.41
1:B:339:ASN:O	2:B:468:HOH:O	2.21	0.41
1:E:226:ASN:ND2	1:H:144:ARG:HE	2.19	0.41
1:E:277:GLY:HA2	1:E:278:PRO:HA	1.75	0.41
1:E:320:HIS:HD2	2:E:622:HOH:O	2.03	0.41
1:F:372:MET:HG2	1:F:373:GLY:H	1.85	0.41
1:H:104:LEU:HD12	1:H:143:PHE:HE2	1.86	0.41
1:H:259:LEU:HD22	1:H:423:TYR:CD1	2.55	0.41
1:H:324:HIS:CD2	1:H:324:HIS:N	2.89	0.41
1:H:333:VAL:HA	1:H:393:ILE:HG22	2.02	0.41
1:K:112:ALA:O	1:K:113:LEU:HB2	2.20	0.41
1:L:335:LYS:HZ3	1:L:365:SER:HB2	1.85	0.41
1:C:146:ALA:HA	1:F:405:GLU:CG	2.51	0.41
1:C:422:PHE:C	1:C:424:ALA:H	2.24	0.41
1:D:120:ARG:HB2	1:D:220:ALA:H	1.86	0.41
1:H:331:GLY:HA2	1:H:332:PRO:HD3	1.93	0.41
1:I:150:ILE:C	1:I:152:ASN:N	2.72	0.41
1:I:320:HIS:CD2	2:I:576:HOH:O	2.73	0.41
1:J:270:CYS:O	1:J:271:SER:CB	2.68	0.41
1:K:36:ARG:CB	2:K:574:HOH:O	2.68	0.41
1:K:238:LEU:C	1:K:240:SER:H	2.24	0.41
1:A:150:ILE:C	1:A:152:ASN:N	2.74	0.41
1:A:213:SER:O	1:A:214:PHE:HB2	2.20	0.41
1:B:135:LYS:CD	2:B:629:HOH:O	2.67	0.41
1:B:170:GLN:NE2	1:C:369:ARG:HE	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:PHE:HD1	1:B:399:ALA:H	1.69	0.41
1:E:378:ILE:CG2	2:E:504:HOH:O	2.52	0.41
1:F:71:PRO:HD2	1:F:74:SER:HB3	2.03	0.41
1:F:75:GLY:O	1:F:258:ILE:HD11	2.21	0.41
1:F:324:HIS:H	1:F:324:HIS:CD2	2.39	0.41
1:F:338:SER:HA	1:H:109:TYR:HA	2.03	0.41
1:F:392:ASP:N	2:F:506:HOH:O	2.53	0.41
1:F:422:PHE:C	1:F:424:ALA:H	2.24	0.41
1:G:124:LEU:O	1:G:125:ALA:HB3	2.20	0.41
1:G:150:ILE:CD1	2:J:461:HOH:O	2.64	0.41
1:G:345:ASN:H	1:G:348:THR:HB	1.85	0.41
1:H:151:PRO:HA	2:H:631:HOH:O	2.20	0.41
1:H:238:LEU:C	1:H:240:SER:H	2.24	0.41
1:H:345:ASN:H	1:H:348:THR:HB	1.86	0.41
1:I:65:ARG:O	1:I:258:ILE:HA	2.21	0.41
1:I:176:ILE:HB	2:I:480:HOH:O	2.20	0.41
1:I:235:LEU:HD21	1:I:403:ILE:HG22	2.03	0.41
1:J:223:VAL:HG22	1:J:235:LEU:HB3	2.03	0.41
1:K:75:GLY:O	1:K:258:ILE:HD11	2.20	0.41
1:K:94:PRO:HB2	1:K:105:GLY:N	2.36	0.41
1:L:366:PHE:HZ	2:L:621:HOH:O	2.03	0.41
1:L:401:HIS:HE1	2:L:567:HOH:O	2.03	0.41
1:B:335:LYS:HZ3	1:B:365:SER:HB2	1.86	0.41
1:D:272:HIS:HB3	1:D:273:CYS:H	1.68	0.41
1:E:65:ARG:CG	2:E:574:HOH:O	2.69	0.41
1:H:150:ILE:C	1:H:152:ASN:N	2.74	0.41
1:I:240:SER:HA	2:I:690:HOH:O	2.20	0.41
1:K:326:PRO:HD2	1:K:364:GLN:HE22	1.86	0.41
1:A:182:PRO:HB3	2:A:552:HOH:O	2.21	0.40
1:A:303:LEU:O	1:A:390:THR:HA	2.22	0.40
1:A:403:ILE:HG23	2:A:543:HOH:O	2.20	0.40
1:A:417:LYS:HD2	2:A:621:HOH:O	2.20	0.40
1:C:237:ASN:HA	1:C:240:SER:HB3	2.03	0.40
2:C:486:HOH:O	1:F:229:PHE:HD1	1.86	0.40
1:D:174:PRO:HA	1:D:175:PRO:HD3	1.80	0.40
1:D:305:SER:HB3	1:D:380:PRO:HG2	2.03	0.40
1:E:345:ASN:H	1:E:348:THR:HB	1.87	0.40
1:F:378:ILE:HD13	1:F:378:ILE:H	1.85	0.40
1:H:16:SER:N	1:H:17:PRO:HD2	2.35	0.40
1:H:65:ARG:O	1:H:258:ILE:HA	2.21	0.40
1:I:180:LEU:O	2:I:497:HOH:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:137:GLU:CG	2:J:509:HOH:O	2.65	0.40
1:J:229:PHE:HB2	1:J:230:ILE:H	1.68	0.40
1:J:299:GLN:NE2	2:J:495:HOH:O	2.50	0.40
1:L:395:LEU:HD21	1:L:415:LEU:HB2	2.03	0.40
1:A:77:ARG:HG2	2:A:651:HOH:O	2.20	0.40
1:A:94:PRO:HB2	1:A:105:GLY:N	2.37	0.40
1:C:26:LEU:HG	1:C:27:ALA:N	2.28	0.40
1:E:13:LEU:HB3	2:E:621:HOH:O	2.20	0.40
1:E:235:LEU:HD23	1:E:236:ASP:N	2.36	0.40
1:G:235:LEU:HD21	1:G:403:ILE:HG22	2.02	0.40
1:G:280:LEU:HD21	2:G:613:HOH:O	2.21	0.40
1:H:222:VAL:CG2	2:H:520:HOH:O	2.61	0.40
1:H:335:LYS:HZ2	1:H:335:LYS:HB2	1.86	0.40
1:J:65:ARG:NH2	1:J:255:GLU:HG3	2.33	0.40
1:J:264:HIS:CD2	2:J:542:HOH:O	2.74	0.40
2:J:495:HOH:O	1:L:56:ARG:HD2	2.19	0.40
1:K:109:TYR:HA	1:L:338:SER:HA	2.02	0.40
1:K:177:ILE:HG23	1:K:178:ALA:H	1.85	0.40
1:C:21:HIS:NE2	1:C:241:CYS:HB3	2.36	0.40
1:C:235:LEU:HD12	1:C:404:ARG:HH11	1.86	0.40
1:E:120:ARG:HH22	1:H:224:GLY:HA3	1.86	0.40
1:E:285:ARG:CZ	2:E:566:HOH:O	2.67	0.40
1:E:422:PHE:C	1:E:424:ALA:H	2.23	0.40
1:F:65:ARG:NH2	2:F:527:HOH:O	2.53	0.40
1:G:104:LEU:HD12	1:G:143:PHE:HE2	1.86	0.40
1:G:226:ASN:ND2	1:J:144:ARG:HE	2.19	0.40
1:G:339:ASN:HB3	2:G:490:HOH:O	2.21	0.40
1:H:21:HIS:NE2	1:H:241:CYS:HB3	2.36	0.40
1:H:288:LEU:HD22	1:H:289:PRO:HD2	2.02	0.40
1:J:369:ARG:HB3	1:L:170:GLN:NE2	2.36	0.40
1:L:249:LEU:HD11	1:L:416:VAL:CA	2.51	0.40
1:L:311:GLY:HA3	1:L:325:GLY:O	2.20	0.40
1:A:178:ALA:HA	2:A:668:HOH:O	2.20	0.40
1:A:237:ASN:HA	1:A:240:SER:HB3	2.04	0.40
1:B:18:THR:HG23	1:B:223:VAL:HB	2.04	0.40
1:B:122:LEU:HD11	1:B:138:SER:HB2	2.03	0.40
1:D:30:LEU:HD22	1:D:83:THR:HG22	2.04	0.40
1:E:249:LEU:HD11	1:E:416:VAL:HA	2.03	0.40
1:F:26:LEU:HB2	1:F:124:LEU:HD11	2.03	0.40
1:F:303:LEU:O	1:F:390:THR:HA	2.21	0.40
1:G:150:ILE:C	1:G:152:ASN:N	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:324:HIS:H	1:G:324:HIS:CD2	2.39	0.40
1:J:104:LEU:HD12	1:J:143:PHE:HE2	1.85	0.40
1:K:151:PRO:CB	2:K:597:HOH:O	2.59	0.40
1:K:210:TYR:HD1	2:K:592:HOH:O	2.04	0.40
1:L:104:LEU:HD12	1:L:143:PHE:HE2	1.87	0.40
1:A:71:PRO:HD2	1:A:74:SER:HB3	2.03	0.40
1:A:109:TYR:HA	1:E:338:SER:HA	2.02	0.40
1:A:235:LEU:HD23	1:A:236:ASP:N	2.36	0.40
1:B:16:SER:N	1:B:17:PRO:HD2	2.35	0.40
1:B:101:PHE:CD2	1:B:179:GLN:HG2	2.49	0.40
1:B:119:ASP:HA	2:B:694:HOH:O	2.21	0.40
1:E:406:LEU:N	2:E:505:HOH:O	2.47	0.40
1:F:16:SER:N	1:F:17:PRO:HD2	2.36	0.40
1:G:146:ALA:HA	1:J:405:GLU:CG	2.52	0.40
1:G:238:LEU:C	1:G:240:SER:H	2.23	0.40
1:G:337:ASN:HA	1:G:341:ARG:HG2	2.03	0.40
1:I:55:THR:CB	2:I:511:HOH:O	2.50	0.40
1:I:270:CYS:O	1:I:271:SER:CB	2.69	0.40
1:I:406:LEU:CA	2:I:435:HOH:O	2.65	0.40
1:J:248:LEU:HG	2:J:647:HOH:O	2.20	0.40
1:J:277:GLY:HA2	1:J:278:PRO:HA	1.77	0.40
1:K:213:SER:HB2	2:K:568:HOH:O	2.22	0.40
1:K:417:LYS:HD3	2:K:695:HOH:O	2.19	0.40
1:L:248:LEU:HG	2:L:630:HOH:O	2.21	0.40
1:L:288:LEU:HD22	1:L:289:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	369/428 (86%)	246 (67%)	82 (22%)	41 (11%)	0 2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	369/428 (86%)	241 (65%)	84 (23%)	44 (12%)	0	1
1	C	369/428 (86%)	245 (66%)	81 (22%)	43 (12%)	0	1
1	D	369/428 (86%)	240 (65%)	86 (23%)	43 (12%)	0	1
1	E	369/428 (86%)	243 (66%)	84 (23%)	42 (11%)	0	2
1	F	369/428 (86%)	243 (66%)	85 (23%)	41 (11%)	0	2
1	G	369/428 (86%)	242 (66%)	90 (24%)	37 (10%)	0	2
1	H	369/428 (86%)	245 (66%)	86 (23%)	38 (10%)	0	2
1	I	369/428 (86%)	240 (65%)	88 (24%)	41 (11%)	0	2
1	J	369/428 (86%)	241 (65%)	85 (23%)	43 (12%)	0	1
1	K	369/428 (86%)	244 (66%)	83 (22%)	42 (11%)	0	2
1	L	369/428 (86%)	244 (66%)	83 (22%)	42 (11%)	0	2
All	All	4428/5136 (86%)	2914 (66%)	1017 (23%)	497 (11%)	0	2

All (497) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	PRO
1	A	125	ALA
1	A	131	ARG
1	A	207	VAL
1	A	214	PHE
1	A	289	PRO
1	A	361	VAL
1	A	381	ILE
1	A	406	LEU
1	A	407	ALA
1	B	116	PRO
1	B	125	ALA
1	B	131	ARG
1	B	207	VAL
1	B	214	PHE
1	B	221	ALA
1	B	289	PRO
1	B	361	VAL
1	B	381	ILE
1	B	406	LEU
1	C	116	PRO
1	C	125	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	131	ARG
1	C	207	VAL
1	C	289	PRO
1	C	361	VAL
1	C	381	ILE
1	C	406	LEU
1	D	116	PRO
1	D	125	ALA
1	D	131	ARG
1	D	207	VAL
1	D	213	SER
1	D	289	PRO
1	D	338	SER
1	D	361	VAL
1	D	381	ILE
1	E	116	PRO
1	E	125	ALA
1	E	131	ARG
1	E	207	VAL
1	E	271	SER
1	E	289	PRO
1	E	361	VAL
1	E	381	ILE
1	E	406	LEU
1	F	116	PRO
1	F	125	ALA
1	F	131	ARG
1	F	207	VAL
1	F	289	PRO
1	F	361	VAL
1	F	381	ILE
1	F	406	LEU
1	G	116	PRO
1	G	125	ALA
1	G	131	ARG
1	G	207	VAL
1	G	221	ALA
1	G	272	HIS
1	G	289	PRO
1	G	361	VAL
1	G	381	ILE
1	H	116	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	125	ALA
1	H	131	ARG
1	H	207	VAL
1	H	289	PRO
1	H	361	VAL
1	H	381	ILE
1	I	116	PRO
1	I	125	ALA
1	I	131	ARG
1	I	207	VAL
1	I	289	PRO
1	I	361	VAL
1	I	381	ILE
1	I	406	LEU
1	J	116	PRO
1	J	125	ALA
1	J	131	ARG
1	J	207	VAL
1	J	213	SER
1	J	214	PHE
1	J	289	PRO
1	J	361	VAL
1	J	381	ILE
1	K	116	PRO
1	K	125	ALA
1	K	131	ARG
1	K	207	VAL
1	K	289	PRO
1	K	361	VAL
1	K	381	ILE
1	L	116	PRO
1	L	125	ALA
1	L	131	ARG
1	L	207	VAL
1	L	214	PHE
1	L	289	PRO
1	L	361	VAL
1	L	381	ILE
1	L	406	LEU
1	A	170	GLN
1	A	208	LEU
1	A	213	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	221	ALA
1	A	271	SER
1	A	272	HIS
1	A	295	SER
1	A	322	ALA
1	A	338	SER
1	A	343	ALA
1	A	344	THR
1	A	404	ARG
1	B	170	GLN
1	B	213	SER
1	B	271	SER
1	B	272	HIS
1	B	295	SER
1	B	338	SER
1	B	343	ALA
1	B	344	THR
1	C	170	GLN
1	C	208	LEU
1	C	271	SER
1	C	272	HIS
1	C	322	ALA
1	C	338	SER
1	C	343	ALA
1	C	344	THR
1	C	407	ALA
1	D	170	GLN
1	D	221	ALA
1	D	272	HIS
1	D	295	SER
1	D	322	ALA
1	D	343	ALA
1	D	406	LEU
1	E	170	GLN
1	E	221	ALA
1	E	272	HIS
1	E	295	SER
1	E	322	ALA
1	E	338	SER
1	E	343	ALA
1	E	344	THR
1	E	404	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	407	ALA
1	F	170	GLN
1	F	221	ALA
1	F	271	SER
1	F	272	HIS
1	F	322	ALA
1	F	338	SER
1	F	343	ALA
1	F	344	THR
1	F	404	ARG
1	G	170	GLN
1	G	271	SER
1	G	322	ALA
1	G	338	SER
1	G	343	ALA
1	G	344	THR
1	G	406	LEU
1	H	170	GLN
1	H	221	ALA
1	H	272	HIS
1	H	295	SER
1	H	322	ALA
1	H	338	SER
1	H	343	ALA
1	H	344	THR
1	H	404	ARG
1	H	406	LEU
1	I	170	GLN
1	I	221	ALA
1	I	271	SER
1	I	272	HIS
1	I	295	SER
1	I	322	ALA
1	I	338	SER
1	I	343	ALA
1	J	170	GLN
1	J	221	ALA
1	J	271	SER
1	J	272	HIS
1	J	295	SER
1	J	322	ALA
1	J	338	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	343	ALA
1	J	344	THR
1	J	404	ARG
1	J	406	LEU
1	J	407	ALA
1	K	170	GLN
1	K	205	ASP
1	K	208	LEU
1	K	213	SER
1	K	221	ALA
1	K	271	SER
1	K	272	HIS
1	K	322	ALA
1	K	338	SER
1	K	343	ALA
1	K	404	ARG
1	K	406	LEU
1	L	170	GLN
1	L	213	SER
1	L	221	ALA
1	L	271	SER
1	L	272	HIS
1	L	295	SER
1	L	322	ALA
1	L	338	SER
1	L	343	ALA
1	L	404	ARG
1	L	407	ALA
1	A	114	PHE
1	A	118	PHE
1	A	121	ASP
1	A	140	LEU
1	A	205	ASP
1	A	244	GLY
1	A	287	LEU
1	B	114	PHE
1	B	121	ASP
1	B	205	ASP
1	B	208	LEU
1	B	287	LEU
1	B	322	ALA
1	B	404	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	114	PHE
1	C	118	PHE
1	C	121	ASP
1	C	151	PRO
1	C	205	ASP
1	C	221	ALA
1	C	244	GLY
1	C	287	LEU
1	C	295	SER
1	C	404	ARG
1	D	114	PHE
1	D	121	ASP
1	D	140	LEU
1	D	151	PRO
1	D	205	ASP
1	D	208	LEU
1	D	244	GLY
1	D	271	SER
1	D	287	LEU
1	D	325	GLY
1	D	344	THR
1	D	404	ARG
1	E	114	PHE
1	E	118	PHE
1	E	140	LEU
1	E	151	PRO
1	E	205	ASP
1	E	208	LEU
1	E	244	GLY
1	E	287	LEU
1	F	114	PHE
1	F	118	PHE
1	F	121	ASP
1	F	140	LEU
1	F	151	PRO
1	F	205	ASP
1	F	208	LEU
1	F	287	LEU
1	F	295	SER
1	F	407	ALA
1	G	114	PHE
1	G	121	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	151	PRO
1	G	205	ASP
1	G	208	LEU
1	G	287	LEU
1	G	295	SER
1	G	404	ARG
1	H	114	PHE
1	H	118	PHE
1	H	121	ASP
1	H	140	LEU
1	H	151	PRO
1	H	205	ASP
1	H	208	LEU
1	H	214	PHE
1	H	271	SER
1	H	287	LEU
1	I	114	PHE
1	I	121	ASP
1	I	140	LEU
1	I	151	PRO
1	I	205	ASP
1	I	208	LEU
1	I	287	LEU
1	I	325	GLY
1	I	344	THR
1	I	404	ARG
1	I	407	ALA
1	J	114	PHE
1	J	118	PHE
1	J	121	ASP
1	J	151	PRO
1	J	205	ASP
1	J	208	LEU
1	J	244	GLY
1	J	287	LEU
1	K	114	PHE
1	K	118	PHE
1	K	140	LEU
1	K	172	GLU
1	K	244	GLY
1	K	287	LEU
1	K	344	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	375	GLY
1	K	407	ALA
1	L	72	LEU
1	L	114	PHE
1	L	121	ASP
1	L	205	ASP
1	L	208	LEU
1	L	287	LEU
1	L	344	THR
1	A	56	ARG
1	A	72	LEU
1	A	92	PRO
1	A	151	PRO
1	A	341	ARG
1	A	360	GLU
1	B	56	ARG
1	B	118	PHE
1	B	140	LEU
1	B	151	PRO
1	B	244	GLY
1	B	325	GLY
1	B	341	ARG
1	B	360	GLU
1	B	423	TYR
1	C	140	LEU
1	C	172	GLU
1	C	341	ARG
1	C	360	GLU
1	C	367	VAL
1	D	56	ARG
1	D	72	LEU
1	D	118	PHE
1	D	220	ALA
1	D	360	GLU
1	D	407	ALA
1	E	56	ARG
1	E	92	PRO
1	E	121	ASP
1	E	325	GLY
1	E	341	ARG
1	E	360	GLU
1	E	423	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	172	GLU
1	F	244	GLY
1	F	360	GLU
1	G	72	LEU
1	G	118	PHE
1	G	140	LEU
1	G	244	GLY
1	G	325	GLY
1	G	360	GLU
1	G	407	ALA
1	H	56	ARG
1	H	244	GLY
1	H	325	GLY
1	H	341	ARG
1	H	360	GLU
1	H	407	ALA
1	I	72	LEU
1	I	118	PHE
1	I	220	ALA
1	I	244	GLY
1	I	341	ARG
1	I	360	GLU
1	J	72	LEU
1	J	341	ARG
1	J	360	GLU
1	K	56	ARG
1	K	92	PRO
1	K	121	ASP
1	K	151	PRO
1	K	295	SER
1	K	325	GLY
1	K	341	ARG
1	K	360	GLU
1	L	56	ARG
1	L	118	PHE
1	L	151	PRO
1	L	244	GLY
1	L	341	ARG
1	L	360	GLU
1	A	288	LEU
1	A	325	GLY
1	A	405	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	72	LEU
1	B	220	ALA
1	B	233	ALA
1	B	288	LEU
1	B	367	VAL
1	B	405	GLU
1	B	407	ALA
1	C	56	ARG
1	C	72	LEU
1	C	92	PRO
1	C	233	ALA
1	C	288	LEU
1	C	325	GLY
1	C	405	GLU
1	D	92	PRO
1	D	237	ASN
1	D	288	LEU
1	D	341	ARG
1	E	72	LEU
1	E	288	LEU
1	E	367	VAL
1	E	375	GLY
1	E	405	GLU
1	F	56	ARG
1	F	72	LEU
1	F	213	SER
1	F	288	LEU
1	F	325	GLY
1	F	341	ARG
1	F	405	GLU
1	G	56	ARG
1	G	92	PRO
1	G	288	LEU
1	G	367	VAL
1	G	405	GLU
1	H	72	LEU
1	H	92	PRO
1	H	288	LEU
1	H	367	VAL
1	H	405	GLU
1	I	56	ARG
1	I	92	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	288	LEU
1	I	367	VAL
1	I	405	GLU
1	I	423	TYR
1	J	56	ARG
1	J	92	PRO
1	J	140	LEU
1	J	288	LEU
1	J	367	VAL
1	J	405	GLU
1	K	220	ALA
1	K	288	LEU
1	K	367	VAL
1	L	92	PRO
1	L	140	LEU
1	L	288	LEU
1	L	325	GLY
1	L	405	GLU
1	A	367	VAL
1	B	92	PRO
1	C	237	ASN
1	D	367	VAL
1	D	405	GLU
1	E	237	ASN
1	F	92	PRO
1	F	367	VAL
1	I	379	GLY
1	J	233	ALA
1	J	325	GLY
1	J	375	GLY
1	K	405	GLU
1	L	367	VAL
1	L	423	TYR
1	D	375	GLY
1	D	380	PRO
1	E	16	SER
1	A	16	SER
1	A	379	GLY
1	B	16	SER
1	C	16	SER
1	C	375	GLY
1	C	379	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	94	PRO
1	F	94	PRO
1	G	16	SER
1	K	16	SER
1	K	94	PRO
1	L	16	SER
1	B	94	PRO
1	D	16	SER
1	F	16	SER
1	I	16	SER
1	J	16	SER
1	J	94	PRO
1	L	375	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/344 (88%)	268 (88%)	35 (12%)	5	23
1	B	303/344 (88%)	266 (88%)	37 (12%)	5	21
1	C	303/344 (88%)	266 (88%)	37 (12%)	5	21
1	D	303/344 (88%)	269 (89%)	34 (11%)	6	24
1	E	303/344 (88%)	266 (88%)	37 (12%)	5	21
1	F	303/344 (88%)	268 (88%)	35 (12%)	5	23
1	G	303/344 (88%)	267 (88%)	36 (12%)	5	22
1	H	303/344 (88%)	268 (88%)	35 (12%)	5	23
1	I	303/344 (88%)	264 (87%)	39 (13%)	4	19
1	J	303/344 (88%)	269 (89%)	34 (11%)	6	24
1	K	303/344 (88%)	266 (88%)	37 (12%)	5	21
1	L	303/344 (88%)	268 (88%)	35 (12%)	5	23
All	All	3636/4128 (88%)	3205 (88%)	431 (12%)	5	22

All (431) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	51	ARG
1	A	65	ARG
1	A	73	GLU
1	A	122	LEU
1	A	123	SER
1	A	140	LEU
1	A	149	VAL
1	A	213	SER
1	A	215	TYR
1	A	218	GLN
1	A	241	CYS
1	A	249	LEU
1	A	258	ILE
1	A	284	LEU
1	A	286	ARG
1	A	288	LEU
1	A	294	PHE
1	A	300	ARG
1	A	305	SER
1	A	323	ASN
1	A	337	ASN
1	A	341	ARG
1	A	346	SER
1	A	361	VAL
1	A	366	PHE
1	A	367	VAL
1	A	378	ILE
1	A	382	THR
1	A	398	PHE
1	A	403	ILE
1	A	404	ARG
1	A	410	HIS
1	A	411	ASP
1	A	412	LEU
1	B	13	LEU
1	B	51	ARG
1	B	65	ARG
1	B	73	GLU
1	B	122	LEU
1	B	123	SER
1	B	140	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	208	LEU
1	B	209	ASP
1	B	213	SER
1	B	215	TYR
1	B	218	GLN
1	B	241	CYS
1	B	249	LEU
1	B	258	ILE
1	B	284	LEU
1	B	286	ARG
1	B	288	LEU
1	B	294	PHE
1	B	300	ARG
1	B	305	SER
1	B	323	ASN
1	B	324	HIS
1	B	337	ASN
1	B	341	ARG
1	B	346	SER
1	B	361	VAL
1	B	366	PHE
1	B	367	VAL
1	B	378	ILE
1	B	382	THR
1	B	398	PHE
1	B	403	ILE
1	B	404	ARG
1	B	410	HIS
1	B	411	ASP
1	B	412	LEU
1	C	13	LEU
1	C	51	ARG
1	C	65	ARG
1	C	73	GLU
1	C	122	LEU
1	C	123	SER
1	C	149	VAL
1	C	180	LEU
1	C	208	LEU
1	C	209	ASP
1	C	213	SER
1	C	215	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	218	GLN
1	C	241	CYS
1	C	249	LEU
1	C	258	ILE
1	C	284	LEU
1	C	286	ARG
1	C	288	LEU
1	C	294	PHE
1	C	300	ARG
1	C	323	ASN
1	C	324	HIS
1	C	337	ASN
1	C	341	ARG
1	C	346	SER
1	C	361	VAL
1	C	366	PHE
1	C	367	VAL
1	C	378	ILE
1	C	382	THR
1	C	398	PHE
1	C	403	ILE
1	C	404	ARG
1	C	410	HIS
1	C	411	ASP
1	C	412	LEU
1	D	51	ARG
1	D	65	ARG
1	D	122	LEU
1	D	140	LEU
1	D	149	VAL
1	D	203	THR
1	D	208	LEU
1	D	214	PHE
1	D	215	TYR
1	D	218	GLN
1	D	241	CYS
1	D	249	LEU
1	D	258	ILE
1	D	284	LEU
1	D	286	ARG
1	D	288	LEU
1	D	294	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	300	ARG
1	D	323	ASN
1	D	324	HIS
1	D	337	ASN
1	D	341	ARG
1	D	346	SER
1	D	361	VAL
1	D	366	PHE
1	D	367	VAL
1	D	378	ILE
1	D	382	THR
1	D	398	PHE
1	D	403	ILE
1	D	404	ARG
1	D	410	HIS
1	D	411	ASP
1	D	412	LEU
1	E	11	ASP
1	E	51	ARG
1	E	55	THR
1	E	65	ARG
1	E	73	GLU
1	E	122	LEU
1	E	123	SER
1	E	140	LEU
1	E	149	VAL
1	E	208	LEU
1	E	213	SER
1	E	215	TYR
1	E	218	GLN
1	E	241	CYS
1	E	249	LEU
1	E	258	ILE
1	E	284	LEU
1	E	286	ARG
1	E	288	LEU
1	E	294	PHE
1	E	300	ARG
1	E	305	SER
1	E	323	ASN
1	E	324	HIS
1	E	337	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	341	ARG
1	E	361	VAL
1	E	366	PHE
1	E	367	VAL
1	E	378	ILE
1	E	382	THR
1	E	398	PHE
1	E	403	ILE
1	E	404	ARG
1	E	410	HIS
1	E	411	ASP
1	E	412	LEU
1	F	11	ASP
1	F	51	ARG
1	F	64	ILE
1	F	65	ARG
1	F	73	GLU
1	F	122	LEU
1	F	123	SER
1	F	140	LEU
1	F	209	ASP
1	F	215	TYR
1	F	218	GLN
1	F	241	CYS
1	F	249	LEU
1	F	258	ILE
1	F	284	LEU
1	F	286	ARG
1	F	288	LEU
1	F	294	PHE
1	F	300	ARG
1	F	323	ASN
1	F	324	HIS
1	F	337	ASN
1	F	341	ARG
1	F	346	SER
1	F	361	VAL
1	F	366	PHE
1	F	367	VAL
1	F	378	ILE
1	F	382	THR
1	F	398	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	403	ILE
1	F	404	ARG
1	F	410	HIS
1	F	411	ASP
1	F	412	LEU
1	G	11	ASP
1	G	13	LEU
1	G	51	ARG
1	G	65	ARG
1	G	73	GLU
1	G	122	LEU
1	G	123	SER
1	G	140	LEU
1	G	208	LEU
1	G	209	ASP
1	G	215	TYR
1	G	218	GLN
1	G	241	CYS
1	G	249	LEU
1	G	258	ILE
1	G	284	LEU
1	G	286	ARG
1	G	288	LEU
1	G	294	PHE
1	G	300	ARG
1	G	323	ASN
1	G	324	HIS
1	G	337	ASN
1	G	341	ARG
1	G	346	SER
1	G	361	VAL
1	G	366	PHE
1	G	367	VAL
1	G	378	ILE
1	G	382	THR
1	G	398	PHE
1	G	403	ILE
1	G	404	ARG
1	G	410	HIS
1	G	411	ASP
1	G	412	LEU
1	H	51	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	65	ARG
1	H	73	GLU
1	H	122	LEU
1	H	123	SER
1	H	140	LEU
1	H	208	LEU
1	H	209	ASP
1	H	213	SER
1	H	215	TYR
1	H	218	GLN
1	H	241	CYS
1	H	249	LEU
1	H	258	ILE
1	H	284	LEU
1	H	286	ARG
1	H	288	LEU
1	H	294	PHE
1	H	300	ARG
1	H	323	ASN
1	H	324	HIS
1	H	337	ASN
1	H	341	ARG
1	H	346	SER
1	H	361	VAL
1	H	366	PHE
1	H	367	VAL
1	H	378	ILE
1	H	382	THR
1	H	398	PHE
1	H	403	ILE
1	H	404	ARG
1	H	410	HIS
1	H	411	ASP
1	H	412	LEU
1	I	10	ILE
1	I	13	LEU
1	I	51	ARG
1	I	55	THR
1	I	65	ARG
1	I	73	GLU
1	I	122	LEU
1	I	123	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	140	LEU
1	I	149	VAL
1	I	208	LEU
1	I	209	ASP
1	I	213	SER
1	I	215	TYR
1	I	218	GLN
1	I	241	CYS
1	I	249	LEU
1	I	258	ILE
1	I	284	LEU
1	I	286	ARG
1	I	288	LEU
1	I	294	PHE
1	I	300	ARG
1	I	323	ASN
1	I	324	HIS
1	I	337	ASN
1	I	341	ARG
1	I	346	SER
1	I	361	VAL
1	I	366	PHE
1	I	367	VAL
1	I	378	ILE
1	I	382	THR
1	I	398	PHE
1	I	403	ILE
1	I	404	ARG
1	I	410	HIS
1	I	411	ASP
1	I	412	LEU
1	J	13	LEU
1	J	51	ARG
1	J	65	ARG
1	J	73	GLU
1	J	122	LEU
1	J	123	SER
1	J	149	VAL
1	J	180	LEU
1	J	208	LEU
1	J	215	TYR
1	J	218	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	241	CYS
1	J	249	LEU
1	J	258	ILE
1	J	284	LEU
1	J	286	ARG
1	J	288	LEU
1	J	294	PHE
1	J	300	ARG
1	J	305	SER
1	J	323	ASN
1	J	337	ASN
1	J	341	ARG
1	J	361	VAL
1	J	366	PHE
1	J	367	VAL
1	J	378	ILE
1	J	382	THR
1	J	398	PHE
1	J	403	ILE
1	J	404	ARG
1	J	410	HIS
1	J	411	ASP
1	J	412	LEU
1	K	13	LEU
1	K	51	ARG
1	K	55	THR
1	K	65	ARG
1	K	73	GLU
1	K	122	LEU
1	K	123	SER
1	K	149	VAL
1	K	208	LEU
1	K	214	PHE
1	K	215	TYR
1	K	218	GLN
1	K	241	CYS
1	K	249	LEU
1	K	258	ILE
1	K	284	LEU
1	K	286	ARG
1	K	288	LEU
1	K	294	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	300	ARG
1	K	323	ASN
1	K	324	HIS
1	K	337	ASN
1	K	341	ARG
1	K	346	SER
1	K	355	LEU
1	K	361	VAL
1	K	366	PHE
1	K	367	VAL
1	K	378	ILE
1	K	382	THR
1	K	398	PHE
1	K	403	ILE
1	K	404	ARG
1	K	410	HIS
1	K	411	ASP
1	K	412	LEU
1	L	13	LEU
1	L	51	ARG
1	L	65	ARG
1	L	73	GLU
1	L	122	LEU
1	L	123	SER
1	L	149	VAL
1	L	208	LEU
1	L	209	ASP
1	L	213	SER
1	L	215	TYR
1	L	218	GLN
1	L	241	CYS
1	L	249	LEU
1	L	258	ILE
1	L	284	LEU
1	L	286	ARG
1	L	288	LEU
1	L	294	PHE
1	L	300	ARG
1	L	323	ASN
1	L	337	ASN
1	L	341	ARG
1	L	346	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	361	VAL
1	L	366	PHE
1	L	367	VAL
1	L	378	ILE
1	L	382	THR
1	L	398	PHE
1	L	403	ILE
1	L	404	ARG
1	L	410	HIS
1	L	411	ASP
1	L	412	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	A	170	GLN
1	A	226	ASN
1	A	237	ASN
1	A	242	HIS
1	A	264	HIS
1	A	272	HIS
1	A	299	GLN
1	A	308	ASN
1	A	315	ASN
1	A	339	ASN
1	A	357	GLN
1	A	364	GLN
1	A	385	GLN
1	A	410	HIS
1	B	152	ASN
1	B	170	GLN
1	B	226	ASN
1	B	237	ASN
1	B	242	HIS
1	B	272	HIS
1	B	282	GLN
1	B	308	ASN
1	B	310	HIS
1	B	315	ASN
1	B	354	HIS
1	B	357	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	364	GLN
1	B	385	GLN
1	C	152	ASN
1	C	170	GLN
1	C	226	ASN
1	C	237	ASN
1	C	242	HIS
1	C	264	HIS
1	C	308	ASN
1	C	310	HIS
1	C	315	ASN
1	C	354	HIS
1	C	357	GLN
1	C	385	GLN
1	D	170	GLN
1	D	226	ASN
1	D	237	ASN
1	D	242	HIS
1	D	272	HIS
1	D	299	GLN
1	D	308	ASN
1	D	315	ASN
1	D	320	HIS
1	D	339	ASN
1	D	414	HIS
1	E	93	ASN
1	E	133	ASN
1	E	152	ASN
1	E	170	GLN
1	E	226	ASN
1	E	237	ASN
1	E	264	HIS
1	E	272	HIS
1	E	299	GLN
1	E	315	ASN
1	E	320	HIS
1	E	339	ASN
1	E	364	GLN
1	E	385	GLN
1	F	152	ASN
1	F	170	GLN
1	F	237	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	242	HIS
1	F	272	HIS
1	F	299	GLN
1	F	315	ASN
1	F	385	GLN
1	G	152	ASN
1	G	170	GLN
1	G	237	ASN
1	G	242	HIS
1	G	315	ASN
1	G	337	ASN
1	G	339	ASN
1	G	385	GLN
1	H	170	GLN
1	H	226	ASN
1	H	237	ASN
1	H	242	HIS
1	H	264	HIS
1	H	272	HIS
1	H	308	ASN
1	H	315	ASN
1	H	364	GLN
1	I	152	ASN
1	I	154	ASN
1	I	168	ASN
1	I	170	GLN
1	I	237	ASN
1	I	242	HIS
1	I	264	HIS
1	I	272	HIS
1	I	308	ASN
1	I	315	ASN
1	I	364	GLN
1	I	385	GLN
1	J	152	ASN
1	J	170	GLN
1	J	226	ASN
1	J	237	ASN
1	J	242	HIS
1	J	264	HIS
1	J	272	HIS
1	J	308	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	315	ASN
1	J	339	ASN
1	J	357	GLN
1	J	364	GLN
1	J	385	GLN
1	K	152	ASN
1	K	154	ASN
1	K	168	ASN
1	K	170	GLN
1	K	226	ASN
1	K	237	ASN
1	K	242	HIS
1	K	264	HIS
1	K	308	ASN
1	K	315	ASN
1	K	320	HIS
1	K	339	ASN
1	K	364	GLN
1	K	385	GLN
1	L	152	ASN
1	L	170	GLN
1	L	237	ASN
1	L	242	HIS
1	L	264	HIS
1	L	272	HIS
1	L	282	GLN
1	L	299	GLN
1	L	308	ASN
1	L	315	ASN
1	L	364	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.