Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 PM GMT

PDB ID	:	4ANI
Title	:	Structural basis for the intermolecular communication between DnaK and GrpE in the DnaK chaperone system from Geobacillus kaustophilus HTA426
Authors	:	Wu, C.-C.; Naveen, V.; Chien, C.-H.; Chang, Y.-W.; Hsiao, C.-D.
Deposited on	:	2012-03-19
Resolution	:	4.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

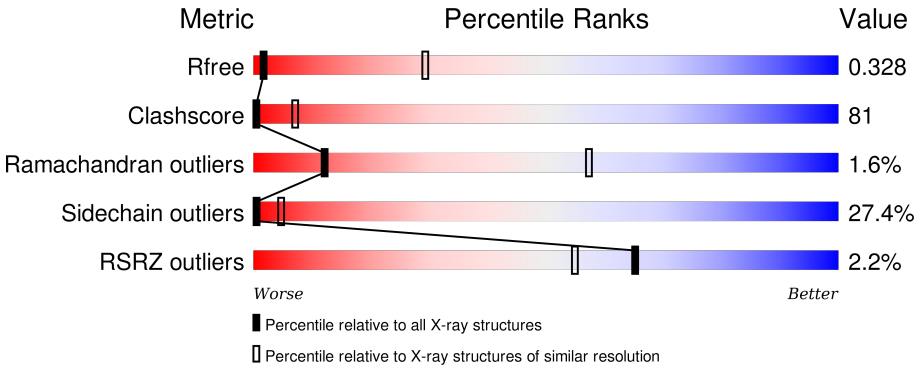
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.09 Å.

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



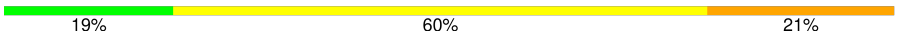
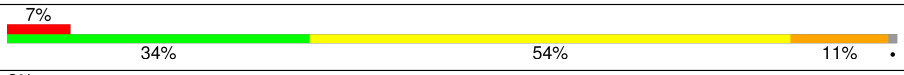
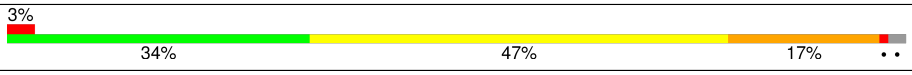
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	213	12% 45% 15% • 27%
1	B	213	17% 38% 16% • 28%
1	E	213	4% 32% 25% 6% 37%
1	F	213	33% 22% 6% 39%
2	C	509	24% 55% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	509	
2	G	509	
2	H	509	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18889 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 PROTEIN GRPE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1242	778	215	243	6			
1	B	154	Total	C	N	O	S	0	0	0
			1240	779	216	239	6			
1	E	135	Total	C	N	O	S	0	0	0
			820	498	160	160	2			
1	F	130	Total	C	N	O	S	0	0	0
			815	496	159	158	2			

- Molecule 2 is a protein called CHAPERONE PROTEIN DNAK.

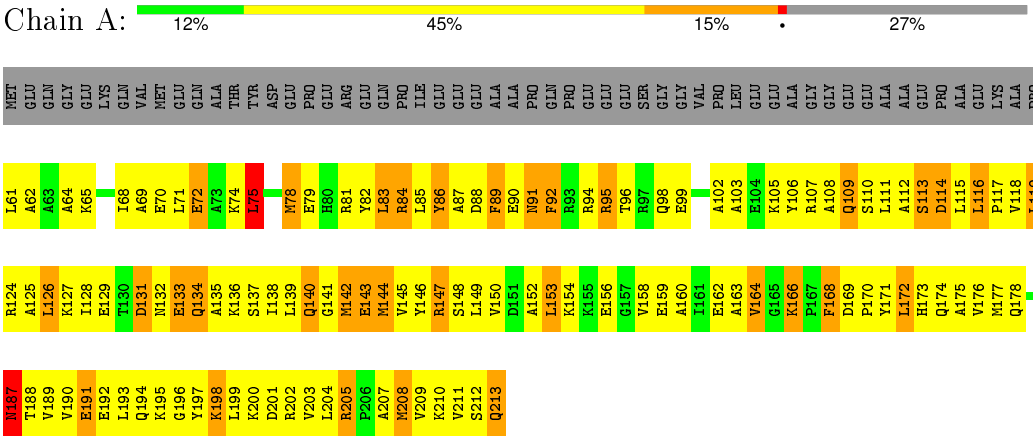
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	509	Total	C	N	O	S	0	0	0
			3862	2410	670	773	9			
2	D	509	Total	C	N	O	S	0	0	0
			3864	2413	671	771	9			
2	G	502	Total	C	N	O	S	0	0	0
			3527	2178	627	716	6			
2	H	501	Total	C	N	O	S	0	0	0
			3519	2176	624	712	7			

3 Residue-property plots (i)

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

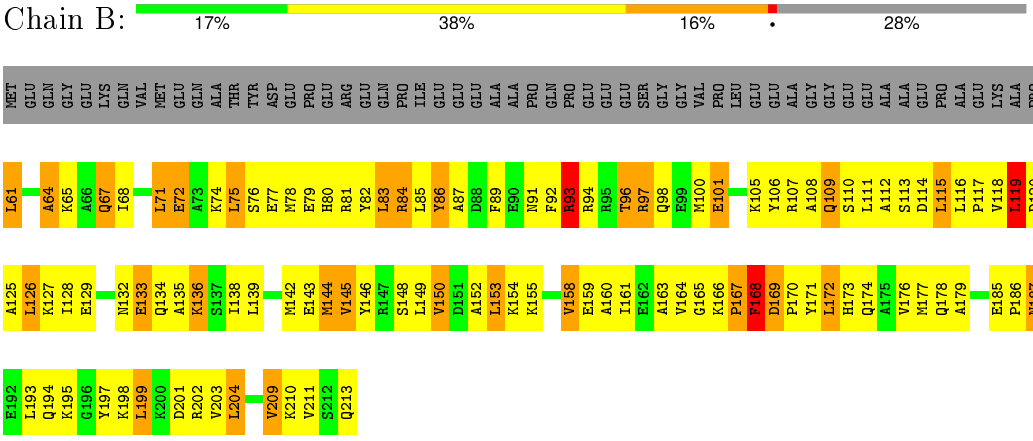
- Molecule 1: PROTEIN GRPE

Chain A:



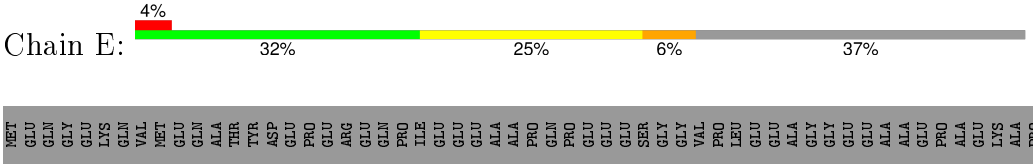
- Molecule 1: PROTEIN GRPE

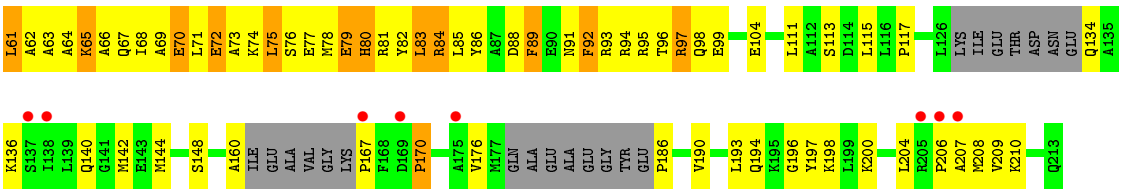
Chain B:



- Molecule 1: PROTEIN GRPE

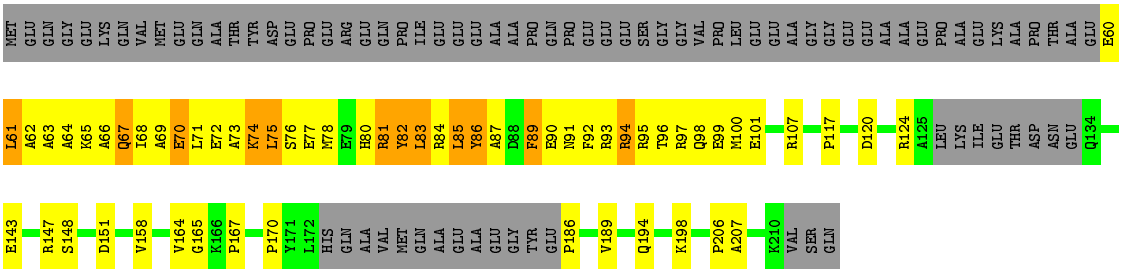
Chain E:





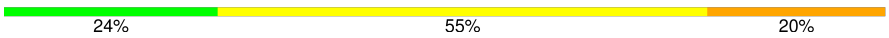
• Molecule 1: PROTEIN GRPE

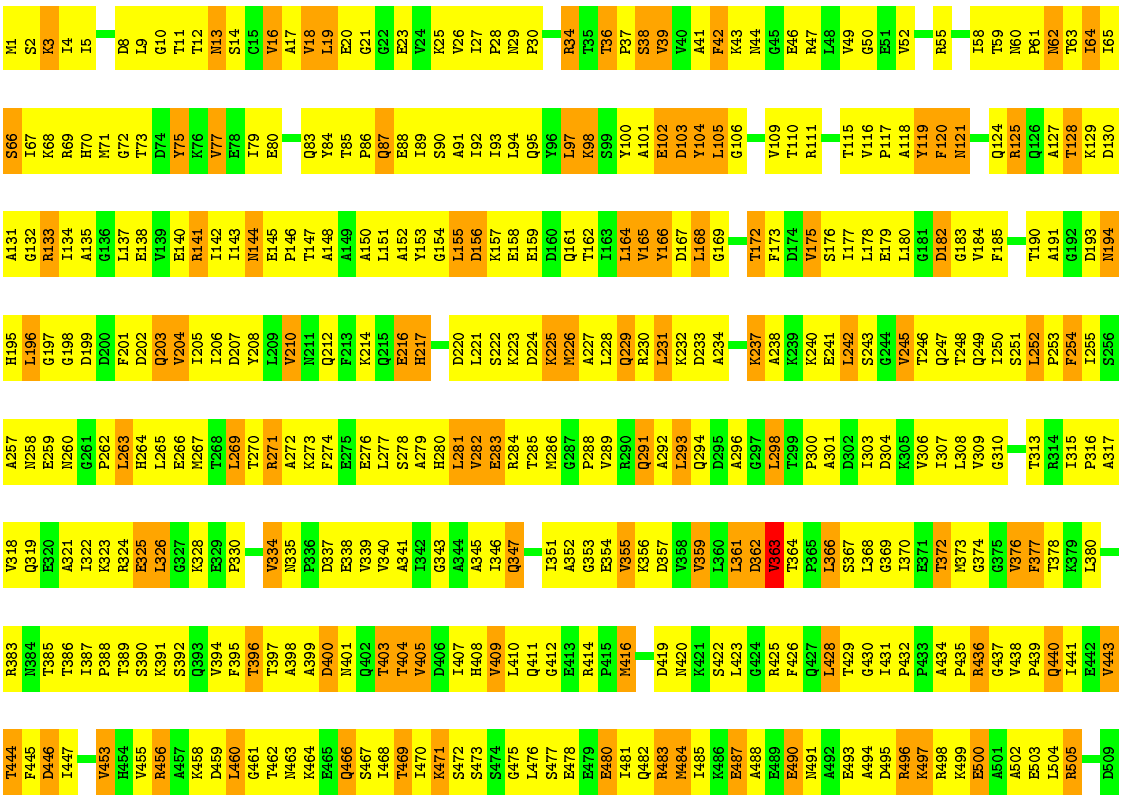
Chain F:



• Molecule 2: CHAPERONE PROTEIN DNAK

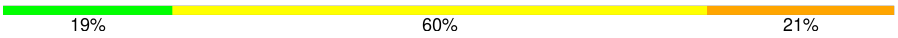
Chain C:

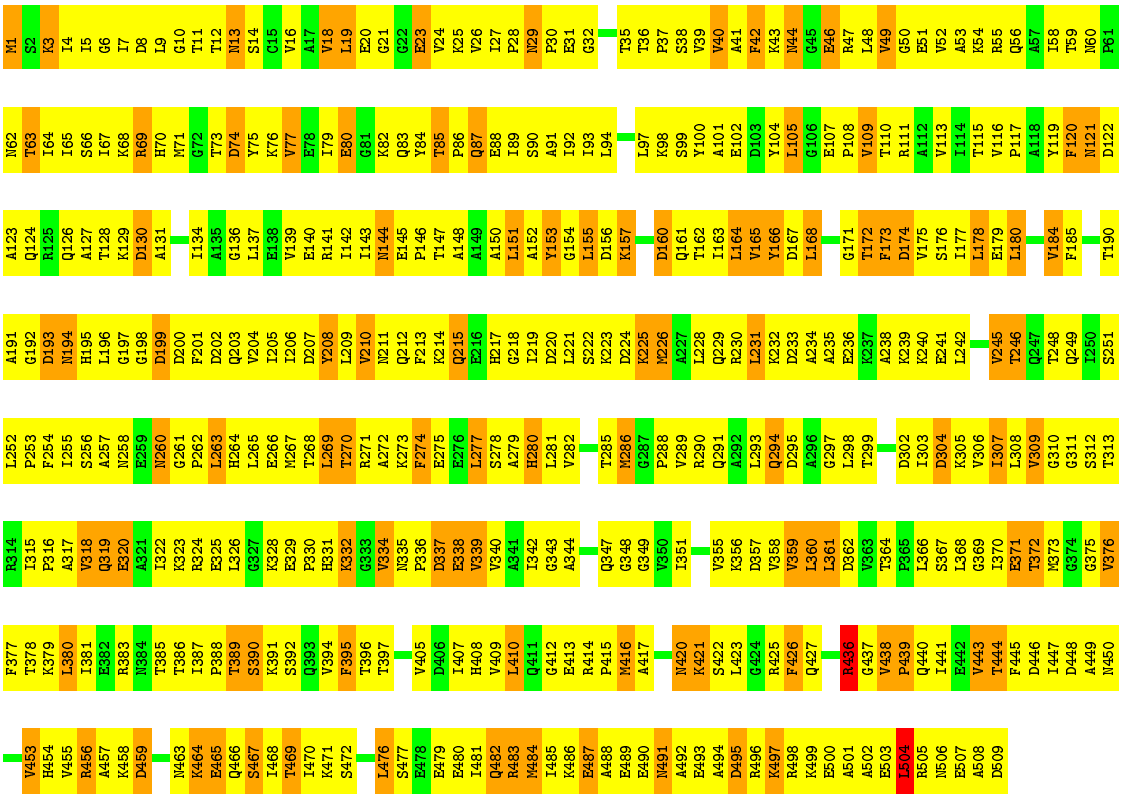




• Molecule 2: CHAPERONE PROTEIN DNAK

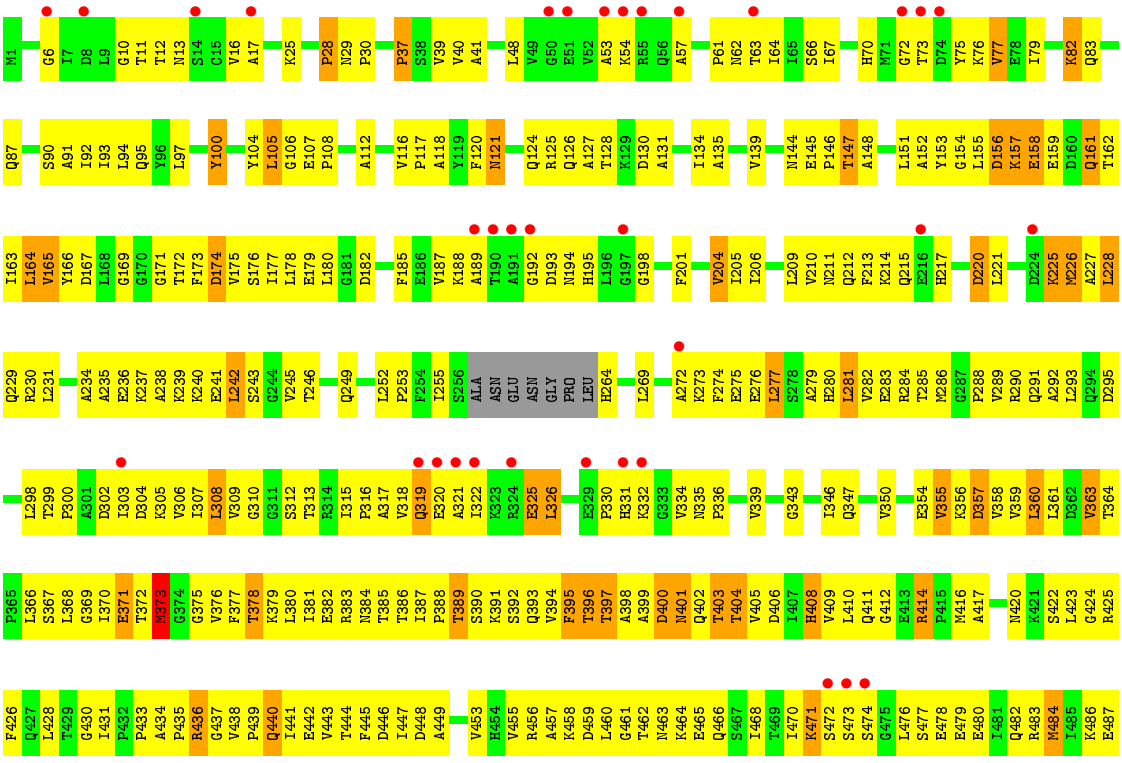
Chain D:



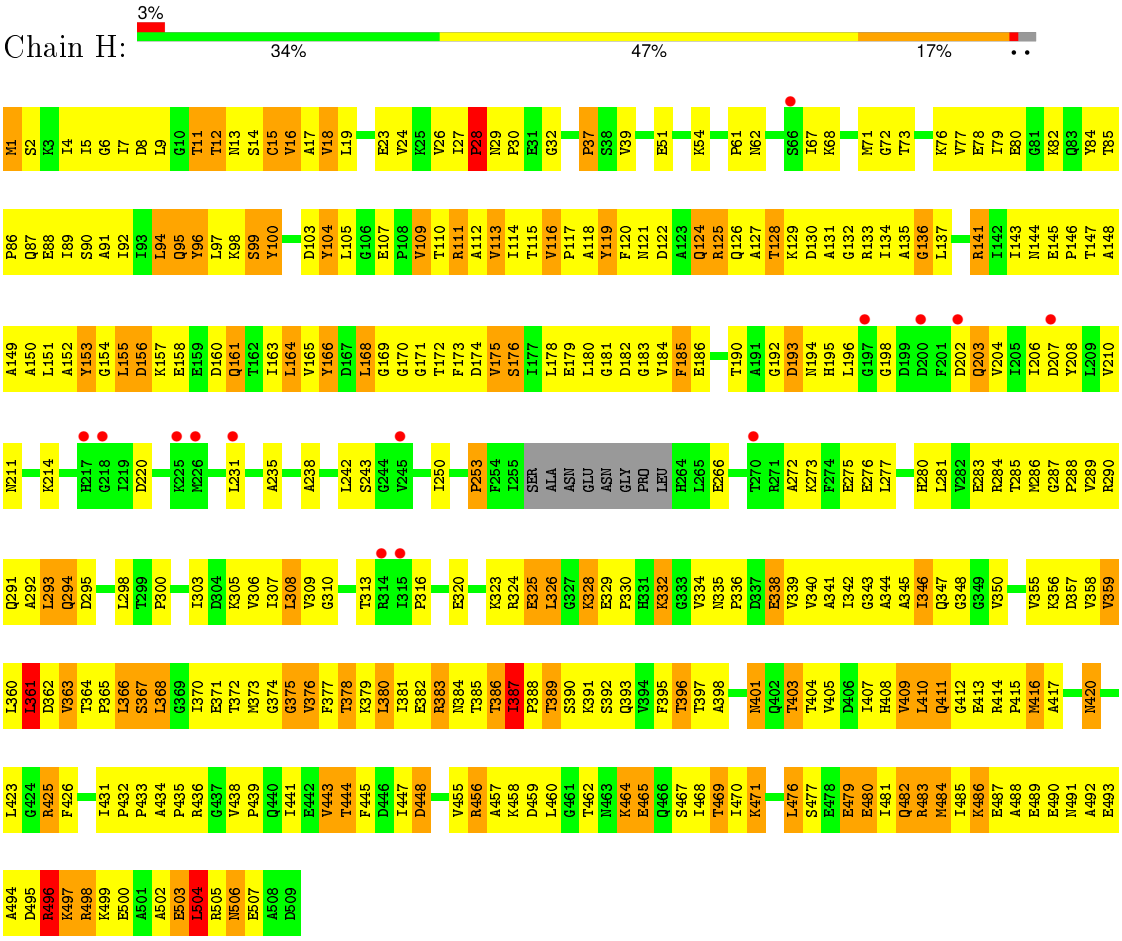


• Molecule 2: CHAPERONE PROTEIN DNAK

Chain G:



• Molecule 2: CHAPERONE PROTEIN DNAK



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	279.98Å 279.98Å 278.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.22 – 4.09 26.22 – 4.09	Depositor EDS
% Data completeness (in resolution range)	94.8 (26.22-4.09) 94.8 (26.22-4.09)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.25 (at 4.10Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.274 , 0.347 0.251 , 0.328	Depositor DCC
R_{free} test set	2083 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	143.4	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 133.3	EDS
Estimated twinning fraction	0.027 for l,-k,h 0.016 for -h,-l,-k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 41252 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	18889	wwPDB-VP
Average B, all atoms (Å^2)	207.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.75	0/1258	0.90	1/1691 (0.1%)
1	B	0.74	0/1257	0.93	2/1688 (0.1%)
1	E	0.64	0/821	0.84	5/1117 (0.4%)
1	F	0.64	0/818	0.84	5/1110 (0.5%)
2	C	0.70	1/3912 (0.0%)	0.86	3/5296 (0.1%)
2	D	0.72	0/3914	0.87	0/5299
2	G	0.67	0/3564	0.85	8/4834 (0.2%)
2	H	0.70	1/3556 (0.0%)	0.92	15/4832 (0.3%)
All	All	0.70	2/19100 (0.0%)	0.88	39/25867 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	D	0	2
2	H	0	2
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	141	ARG	CZ-NH1	-6.64	1.24	1.33
2	C	64	ILE	CB-CG2	-5.03	1.37	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	141	ARG	NE-CZ-NH2	10.76	125.68	120.30
2	H	361	LEU	CB-CG-CD1	-7.35	98.50	111.00
2	H	387	ILE	CG1-CB-CG2	-7.13	95.71	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	117	PRO	N-CA-CB	7.10	111.82	103.30
2	G	108	PRO	N-CA-CB	6.86	111.53	103.30
2	H	30	PRO	N-CA-CB	6.64	111.27	103.30
2	H	300	PRO	N-CA-CB	6.55	111.17	103.30
1	E	167	PRO	N-CA-CB	6.55	111.16	103.30
2	G	61	PRO	N-CA-CB	6.42	111.01	103.30
1	F	206	PRO	N-CA-CB	6.40	110.98	103.30
1	E	206	PRO	N-CA-CB	6.32	110.88	103.30
1	E	186	PRO	N-CA-CB	6.31	110.87	103.30
2	H	61	PRO	N-CA-CB	6.28	110.84	103.30
1	F	186	PRO	N-CA-CB	6.14	110.67	103.30
1	E	117	PRO	N-CA-CB	6.10	110.62	103.30
2	H	28	PRO	N-CA-CB	6.09	110.61	103.30
1	E	170	PRO	N-CA-CB	5.97	110.47	103.30
1	F	117	PRO	N-CA-CB	5.88	110.35	103.30
1	F	167	PRO	N-CA-CB	5.87	110.34	103.30
2	G	253	PRO	N-CA-CB	5.87	110.34	103.30
2	G	30	PRO	N-CA-CB	5.78	110.24	103.30
2	H	164	LEU	CA-CB-CG	5.68	128.37	115.30
2	C	353	GLY	N-CA-C	5.62	127.14	113.10
1	B	119	LEU	CA-CB-CG	-5.61	102.40	115.30
2	G	28	PRO	N-CA-CB	5.60	110.02	103.30
1	B	61	LEU	CA-CB-CG	5.58	128.14	115.30
1	F	170	PRO	N-CA-CB	5.52	109.93	103.30
2	H	375	GLY	N-CA-C	-5.39	99.62	113.10
2	H	253	PRO	N-CA-CB	5.36	109.73	103.30
2	H	37	PRO	N-CA-CB	5.32	109.68	103.30
2	H	136	GLY	N-CA-C	-5.31	99.82	113.10
2	G	37	PRO	N-CA-CB	5.26	109.61	103.30
2	H	141	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
2	C	263	LEU	CA-CB-CG	5.16	127.16	115.30
2	G	228	LEU	CA-CB-CG	5.15	127.15	115.30
2	C	175	VAL	CB-CA-C	-5.14	101.63	111.40
1	A	116	LEU	CA-CB-CG	-5.13	103.50	115.30
2	H	308	LEU	CA-CB-CG	5.03	126.88	115.30
2	H	504	LEU	CA-CB-CG	5.03	126.86	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	167	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	D	394	VAL	Peptide
2	D	436	ARG	Peptide
2	H	477	SER	Peptide
2	H	496	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1242	0	1239	264	0
1	B	1240	0	1246	243	0
1	E	820	0	567	85	0
1	F	815	0	588	79	0
2	C	3862	0	3901	638	0
2	D	3864	0	3909	766	0
2	G	3527	0	3217	518	0
2	H	3519	0	3231	544	0
All	All	18889	0	17898	2971	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 81.

All (2971) 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)
2:C:67:ILE:CD1	2:C:89:ILE:HG21	1.51	1.40
2:G:152:ALA:HA	2:G:346:ILE:CD1	1.51	1.39
2:H:141:ARG:NH1	2:H:143:ILE:HD11	1.40	1.36
2:H:67:ILE:CD1	2:H:89:ILE:HG21	1.57	1.31
2:D:426:PHE:HB3	2:D:468:ILE:CD1	1.61	1.30
2:C:129:LYS:HG3	2:C:142:ILE:CD1	1.60	1.30
2:H:387:ILE:HG22	2:H:388:PRO:CD	1.60	1.30
2:D:67:ILE:CD1	2:D:89:ILE:HG21	1.62	1.30
2:D:252:LEU:CD1	2:D:255:ILE:HG12	1.63	1.29
2:D:252:LEU:O	2:D:255:ILE:HG13	1.28	1.27
2:G:442:GLU:O	2:G:457:ALA:HA	1.35	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:ARG:NH1	2:H:143:ILE:CD1	1.99	1.24
2:C:255:ILE:CD1	2:C:265:LEU:HB2	1.68	1.23
2:H:339:VAL:HG23	2:H:342:ILE:CD1	1.70	1.22
2:H:339:VAL:CG2	2:H:342:ILE:HD12	1.71	1.20
1:B:84:ARG:HD3	2:C:388:PRO:O	1.42	1.20
2:H:141:ARG:HH11	2:H:143:ILE:CD1	1.54	1.19
2:D:426:PHE:CB	2:D:468:ILE:HD11	1.70	1.19
2:C:4:ILE:HD12	2:C:352:ALA:HB2	1.20	1.19
2:G:319:GLN:NE2	2:G:330:PRO:HG3	1.58	1.18
2:C:67:ILE:HD13	2:C:89:ILE:HG21	1.25	1.17
1:B:91:ASN:ND2	2:C:386:THR:HB	1.57	1.17
2:C:64:ILE:CG2	2:C:67:ILE:HD11	1.73	1.17
2:G:243:SER:OG	2:G:315:ILE:HG12	1.46	1.16
2:D:98:LYS:HD2	2:D:137:LEU:HD21	1.21	1.15
2:H:483:ARG:HH11	2:H:483:ARG:HG2	1.12	1.15
2:C:13:ASN:HB3	2:C:37:PRO:HA	1.17	1.15
2:G:443:VAL:HA	2:G:456:ARG:O	1.42	1.14
2:C:255:ILE:HD11	2:C:265:LEU:CB	1.78	1.14
1:B:122:PHE:HA	1:B:146:TYR:CE2	1.83	1.14
1:A:106:TYR:CD2	1:A:202:ARG:HD2	1.83	1.13
2:D:252:LEU:HD12	2:D:255:ILE:CG1	1.78	1.12
2:G:166:TYR:O	2:G:309:VAL:HB	1.49	1.12
2:D:361:LEU:CD2	2:D:387:ILE:HD11	1.79	1.12
2:D:387:ILE:CG2	2:D:388:PRO:HD2	1.80	1.12
2:D:387:ILE:HG23	2:D:388:PRO:HD2	1.29	1.12
2:G:371:GLU:HG3	2:G:408:HIS:HB3	1.30	1.12
2:G:426:PHE:HE2	2:G:466:GLN:HB3	1.15	1.12
2:G:372:THR:HB	2:G:376:VAL:HG13	1.32	1.11
2:D:255:ILE:HD12	2:D:265:LEU:CB	1.78	1.11
2:D:255:ILE:HD12	2:D:265:LEU:HB2	1.22	1.11
2:C:129:LYS:HG3	2:C:142:ILE:HD11	1.12	1.10
2:H:67:ILE:CD1	2:H:89:ILE:HD13	1.81	1.09
1:B:123:GLU:O	1:B:127:LYS:HB2	1.52	1.09
2:G:370:ILE:HG22	2:G:371:GLU:H	1.17	1.09
1:E:96:THR:HA	1:E:99:GLU:HG3	1.29	1.09
2:D:19:LEU:HB2	2:D:24:VAL:HG22	1.25	1.09
2:D:361:LEU:HD21	2:D:387:ILE:HD11	1.14	1.09
2:D:359:VAL:HG22	2:D:360:LEU:H	1.08	1.09
2:G:319:GLN:HE22	2:G:330:PRO:CG	1.66	1.09
1:F:91:ASN:HD21	2:G:385:THR:HG23	1.12	1.09
2:D:366:LEU:HD13	2:D:481:ILE:HG23	1.22	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PHE:CE1	1:B:146:TYR:HB3	1.89	1.08
2:H:361:LEU:HD13	2:H:387:ILE:HG13	1.31	1.08
2:D:5:ILE:HD12	2:D:109:VAL:HG21	1.13	1.08
2:G:334:VAL:HG21	2:G:339:VAL:HG23	1.30	1.08
2:C:64:ILE:HG21	2:C:67:ILE:HD11	1.11	1.08
1:B:91:ASN:HD21	2:C:386:THR:HB	0.93	1.08
2:D:5:ILE:CD1	2:D:109:VAL:HG21	1.82	1.08
2:D:173:PHE:HD1	2:D:174:ASP:N	1.51	1.08
2:D:121:ASN:OD1	2:D:124:GLN:HG3	1.52	1.07
2:D:173:PHE:HD2	2:D:196:LEU:HD23	1.15	1.07
2:D:65:ILE:HG22	2:D:66:SER:H	1.11	1.07
2:G:152:ALA:HA	2:G:346:ILE:HD11	1.07	1.07
2:H:339:VAL:HG23	2:H:342:ILE:HD12	1.08	1.07
2:D:37:PRO:HG3	2:D:51:GLU:HG2	1.35	1.07
2:G:381:ILE:HD13	2:G:447:ILE:HD11	1.34	1.06
2:C:98:LYS:HD2	2:C:137:LEU:HD21	1.33	1.06
2:D:372:THR:HG23	2:D:376:VAL:HG13	1.34	1.05
2:H:387:ILE:HG22	2:H:388:PRO:HD3	1.07	1.05
2:D:13:ASN:HB3	2:D:37:PRO:HA	1.07	1.05
2:D:273:LYS:O	2:D:277:LEU:HB2	1.56	1.05
1:A:199:LEU:HB2	1:A:204:LEU:HD11	1.38	1.05
2:C:409:VAL:HG11	2:C:470:ILE:CD1	1.87	1.05
2:D:64:ILE:HG21	2:D:67:ILE:HD11	1.07	1.05
2:D:1:MET:HA	2:D:111:ARG:HH21	1.15	1.05
2:C:370:ILE:HG21	2:C:407:ILE:HG23	1.35	1.05
2:H:361:LEU:CD1	2:H:387:ILE:HG13	1.87	1.04
2:D:252:LEU:HB3	2:D:255:ILE:HD11	1.07	1.04
2:D:252:LEU:O	2:D:255:ILE:CG1	2.05	1.04
2:D:251:SER:OG	2:D:253:PRO:HD3	1.56	1.04
2:C:110:THR:HG23	2:C:111:ARG:HG3	1.34	1.04
2:H:377:PHE:N	2:H:417:ALA:HB2	1.72	1.04
2:C:409:VAL:HG11	2:C:470:ILE:HD11	1.09	1.03
1:B:121:ASN:HA	1:B:124:ARG:HB2	1.41	1.02
2:C:396:THR:OG1	2:C:437:GLY:HA2	1.59	1.02
2:G:383:ARG:HD2	2:G:384:ASN:N	1.75	1.02
1:A:138:ILE:HG21	1:B:139:LEU:HD21	1.40	1.02
2:D:173:PHE:HE2	2:D:285:THR:HG23	1.20	1.02
1:A:58:ALA:HA	1:A:61:LEU:HB2	1.38	1.02
2:H:98:LYS:HD2	2:H:137:LEU:HD21	1.40	1.02
2:D:366:LEU:CD1	2:D:481:ILE:HG23	1.90	1.01
1:B:165:GLY:H	1:B:189:VAL:HG12	1.24	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:416:MET:HE3	2:G:417:ALA:H	1.26	1.01
1:A:126:LEU:HD13	1:A:127:LYS:HG3	1.42	1.01
2:D:67:ILE:HD11	2:D:89:ILE:HG21	1.42	1.01
2:C:64:ILE:HD13	2:C:89:ILE:CD1	1.90	1.01
2:C:4:ILE:CD1	2:C:352:ALA:HB2	1.91	1.01
2:D:319:GLN:HE21	2:D:330:PRO:HG2	1.18	1.01
2:H:67:ILE:HD12	2:H:89:ILE:HG21	1.37	1.00
2:C:255:ILE:HD11	2:C:265:LEU:HB2	1.31	1.00
2:D:252:LEU:HB3	2:D:255:ILE:CD1	1.91	1.00
2:D:386:THR:HG23	2:D:387:ILE:O	1.59	1.00
1:A:89:PHE:HD2	1:B:89:PHE:HD1	1.05	1.00
2:C:64:ILE:HG21	2:C:67:ILE:CD1	1.90	1.00
1:A:89:PHE:CD2	1:B:89:PHE:HD1	1.77	1.00
2:G:380:LEU:HD12	2:G:445:PHE:CE2	1.98	0.99
2:D:12:THR:HG21	2:D:171:GLY:H	1.25	0.99
1:A:119:LEU:HD11	1:A:197:TYR:OH	1.63	0.99
1:A:89:PHE:HD2	1:B:89:PHE:CD1	1.80	0.99
2:G:390:SER:HB3	2:G:446:ASP:HA	1.42	0.99
2:D:426:PHE:HB3	2:D:468:ILE:HD11	1.03	0.98
2:D:64:ILE:CG2	2:D:67:ILE:HD11	1.92	0.98
2:H:334:VAL:C	2:H:336:PRO:HD3	1.83	0.98
2:C:73:THR:HG23	2:C:75:TYR:H	1.28	0.98
2:H:376:VAL:C	2:H:417:ALA:HB2	1.84	0.98
2:H:127:ALA:O	2:H:130:ASP:HB2	1.62	0.98
2:H:202:ASP:O	2:H:206:ILE:HG13	1.60	0.98
2:C:180:LEU:HB2	2:C:185:PHE:HE1	1.29	0.98
2:G:152:ALA:CA	2:G:346:ILE:CD1	2.42	0.97
2:H:9:LEU:HD11	2:H:94:LEU:HD21	1.45	0.97
1:B:116:LEU:HD13	1:B:197:TYR:HD2	1.30	0.97
2:C:426:PHE:HD2	2:C:468:ILE:HD12	1.30	0.97
2:D:117:PRO:HG2	2:D:120:PHE:CD1	1.99	0.97
1:B:126:LEU:H	1:B:126:LEU:HD23	1.29	0.97
2:G:381:ILE:CD1	2:G:447:ILE:HD11	1.95	0.96
2:C:166:TYR:CE1	2:C:173:PHE:HE1	1.81	0.96
1:B:177:MET:HB3	1:B:210:LYS:HG3	1.44	0.96
2:D:64:ILE:HG21	2:D:67:ILE:CD1	1.94	0.96
2:D:141:ARG:CZ	2:D:143:ILE:HD11	1.94	0.96
2:H:166:TYR:HA	2:H:175:VAL:HG12	1.48	0.96
2:C:395:PHE:HA	2:H:360:LEU:HA	1.44	0.96
2:D:157:LYS:HA	2:D:157:LYS:HE3	1.44	0.96
2:G:396:THR:OG1	2:G:437:GLY:HA2	1.65	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:249:GLN:HA	2:G:269:LEU:H	1.30	0.96
2:D:209:LEU:HD11	2:D:265:LEU:HD11	1.45	0.96
2:D:252:LEU:CB	2:D:255:ILE:HD11	1.96	0.95
2:C:62:ASN:HB3	2:C:79:ILE:HD13	1.49	0.95
2:D:307:ILE:HG22	2:D:308:LEU:H	1.28	0.95
2:C:387:ILE:HG23	2:C:447:ILE:CG2	1.97	0.95
1:F:65:LYS:HA	1:F:68:ILE:HD12	1.48	0.95
2:G:145:GLU:HB2	2:G:146:PRO:HD3	1.46	0.95
2:D:323:LYS:HD2	2:D:329:GLU:HA	1.48	0.95
2:C:196:LEU:HD12	2:C:197:GLY:N	1.82	0.95
1:A:78:MET:HB3	1:A:82:TYR:CZ	2.01	0.95
1:E:84:ARG:HH21	2:G:354:GLU:H	1.09	0.94
1:B:128:ILE:HD13	2:D:262:PRO:HG3	1.49	0.94
2:G:165:VAL:HG22	2:G:176:SER:H	1.32	0.94
2:D:67:ILE:CD1	2:D:89:ILE:CG2	2.45	0.94
2:C:67:ILE:CD1	2:C:89:ILE:CG2	2.44	0.94
2:G:498:ARG:NH1	2:G:498:ARG:HB2	1.82	0.94
2:G:370:ILE:CG2	2:G:371:GLU:H	1.79	0.94
2:D:153:TYR:HB3	2:D:155:LEU:HD11	1.48	0.93
2:D:255:ILE:CD1	2:D:265:LEU:CB	2.46	0.93
1:A:75:LEU:HD13	1:A:79:GLU:OE2	1.66	0.93
2:G:73:THR:HG22	2:G:75:TYR:H	1.32	0.93
2:D:173:PHE:CD2	2:D:196:LEU:HD23	2.03	0.93
2:D:309:VAL:HG12	2:D:310:GLY:H	1.34	0.93
1:A:95:ARG:HD3	2:C:104:TYR:CE1	2.04	0.93
2:H:148:ALA:HB1	2:H:340:VAL:HG13	1.51	0.93
2:H:387:ILE:CG2	2:H:388:PRO:HD3	1.99	0.93
2:D:257:ALA:HB2	2:D:262:PRO:HA	1.50	0.92
2:G:361:LEU:HB3	2:G:387:ILE:HD12	1.51	0.92
2:C:462:THR:HG21	2:C:464:LYS:HB2	1.49	0.92
2:D:1:MET:HA	2:D:111:ARG:NH2	1.84	0.92
1:A:106:TYR:HD2	1:A:202:ARG:HD2	1.29	0.92
2:H:483:ARG:NH1	2:H:483:ARG:HG2	1.73	0.92
1:A:89:PHE:CD2	1:B:89:PHE:CD1	2.57	0.92
1:A:71:LEU:HB3	1:B:71:LEU:HD12	1.49	0.92
2:H:386:THR:HG23	2:H:387:ILE:O	1.68	0.92
2:H:372:THR:HG23	2:H:376:VAL:HG13	1.49	0.92
2:D:64:ILE:HD13	2:D:89:ILE:CD1	2.00	0.92
2:D:323:LYS:HB2	2:D:330:PRO:HD3	1.52	0.92
2:G:308:LEU:HD11	2:G:319:GLN:NE2	1.85	0.92
1:B:122:PHE:HE1	1:B:146:TYR:HB3	1.34	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PHE:HD1	1:B:146:TYR:CG	1.88	0.91
2:D:307:ILE:HG22	2:D:308:LEU:N	1.84	0.91
2:C:129:LYS:CG	2:C:142:ILE:HD11	1.99	0.91
2:G:426:PHE:CE2	2:G:466:GLN:HB3	2.04	0.91
2:C:4:ILE:HA	2:C:111:ARG:O	1.70	0.91
2:G:280:HIS:CE1	2:G:281:LEU:HG	2.05	0.91
2:D:65:ILE:HG22	2:D:66:SER:N	1.85	0.91
2:H:67:ILE:HD13	2:H:89:ILE:HD13	1.53	0.91
1:B:91:ASN:HD21	2:C:386:THR:CB	1.81	0.90
2:D:468:ILE:HG22	2:D:469:THR:N	1.83	0.90
2:C:97:LEU:HD12	2:C:100:TYR:HE1	1.37	0.90
2:H:27:ILE:HG22	2:H:28:PRO:N	1.86	0.90
2:D:257:ALA:HB1	2:D:261:GLY:O	1.72	0.90
2:D:322:ILE:HG22	2:D:326:LEU:HD22	1.51	0.90
1:A:106:TYR:HD2	1:A:202:ARG:HH11	1.10	0.90
2:G:370:ILE:HG22	2:G:371:GLU:N	1.85	0.90
2:H:67:ILE:HD13	2:H:89:ILE:HG21	1.51	0.90
2:G:381:ILE:HD13	2:G:447:ILE:CD1	2.00	0.90
2:G:205:ILE:HG21	2:G:235:ALA:HB1	1.52	0.90
2:C:18:VAL:HG11	2:C:27:ILE:HD11	1.54	0.90
2:G:334:VAL:HG21	2:G:339:VAL:CG2	2.01	0.90
2:D:126:GLN:O	2:D:130:ASP:HB2	1.73	0.89
2:H:381:ILE:HD13	2:H:447:ILE:HD12	1.55	0.89
2:C:423:LEU:HD13	2:C:470:ILE:HG21	1.54	0.89
2:C:34:ARG:HH11	2:C:34:ARG:H	1.17	0.89
2:C:26:VAL:O	2:C:28:PRO:HD3	1.71	0.89
1:B:125:ALA:HA	2:D:254:PHE:CE2	2.07	0.89
2:H:366:LEU:HD22	2:H:481:ILE:HG12	1.52	0.89
2:H:308:LEU:HD13	2:H:330:PRO:HG3	1.54	0.89
2:G:414:ARG:NH2	2:G:494:ALA:H	1.69	0.89
2:C:462:THR:HB	2:C:464:LYS:H	1.36	0.89
2:G:281:LEU:HA	2:G:284:ARG:HG3	1.52	0.89
2:C:85:THR:OG1	2:C:88:GLU:HG3	1.71	0.88
2:H:141:ARG:HH11	2:H:143:ILE:HD12	1.38	0.88
2:D:407:ILE:HD12	2:D:426:PHE:CE2	2.08	0.88
2:H:468:ILE:HG22	2:H:469:THR:N	1.88	0.88
2:G:151:LEU:HD12	2:G:154:GLY:HA2	1.55	0.88
2:H:153:TYR:HB3	2:H:155:LEU:HD11	1.55	0.88
2:H:67:ILE:CD1	2:H:89:ILE:CG2	2.50	0.88
2:C:129:LYS:HG3	2:C:142:ILE:HD12	1.55	0.88
2:D:155:LEU:H	2:D:155:LEU:HD22	1.36	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:205:ILE:O	2:G:209:LEU:HG	1.73	0.88
2:H:152:ALA:HB2	2:H:342:ILE:HG21	1.54	0.88
2:H:76:LYS:HB3	2:H:84:TYR:O	1.72	0.88
2:D:255:ILE:CD1	2:D:265:LEU:HB3	2.04	0.88
2:D:370:ILE:HG13	2:D:445:PHE:HZ	1.39	0.88
2:C:67:ILE:HD13	2:C:89:ILE:CG2	2.02	0.87
2:H:387:ILE:CG2	2:H:388:PRO:CD	2.51	0.87
2:G:152:ALA:CA	2:G:346:ILE:HD11	1.99	0.87
2:H:334:VAL:O	2:H:336:PRO:HD3	1.74	0.87
1:A:92:PHE:HD1	1:A:92:PHE:O	1.57	0.87
1:A:116:LEU:HD13	1:A:197:TYR:HD2	1.37	0.87
2:H:15:CYS:O	2:H:341:ALA:HB2	1.74	0.87
2:D:359:VAL:HG22	2:D:360:LEU:N	1.89	0.87
2:H:67:ILE:HD13	2:H:89:ILE:CD1	2.04	0.87
1:B:122:PHE:HD1	1:B:146:TYR:CD2	1.93	0.87
2:D:173:PHE:CE2	2:D:285:THR:HG23	2.09	0.87
2:C:65:ILE:HG22	2:C:66:SER:OG	1.73	0.87
2:C:152:ALA:HA	2:C:346:ILE:HD12	1.56	0.87
1:F:158:VAL:HA	1:F:198:LYS:O	1.72	0.87
2:C:255:ILE:HD12	2:C:265:LEU:HB2	1.55	0.87
1:F:91:ASN:ND2	2:G:385:THR:HG23	1.88	0.87
2:G:426:PHE:CG	2:G:468:ILE:HD11	2.10	0.87
2:C:255:ILE:HD11	2:C:265:LEU:HB3	1.56	0.87
1:F:86:TYR:HE2	2:G:359:VAL:HG22	1.40	0.86
1:B:65:LYS:HA	1:B:68:ILE:HD12	1.57	0.86
2:D:255:ILE:CD1	2:D:265:LEU:HB2	2.03	0.86
2:H:141:ARG:NH1	2:H:143:ILE:HD12	1.88	0.86
2:D:173:PHE:CD1	2:D:174:ASP:N	2.41	0.86
2:H:414:ARG:HG2	2:H:488:ALA:HB2	1.57	0.86
2:C:129:LYS:CG	2:C:142:ILE:CD1	2.52	0.86
2:H:132:GLY:O	2:H:135:ALA:HB3	1.74	0.86
2:D:298:LEU:HD12	2:D:302:ASP:HB3	1.57	0.86
2:G:361:LEU:HD22	2:G:387:ILE:CD1	2.05	0.86
2:H:119:TYR:HB3	2:H:190:THR:HG21	1.55	0.86
2:G:162:THR:OG1	2:G:303:ILE:HA	1.76	0.86
2:D:322:ILE:CG2	2:D:326:LEU:HD22	2.06	0.86
2:C:366:LEU:HD23	2:C:383:ARG:HG3	1.55	0.86
2:G:281:LEU:HB3	2:G:284:ARG:HD3	1.56	0.86
2:D:257:ALA:HA	2:D:263:LEU:HB2	1.55	0.86
2:C:180:LEU:HB2	2:C:185:PHE:CE1	2.10	0.86
2:H:210:VAL:O	2:H:214:LYS:HG3	1.76	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:HD12	1:B:197:TYR:OH	1.76	0.86
1:B:161:ILE:HD11	1:B:198:LYS:HB3	1.58	0.86
2:H:496:ARG:HE	2:H:496:ARG:C	1.79	0.86
2:D:98:LYS:HB2	2:D:137:LEU:HD11	1.58	0.85
2:H:306:VAL:HG21	2:H:326:LEU:HD23	1.59	0.85
2:C:64:ILE:CG2	2:C:67:ILE:CD1	2.53	0.85
2:H:381:ILE:HD13	2:H:447:ILE:CD1	2.06	0.85
1:B:189:VAL:HA	1:B:211:VAL:HG23	1.58	0.85
1:A:177:MET:HG2	2:C:225:LYS:HZ3	1.39	0.85
2:G:409:VAL:HG22	2:G:423:LEU:HD12	1.55	0.85
2:C:62:ASN:HB3	2:C:79:ILE:CD1	2.07	0.85
1:A:70:GLU:HB3	1:A:74:LYS:HE3	1.57	0.85
2:H:426:PHE:HB3	2:H:468:ILE:CD1	2.06	0.85
2:G:210:VAL:HG12	2:G:221:LEU:HD12	1.59	0.85
2:G:152:ALA:HA	2:G:346:ILE:HD12	1.55	0.85
2:D:102:GLU:HG2	2:D:108:PRO:HA	1.59	0.85
2:D:67:ILE:HD12	2:D:89:ILE:HG21	1.57	0.85
2:D:208:TYR:CE1	2:D:212:GLN:HG3	2.12	0.84
2:D:98:LYS:CD	2:D:137:LEU:HD21	2.07	0.84
2:C:77:VAL:O	2:C:83:GLN:HA	1.75	0.84
2:C:366:LEU:HD13	2:C:412:GLY:HA2	1.58	0.84
1:A:78:MET:O	1:A:82:TYR:CG	2.29	0.84
2:C:13:ASN:HB3	2:C:37:PRO:CA	2.05	0.84
2:D:65:ILE:CG2	2:D:66:SER:H	1.90	0.84
2:C:426:PHE:HB3	2:C:468:ILE:HD11	1.57	0.84
2:H:496:ARG:HA	2:H:498:ARG:HG2	1.57	0.84
2:D:200:ASP:O	2:D:281:LEU:HD21	1.78	0.84
2:G:205:ILE:CG2	2:G:235:ALA:HB1	2.08	0.84
2:D:79:ILE:HD12	2:D:84:TYR:CD2	2.13	0.84
2:G:366:LEU:HB2	2:G:411:GLN:HE21	1.42	0.84
2:C:150:ALA:HA	2:C:307:ILE:HD13	1.56	0.84
2:C:47:ARG:HH11	2:C:92:ILE:HG12	1.42	0.83
2:D:117:PRO:HG2	2:D:120:PHE:HD1	1.41	0.83
2:D:307:ILE:CG2	2:D:308:LEU:H	1.91	0.83
1:B:204:LEU:HD12	1:B:204:LEU:H	1.41	0.83
1:B:144:MET:SD	2:C:266:GLU:OE2	2.36	0.83
1:F:91:ASN:HD21	2:G:385:THR:CG2	1.90	0.83
1:E:62:ALA:HA	1:E:65:LYS:HE3	1.61	0.83
2:D:319:GLN:NE2	2:D:330:PRO:HG2	1.93	0.83
2:H:361:LEU:CD1	2:H:387:ILE:CG1	2.57	0.83
2:G:426:PHE:CD1	2:G:468:ILE:HD11	2.13	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:ILE:HD12	2:D:109:VAL:CG2	2.05	0.83
2:D:370:ILE:CG1	2:D:445:PHE:HZ	1.91	0.83
2:H:67:ILE:HD11	2:H:89:ILE:HD13	1.59	0.83
2:G:177:ILE:HD12	2:G:292:ALA:HB1	1.60	0.83
2:H:493:GLU:O	2:H:496:ARG:HD3	1.79	0.83
2:D:64:ILE:HD13	2:D:89:ILE:HD13	1.59	0.83
2:D:13:ASN:CB	2:D:37:PRO:HA	2.02	0.83
2:C:496:ARG:O	2:C:499:LYS:HB3	1.79	0.83
2:G:166:TYR:HA	2:G:175:VAL:HG12	1.61	0.83
1:A:89:PHE:HB2	1:B:89:PHE:CD1	2.13	0.83
2:D:416:MET:HE3	2:D:417:ALA:H	1.44	0.83
2:D:335:ASN:HB3	2:D:338:GLU:OE2	1.77	0.83
2:D:208:TYR:O	2:D:212:GLN:HG2	1.78	0.82
2:C:387:ILE:HG23	2:C:447:ILE:HG21	1.59	0.82
2:G:377:PHE:HB2	2:G:410:LEU:HD12	1.62	0.82
2:H:377:PHE:HB2	2:H:417:ALA:HA	1.60	0.82
1:E:89:PHE:HD1	1:E:89:PHE:C	1.81	0.82
2:H:165:VAL:HG13	2:H:176:SER:O	1.79	0.82
2:H:135:ALA:HB3	2:H:137:LEU:HB2	1.61	0.82
2:D:161:GLN:HE21	2:D:163:ILE:HD11	1.43	0.82
2:C:198:GLY:O	2:C:201:PHE:HB2	1.79	0.82
1:A:58:ALA:N	1:A:61:LEU:HD12	1.93	0.82
2:H:496:ARG:HE	2:H:496:ARG:CA	1.90	0.82
2:G:462:THR:CG2	2:G:464:LYS:HB2	2.08	0.82
2:H:476:LEU:HD23	2:H:476:LEU:H	1.43	0.82
2:C:29:ASN:ND2	2:C:36:THR:HG23	1.94	0.82
2:D:361:LEU:CD2	2:D:387:ILE:CD1	2.57	0.82
2:D:482:GLN:OE1	2:G:391:LYS:HA	1.79	0.82
1:F:62:ALA:HB1	1:F:65:LYS:HD2	1.62	0.82
2:C:205:ILE:HD11	2:C:274:PHE:CE2	2.15	0.82
2:G:164:LEU:O	2:G:306:VAL:HG13	1.79	0.82
2:G:173:PHE:CZ	2:G:175:VAL:HG13	2.15	0.82
2:C:13:ASN:CB	2:C:37:PRO:HA	2.06	0.82
2:G:390:SER:CB	2:G:446:ASP:HA	2.09	0.82
2:G:300:PRO:HB3	2:G:326:LEU:HD12	1.62	0.82
1:A:191:GLU:HG2	1:A:210:LYS:HD2	1.59	0.82
2:H:135:ALA:HB1	2:H:137:LEU:HD12	1.62	0.81
2:D:164:LEU:HD22	2:D:176:SER:O	1.79	0.81
1:B:198:LYS:HB2	1:B:203:VAL:HG22	1.60	0.81
1:A:140:GLN:HA	1:A:143:GLU:OE2	1.80	0.81
2:H:116:VAL:HG12	2:H:117:PRO:CD	2.11	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:4:ILE:HD12	2:C:352:ALA:CB	2.07	0.81
2:G:370:ILE:HG23	2:G:408:HIS:O	1.79	0.81
2:D:13:ASN:HB3	2:D:37:PRO:CA	2.02	0.81
2:H:97:LEU:HG	2:H:100:TYR:HE1	1.46	0.81
2:D:309:VAL:HG12	2:D:310:GLY:N	1.94	0.81
2:D:62:ASN:HD21	2:D:80:GLU:CD	1.82	0.81
2:D:121:ASN:HD21	2:D:123:ALA:H	1.28	0.81
2:G:293:LEU:HD13	2:G:300:PRO:HG3	1.61	0.81
2:H:12:THR:HG23	2:H:13:ASN:H	1.45	0.81
2:G:131:ALA:HA	2:G:134:ILE:CG1	2.11	0.81
2:G:319:GLN:HE22	2:G:330:PRO:HG3	0.72	0.81
2:D:426:PHE:HB3	2:D:468:ILE:HD12	1.63	0.81
2:H:483:ARG:HH11	2:H:483:ARG:CG	1.92	0.81
2:G:165:VAL:HG13	2:G:176:SER:O	1.80	0.81
2:D:387:ILE:CG2	2:D:388:PRO:CD	2.59	0.81
2:G:445:PHE:HA	2:G:455:VAL:HG22	1.63	0.81
2:D:291:GLN:O	2:D:295:ASP:HB2	1.79	0.81
1:E:75:LEU:HA	1:E:78:MET:HG3	1.63	0.80
2:H:202:ASP:O	2:H:206:ILE:CG1	2.27	0.80
2:C:462:THR:CG2	2:C:464:LYS:HB2	2.11	0.80
2:C:66:SER:O	2:C:69:ARG:HG3	1.82	0.80
2:C:145:GLU:HB2	2:C:146:PRO:HD3	1.62	0.80
2:D:397:THR:HG21	2:D:436:ARG:HA	1.63	0.80
2:C:229:GLN:HE21	2:C:229:GLN:HA	1.45	0.80
2:C:447:ILE:HG12	2:C:453:VAL:HB	1.62	0.80
1:A:116:LEU:HD22	1:A:197:TYR:CE2	2.16	0.80
2:H:2:SER:HA	2:H:107:GLU:OE2	1.79	0.80
2:H:84:TYR:HD1	2:H:88:GLU:OE2	1.65	0.80
1:A:138:ILE:CG2	1:B:139:LEU:HD21	2.11	0.80
2:C:326:LEU:N	2:C:326:LEU:HD13	1.97	0.80
1:F:72:GLU:O	1:F:75:LEU:HB3	1.83	0.80
2:C:387:ILE:CG2	2:C:447:ILE:HG22	2.11	0.79
1:B:149:LEU:HD23	1:B:149:LEU:C	2.03	0.79
1:B:165:GLY:H	1:B:189:VAL:CG1	1.95	0.79
2:H:426:PHE:HB3	2:H:468:ILE:HD11	1.61	0.79
2:G:470:ILE:HG22	2:G:471:LYS:N	1.97	0.79
2:H:280:HIS:O	2:H:284:ARG:HG3	1.80	0.79
2:D:266:GLU:O	2:D:267:MET:HB3	1.81	0.79
2:G:177:ILE:CD1	2:G:292:ALA:HB1	2.11	0.79
2:C:426:PHE:CD2	2:C:468:ILE:HD12	2.15	0.79
2:H:435:PRO:O	2:H:438:VAL:HG22	1.81	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:ALA:HB3	2:H:341:ALA:O	1.82	0.79
2:D:480:GLU:OE1	1:E:93:ARG:HD2	1.82	0.79
2:C:68:LYS:NZ	2:C:117:PRO:HG3	1.97	0.79
2:D:388:PRO:HB3	2:D:448:ASP:HA	1.65	0.79
2:D:370:ILE:HG13	2:D:445:PHE:CZ	2.17	0.79
2:D:370:ILE:HG22	2:D:371:GLU:O	1.82	0.79
1:F:143:GLU:O	1:F:147:ARG:CB	2.30	0.79
1:B:125:ALA:HA	2:D:254:PHE:HE2	1.47	0.79
2:D:121:ASN:ND2	2:D:123:ALA:H	1.81	0.79
2:D:503:GLU:HA	2:D:505:ARG:HG2	1.65	0.79
2:D:464:LYS:HE3	2:D:466:GLN:HE21	1.48	0.79
2:C:67:ILE:HD11	2:C:89:ILE:HG21	1.62	0.79
2:D:361:LEU:HD22	2:D:387:ILE:CG1	2.13	0.79
2:G:370:ILE:HD11	2:G:445:PHE:CE1	2.17	0.79
1:A:171:TYR:CD1	2:C:52:VAL:HG21	2.18	0.79
2:G:500:GLU:HA	2:G:503:GLU:HG3	1.65	0.79
2:D:70:HIS:CE1	2:D:75:TYR:CE2	2.70	0.79
1:A:193:LEU:HG	1:A:209:VAL:HA	1.65	0.79
2:C:150:ALA:HA	2:C:307:ILE:CD1	2.13	0.78
2:D:152:ALA:HB1	2:D:334:VAL:HG11	1.62	0.78
2:C:387:ILE:HG23	2:C:447:ILE:HG22	1.65	0.78
2:G:383:ARG:HD2	2:G:384:ASN:H	1.48	0.78
1:A:135:ALA:HB1	1:B:135:ALA:HB3	1.65	0.78
2:H:370:ILE:HD13	2:H:407:ILE:HG23	1.66	0.78
1:B:153:LEU:HD12	1:B:158:VAL:HG11	1.64	0.78
2:H:67:ILE:CG2	2:H:86:PRO:HB3	2.14	0.78
1:B:122:PHE:CD1	1:B:146:TYR:HB3	2.19	0.78
1:F:98:GLN:O	1:F:101:GLU:HB2	1.83	0.78
2:C:164:LEU:HB3	2:C:306:VAL:HG22	1.66	0.78
2:C:296:ALA:HB1	2:C:298:LEU:HD22	1.65	0.78
2:C:414:ARG:HD3	2:C:419:ASP:HB3	1.65	0.78
2:H:376:VAL:HA	2:H:416:MET:O	1.83	0.78
2:H:496:ARG:H	2:H:496:ARG:CD	1.96	0.78
1:E:89:PHE:C	1:E:89:PHE:CD1	2.53	0.78
2:D:468:ILE:CG2	2:D:469:THR:N	2.46	0.78
2:H:494:ALA:HA	2:H:496:ARG:NH1	1.99	0.78
2:H:409:VAL:HG21	2:H:470:ILE:HD11	1.65	0.78
1:B:143:GLU:O	1:B:143:GLU:HG3	1.82	0.77
2:D:204:VAL:HG22	2:D:277:LEU:HD13	1.64	0.77
2:C:226:MET:O	2:C:229:GLN:HB3	1.83	0.77
2:C:168:LEU:HB2	2:C:173:PHE:HD1	1.48	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:MET:O	1:B:210:LYS:HA	1.84	0.77
2:C:64:ILE:HD13	2:C:89:ILE:HD13	1.65	0.77
2:G:206:ILE:HG23	2:G:231:LEU:HD23	1.65	0.77
2:G:462:THR:HG21	2:G:464:LYS:HB2	1.65	0.77
2:C:477:SER:O	2:C:480:GLU:HG3	1.83	0.77
2:D:208:TYR:HB2	2:D:277:LEU:HD11	1.64	0.77
2:H:5:ILE:HG12	2:H:18:VAL:HB	1.66	0.77
2:C:396:THR:HB	2:C:439:PRO:O	1.83	0.77
2:D:388:PRO:HG3	2:D:449:ALA:HA	1.66	0.77
1:F:62:ALA:CB	1:F:65:LYS:HD2	2.13	0.77
1:E:83:LEU:HA	1:E:86:TYR:CD1	2.19	0.77
1:B:199:LEU:HB2	1:B:204:LEU:HD11	1.65	0.77
2:G:76:LYS:HD2	2:G:83:GLN:HE22	1.48	0.77
2:D:290:ARG:HA	2:D:293:LEU:HG	1.67	0.77
2:D:421:LYS:HG3	2:D:422:SER:N	2.00	0.77
2:D:483:ARG:HG2	2:D:483:ARG:HH11	1.48	0.77
1:B:124:ARG:HH12	2:D:230:ARG:CZ	1.98	0.77
2:C:147:THR:HG23	2:C:185:PHE:HD2	1.49	0.77
1:F:67:GLN:O	1:F:71:LEU:HG	1.84	0.77
1:B:128:ILE:CD1	2:D:262:PRO:HG3	2.15	0.77
2:D:504:LEU:HD13	2:D:507:GLU:HB3	1.66	0.77
2:D:372:THR:CG2	2:D:376:VAL:HG13	2.12	0.77
2:C:132:GLY:O	2:C:135:ALA:HB3	1.84	0.77
2:G:243:SER:OG	2:G:315:ILE:CG1	2.29	0.77
2:G:389:THR:O	2:G:447:ILE:HB	1.85	0.77
1:A:116:LEU:HD13	1:A:197:TYR:CD2	2.20	0.77
2:D:88:GLU:O	2:D:91:ALA:HB3	1.85	0.76
2:D:79:ILE:HD12	2:D:84:TYR:HD2	1.47	0.76
2:H:27:ILE:CG2	2:H:28:PRO:N	2.49	0.76
2:H:86:PRO:HA	2:H:89:ILE:HD12	1.67	0.76
2:H:502:ALA:C	2:H:504:LEU:H	1.88	0.76
2:H:387:ILE:HG22	2:H:388:PRO:N	1.99	0.76
2:G:416:MET:CE	2:G:417:ALA:H	1.98	0.76
2:D:205:ILE:HD11	2:D:274:PHE:CE2	2.20	0.76
1:B:160:ALA:HA	1:B:197:TYR:HD1	1.50	0.76
1:B:158:VAL:O	1:B:158:VAL:HG12	1.85	0.76
2:C:471:LYS:H	2:C:471:LYS:HD3	1.49	0.76
2:C:102:GLU:HG3	2:C:109:VAL:HG12	1.67	0.76
2:D:285:THR:O	2:D:288:PRO:HD2	1.86	0.76
2:C:105:LEU:N	2:C:105:LEU:HD13	2.00	0.76
2:C:366:LEU:HD22	2:C:367:SER:H	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:LEU:HD12	2:C:100:TYR:CE1	2.20	0.76
2:D:206:ILE:O	2:D:210:VAL:HG12	1.85	0.75
2:D:252:LEU:HD12	2:D:255:ILE:HG12	0.82	0.75
1:A:128:ILE:HG22	1:A:128:ILE:O	1.86	0.75
2:C:242:LEU:HD21	2:C:269:LEU:HG	1.67	0.75
2:G:397:THR:CB	2:G:437:GLY:H	1.99	0.75
1:A:135:ALA:HB1	1:B:135:ALA:CB	2.16	0.75
2:C:152:ALA:HA	2:C:346:ILE:CD1	2.17	0.75
2:D:42:PHE:CE1	2:D:79:ILE:HD13	2.21	0.75
1:B:84:ARG:CZ	2:C:389:THR:HA	2.17	0.75
2:C:16:VAL:HG22	2:C:16:VAL:O	1.85	0.75
2:C:414:ARG:HH21	2:C:494:ALA:HB2	1.52	0.75
2:G:151:LEU:O	2:G:346:ILE:HD13	1.86	0.75
2:H:147:THR:HG22	2:H:185:PHE:CD2	2.21	0.75
2:G:462:THR:HB	2:G:464:LYS:H	1.52	0.75
2:C:151:LEU:CD2	2:C:347:GLN:HG2	2.16	0.75
2:H:503:GLU:C	2:H:505:ARG:N	2.34	0.75
2:D:205:ILE:HD11	2:D:274:PHE:HE2	1.50	0.75
1:A:145:VAL:HG13	1:B:118:VAL:HG22	1.69	0.75
1:E:82:TYR:O	1:E:86:TYR:CE1	2.40	0.75
2:H:67:ILE:HG23	2:H:86:PRO:HB3	1.68	0.74
1:B:172:LEU:N	1:B:172:LEU:HD23	2.02	0.74
2:H:7:ILE:HG12	2:H:16:VAL:HB	1.69	0.74
1:E:92:PHE:HA	1:E:95:ARG:HB2	1.68	0.74
2:C:410:LEU:HD23	2:C:422:SER:HA	1.69	0.74
1:A:160:ALA:HA	1:A:197:TYR:HD1	1.53	0.74
1:F:86:TYR:CE2	2:G:359:VAL:HG22	2.22	0.74
2:C:370:ILE:CG2	2:C:407:ILE:HG23	2.16	0.74
2:D:164:LEU:HB3	2:D:306:VAL:HG22	1.67	0.74
2:C:42:PHE:CD1	2:C:42:PHE:N	2.54	0.74
2:H:148:ALA:CB	2:H:340:VAL:HG13	2.17	0.74
2:H:455:VAL:O	2:H:467:SER:HB2	1.86	0.74
2:C:362:ASP:O	2:C:363:VAL:HG13	1.86	0.74
2:G:243:SER:HA	2:G:316:PRO:HD2	1.68	0.74
2:C:80:GLU:OE1	2:C:80:GLU:HA	1.87	0.74
2:D:19:LEU:HD23	2:D:19:LEU:O	1.87	0.74
2:G:426:PHE:HB3	2:G:468:ILE:HD11	1.68	0.74
1:B:132:ASN:O	1:B:133:GLU:HG3	1.87	0.74
2:C:246:THR:O	2:C:247:GLN:HG3	1.88	0.74
2:C:440:GLN:HB2	2:C:460:LEU:HB2	1.69	0.74
2:H:339:VAL:O	2:H:342:ILE:HB	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:359:VAL:CG2	2:D:360:LEU:H	1.93	0.74
2:C:426:PHE:HB3	2:C:468:ILE:CD1	2.16	0.74
2:C:168:LEU:HD12	2:C:169:GLY:O	1.87	0.74
2:C:390:SER:HB3	2:C:446:ASP:OD1	1.88	0.74
2:H:151:LEU:O	2:H:346:ILE:HD13	1.86	0.74
2:D:269:LEU:HD12	2:D:270:THR:N	2.02	0.74
1:A:95:ARG:HD3	2:C:104:TYR:HE1	1.52	0.74
2:C:325:GLU:C	2:C:326:LEU:HD13	2.07	0.74
2:H:334:VAL:HG23	2:H:336:PRO:HG3	1.69	0.74
2:G:377:PHE:CE1	2:G:410:LEU:HB2	2.22	0.74
2:C:403:THR:HG23	2:C:404:THR:HG22	1.68	0.74
2:H:361:LEU:HD13	2:H:387:ILE:CG1	2.14	0.74
1:B:122:PHE:CD1	1:B:146:TYR:CD2	2.76	0.74
2:G:426:PHE:CD1	2:G:468:ILE:CD1	2.70	0.74
2:H:323:LYS:HB2	2:H:329:GLU:HB2	1.69	0.74
2:D:484:MET:O	2:D:484:MET:HE2	1.86	0.73
2:D:210:VAL:HG23	2:D:221:LEU:CD1	2.19	0.73
2:D:325:GLU:C	2:D:326:LEU:HD12	2.09	0.73
2:D:178:LEU:N	2:D:178:LEU:HD12	2.03	0.73
1:B:126:LEU:HD13	1:B:143:GLU:OE1	1.87	0.73
1:B:84:ARG:NH1	2:C:389:THR:HA	2.04	0.73
2:G:281:LEU:HA	2:G:284:ARG:CG	2.18	0.73
2:C:38:SER:HB3	2:C:93:ILE:HD13	1.69	0.73
2:C:487:GLU:HA	2:C:490:GLU:HB2	1.70	0.73
2:C:173:PHE:CZ	2:C:285:THR:HG23	2.24	0.73
2:D:370:ILE:HD11	2:D:445:PHE:CE1	2.23	0.73
2:C:269:LEU:HD12	2:C:270:THR:N	2.03	0.73
2:H:116:VAL:HG12	2:H:117:PRO:HD2	1.70	0.73
2:H:286:MET:HB3	2:H:290:ARG:CZ	2.19	0.73
2:G:409:VAL:HG13	2:G:424:GLY:H	1.54	0.73
1:A:78:MET:O	1:A:82:TYR:CD2	2.42	0.73
2:D:116:VAL:HG11	2:D:128:THR:HG21	1.70	0.73
1:E:84:ARG:NH2	2:G:354:GLU:H	1.87	0.73
2:H:67:ILE:HD13	2:H:89:ILE:CG2	2.18	0.73
2:D:213:PHE:HD2	2:D:221:LEU:HD21	1.54	0.73
2:C:196:LEU:HD21	2:C:285:THR:OG1	1.89	0.73
2:G:505:ARG:HG2	2:G:505:ARG:O	1.87	0.73
2:G:286:MET:SD	2:G:325:GLU:HG3	2.28	0.73
2:H:292:ALA:HA	2:H:295:ASP:OD2	1.87	0.73
2:H:166:TYR:HA	2:H:175:VAL:CG1	2.19	0.72
2:H:468:ILE:CG2	2:H:469:THR:N	2.52	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:MET:HG2	2:C:225:LYS:NZ	2.04	0.72
2:C:153:TYR:HE1	2:C:334:VAL:CG1	2.02	0.72
2:H:155:LEU:HD22	2:H:155:LEU:H	1.54	0.72
2:H:468:ILE:HG22	2:H:469:THR:H	1.50	0.72
2:H:361:LEU:HD11	2:H:387:ILE:CG1	2.17	0.72
2:G:381:ILE:CD1	2:G:447:ILE:CD1	2.63	0.72
2:H:281:LEU:HA	2:H:284:ARG:HD3	1.70	0.72
2:D:500:GLU:HA	2:D:503:GLU:HB2	1.69	0.72
1:A:131:ASP:HB3	1:A:136:LYS:HE3	1.70	0.72
2:C:67:ILE:HD12	2:C:89:ILE:HG21	1.62	0.72
2:H:114:ILE:HG22	2:H:115:THR:N	2.04	0.72
2:G:239:LYS:CG	2:G:315:ILE:HD11	2.18	0.72
2:D:325:GLU:O	2:D:326:LEU:HD12	1.89	0.72
2:C:70:HIS:CD2	2:C:75:TYR:CE2	2.78	0.72
2:G:77:VAL:HG11	2:G:79:ILE:HD12	1.70	0.72
2:D:366:LEU:HD13	2:D:481:ILE:CG2	2.13	0.72
2:H:468:ILE:CG2	2:H:469:THR:H	2.02	0.72
2:D:498:ARG:O	2:D:501:ALA:HB3	1.89	0.72
1:A:172:LEU:N	1:A:172:LEU:HD23	2.04	0.72
2:H:364:THR:O	2:H:366:LEU:N	2.23	0.72
1:E:77:GLU:OE2	1:E:81:ARG:HD2	1.89	0.72
2:G:77:VAL:HG11	2:G:79:ILE:CD1	2.20	0.72
2:C:254:PHE:CE1	2:C:264:HIS:HE1	2.08	0.72
2:H:309:VAL:HA	2:H:336:PRO:HB3	1.70	0.72
2:D:117:PRO:CG	2:D:120:PHE:CD1	2.73	0.72
1:A:126:LEU:CD1	1:A:127:LYS:HG3	2.19	0.72
1:A:79:GLU:HA	1:A:82:TYR:CD2	2.24	0.72
2:H:146:PRO:HB3	2:H:165:VAL:HG11	1.71	0.72
2:D:322:ILE:O	2:D:326:LEU:HD13	1.89	0.72
2:H:13:ASN:OD1	2:H:37:PRO:HA	1.90	0.72
2:D:305:LYS:HD3	2:D:331:HIS:NE2	2.04	0.71
2:G:121:ASN:HA	2:G:125:ARG:HH21	1.53	0.71
2:D:102:GLU:HG3	2:D:109:VAL:HG13	1.72	0.71
2:H:365:PRO:HB2	2:H:481:ILE:CD1	2.20	0.71
1:E:85:LEU:HG	1:F:82:TYR:CZ	2.26	0.71
2:G:169:GLY:HA3	2:G:172:THR:HG23	1.72	0.71
2:C:257:ALA:CA	2:C:263:LEU:HD12	2.20	0.71
2:H:339:VAL:CB	2:H:342:ILE:HD12	2.19	0.71
2:G:161:GLN:HB2	2:G:304:ASP:HB2	1.73	0.71
2:D:409:VAL:HG21	2:D:470:ILE:HD11	1.71	0.71
2:D:319:GLN:HE21	2:D:330:PRO:CG	1.98	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:LYS:HG2	2:D:329:GLU:H	1.55	0.71
2:H:151:LEU:O	2:H:346:ILE:CD1	2.39	0.71
2:C:87:GLN:O	2:C:91:ALA:HB2	1.91	0.71
2:G:442:GLU:O	2:G:457:ALA:CA	2.29	0.71
2:G:293:LEU:CD1	2:G:300:PRO:HG3	2.20	0.71
2:D:173:PHE:HD1	2:D:174:ASP:H	1.37	0.71
2:G:459:ASP:OD1	2:G:460:LEU:N	2.24	0.71
2:H:141:ARG:HH12	2:H:143:ILE:CD1	2.03	0.71
2:C:18:VAL:CG1	2:C:27:ILE:HD11	2.21	0.71
2:H:84:TYR:CD1	2:H:88:GLU:OE2	2.44	0.71
1:F:82:TYR:O	1:F:85:LEU:HB2	1.91	0.71
2:G:238:ALA:O	2:G:242:LEU:HD22	1.91	0.71
2:C:115:THR:HA	2:C:143:ILE:O	1.90	0.71
1:F:84:ARG:HD2	2:G:388:PRO:O	1.91	0.71
2:G:470:ILE:HG22	2:G:471:LYS:H	1.53	0.71
2:C:151:LEU:HD21	2:C:347:GLN:HG2	1.72	0.71
2:C:475:GLY:O	2:C:476:LEU:HD22	1.91	0.71
2:C:27:ILE:HG12	2:C:104:TYR:HD2	1.55	0.70
1:A:89:PHE:C	1:A:89:PHE:CD1	2.64	0.70
2:G:397:THR:OG1	2:G:437:GLY:N	2.24	0.70
2:H:464:LYS:NZ	2:H:464:LYS:HB2	2.06	0.70
2:D:166:TYR:HD1	2:D:166:TYR:C	1.94	0.70
2:C:280:HIS:NE2	2:C:281:LEU:HD13	2.06	0.70
1:B:67:GLN:CA	1:B:67:GLN:HE21	2.04	0.70
2:D:58:ILE:HG22	2:D:58:ILE:O	1.90	0.70
2:H:153:TYR:O	2:H:155:LEU:HD13	1.90	0.70
2:D:208:TYR:HE1	2:D:212:GLN:HG3	1.54	0.70
1:B:144:MET:CE	1:B:144:MET:HA	2.21	0.70
1:B:116:LEU:CD1	1:B:197:TYR:HD2	2.03	0.70
1:A:115:LEU:HD23	1:A:153:LEU:HD21	1.74	0.70
1:E:82:TYR:O	1:E:86:TYR:HE1	1.73	0.70
2:D:225:LYS:H	2:D:225:LYS:CD	2.03	0.70
2:D:225:LYS:H	2:D:225:LYS:HD2	1.56	0.70
1:A:144:MET:SD	2:D:253:PRO:HB3	2.32	0.70
2:C:10:GLY:HA3	2:C:13:ASN:O	1.91	0.70
1:E:78:MET:O	1:E:82:TYR:CG	2.44	0.70
2:C:377:PHE:CD1	2:C:377:PHE:O	2.45	0.70
2:C:396:THR:OG1	2:C:437:GLY:CA	2.39	0.70
2:G:377:PHE:CD1	2:G:410:LEU:HB2	2.25	0.70
2:D:414:ARG:CZ	2:D:491:ASN:HD21	2.03	0.70
2:G:500:GLU:HA	2:G:503:GLU:CG	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:ARG:O	2:D:48:LEU:HD23	1.92	0.70
2:D:87:GLN:CD	2:D:87:GLN:H	1.92	0.70
2:C:100:TYR:O	2:C:103:ASP:HB2	1.91	0.70
2:D:388:PRO:HB3	2:D:448:ASP:CA	2.20	0.70
1:A:78:MET:HB3	1:A:82:TYR:CE2	2.25	0.70
2:G:443:VAL:CA	2:G:456:ARG:O	2.33	0.70
1:F:74:LYS:O	1:F:78:MET:HB2	1.89	0.70
2:D:426:PHE:HB2	2:D:468:ILE:HD11	1.72	0.70
2:D:409:VAL:CG2	2:D:470:ILE:HD11	2.20	0.70
2:H:115:THR:HG21	2:H:340:VAL:HG11	1.73	0.70
2:D:409:VAL:O	2:D:409:VAL:HG23	1.92	0.70
2:H:149:ALA:CB	2:H:339:VAL:HG13	2.22	0.70
2:C:8:ASP:HA	2:C:115:THR:HG22	1.73	0.70
2:C:225:LYS:O	2:C:228:LEU:HB3	1.91	0.70
2:D:387:ILE:HG22	2:D:388:PRO:CD	2.22	0.70
1:B:190:VAL:HG12	1:B:191:GLU:N	2.06	0.70
2:C:394:VAL:HG21	2:H:363:VAL:HG11	1.74	0.69
1:A:139:LEU:HD21	1:B:138:ILE:HG21	1.71	0.69
1:E:65:LYS:HA	1:E:68:ILE:HB	1.74	0.69
2:C:153:TYR:CE1	2:C:334:VAL:CG1	2.75	0.69
2:C:224:ASP:OD2	2:C:227:ALA:HB2	1.92	0.69
1:A:192:GLU:HA	1:A:209:VAL:HG12	1.72	0.69
2:D:497:LYS:O	2:D:499:LYS:N	2.25	0.69
1:A:171:TYR:CE1	2:C:52:VAL:HG21	2.27	0.69
2:C:266:GLU:O	2:C:267:MET:HB3	1.90	0.69
2:D:414:ARG:HB3	2:D:415:PRO:HD2	1.74	0.69
2:C:408:HIS:CE1	2:C:425:ARG:NH2	2.60	0.69
1:A:58:ALA:CA	1:A:61:LEU:HB2	2.20	0.69
2:C:166:TYR:OH	2:C:285:THR:HG21	1.93	0.69
2:H:12:THR:HB	2:H:171:GLY:H	1.58	0.69
1:A:168:PHE:CB	1:A:189:VAL:HG22	2.22	0.69
2:C:64:ILE:CG2	2:C:67:ILE:CG1	2.70	0.69
2:D:480:GLU:O	2:D:484:MET:HG3	1.92	0.69
2:H:149:ALA:HB1	2:H:339:VAL:HG13	1.73	0.69
1:A:106:TYR:HD2	1:A:202:ARG:NH1	1.86	0.69
2:G:387:ILE:HG22	2:G:448:ASP:O	1.93	0.69
2:C:34:ARG:H	2:C:34:ARG:NH1	1.90	0.69
2:H:496:ARG:HA	2:H:498:ARG:CG	2.22	0.69
2:G:462:THR:O	2:G:463:ASN:HB2	1.91	0.69
2:H:367:SER:C	2:H:368:LEU:HD23	2.13	0.69
2:D:251:SER:HB2	2:D:266:GLU:OE2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:496:ARG:NE	2:H:496:ARG:CA	2.54	0.69
2:C:64:ILE:HG21	2:C:89:ILE:HD13	1.74	0.69
1:B:122:PHE:CD1	1:B:146:TYR:CG	2.76	0.69
2:H:109:VAL:HG23	2:H:111:ARG:O	1.91	0.69
2:D:161:GLN:NE2	2:D:163:ILE:HD11	2.07	0.69
2:G:164:LEU:H	2:G:306:VAL:HG22	1.57	0.69
2:H:100:TYR:HA	2:H:103:ASP:OD2	1.93	0.69
1:E:84:ARG:HH21	2:G:354:GLU:N	1.86	0.69
2:G:283:GLU:OE1	2:G:286:MET:HG3	1.93	0.69
2:C:484:MET:HE2	2:C:484:MET:HA	1.75	0.69
2:D:408:HIS:CD2	2:D:425:ARG:HH11	2.11	0.69
2:C:392:SER:OG	2:C:444:THR:HB	1.93	0.69
2:D:242:LEU:HD12	2:D:271:ARG:HD3	1.74	0.69
2:D:279:ALA:O	2:D:282:VAL:HB	1.92	0.69
2:D:116:VAL:HB	2:D:117:PRO:HD2	1.74	0.69
2:C:166:TYR:CE1	2:C:173:PHE:CE1	2.74	0.69
2:D:483:ARG:HG2	2:D:483:ARG:NH1	2.05	0.69
2:D:269:LEU:HD12	2:D:270:THR:H	1.58	0.69
2:H:87:GLN:CG	2:H:127:ALA:HB1	2.23	0.69
2:G:398:ALA:CB	2:G:402:GLN:HE22	2.06	0.69
2:C:273:LYS:O	2:C:276:GLU:HB2	1.92	0.68
2:H:281:LEU:O	2:H:284:ARG:HB2	1.93	0.68
2:D:175:VAL:HG11	2:D:289:VAL:HG22	1.75	0.68
1:A:135:ALA:CB	1:B:135:ALA:HB3	2.23	0.68
1:B:179:ALA:HB2	1:B:210:LYS:HG2	1.75	0.68
2:H:92:ILE:HG23	2:H:95:GLN:HE22	1.59	0.68
2:C:159:GLU:CD	2:C:159:GLU:H	1.97	0.68
2:D:87:GLN:O	2:D:91:ALA:HB2	1.93	0.68
2:D:414:ARG:NE	2:D:491:ASN:HD21	1.91	0.68
1:A:160:ALA:HB2	1:A:197:TYR:HE1	1.58	0.68
1:E:194:GLN:H	1:E:208:MET:CB	2.06	0.68
1:B:119:LEU:O	1:B:122:PHE:HB3	1.93	0.68
1:E:78:MET:O	1:E:82:TYR:HB2	1.92	0.68
2:D:379:LYS:HD3	2:D:379:LYS:H	1.57	0.68
2:G:157:LYS:HD2	2:G:158:GLU:HG2	1.73	0.68
1:A:141:GLY:HA2	2:D:264:HIS:CE1	2.28	0.68
2:G:370:ILE:HG12	2:G:409:VAL:HB	1.75	0.68
2:H:377:PHE:HB2	2:H:417:ALA:CA	2.24	0.68
1:B:160:ALA:HB2	1:B:197:TYR:HE1	1.59	0.68
2:G:300:PRO:HB3	2:G:326:LEU:CD1	2.23	0.68
2:D:503:GLU:C	2:D:505:ARG:N	2.44	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:76:LYS:HD2	2:G:83:GLN:NE2	2.07	0.68
1:A:142:MET:N	1:A:142:MET:SD	2.67	0.68
2:C:387:ILE:O	2:C:389:THR:N	2.27	0.68
2:D:151:LEU:HA	2:D:154:GLY:HA2	1.75	0.68
1:A:109:GLN:HG3	1:A:199:LEU:CD1	2.24	0.68
2:G:334:VAL:HG22	2:G:335:ASN:H	1.59	0.68
2:G:483:ARG:NH1	2:G:486:LYS:NZ	2.42	0.68
2:G:315:ILE:HG22	2:G:317:ALA:H	1.58	0.67
2:H:51:GLU:HA	2:H:54:LYS:CB	2.23	0.67
2:C:398:ALA:HB2	2:H:357:ASP:O	1.93	0.67
2:D:257:ALA:CB	2:D:262:PRO:HA	2.21	0.67
2:G:364:THR:HB	2:G:385:THR:H	1.59	0.67
2:H:306:VAL:HG12	2:H:307:ILE:N	2.08	0.67
2:D:277:LEU:O	2:D:277:LEU:HD22	1.95	0.67
2:D:116:VAL:O	2:D:144:ASN:HA	1.94	0.67
1:E:82:TYR:CE2	1:F:78:MET:HB3	2.30	0.67
1:A:170:PRO:HA	1:A:173:HIS:O	1.94	0.67
1:A:168:PHE:HB2	1:A:189:VAL:HG22	1.76	0.67
1:A:166:LYS:O	1:A:189:VAL:HG23	1.94	0.67
2:C:359:VAL:HG12	2:C:362:ASP:OD2	1.94	0.67
2:G:382:GLU:CD	2:G:383:ARG:H	1.97	0.67
2:C:159:GLU:O	2:C:161:GLN:HG2	1.95	0.67
2:D:426:PHE:CB	2:D:468:ILE:CD1	2.45	0.67
1:A:115:LEU:CD2	1:A:153:LEU:HD21	2.25	0.67
2:H:460:LEU:N	2:H:460:LEU:HD22	2.09	0.67
1:A:122:PHE:CB	1:A:146:TYR:CD2	2.78	0.67
2:H:329:GLU:OE2	2:H:330:PRO:HG2	1.94	0.67
2:D:213:PHE:CD2	2:D:221:LEU:HD21	2.29	0.67
1:F:68:ILE:O	1:F:72:GLU:HG3	1.94	0.67
2:G:255:ILE:CB	2:G:264:HIS:HA	2.24	0.67
2:G:273:LYS:HD2	2:G:276:GLU:OE2	1.95	0.67
2:G:426:PHE:CB	2:G:468:ILE:HD11	2.24	0.67
1:E:75:LEU:O	1:E:78:MET:HB2	1.94	0.67
2:G:73:THR:HG22	2:G:75:TYR:N	2.08	0.67
2:H:204:VAL:O	2:H:208:TYR:HB2	1.95	0.67
2:G:369:GLY:HA3	2:G:378:THR:O	1.95	0.67
2:G:369:GLY:O	2:G:409:VAL:HG23	1.93	0.67
2:D:359:VAL:O	2:G:395:PHE:HB3	1.95	0.67
2:H:88:GLU:HA	2:H:91:ALA:HB3	1.76	0.67
1:F:61:LEU:HD23	1:F:61:LEU:N	2.08	0.67
2:D:426:PHE:CD1	2:D:427:GLN:N	2.63	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:ILE:HG22	2:D:388:PRO:HD2	1.74	0.67
2:G:414:ARG:CZ	2:G:494:ALA:HB3	2.24	0.67
2:D:315:ILE:HG23	2:D:316:PRO:HD2	1.76	0.67
1:A:87:ALA:O	1:A:91:ASN:HB2	1.95	0.67
2:G:210:VAL:HB	2:G:214:LYS:NZ	2.09	0.67
2:G:206:ILE:O	2:G:210:VAL:HG13	1.94	0.67
2:D:507:GLU:HA	2:D:507:GLU:OE1	1.93	0.67
2:D:16:VAL:O	2:D:16:VAL:HG22	1.92	0.67
2:H:387:ILE:O	2:H:388:PRO:C	2.30	0.66
2:H:334:VAL:HG23	2:H:336:PRO:CG	2.24	0.66
1:A:116:LEU:HD22	1:A:197:TYR:CD2	2.31	0.66
2:G:497:LYS:O	2:G:500:GLU:HG2	1.95	0.66
2:G:162:THR:O	2:G:303:ILE:HG23	1.95	0.66
2:D:105:LEU:C	2:D:107:GLU:H	1.96	0.66
2:D:12:THR:HG21	2:D:171:GLY:N	2.05	0.66
2:C:205:ILE:HD11	2:C:274:PHE:HE2	1.58	0.66
2:C:153:TYR:OH	2:C:334:VAL:HG12	1.95	0.66
1:B:193:LEU:HD21	2:D:226:MET:HG2	1.77	0.66
2:C:265:LEU:HD23	2:C:266:GLU:N	2.09	0.66
2:D:129:LYS:HB2	2:D:142:ILE:CD1	2.26	0.66
2:H:4:ILE:HG22	2:H:348:GLY:O	1.95	0.66
2:H:116:VAL:HG12	2:H:117:PRO:HD3	1.76	0.66
2:C:368:LEU:HD21	2:C:411:GLN:HB2	1.78	0.66
2:D:173:PHE:CD1	2:D:173:PHE:C	2.68	0.66
2:H:365:PRO:HB2	2:H:481:ILE:HD13	1.75	0.66
2:G:205:ILE:HG21	2:G:235:ALA:CB	2.25	0.66
2:H:156:ASP:HA	2:H:180:LEU:HD11	1.77	0.66
2:D:252:LEU:O	2:D:255:ILE:CD1	2.44	0.66
1:A:192:GLU:OE2	1:A:195:LYS:HA	1.95	0.66
2:G:153:TYR:CZ	2:G:334:VAL:HB	2.30	0.66
2:G:400:ASP:C	2:G:401:ASN:HD22	1.99	0.66
2:G:462:THR:HG22	2:G:464:LYS:HB2	1.78	0.66
2:H:115:THR:HG21	2:H:340:VAL:CG1	2.26	0.66
2:D:166:TYR:C	2:D:166:TYR:CD1	2.68	0.66
2:C:364:THR:HG23	2:C:385:THR:O	1.95	0.66
2:C:101:ALA:O	2:C:105:LEU:HD22	1.96	0.66
2:H:503:GLU:C	2:H:505:ARG:H	1.97	0.66
2:H:361:LEU:HD22	2:H:387:ILE:HD11	1.77	0.66
2:D:280:HIS:NE2	2:D:281:LEU:HD13	2.10	0.66
1:B:86:TYR:HE2	2:C:359:VAL:HG21	1.61	0.66
2:D:493:GLU:HA	2:D:495:ASP:OD1	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:ARG:HB3	2:C:133:ARG:NH1	2.10	0.66
2:C:396:THR:HG1	2:C:437:GLY:HA2	1.57	0.66
2:C:254:PHE:CD1	2:C:254:PHE:N	2.63	0.66
2:G:166:TYR:OH	2:G:318:VAL:HG21	1.96	0.66
2:G:498:ARG:HH11	2:G:498:ARG:HB2	1.58	0.66
1:A:121:ASN:HD22	1:B:145:VAL:HG23	1.61	0.65
2:H:29:ASN:HA	2:H:100:TYR:CD2	2.31	0.65
2:D:444:THR:O	2:D:445:PHE:HD1	1.78	0.65
2:C:471:LYS:HZ2	2:C:471:LYS:H	1.44	0.65
2:D:162:THR:OG1	2:D:179:GLU:HG2	1.95	0.65
2:D:355:VAL:HG21	2:G:399:ALA:HB3	1.79	0.65
1:B:100:MET:O	1:B:101:GLU:C	2.35	0.65
2:G:145:GLU:O	2:G:148:ALA:HB3	1.96	0.65
2:G:164:LEU:HD21	2:G:175:VAL:HB	1.78	0.65
1:B:112:ALA:O	1:B:115:LEU:N	2.28	0.65
2:C:367:SER:HB2	2:C:412:GLY:O	1.96	0.65
2:H:2:SER:OG	2:H:110:THR:HB	1.96	0.65
2:C:471:LYS:HB2	2:C:471:LYS:HZ3	1.60	0.65
2:C:216:GLU:HB3	2:C:217:HIS:ND1	2.10	0.65
2:D:453:VAL:O	2:D:453:VAL:HG22	1.96	0.65
2:D:193:ASP:OD1	2:D:194:ASN:N	2.29	0.65
2:D:366:LEU:O	2:D:368:LEU:HD23	1.96	0.65
1:B:121:ASN:CA	1:B:124:ARG:HB2	2.23	0.65
2:D:218:GLY:O	2:D:219:ILE:HG13	1.96	0.65
2:H:364:THR:HG22	2:H:366:LEU:O	1.96	0.65
2:D:153:TYR:O	2:D:155:LEU:HD13	1.95	0.65
2:H:414:ARG:HG2	2:H:488:ALA:CB	2.27	0.65
2:D:64:ILE:CG2	2:D:67:ILE:CG1	2.74	0.65
2:D:210:VAL:HG23	2:D:221:LEU:HD12	1.77	0.65
2:H:339:VAL:CA	2:H:342:ILE:HD12	2.26	0.65
2:D:437:GLY:C	2:D:439:PRO:HD3	2.17	0.65
2:G:281:LEU:HA	2:G:284:ARG:CD	2.26	0.65
2:D:323:LYS:HG3	2:D:328:LYS:O	1.96	0.65
2:H:96:TYR:HA	2:H:99:SER:HB2	1.79	0.65
2:C:140:GLU:O	2:C:141:ARG:HB2	1.97	0.65
2:C:85:THR:HG1	2:C:88:GLU:HG3	1.60	0.65
1:B:185:GLU:O	1:B:188:THR:HB	1.97	0.65
2:C:431:ILE:HG23	2:C:432:PRO:HD2	1.78	0.65
2:D:26:VAL:O	2:D:26:VAL:HG23	1.97	0.65
2:G:225:LYS:HB3	2:G:225:LYS:NZ	2.12	0.65
2:C:64:ILE:HG22	2:C:67:ILE:HD11	1.75	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:MET:SD	2:D:268:THR:C	2.74	0.65
2:G:408:HIS:CE1	2:G:425:ARG:HB2	2.31	0.65
2:G:462:THR:HG21	2:G:464:LYS:CB	2.26	0.65
2:H:147:THR:CG2	2:H:185:PHE:HD2	2.09	0.65
2:C:145:GLU:O	2:C:148:ALA:HB3	1.97	0.65
2:G:507:GLU:O	2:G:507:GLU:HG3	1.95	0.65
2:C:63:THR:HG22	2:C:63:THR:O	1.95	0.65
2:C:357:ASP:HB3	2:C:359:VAL:HG23	1.78	0.65
2:C:164:LEU:HD22	2:C:165:VAL:N	2.11	0.65
2:D:508:ALA:O	2:D:509:ASP:HB2	1.97	0.65
2:H:361:LEU:CD2	2:H:387:ILE:CD1	2.74	0.64
2:G:116:VAL:O	2:G:145:GLU:N	2.22	0.64
2:D:4:ILE:HG12	2:D:111:ARG:HB3	1.79	0.64
1:B:189:VAL:CA	1:B:211:VAL:HG23	2.26	0.64
2:H:235:ALA:O	2:H:238:ALA:HB3	1.96	0.64
1:F:82:TYR:O	1:F:85:LEU:N	2.30	0.64
2:D:214:LYS:HG3	2:D:215:GLN:N	2.12	0.64
2:D:231:LEU:O	2:D:232:LYS:C	2.35	0.64
2:G:366:LEU:HD13	2:G:412:GLY:HA2	1.78	0.64
2:D:55:ARG:HG3	2:D:55:ARG:HH11	1.61	0.64
2:C:152:ALA:HB2	2:C:343:GLY:CA	2.26	0.64
1:E:58:ALA:O	1:E:61:LEU:HG	1.98	0.64
2:G:308:LEU:CD1	2:G:319:GLN:NE2	2.59	0.64
2:D:173:PHE:HD2	2:D:196:LEU:CD2	2.02	0.64
2:D:339:VAL:O	2:D:342:ILE:HB	1.97	0.64
2:D:483:ARG:O	2:D:486:LYS:HG3	1.96	0.64
2:G:272:ALA:HA	2:G:275:GLU:HB2	1.79	0.64
2:D:388:PRO:CB	2:D:448:ASP:HA	2.28	0.64
2:H:72:GLY:HA3	2:H:124:GLN:HA	1.78	0.64
1:E:91:ASN:O	1:E:94:ARG:HB3	1.97	0.64
2:G:144:ASN:ND2	2:G:147:THR:H	1.95	0.64
2:G:146:PRO:HB3	2:G:165:VAL:HG11	1.79	0.64
2:C:5:ILE:HG12	2:C:18:VAL:HB	1.79	0.64
1:A:89:PHE:HB2	1:B:89:PHE:HD1	1.60	0.64
2:G:144:ASN:OD1	2:G:147:THR:HB	1.97	0.64
2:H:401:ASN:HA	2:H:434:ALA:O	1.98	0.64
1:E:96:THR:CA	1:E:99:GLU:HG3	2.16	0.64
1:B:165:GLY:N	1:B:189:VAL:HG12	2.05	0.64
2:H:416:MET:O	2:H:417:ALA:HB3	1.97	0.64
2:H:87:GLN:HG2	2:H:127:ALA:HB1	1.79	0.64
2:G:396:THR:OG1	2:G:437:GLY:CA	2.43	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:O	1:B:82:TYR:CE2	2.51	0.64
2:D:444:THR:HG23	2:D:456:ARG:HB3	1.79	0.64
2:H:374:GLY:N	2:H:375:GLY:HA2	2.13	0.64
2:D:249:GLN:HG2	2:D:267:MET:O	1.98	0.64
2:C:68:LYS:HG2	2:C:68:LYS:O	1.97	0.64
2:H:420:ASN:H	2:H:420:ASN:ND2	1.96	0.64
2:H:8:ASP:HB3	2:H:340:VAL:CG1	2.28	0.64
2:D:361:LEU:HD13	2:D:387:ILE:HG13	1.78	0.64
2:G:166:TYR:O	2:G:309:VAL:CB	2.38	0.64
1:A:107:ARG:CB	1:B:107:ARG:HG2	2.28	0.64
2:C:64:ILE:HD13	2:C:89:ILE:HD11	1.78	0.64
2:C:47:ARG:NH1	2:C:92:ILE:HG12	2.13	0.64
2:C:144:ASN:O	2:C:145:GLU:C	2.34	0.64
2:D:166:TYR:CE2	2:D:322:ILE:HD11	2.33	0.64
1:A:89:PHE:HD1	1:A:90:GLU:N	1.95	0.64
2:C:158:GLU:HG2	2:C:159:GLU:OE1	1.99	0.64
2:G:67:ILE:O	2:G:67:ILE:HG22	1.97	0.64
2:D:198:GLY:O	2:D:201:PHE:N	2.22	0.63
2:D:203:GLN:O	2:D:206:ILE:N	2.31	0.63
2:G:325:GLU:HB3	2:G:326:LEU:HD22	1.79	0.63
2:D:503:GLU:C	2:D:505:ARG:H	1.98	0.63
2:H:409:VAL:CG2	2:H:409:VAL:O	2.46	0.63
2:C:17:ALA:HB3	2:C:341:ALA:O	1.98	0.63
1:B:84:ARG:CD	2:C:388:PRO:O	2.34	0.63
2:C:180:LEU:HD13	2:C:185:PHE:CE1	2.34	0.63
2:H:9:LEU:CD1	2:H:94:LEU:HD21	2.25	0.63
2:D:370:ILE:CG1	2:D:445:PHE:CZ	2.79	0.63
1:B:65:LYS:O	1:B:68:ILE:HB	1.99	0.63
2:H:377:PHE:CA	2:H:417:ALA:HB2	2.28	0.63
2:D:322:ILE:CG2	2:D:326:LEU:CD2	2.77	0.63
2:H:100:TYR:HA	2:H:103:ASP:CG	2.19	0.63
2:C:416:MET:HE2	2:C:497:LYS:HB3	1.81	0.63
2:C:502:ALA:O	2:C:505:ARG:HB3	1.98	0.63
2:C:238:ALA:O	2:C:242:LEU:HB2	1.98	0.63
2:H:502:ALA:C	2:H:504:LEU:N	2.50	0.63
2:G:162:THR:HG22	2:G:179:GLU:HG2	1.80	0.63
1:B:123:GLU:O	1:B:127:LYS:CB	2.39	0.63
2:D:385:THR:HG22	2:D:386:THR:HG22	1.80	0.63
2:D:388:PRO:CG	2:D:449:ALA:HA	2.28	0.63
2:D:369:GLY:HA3	2:D:377:PHE:HE1	1.64	0.63
2:D:454:HIS:O	2:D:455:VAL:HG23	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:398:ALA:HB3	2:G:402:GLN:NE2	2.12	0.63
2:H:243:SER:CB	2:H:316:PRO:HD3	2.28	0.63
2:H:346:ILE:O	2:H:350:VAL:HG23	1.97	0.63
2:H:67:ILE:HD13	2:H:89:ILE:CB	2.27	0.63
2:G:498:ARG:HB2	2:G:498:ARG:CZ	2.28	0.63
2:C:257:ALA:N	2:C:263:LEU:HD12	2.13	0.63
1:A:162:GLU:N	1:A:162:GLU:OE1	2.31	0.63
1:A:122:PHE:CB	1:A:146:TYR:CG	2.82	0.63
2:C:1:MET:HG3	2:C:2:SER:H	1.63	0.63
2:G:309:VAL:HG12	2:G:310:GLY:N	2.12	0.63
2:D:3:LYS:HD2	2:D:107:GLU:OE2	1.98	0.63
1:A:105:LYS:HD3	1:A:200:LYS:NZ	2.13	0.63
2:G:372:THR:HG22	2:G:373:MET:N	2.14	0.63
2:H:448:ASP:C	2:H:448:ASP:OD1	2.37	0.63
2:H:8:ASP:HB3	2:H:340:VAL:HG12	1.81	0.63
2:G:164:LEU:HB2	2:G:177:ILE:HG12	1.81	0.63
2:C:97:LEU:CD1	2:C:100:TYR:HE1	2.09	0.63
2:G:363:VAL:HG12	2:G:384:ASN:O	1.99	0.63
2:C:73:THR:HG23	2:C:75:TYR:N	2.09	0.63
2:C:180:LEU:CB	2:C:185:PHE:HE1	2.07	0.63
2:C:164:LEU:O	2:C:164:LEU:HD13	1.98	0.63
2:C:414:ARG:NH2	2:C:494:ALA:HB2	2.12	0.63
2:D:224:ASP:OD2	2:D:226:MET:HB2	1.99	0.63
2:C:18:VAL:CG2	2:C:19:LEU:N	2.62	0.63
2:G:361:LEU:HD22	2:G:387:ILE:HD11	1.80	0.63
2:H:24:VAL:HG11	2:H:345:ALA:CB	2.29	0.63
2:G:465:GLU:HG3	2:G:465:GLU:O	1.97	0.63
1:A:109:GLN:HG3	1:A:199:LEU:HD13	1.80	0.63
2:D:119:TYR:HB3	2:D:190:THR:HG21	1.80	0.63
2:D:414:ARG:CZ	2:D:491:ASN:ND2	2.61	0.63
1:A:92:PHE:HD1	1:A:92:PHE:C	2.01	0.63
1:A:112:ALA:O	1:A:116:LEU:HG	1.99	0.63
1:A:119:LEU:HD11	1:A:197:TYR:CZ	2.33	0.63
2:H:408:HIS:CE1	2:H:425:ARG:NH2	2.66	0.63
2:H:426:PHE:CB	2:H:468:ILE:HD11	2.28	0.63
2:H:426:PHE:HB3	2:H:468:ILE:HD12	1.81	0.63
2:G:470:ILE:CG2	2:G:471:LYS:H	2.11	0.63
2:H:392:SER:HB2	2:H:444:THR:HB	1.79	0.63
2:H:151:LEU:HB3	2:H:343:GLY:HA2	1.81	0.62
1:A:84:ARG:NH2	2:C:354:GLU:HB2	2.13	0.62
2:D:164:LEU:HD13	2:D:164:LEU:C	2.18	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:444:THR:C	2:D:445:PHE:HD1	2.01	0.62
1:B:198:LYS:CB	1:B:203:VAL:HG22	2.28	0.62
2:G:458:LYS:HB2	2:G:465:GLU:CB	2.29	0.62
2:D:391:LYS:HG3	2:D:392:SER:N	2.14	0.62
1:B:178:GLN:HG3	1:B:213:GLN:HB3	1.80	0.62
2:H:361:LEU:CD1	2:H:387:ILE:CD1	2.77	0.62
2:G:280:HIS:CE1	2:G:281:LEU:CG	2.82	0.62
2:D:155:LEU:N	2:D:155:LEU:HD22	2.13	0.62
2:G:397:THR:OG1	2:G:439:PRO:HD2	1.98	0.62
2:D:307:ILE:CG2	2:D:308:LEU:N	2.51	0.62
2:H:308:LEU:HB2	2:H:330:PRO:HB2	1.81	0.62
2:D:11:THR:N	2:D:68:LYS:HZ2	1.96	0.62
2:H:383:ARG:HG2	2:H:384:ASN:ND2	2.14	0.62
2:H:361:LEU:HD21	2:H:387:ILE:HD12	1.80	0.62
2:D:230:ARG:NH2	2:D:252:LEU:HD13	2.14	0.62
2:C:370:ILE:HG23	2:C:408:HIS:O	1.99	0.62
2:H:308:LEU:HD22	2:H:330:PRO:HG2	1.80	0.62
1:A:141:GLY:CA	2:D:264:HIS:CE1	2.82	0.62
1:A:99:GLU:O	1:A:102:ALA:HB3	1.99	0.62
2:G:151:LEU:HD12	2:G:154:GLY:CA	2.27	0.62
2:G:157:LYS:CD	2:G:158:GLU:HG2	2.29	0.62
2:C:129:LYS:CG	2:C:142:ILE:HD12	2.27	0.62
2:D:388:PRO:CD	2:D:449:ALA:HA	2.29	0.62
1:F:87:ALA:HA	2:G:386:THR:HB	1.81	0.62
2:G:29:ASN:HA	2:G:100:TYR:CD2	2.35	0.62
2:D:468:ILE:CG2	2:D:469:THR:H	2.12	0.62
2:H:385:THR:HG21	2:H:389:THR:HG21	1.81	0.62
2:C:153:TYR:HE1	2:C:334:VAL:HG11	1.64	0.62
2:C:334:VAL:HG11	2:C:339:VAL:HG23	1.81	0.62
2:C:313:THR:O	2:C:319:GLN:NE2	2.32	0.62
2:H:71:MET:CE	2:H:128:THR:HG23	2.30	0.62
1:E:74:LYS:O	1:E:78:MET:HG2	1.99	0.62
2:H:308:LEU:HD13	2:H:330:PRO:CG	2.28	0.62
2:D:152:ALA:CB	2:D:334:VAL:HG11	2.28	0.62
2:G:470:ILE:CG2	2:G:471:LYS:N	2.62	0.62
2:H:92:ILE:HG23	2:H:95:GLN:NE2	2.15	0.62
2:C:251:SER:O	2:C:252:LEU:HD13	1.99	0.62
2:D:140:GLU:HB3	2:D:351:ILE:HG21	1.82	0.62
2:C:270:THR:HB	2:C:273:LYS:H	1.64	0.62
2:G:409:VAL:HG13	2:G:423:LEU:HB2	1.81	0.62
2:H:207:ASP:HA	2:H:210:VAL:HG22	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:PHE:HD1	1:E:89:PHE:O	1.83	0.62
2:H:281:LEU:HD12	2:H:284:ARG:NH1	2.14	0.62
2:C:459:ASP:OD1	2:C:460:LEU:N	2.33	0.62
1:F:61:LEU:HD23	1:F:61:LEU:H	1.65	0.62
2:D:63:THR:HG22	2:D:63:THR:O	2.00	0.62
1:A:92:PHE:CD1	1:A:92:PHE:O	2.46	0.62
2:C:43:LYS:HZ3	2:C:60:ASN:HA	1.64	0.62
2:D:131:ALA:HA	2:D:134:ILE:HD12	1.82	0.62
2:C:500:GLU:HA	2:C:503:GLU:HG2	1.80	0.62
2:C:154:GLY:O	2:C:156:ASP:N	2.33	0.62
2:C:355:VAL:HG23	2:C:356:LYS:N	2.14	0.62
2:D:337:ASP:N	2:D:337:ASP:OD1	2.31	0.62
2:C:499:LYS:HG2	2:C:500:GLU:OE1	2.00	0.62
1:B:86:TYR:CE2	2:C:359:VAL:HG21	2.35	0.61
2:H:114:ILE:CG2	2:H:115:THR:N	2.62	0.61
2:G:145:GLU:CB	2:G:146:PRO:HD3	2.25	0.61
2:G:192:GLY:N	2:G:288:PRO:HB3	2.16	0.61
2:C:172:THR:O	2:C:172:THR:OG1	2.16	0.61
2:D:257:ALA:HB1	2:D:261:GLY:C	2.20	0.61
2:H:98:LYS:CD	2:H:137:LEU:HD21	2.25	0.61
1:E:78:MET:O	1:E:82:TYR:CB	2.48	0.61
2:D:193:ASP:OD1	2:D:193:ASP:C	2.38	0.61
2:D:64:ILE:HG21	2:D:67:ILE:CG1	2.30	0.61
2:C:246:THR:C	2:C:247:GLN:HG3	2.18	0.61
1:A:62:ALA:HA	1:A:65:LYS:HE2	1.81	0.61
1:A:88:ASP:OD2	2:C:20:GLU:HA	1.99	0.61
2:C:68:LYS:HZ3	2:C:117:PRO:HG3	1.66	0.61
2:H:376:VAL:C	2:H:417:ALA:CB	2.65	0.61
2:C:426:PHE:HD2	2:C:468:ILE:CD1	2.09	0.61
2:D:298:LEU:HD12	2:D:302:ASP:CB	2.30	0.61
2:C:497:LYS:C	2:C:499:LYS:N	2.53	0.61
2:C:471:LYS:N	2:C:471:LYS:HZ2	1.98	0.61
2:D:252:LEU:CD1	2:D:255:ILE:CG1	2.56	0.61
2:G:372:THR:CB	2:G:376:VAL:HG13	2.21	0.61
1:E:96:THR:HA	1:E:99:GLU:CG	2.19	0.61
1:A:160:ALA:HB2	1:A:197:TYR:CE1	2.36	0.61
2:G:461:GLY:O	2:H:391:LYS:HD3	1.99	0.61
2:D:199:ASP:N	2:D:199:ASP:OD1	2.27	0.61
1:A:89:PHE:O	1:A:92:PHE:N	2.33	0.61
2:C:151:LEU:O	2:C:154:GLY:N	2.33	0.61
2:D:230:ARG:NE	2:D:252:LEU:HD11	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:239:LYS:HA	2:G:242:LEU:HD22	1.82	0.61
2:H:100:TYR:O	2:H:103:ASP:HB2	2.00	0.61
1:B:67:GLN:HA	1:B:67:GLN:HE21	1.65	0.61
1:A:168:PHE:HD2	1:A:173:HIS:HB2	1.65	0.61
2:G:243:SER:HA	2:G:316:PRO:CD	2.30	0.61
2:G:371:GLU:HB2	2:G:408:HIS:O	2.00	0.61
2:H:208:TYR:OH	2:H:273:LYS:HD2	2.01	0.61
1:F:73:ALA:O	1:F:77:GLU:HB2	2.00	0.61
2:C:64:ILE:HD13	2:C:89:ILE:CG1	2.31	0.61
2:C:372:THR:CG2	2:C:378:THR:OG1	2.48	0.61
2:D:102:GLU:HG3	2:D:109:VAL:CG1	2.30	0.61
2:D:105:LEU:HB3	2:D:107:GLU:HB3	1.83	0.61
2:G:205:ILE:O	2:G:209:LEU:CG	2.47	0.61
2:D:7:ILE:O	2:D:115:THR:HG22	2.00	0.61
2:D:364:THR:O	2:D:364:THR:HG22	2.01	0.61
2:G:307:ILE:HG22	2:G:308:LEU:N	2.16	0.60
2:H:72:GLY:H	2:H:87:GLN:NE2	1.98	0.60
2:H:4:ILE:HD11	2:H:111:ARG:HH11	1.66	0.60
2:H:306:VAL:HG12	2:H:307:ILE:H	1.63	0.60
1:E:75:LEU:HA	1:E:78:MET:CG	2.31	0.60
2:D:370:ILE:HD11	2:D:445:PHE:HE1	1.64	0.60
1:A:168:PHE:CZ	1:A:175:ALA:HB2	2.35	0.60
2:H:125:ARG:HA	2:H:128:THR:OG1	2.00	0.60
1:E:81:ARG:HG3	1:E:82:TYR:N	2.15	0.60
2:D:224:ASP:OD1	2:D:226:MET:HB2	2.00	0.60
1:B:126:LEU:H	1:B:126:LEU:CD2	2.06	0.60
1:A:119:LEU:C	1:A:119:LEU:HD13	2.21	0.60
2:G:477:SER:O	2:G:480:GLU:HG3	2.01	0.60
2:H:184:VAL:HG12	2:H:185:PHE:N	2.16	0.60
2:G:163:ILE:HG12	2:G:305:LYS:O	2.02	0.60
2:G:458:LYS:HG2	2:G:459:ASP:O	2.00	0.60
2:G:162:THR:O	2:G:163:ILE:HG13	2.00	0.60
2:C:321:ALA:O	2:C:325:GLU:HB2	2.01	0.60
1:A:71:LEU:CB	1:B:71:LEU:HD12	2.29	0.60
2:D:483:ARG:NH1	2:D:486:LYS:HD3	2.17	0.60
1:E:190:VAL:CB	1:E:210:LYS:O	2.49	0.60
2:D:497:LYS:HD3	2:D:498:ARG:N	2.16	0.60
2:D:391:LYS:HG3	2:D:392:SER:H	1.66	0.60
2:D:67:ILE:O	2:D:69:ARG:N	2.34	0.60
2:D:208:TYR:C	2:D:208:TYR:CD1	2.74	0.60
2:D:255:ILE:HD11	2:D:265:LEU:HB3	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:455:VAL:CG1	2:D:456:ARG:N	2.65	0.60
2:G:210:VAL:HB	2:G:214:LYS:HZ1	1.67	0.60
2:H:505:ARG:O	2:H:507:GLU:N	2.34	0.60
2:C:64:ILE:HG22	2:C:67:ILE:CG1	2.32	0.60
2:H:335:ASN:O	2:H:339:VAL:HB	2.01	0.60
2:H:367:SER:HB3	2:H:383:ARG:HA	1.83	0.60
2:H:128:THR:O	2:H:129:LYS:C	2.39	0.60
2:C:199:ASP:O	2:C:202:ASP:HB2	2.02	0.60
2:D:70:HIS:ND1	2:D:75:TYR:CE2	2.70	0.60
2:C:334:VAL:HG11	2:C:339:VAL:CG2	2.32	0.60
2:D:476:LEU:HB2	2:D:480:GLU:CD	2.23	0.59
2:D:361:LEU:CD2	2:D:387:ILE:CG1	2.80	0.59
2:G:370:ILE:HD11	2:G:445:PHE:HE1	1.63	0.59
1:A:177:MET:SD	1:A:210:LYS:HE3	2.41	0.59
2:D:193:ASP:OD1	2:D:195:HIS:N	2.32	0.59
2:D:280:HIS:CD2	2:D:281:LEU:HD13	2.37	0.59
1:B:122:PHE:CD1	1:B:146:TYR:CB	2.84	0.59
2:H:376:VAL:CG2	2:H:377:PHE:N	2.65	0.59
2:H:16:VAL:CG2	2:H:27:ILE:HD12	2.32	0.59
1:B:199:LEU:N	1:B:204:LEU:HD11	2.17	0.59
2:H:496:ARG:NE	2:H:496:ARG:N	2.49	0.59
1:F:89:PHE:O	1:F:92:PHE:HD1	1.85	0.59
2:C:380:LEU:HD12	2:C:445:PHE:CE1	2.36	0.59
2:D:471:LYS:H	2:D:471:LYS:HD2	1.66	0.59
2:G:205:ILE:HG22	2:G:209:LEU:HD11	1.84	0.59
2:C:497:LYS:HA	2:C:500:GLU:OE2	2.02	0.59
2:H:141:ARG:NH1	2:H:347:GLN:HE21	1.99	0.59
2:H:143:ILE:HG22	2:H:144:ASN:N	2.17	0.59
2:C:254:PHE:HD1	2:C:254:PHE:N	1.99	0.59
2:C:255:ILE:CD1	2:C:265:LEU:CB	2.47	0.59
2:H:339:VAL:HA	2:H:342:ILE:HD12	1.83	0.59
1:E:63:ALA:HA	1:E:66:ALA:HB3	1.84	0.59
2:C:397:THR:CG2	2:C:436:ARG:HA	2.32	0.59
1:A:153:LEU:HB3	1:A:158:VAL:HB	1.85	0.59
2:C:471:LYS:CD	2:C:471:LYS:H	2.15	0.59
2:H:361:LEU:CD2	2:H:387:ILE:HD12	2.32	0.59
2:H:152:ALA:CB	2:H:342:ILE:HG21	2.31	0.59
2:G:239:LYS:NZ	2:G:312:SER:OG	2.35	0.59
2:D:153:TYR:HB3	2:D:155:LEU:CD1	2.27	0.59
1:A:92:PHE:CZ	1:B:92:PHE:CE1	2.90	0.59
2:H:202:ASP:O	2:H:206:ILE:CD1	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:249:GLN:HA	2:G:269:LEU:N	2.11	0.59
2:D:299:THR:HG23	2:D:302:ASP:OD2	2.02	0.59
2:D:494:ALA:C	2:D:496:ARG:HG2	2.23	0.59
1:A:128:ILE:O	1:A:128:ILE:CG2	2.49	0.59
2:H:324:ARG:HG3	2:H:325:GLU:H	1.68	0.59
2:G:392:SER:OG	2:G:444:THR:HG22	2.01	0.59
2:G:112:ALA:O	2:G:139:VAL:HA	2.03	0.59
2:D:67:ILE:HD12	2:D:89:ILE:CG2	2.24	0.59
2:C:357:ASP:HB3	2:C:359:VAL:CG2	2.33	0.59
2:D:387:ILE:O	2:D:389:THR:HG22	2.02	0.59
2:C:462:THR:O	2:C:463:ASN:HB2	2.02	0.59
2:H:370:ILE:HG22	2:H:371:GLU:N	2.17	0.59
2:H:494:ALA:O	2:H:496:ARG:CZ	2.51	0.59
2:G:211:ASN:HA	2:G:214:LYS:HD2	1.83	0.59
2:H:250:ILE:O	2:H:266:GLU:HA	2.02	0.59
2:H:486:LYS:HZ2	2:H:486:LYS:C	2.06	0.59
2:H:180:LEU:HB2	2:H:185:PHE:HE1	1.68	0.59
2:H:443:VAL:HA	2:H:456:ARG:O	2.03	0.59
2:D:209:LEU:CD1	2:D:265:LEU:HD11	2.27	0.59
2:G:239:LYS:HG2	2:G:315:ILE:HD11	1.83	0.59
2:C:27:ILE:HD13	2:C:101:ALA:HA	1.85	0.59
1:B:110:SER:OG	1:B:111:LEU:N	2.35	0.59
2:G:434:ALA:HB1	2:G:435:PRO:HD2	1.85	0.59
1:A:114:ASP:OD2	1:B:155:LYS:CE	2.50	0.59
2:C:414:ARG:CZ	2:C:419:ASP:OD2	2.51	0.59
2:H:479:GLU:HG3	2:H:480:GLU:N	2.18	0.59
2:G:307:ILE:CG2	2:G:308:LEU:N	2.65	0.59
1:A:199:LEU:HB2	1:A:204:LEU:CD1	2.23	0.59
2:D:312:SER:O	2:D:315:ILE:CD1	2.51	0.59
2:H:243:SER:O	2:H:316:PRO:HG3	2.02	0.59
1:A:199:LEU:O	1:A:200:LYS:C	2.42	0.58
2:G:377:PHE:CD1	2:G:410:LEU:HD12	2.38	0.58
2:D:312:SER:O	2:D:315:ILE:HG13	2.02	0.58
2:H:373:MET:HG2	2:H:398:ALA:HB2	1.85	0.58
1:A:134:GLN:HG2	2:D:260:ASN:O	2.03	0.58
2:G:151:LEU:HA	2:G:154:GLY:HA2	1.84	0.58
2:G:151:LEU:O	2:G:346:ILE:CD1	2.49	0.58
2:H:147:THR:HG22	2:H:185:PHE:HD2	1.66	0.58
2:H:16:VAL:HG22	2:H:27:ILE:HD12	1.83	0.58
2:D:497:LYS:HD3	2:D:498:ARG:CA	2.33	0.58
2:H:156:ASP:HA	2:H:180:LEU:HD21	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:359:VAL:CG1	2:C:362:ASP:OD2	2.51	0.58
2:H:126:GLN:O	2:H:127:ALA:C	2.42	0.58
1:E:67:GLN:OE1	1:F:68:ILE:HD13	2.03	0.58
2:D:455:VAL:HG12	2:D:456:ARG:N	2.17	0.58
2:G:77:VAL:CG1	2:G:79:ILE:HD12	2.32	0.58
2:C:372:THR:HG21	2:C:378:THR:OG1	2.03	0.58
2:H:361:LEU:CD2	2:H:387:ILE:HD11	2.32	0.58
2:D:98:LYS:HD2	2:D:137:LEU:CD2	2.14	0.58
2:C:229:GLN:CA	2:C:229:GLN:HE21	2.15	0.58
1:A:89:PHE:HA	1:B:89:PHE:HE1	1.69	0.58
1:A:92:PHE:HE1	1:A:96:THR:OG1	1.86	0.58
2:C:322:ILE:O	2:C:326:LEU:HD22	2.02	0.58
2:C:347:GLN:O	2:C:351:ILE:HG13	2.03	0.58
1:E:95:ARG:HD2	2:G:104:TYR:CE1	2.38	0.58
2:H:361:LEU:HD11	2:H:387:ILE:CD1	2.33	0.58
2:H:339:VAL:HA	2:H:342:ILE:CD1	2.32	0.58
2:G:491:ASN:ND2	2:G:494:ALA:HB2	2.19	0.58
2:H:119:TYR:CB	2:H:190:THR:HG21	2.31	0.58
2:C:191:ALA:HB1	2:C:288:PRO:HB3	1.84	0.58
2:D:208:TYR:HD1	2:D:208:TYR:C	2.05	0.58
2:C:18:VAL:HG23	2:C:19:LEU:N	2.19	0.58
2:D:359:VAL:H	2:G:395:PHE:HB3	1.69	0.58
1:A:196:GLY:HA3	1:A:207:ALA:HB2	1.86	0.58
2:C:152:ALA:HB2	2:C:343:GLY:N	2.18	0.58
2:C:159:GLU:N	2:C:159:GLU:CD	2.56	0.58
2:D:29:ASN:HD22	2:D:29:ASN:H	1.50	0.58
2:H:67:ILE:CD1	2:H:89:ILE:CD1	2.62	0.58
1:B:123:GLU:OE2	1:B:195:LYS:HD2	2.03	0.58
2:D:385:THR:O	2:D:386:THR:HB	2.02	0.58
1:A:89:PHE:HB2	1:B:89:PHE:CE1	2.39	0.58
2:C:205:ILE:CD1	2:C:274:PHE:HE2	2.17	0.58
2:G:212:GLN:O	2:G:215:GLN:HB3	2.04	0.58
1:B:86:TYR:CE2	2:C:359:VAL:HG11	2.38	0.58
2:G:303:ILE:HG21	2:G:306:VAL:HG23	1.86	0.58
1:A:158:VAL:HG22	1:A:199:LEU:HG	1.84	0.58
2:D:139:VAL:HG12	2:D:141:ARG:N	2.19	0.58
2:H:286:MET:O	2:H:290:ARG:HD2	2.02	0.58
2:H:144:ASN:HB3	2:H:146:PRO:HD2	1.86	0.58
2:D:389:THR:OG1	2:D:390:SER:N	2.34	0.58
2:G:414:ARG:O	2:G:420:ASN:ND2	2.37	0.58
2:C:462:THR:HG21	2:C:464:LYS:CB	2.31	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:396:THR:OG1	2:H:397:THR:N	2.30	0.58
2:D:11:THR:HG23	2:D:68:LYS:HZ2	1.69	0.58
1:A:198:LYS:O	1:A:198:LYS:HG2	2.02	0.58
2:G:394:VAL:HG13	2:G:441:ILE:O	2.03	0.58
2:H:153:TYR:HB3	2:H:155:LEU:CD1	2.31	0.58
2:H:361:LEU:HD11	2:H:387:ILE:HD12	1.85	0.58
2:D:105:LEU:HD13	2:D:105:LEU:N	2.19	0.58
2:H:16:VAL:O	2:H:16:VAL:HG22	2.03	0.58
2:C:396:THR:CG2	2:H:361:LEU:HB2	2.34	0.57
2:D:206:ILE:HD11	2:D:232:LYS:HA	1.85	0.57
2:D:361:LEU:O	2:D:362:ASP:CG	2.41	0.57
2:G:370:ILE:CD1	2:G:445:PHE:CZ	2.86	0.57
2:D:65:ILE:O	2:D:66:SER:C	2.42	0.57
2:C:73:THR:CG2	2:C:75:TYR:HB3	2.34	0.57
1:E:81:ARG:NH1	2:G:355:VAL:HG23	2.19	0.57
2:H:496:ARG:C	2:H:498:ARG:N	2.54	0.57
2:C:499:LYS:O	2:C:502:ALA:HB3	2.03	0.57
2:C:198:GLY:O	2:C:201:PHE:N	2.37	0.57
1:A:131:ASP:CB	1:A:136:LYS:HE3	2.32	0.57
1:A:178:GLN:NE2	1:A:213:GLN:HA	2.18	0.57
2:D:148:ALA:O	2:D:343:GLY:HA3	2.03	0.57
2:D:73:THR:HG22	2:D:74:ASP:N	2.19	0.57
2:G:29:ASN:HA	2:G:100:TYR:CE2	2.39	0.57
2:D:422:SER:O	2:D:423:LEU:HG	2.05	0.57
2:C:29:ASN:HB2	2:C:30:PRO:CD	2.35	0.57
1:B:116:LEU:HD13	1:B:197:TYR:CD2	2.23	0.57
1:A:149:LEU:O	1:A:152:ALA:HB3	2.04	0.57
2:H:124:GLN:O	2:H:127:ALA:HB3	2.05	0.57
2:G:322:ILE:HA	2:G:325:GLU:HB2	1.85	0.57
2:C:414:ARG:HH21	2:C:494:ALA:CB	2.17	0.57
2:H:147:THR:CG2	2:H:185:PHE:CD2	2.86	0.57
2:G:177:ILE:HB	2:G:189:ALA:HB3	1.86	0.57
2:C:193:ASP:OD2	2:C:196:LEU:N	2.36	0.57
2:C:269:LEU:HD11	2:C:274:PHE:HB2	1.86	0.57
2:D:495:ASP:C	2:D:497:LYS:N	2.56	0.57
2:H:289:VAL:O	2:H:293:LEU:HG	2.04	0.57
1:A:185:GLU:HB3	1:A:186:PRO:HD2	1.86	0.57
1:F:84:ARG:O	1:F:87:ALA:HB3	2.05	0.57
2:C:43:LYS:NZ	2:C:61:PRO:HD2	2.20	0.57
2:G:242:LEU:HD23	2:G:274:PHE:CD2	2.40	0.57
1:A:120:ASP:O	1:A:123:GLU:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:SER:O	2:D:39:VAL:CG1	2.53	0.57
2:D:372:THR:OG1	2:D:373:MET:N	2.36	0.57
2:C:70:HIS:O	2:C:73:THR:HG22	2.03	0.57
2:G:151:LEU:HG	2:G:151:LEU:O	2.03	0.57
2:D:256:SER:O	2:D:263:LEU:HB2	2.04	0.57
2:H:71:MET:O	2:H:124:GLN:HB2	2.05	0.57
2:C:426:PHE:CD2	2:C:468:ILE:CD1	2.87	0.57
2:C:505:ARG:NH1	2:C:505:ARG:HG2	2.19	0.57
2:H:397:THR:HG22	2:H:439:PRO:HD2	1.87	0.57
2:G:124:GLN:O	2:G:127:ALA:HB3	2.05	0.57
2:D:230:ARG:CZ	2:D:252:LEU:CD1	2.83	0.57
1:A:109:GLN:O	1:A:110:SER:C	2.43	0.57
2:D:388:PRO:HG3	2:D:449:ALA:CA	2.34	0.57
2:H:166:TYR:CE1	2:H:168:LEU:HD23	2.40	0.57
2:D:504:LEU:HD13	2:D:507:GLU:CB	2.33	0.57
1:A:114:ASP:OD2	1:B:155:LYS:HE3	2.04	0.57
2:G:398:ALA:HB2	2:G:402:GLN:HE22	1.69	0.57
2:D:210:VAL:HG23	2:D:221:LEU:HD13	1.85	0.57
2:C:18:VAL:CG1	2:C:27:ILE:CD1	2.83	0.57
2:C:370:ILE:HD13	2:C:407:ILE:CG2	2.34	0.57
2:D:151:LEU:N	2:D:151:LEU:CD1	2.66	0.57
2:C:175:VAL:HG12	2:C:176:SER:N	2.19	0.57
1:A:125:ALA:O	1:A:128:ILE:HG13	2.04	0.57
2:C:241:GLU:O	2:C:245:VAL:HG13	2.05	0.57
2:G:241:GLU:O	2:G:245:VAL:N	2.37	0.57
2:H:495:ASP:C	2:H:497:LYS:H	2.06	0.57
1:A:174:GLN:HB2	2:C:55:ARG:HD2	1.85	0.57
1:B:92:PHE:CG	1:B:93:ARG:N	2.73	0.57
2:G:400:ASP:N	2:G:436:ARG:HB3	2.19	0.57
1:A:78:MET:SD	1:A:82:TYR:OH	2.62	0.57
2:C:243:SER:O	2:C:271:ARG:NH1	2.38	0.57
2:H:96:TYR:O	2:H:99:SER:N	2.38	0.57
1:F:120:ASP:O	1:F:124:ARG:CB	2.53	0.57
2:C:87:GLN:HB3	2:C:134:ILE:HD12	1.87	0.56
2:D:64:ILE:CG2	2:D:67:ILE:CD1	2.69	0.56
2:D:137:LEU:N	2:D:137:LEU:HD23	2.19	0.56
2:C:116:VAL:O	2:C:144:ASN:HA	2.04	0.56
2:C:8:ASP:O	2:C:14:SER:HB3	2.04	0.56
2:G:387:ILE:HG21	2:G:449:ALA:O	2.05	0.56
1:B:169:ASP:C	1:B:171:TYR:N	2.55	0.56
2:D:13:ASN:HA	2:D:38:SER:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:TYR:CE2	2:D:322:ILE:CD1	2.88	0.56
1:B:132:ASN:C	1:B:133:GLU:HG3	2.25	0.56
2:C:405:VAL:HG11	2:C:441:ILE:HD13	1.86	0.56
2:D:379:LYS:O	2:D:380:LEU:HD23	2.05	0.56
1:A:68:ILE:O	1:A:72:GLU:HG3	2.05	0.56
2:H:8:ASP:O	2:H:14:SER:HB3	2.04	0.56
2:G:164:LEU:HD22	2:G:165:VAL:N	2.21	0.56
2:C:29:ASN:HA	2:C:100:TYR:CD2	2.39	0.56
2:D:285:THR:HB	2:D:286:MET:SD	2.44	0.56
1:A:133:GLU:CD	1:B:133:GLU:OE1	2.44	0.56
2:D:58:ILE:CG2	2:D:58:ILE:O	2.53	0.56
2:H:420:ASN:H	2:H:420:ASN:HD22	1.52	0.56
2:D:421:LYS:HZ1	2:D:480:GLU:CD	2.08	0.56
2:D:67:ILE:HD13	2:D:89:ILE:CB	2.35	0.56
2:D:70:HIS:O	2:D:86:PRO:HG2	2.05	0.56
1:A:106:TYR:CD1	1:A:106:TYR:N	2.71	0.56
2:D:38:SER:O	2:D:39:VAL:HG12	2.05	0.56
2:C:370:ILE:HD13	2:C:407:ILE:HG21	1.87	0.56
2:D:318:VAL:HG12	2:D:322:ILE:HD11	1.87	0.56
2:H:71:MET:HE2	2:H:128:THR:HG23	1.87	0.56
2:C:152:ALA:HB2	2:C:343:GLY:HA2	1.86	0.56
2:G:91:ALA:O	2:G:135:ALA:HB2	2.05	0.56
2:G:125:ARG:HA	2:G:128:THR:HG23	1.86	0.56
2:C:133:ARG:HB3	2:C:133:ARG:HH11	1.68	0.56
2:H:114:ILE:CG2	2:H:115:THR:H	2.19	0.56
2:H:368:LEU:HD23	2:H:368:LEU:N	2.20	0.56
2:D:42:PHE:CE1	2:D:79:ILE:CD1	2.89	0.56
2:C:497:LYS:C	2:C:499:LYS:H	2.07	0.56
2:G:492:ALA:O	2:G:493:GLU:HG2	2.06	0.56
2:H:367:SER:HB3	2:H:383:ARG:CA	2.35	0.56
2:G:371:GLU:CG	2:G:408:HIS:HB3	2.20	0.56
1:B:94:ARG:NH1	1:B:98:GLN:NE2	2.54	0.56
2:C:366:LEU:HA	2:C:383:ARG:CG	2.35	0.56
2:D:339:VAL:HG12	2:D:340:VAL:N	2.19	0.56
2:G:279:ALA:O	2:G:282:VAL:HG12	2.05	0.56
1:A:203:VAL:HG12	1:A:203:VAL:O	2.05	0.56
2:G:120:PHE:HA	2:G:124:GLN:NE2	2.20	0.56
2:C:505:ARG:HH11	2:C:505:ARG:HG2	1.71	0.56
2:D:161:GLN:N	2:D:180:LEU:HD23	2.20	0.56
2:G:462:THR:CB	2:G:464:LYS:H	2.17	0.56
2:C:471:LYS:NZ	2:C:471:LYS:HB2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:GLY:C	2:C:156:ASP:H	2.08	0.56
2:H:147:THR:HA	2:H:150:ALA:HB3	1.87	0.56
2:C:397:THR:HG22	2:C:437:GLY:H	1.71	0.56
2:D:201:PHE:CE1	2:D:281:LEU:HD23	2.40	0.56
2:D:121:ASN:N	2:D:124:GLN:OE1	2.39	0.56
2:D:143:ILE:HG22	2:D:144:ASN:N	2.20	0.56
2:C:408:HIS:NE2	2:C:422:SER:OG	2.33	0.56
2:C:79:ILE:HG22	2:C:80:GLU:HG2	1.87	0.56
2:G:501:ALA:O	2:G:504:LEU:HD23	2.04	0.56
1:A:71:LEU:HG	1:A:74:LYS:HD2	1.87	0.56
2:H:273:LYS:HD3	2:H:276:GLU:CD	2.26	0.56
2:D:256:SER:O	2:D:263:LEU:CB	2.54	0.56
2:G:308:LEU:HD13	2:G:330:PRO:CG	2.35	0.56
2:D:105:LEU:C	2:D:107:GLU:N	2.59	0.56
1:E:66:ALA:O	1:E:69:ALA:HB3	2.06	0.56
2:D:14:SER:O	2:D:36:THR:CG2	2.53	0.56
1:F:98:GLN:HA	1:F:101:GLU:CD	2.25	0.56
2:D:21:GLY:C	2:D:23:GLU:H	2.09	0.56
2:H:67:ILE:CG1	2:H:89:ILE:HD13	2.35	0.56
2:D:220:ASP:O	2:D:223:LYS:HG2	2.06	0.56
1:F:86:TYR:CE2	2:G:359:VAL:HG13	2.40	0.56
2:D:338:GLU:O	2:D:339:VAL:C	2.44	0.56
1:A:88:ASP:OD1	2:C:3:LYS:HE2	2.06	0.56
1:A:121:ASN:HD22	1:B:145:VAL:CG2	2.19	0.56
2:D:65:ILE:CG2	2:D:66:SER:N	2.54	0.56
2:D:334:VAL:HB	2:D:339:VAL:CG2	2.36	0.56
2:D:499:LYS:HG2	2:D:500:GLU:N	2.21	0.56
2:D:224:ASP:CG	2:D:226:MET:HB2	2.26	0.56
2:C:72:GLY:HA3	2:C:124:GLN:HG2	1.88	0.56
2:G:10:GLY:N	2:G:13:ASN:O	2.37	0.56
2:H:1:MET:O	2:H:1:MET:HG2	2.05	0.56
2:C:5:ILE:HD12	2:C:109:VAL:HG21	1.87	0.55
1:B:165:GLY:O	1:B:188:THR:HG23	2.06	0.55
1:A:138:ILE:HD13	1:B:139:LEU:HD11	1.87	0.55
2:H:166:TYR:HE1	2:H:168:LEU:HD23	1.71	0.55
2:D:416:MET:CE	2:D:417:ALA:H	2.17	0.55
2:D:504:LEU:O	2:D:504:LEU:CD1	2.54	0.55
2:D:146:PRO:HB3	2:D:165:VAL:HG21	1.87	0.55
2:H:435:PRO:O	2:H:439:PRO:HD3	2.05	0.55
1:E:97:ARG:HD2	1:E:97:ARG:O	2.05	0.55
2:G:489:GLU:OE1	2:G:489:GLU:HA	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:347:GLN:HA	2:G:350:VAL:HB	1.87	0.55
2:D:154:GLY:O	2:D:156:ASP:OD1	2.23	0.55
2:H:203:GLN:HE22	2:H:206:ILE:HG21	1.72	0.55
1:F:60:GLU:N	1:F:63:ALA:HB3	2.21	0.55
2:D:130:ASP:O	2:D:134:ILE:HG13	2.05	0.55
2:C:502:ALA:O	2:C:505:ARG:HD3	2.05	0.55
2:D:408:HIS:HB3	2:D:410:LEU:HD21	1.87	0.55
2:H:146:PRO:CB	2:H:178:LEU:HD11	2.36	0.55
2:H:361:LEU:HD11	2:H:387:ILE:HG13	1.77	0.55
2:D:208:TYR:CE1	2:D:212:GLN:CG	2.88	0.55
2:H:339:VAL:HG23	2:H:342:ILE:HD13	1.75	0.55
2:H:149:ALA:HA	2:H:339:VAL:O	2.07	0.55
2:G:164:LEU:CD2	2:G:175:VAL:HB	2.36	0.55
2:G:165:VAL:HG22	2:G:176:SER:N	2.13	0.55
2:D:120:PHE:CE2	2:D:124:GLN:HB3	2.42	0.55
2:D:164:LEU:HD13	2:D:165:VAL:C	2.27	0.55
2:H:94:LEU:HD12	2:H:97:LEU:HB2	1.88	0.55
2:D:483:ARG:HH21	1:F:85:LEU:CD2	2.19	0.55
2:C:155:LEU:HD13	2:C:155:LEU:N	2.21	0.55
2:C:468:ILE:HG22	2:C:469:THR:N	2.21	0.55
2:D:42:PHE:N	2:D:42:PHE:CD1	2.73	0.55
1:A:134:GLN:O	1:A:137:SER:HB3	2.06	0.55
2:D:405:VAL:O	2:D:405:VAL:HG23	2.05	0.55
2:H:15:CYS:SG	2:H:338:GLU:CB	2.95	0.55
2:C:102:GLU:O	2:C:106:GLY:N	2.39	0.55
2:D:315:ILE:HD12	2:D:318:VAL:HG21	1.88	0.55
2:H:7:ILE:HD13	2:H:97:LEU:HD23	1.89	0.55
1:E:72:GLU:HA	1:E:75:LEU:HB2	1.89	0.55
1:E:81:ARG:HG3	1:E:82:TYR:CD1	2.41	0.55
2:D:332:LYS:H	2:D:332:LYS:CD	2.20	0.55
2:D:500:GLU:CA	2:D:503:GLU:HB2	2.37	0.55
1:A:113:SER:OG	1:A:114:ASP:N	2.37	0.55
2:D:10:GLY:HA2	2:D:68:LYS:HZ1	1.71	0.55
2:D:235:ALA:O	2:D:238:ALA:HB3	2.07	0.55
2:D:420:ASN:ND2	2:D:420:ASN:N	2.54	0.55
2:D:421:LYS:HE3	2:D:480:GLU:OE2	2.06	0.55
2:H:381:ILE:CD1	2:H:447:ILE:CD1	2.82	0.55
2:G:366:LEU:HB2	2:G:411:GLN:NE2	2.18	0.55
2:G:411:GLN:HB2	2:G:423:LEU:HD11	1.89	0.55
2:D:322:ILE:HG23	2:D:326:LEU:CD2	2.37	0.55
1:A:89:PHE:C	1:A:89:PHE:HD1	2.10	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LEU:O	1:A:119:LEU:HD13	2.07	0.55
2:C:282:VAL:CG1	2:C:283:GLU:N	2.70	0.55
2:C:17:ALA:O	2:C:345:ALA:HB2	2.07	0.55
2:H:192:GLY:O	2:H:288:PRO:HG3	2.07	0.55
2:H:153:TYR:O	2:H:154:GLY:C	2.44	0.55
2:D:67:ILE:HD13	2:D:89:ILE:CG2	2.34	0.55
1:B:177:MET:HB3	1:B:210:LYS:CG	2.28	0.55
1:F:64:ALA:O	1:F:68:ILE:HG13	2.07	0.55
2:H:397:THR:CG2	2:H:439:PRO:HG2	2.37	0.55
2:G:398:ALA:N	2:G:402:GLN:OE1	2.39	0.55
2:C:368:LEU:CD2	2:C:411:GLN:HB2	2.37	0.55
2:D:25:LYS:HG3	2:D:26:VAL:H	1.71	0.55
1:A:134:GLN:CG	2:D:260:ASN:O	2.54	0.55
2:C:303:ILE:O	2:C:328:LYS:HE3	2.07	0.55
2:H:484:MET:O	2:H:487:GLU:HB3	2.07	0.55
2:G:298:LEU:HB3	2:G:302:ASP:CB	2.37	0.55
2:G:370:ILE:HD11	2:G:445:PHE:CZ	2.41	0.55
2:D:167:ASP:C	2:D:167:ASP:OD1	2.44	0.55
2:C:370:ILE:HG12	2:C:409:VAL:HA	1.88	0.55
1:A:160:ALA:HA	1:A:197:TYR:CD1	2.40	0.55
2:C:168:LEU:HD13	2:C:197:GLY:HA2	1.87	0.55
2:D:370:ILE:HD11	2:D:445:PHE:CZ	2.41	0.55
1:B:161:ILE:CD1	1:B:198:LYS:HB3	2.35	0.55
2:G:440:GLN:HB2	2:G:460:LEU:HG	1.88	0.55
2:D:495:ASP:C	2:D:497:LYS:H	2.09	0.55
2:D:236:GLU:O	2:D:239:LYS:N	2.40	0.55
2:H:387:ILE:CG2	2:H:388:PRO:N	2.69	0.55
2:D:230:ARG:CZ	2:D:252:LEU:HD13	2.37	0.55
2:C:19:LEU:HD23	2:C:19:LEU:O	2.06	0.55
2:G:370:ILE:HG13	2:G:445:PHE:HZ	1.71	0.55
1:A:119:LEU:O	1:A:119:LEU:HD22	2.07	0.55
2:G:205:ILE:HG22	2:G:209:LEU:CD1	2.37	0.55
2:H:496:ARG:NE	2:H:496:ARG:C	2.58	0.55
2:C:151:LEU:C	2:C:154:GLY:H	2.10	0.55
1:E:92:PHE:CE1	1:F:92:PHE:CE2	2.95	0.55
2:G:472:SER:O	2:G:473:SER:HB3	2.07	0.55
2:C:27:ILE:HD13	2:C:101:ALA:CB	2.37	0.54
1:A:91:ASN:O	1:A:94:ARG:N	2.40	0.54
1:A:75:LEU:HG	1:B:75:LEU:CD2	2.37	0.54
2:C:164:LEU:C	2:C:164:LEU:HD22	2.26	0.54
2:D:241:GLU:O	2:D:245:VAL:HG13	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:477:SER:HB3	2:D:481:ILE:CD1	2.37	0.54
2:D:73:THR:HG22	2:D:74:ASP:H	1.71	0.54
2:G:162:THR:C	2:G:163:ILE:HG13	2.28	0.54
2:D:104:TYR:C	2:D:105:LEU:HD13	2.28	0.54
2:C:29:ASN:HD21	2:C:36:THR:HG23	1.70	0.54
2:G:458:LYS:NZ	2:G:465:GLU:HB3	2.22	0.54
2:C:203:GLN:OE1	2:C:203:GLN:HA	2.06	0.54
2:G:91:ALA:HB2	2:G:134:ILE:CG2	2.37	0.54
2:D:505:ARG:HG3	2:D:506:ASN:H	1.71	0.54
2:C:257:ALA:HB2	2:C:262:PRO:HA	1.90	0.54
1:A:168:PHE:HB3	1:A:189:VAL:HG22	1.89	0.54
2:G:405:VAL:HG21	2:G:441:ILE:HD13	1.90	0.54
1:B:160:ALA:HB2	1:B:197:TYR:CE1	2.40	0.54
1:A:105:LYS:HB3	1:A:106:TYR:CD1	2.43	0.54
2:G:414:ARG:NE	2:G:494:ALA:HB3	2.23	0.54
2:D:196:LEU:HD12	2:D:197:GLY:H	1.71	0.54
2:D:141:ARG:NH2	2:D:143:ILE:HD11	2.22	0.54
2:D:322:ILE:HG23	2:D:326:LEU:HD22	1.89	0.54
2:G:249:GLN:CA	2:G:269:LEU:H	2.14	0.54
2:C:80:GLU:CA	2:C:80:GLU:OE1	2.53	0.54
1:E:71:LEU:HB3	1:F:71:LEU:HD12	1.88	0.54
1:B:77:GLU:OE1	1:B:81:ARG:HD3	2.08	0.54
2:D:8:ASP:O	2:D:14:SER:HB3	2.08	0.54
2:D:180:LEU:HA	2:D:184:VAL:O	2.06	0.54
2:D:492:ALA:C	2:D:494:ALA:H	2.08	0.54
2:C:245:VAL:HG22	2:C:247:GLN:H	1.72	0.54
2:G:77:VAL:CG1	2:G:79:ILE:CD1	2.84	0.54
1:A:168:PHE:CD2	1:A:173:HIS:HB2	2.42	0.54
2:G:434:ALA:HB1	2:G:435:PRO:CD	2.37	0.54
2:C:357:ASP:CB	2:C:359:VAL:HG23	2.37	0.54
2:G:428:LEU:HD13	2:G:466:GLN:HB2	1.88	0.54
2:D:289:VAL:O	2:D:293:LEU:HG	2.07	0.54
2:C:20:GLU:O	2:C:21:GLY:C	2.43	0.54
1:B:94:ARG:O	1:B:98:GLN:HB2	2.07	0.54
2:H:29:ASN:HA	2:H:100:TYR:HD2	1.73	0.54
2:G:396:THR:HG1	2:G:437:GLY:HA2	1.70	0.54
1:E:71:LEU:HD23	1:F:71:LEU:HB2	1.87	0.54
2:C:194:ASN:OD1	2:C:194:ASN:C	2.45	0.54
2:H:141:ARG:NH1	2:H:347:GLN:NE2	2.55	0.54
1:B:126:LEU:HD23	1:B:126:LEU:N	2.11	0.54
1:B:123:GLU:HB3	1:B:127:LYS:CE	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:LYS:HG2	1:B:167:PRO:HD3	1.89	0.54
2:C:493:GLU:HA	2:C:493:GLU:OE1	2.07	0.54
2:D:29:ASN:HD22	2:D:29:ASN:N	2.04	0.54
2:C:178:LEU:HD12	2:C:178:LEU:N	2.23	0.54
2:D:86:PRO:HD2	2:D:87:GLN:OE1	2.08	0.54
2:H:481:ILE:C	2:H:483:ARG:N	2.60	0.54
2:G:308:LEU:HD13	2:G:330:PRO:CB	2.38	0.54
2:C:90:SER:O	2:C:94:LEU:HD13	2.07	0.54
2:D:175:VAL:CG2	2:D:191:ALA:HB3	2.38	0.54
2:D:173:PHE:CE1	2:D:175:VAL:HG13	2.43	0.54
1:A:126:LEU:O	1:A:129:GLU:OE2	2.25	0.54
2:D:323:LYS:HG3	2:D:328:LYS:C	2.27	0.54
2:G:357:ASP:OD2	2:G:359:VAL:CG2	2.56	0.54
2:C:270:THR:HG22	2:C:271:ARG:N	2.23	0.54
2:G:64:ILE:CB	2:G:67:ILE:HD11	2.37	0.54
2:G:156:ASP:N	2:G:156:ASP:OD1	2.34	0.54
2:D:477:SER:HB3	2:D:481:ILE:HD12	1.90	0.54
2:D:52:VAL:HA	2:D:55:ARG:NH2	2.23	0.54
1:A:111:LEU:CD1	1:B:111:LEU:HD12	2.37	0.54
2:G:400:ASP:CB	2:G:401:ASN:HD22	2.19	0.54
1:A:79:GLU:HA	1:A:82:TYR:HD2	1.71	0.54
2:H:504:LEU:O	2:H:507:GLU:HB3	2.08	0.54
2:H:471:LYS:H	2:H:471:LYS:HD2	1.71	0.54
2:D:468:ILE:HG22	2:D:469:THR:H	1.67	0.54
2:C:252:LEU:O	2:C:255:ILE:HG13	2.07	0.54
1:A:111:LEU:HD12	1:B:111:LEU:HD12	1.89	0.54
2:G:397:THR:HB	2:G:437:GLY:H	1.72	0.54
2:D:436:ARG:HB3	2:D:436:ARG:CZ	2.38	0.54
2:D:504:LEU:O	2:D:507:GLU:HB3	2.07	0.54
2:C:414:ARG:NH1	2:C:419:ASP:CG	2.61	0.54
2:C:484:MET:HE2	2:C:487:GLU:HB2	1.90	0.54
2:H:464:LYS:HZ2	2:H:464:LYS:HB2	1.72	0.54
1:A:178:GLN:HE21	1:A:213:GLN:HA	1.73	0.54
2:G:155:LEU:HB2	2:G:185:PHE:HZ	1.71	0.54
2:D:209:LEU:HD12	2:D:231:LEU:HD21	1.89	0.54
2:H:334:VAL:CG2	2:H:336:PRO:HG3	2.37	0.54
2:G:163:ILE:HG22	2:G:164:LEU:N	2.23	0.54
2:G:308:LEU:HD13	2:G:330:PRO:HG3	1.89	0.54
1:A:106:TYR:N	1:A:106:TYR:HD1	2.06	0.54
2:D:141:ARG:NE	2:D:143:ILE:HD11	2.23	0.54
2:D:381:ILE:HD13	2:D:447:ILE:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NH2	2:C:354:GLU:CB	2.71	0.53
2:G:498:ARG:O	2:G:501:ALA:HB3	2.07	0.53
2:H:496:ARG:NE	2:H:496:ARG:H	2.05	0.53
2:C:243:SER:O	2:C:316:PRO:HG3	2.08	0.53
2:H:409:VAL:HG23	2:H:409:VAL:O	2.07	0.53
2:D:483:ARG:CG	2:D:483:ARG:HH11	2.20	0.53
2:D:82:LYS:HD2	2:D:83:GLN:H	1.73	0.53
2:C:64:ILE:HG22	2:C:67:ILE:HG13	1.90	0.53
2:G:306:VAL:HG12	2:G:307:ILE:N	2.23	0.53
2:D:161:GLN:H	2:D:180:LEU:HD23	1.72	0.53
1:A:164:VAL:O	1:A:164:VAL:HG12	2.07	0.53
2:C:128:THR:O	2:C:131:ALA:HB3	2.08	0.53
2:H:381:ILE:CD1	2:H:447:ILE:HD11	2.39	0.53
2:D:67:ILE:CD1	2:D:89:ILE:HD13	2.38	0.53
2:G:153:TYR:OH	2:G:334:VAL:HB	2.08	0.53
2:D:192:GLY:HA2	2:D:288:PRO:HB3	1.90	0.53
2:H:173:PHE:CZ	2:H:175:VAL:HG22	2.43	0.53
2:G:321:ALA:O	2:G:325:GLU:HB2	2.09	0.53
2:D:40:VAL:CG2	2:D:41:ALA:N	2.71	0.53
2:G:499:LYS:HG2	2:G:500:GLU:OE1	2.08	0.53
2:C:221:LEU:HD21	2:C:255:ILE:HG22	1.90	0.53
1:E:96:THR:HG23	1:F:100:MET:HE3	1.91	0.53
1:B:77:GLU:O	1:B:81:ARG:HB2	2.09	0.53
2:G:70:HIS:CG	2:G:75:TYR:CG	2.97	0.53
2:G:91:ALA:HB2	2:G:134:ILE:HG22	1.90	0.53
2:H:396:THR:OG1	2:H:439:PRO:HD2	2.08	0.53
2:C:153:TYR:HB3	2:C:155:LEU:HD11	1.91	0.53
2:G:483:ARG:NH1	2:G:486:LYS:HZ3	2.05	0.53
2:C:84:TYR:HA	2:C:88:GLU:OE1	2.07	0.53
2:D:71:MET:SD	2:D:86:PRO:HB2	2.49	0.53
2:G:239:LYS:HG3	2:G:315:ILE:HD11	1.88	0.53
1:B:169:ASP:O	1:B:171:TYR:N	2.42	0.53
2:D:164:LEU:HD12	2:D:306:VAL:HG13	1.89	0.53
1:A:86:TYR:CE2	1:A:90:GLU:OE2	2.61	0.53
2:C:493:GLU:C	2:C:495:ASP:H	2.10	0.53
2:H:438:VAL:HG22	2:H:439:PRO:HD3	1.89	0.53
2:G:433:PRO:O	2:G:434:ALA:HB2	2.09	0.53
2:C:478:GLU:HA	2:C:481:ILE:HD12	1.90	0.53
2:H:389:THR:OG1	2:H:390:SER:N	2.39	0.53
2:D:201:PHE:O	2:D:202:ASP:C	2.46	0.53
2:G:236:GLU:O	2:G:239:LYS:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:243:SER:HB3	2:G:315:ILE:HA	1.90	0.53
2:D:172:THR:OG1	2:D:173:PHE:N	2.39	0.53
1:A:83:LEU:O	1:A:83:LEU:HG	2.08	0.53
2:C:458:LYS:HE2	2:C:463:ASN:HD22	1.73	0.53
2:H:438:VAL:N	2:H:439:PRO:CD	2.71	0.53
2:D:483:ARG:NH2	1:F:85:LEU:HD22	2.23	0.53
2:C:154:GLY:C	2:C:156:ASP:N	2.61	0.53
2:H:204:VAL:HB	2:H:277:LEU:HD22	1.91	0.53
2:C:387:ILE:CG2	2:C:447:ILE:CG2	2.72	0.53
2:G:309:VAL:CG1	2:G:310:GLY:N	2.71	0.53
2:G:281:LEU:CB	2:G:284:ARG:HD3	2.33	0.53
2:G:377:PHE:CB	2:G:410:LEU:HD12	2.36	0.53
2:D:323:LYS:HD2	2:D:329:GLU:CA	2.29	0.53
1:A:75:LEU:CD1	1:A:79:GLU:OE2	2.49	0.53
2:H:85:THR:OG1	2:H:88:GLU:HG3	2.08	0.53
2:D:29:ASN:O	2:D:31:GLU:O	2.26	0.53
1:E:94:ARG:HH12	2:G:106:GLY:HA3	1.74	0.53
2:G:298:LEU:HB3	2:G:302:ASP:OD2	2.07	0.53
2:C:396:THR:OG1	2:C:397:THR:N	2.42	0.53
2:H:416:MET:O	2:H:417:ALA:CB	2.56	0.53
1:A:196:GLY:O	1:A:197:TYR:CD1	2.61	0.53
1:B:190:VAL:CG1	1:B:191:GLU:N	2.72	0.53
2:G:227:ALA:O	2:G:230:ARG:HB3	2.09	0.53
2:D:500:GLU:O	2:D:503:GLU:HB2	2.09	0.53
2:D:25:LYS:HG3	2:D:26:VAL:N	2.24	0.53
2:G:28:PRO:O	2:G:100:TYR:HE2	1.92	0.53
2:C:374:GLY:O	2:C:376:VAL:N	2.42	0.53
2:H:148:ALA:O	2:H:343:GLY:HA3	2.08	0.53
2:H:155:LEU:HD22	2:H:155:LEU:N	2.21	0.53
2:G:242:LEU:N	2:G:242:LEU:HD13	2.24	0.53
2:D:325:GLU:HB3	2:D:326:LEU:CD1	2.38	0.53
2:C:282:VAL:O	2:C:286:MET:HE3	2.09	0.53
2:G:212:GLN:HA	2:G:215:GLN:HB3	1.90	0.53
2:C:428:LEU:HG	2:C:429:THR:N	2.24	0.53
2:H:365:PRO:O	2:H:366:LEU:HD13	2.09	0.53
1:B:160:ALA:HA	1:B:197:TYR:CD1	2.39	0.53
1:A:192:GLU:OE2	1:A:195:LYS:CA	2.57	0.53
2:G:370:ILE:HG12	2:G:409:VAL:CB	2.39	0.53
1:B:96:THR:O	1:B:97:ARG:C	2.47	0.53
1:B:81:ARG:C	1:B:82:TYR:HD1	2.12	0.53
1:E:81:ARG:HD3	1:E:82:TYR:CE1	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:214:LYS:NZ	2:G:221:LEU:H	2.07	0.53
1:A:171:TYR:HD1	2:C:52:VAL:HG21	1.70	0.53
2:G:275:GLU:O	2:G:279:ALA:N	2.43	0.53
2:D:210:VAL:HA	2:D:221:LEU:HD13	1.91	0.52
1:B:139:LEU:N	1:B:139:LEU:HD23	2.24	0.52
2:H:132:GLY:O	2:H:135:ALA:CB	2.51	0.52
2:D:155:LEU:H	2:D:155:LEU:CD2	2.13	0.52
2:C:493:GLU:C	2:C:495:ASP:N	2.61	0.52
2:C:471:LYS:N	2:C:471:LYS:HD3	2.21	0.52
2:C:153:TYR:CE1	2:C:334:VAL:HG12	2.43	0.52
2:C:339:VAL:HG13	2:C:340:VAL:N	2.24	0.52
1:E:193:LEU:N	1:E:208:MET:O	2.42	0.52
2:D:211:ASN:O	2:D:215:GLN:HB2	2.08	0.52
2:D:377:PHE:HD1	2:D:378:THR:N	2.06	0.52
2:D:164:LEU:HD11	2:D:166:TYR:HB2	1.91	0.52
2:H:128:THR:C	2:H:130:ASP:N	2.60	0.52
1:F:60:GLU:N	1:F:63:ALA:CB	2.73	0.52
2:C:153:TYR:CE1	2:C:334:VAL:HB	2.44	0.52
2:H:362:ASP:HB2	2:H:387:ILE:HG12	1.90	0.52
1:B:144:MET:SD	2:C:266:GLU:CD	2.86	0.52
1:A:85:LEU:HB3	1:B:85:LEU:HD12	1.92	0.52
1:A:105:LYS:C	1:A:106:TYR:HD1	2.11	0.52
2:D:286:MET:N	2:D:286:MET:SD	2.77	0.52
1:A:86:TYR:O	1:A:87:ALA:C	2.48	0.52
2:H:370:ILE:HG22	2:H:371:GLU:O	2.10	0.52
1:A:177:MET:HB2	1:A:210:LYS:HA	1.91	0.52
2:G:90:SER:HA	2:G:93:ILE:HD12	1.91	0.52
1:A:186:PRO:O	1:A:188:THR:N	2.42	0.52
2:H:495:ASP:C	2:H:497:LYS:N	2.61	0.52
2:D:485:ILE:O	2:D:488:ALA:N	2.43	0.52
2:C:64:ILE:HG21	2:C:67:ILE:CG1	2.38	0.52
2:H:445:PHE:CE1	2:H:455:VAL:HG22	2.44	0.52
2:D:213:PHE:O	2:D:214:LYS:C	2.45	0.52
2:H:309:VAL:HG22	2:H:339:VAL:HG11	1.92	0.52
2:D:121:ASN:ND2	2:D:123:ALA:N	2.55	0.52
2:D:397:THR:HB	2:D:439:PRO:HG2	1.90	0.52
1:A:178:GLN:HA	1:A:211:VAL:O	2.09	0.52
2:D:43:LYS:NZ	2:D:59:THR:HG21	2.24	0.52
2:H:298:LEU:HD21	2:H:303:ILE:CB	2.40	0.52
2:D:251:SER:CB	2:D:266:GLU:OE2	2.58	0.52
2:G:161:GLN:HA	2:G:304:ASP:OD2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:312:SER:O	2:D:315:ILE:HD11	2.10	0.52
1:A:92:PHE:CD1	1:A:92:PHE:C	2.74	0.52
2:H:448:ASP:O	2:H:448:ASP:OD1	2.26	0.52
2:D:27:ILE:HG12	2:D:104:TYR:CD2	2.45	0.52
2:D:120:PHE:CD2	2:D:124:GLN:HB2	2.44	0.52
2:D:377:PHE:CD1	2:D:378:THR:N	2.78	0.52
2:H:376:VAL:HG23	2:H:377:PHE:N	2.25	0.52
2:D:147:THR:O	2:D:150:ALA:HB3	2.09	0.52
1:A:82:TYR:O	1:B:82:TYR:CD2	2.62	0.52
2:G:398:ALA:HB3	2:G:402:GLN:HE22	1.71	0.52
2:G:430:GLY:O	2:G:431:ILE:C	2.48	0.52
2:C:220:ASP:OD2	2:C:223:LYS:HG3	2.10	0.52
1:E:111:LEU:O	1:E:115:LEU:CB	2.58	0.52
2:D:206:ILE:CD1	2:D:232:LYS:HA	2.39	0.52
2:D:213:PHE:HB3	2:D:221:LEU:HD11	1.92	0.52
2:D:229:GLN:O	2:D:230:ARG:C	2.46	0.52
2:G:193:ASP:OD2	2:G:284:ARG:NH2	2.43	0.52
1:A:194:GLN:HG2	1:A:205:ARG:HH22	1.75	0.52
2:H:4:ILE:HG12	2:H:111:ARG:HD3	1.90	0.52
1:E:71:LEU:HD22	1:F:68:ILE:HA	1.91	0.52
1:B:198:LYS:HA	1:B:204:LEU:HD12	1.91	0.52
2:C:308:LEU:HD11	2:C:330:PRO:CB	2.40	0.52
2:D:416:MET:O	2:D:417:ALA:C	2.46	0.52
1:B:122:PHE:CE1	1:B:146:TYR:CB	2.78	0.52
2:D:282:VAL:O	2:D:286:MET:SD	2.68	0.52
2:D:164:LEU:HD13	2:D:165:VAL:N	2.24	0.52
1:E:75:LEU:O	1:E:78:MET:N	2.42	0.52
2:C:416:MET:CE	2:C:497:LYS:HB3	2.40	0.52
2:D:225:LYS:N	2:D:225:LYS:HD2	2.24	0.52
2:D:426:PHE:HZ	2:D:457:ALA:HB3	1.75	0.52
2:C:253:PRO:C	2:C:254:PHE:HD1	2.12	0.52
2:G:176:SER:O	2:G:178:LEU:HD13	2.10	0.52
1:A:120:ASP:O	1:A:121:ASN:C	2.46	0.52
2:H:4:ILE:CG1	2:H:111:ARG:HD3	2.40	0.52
2:C:279:ALA:O	2:C:282:VAL:HG12	2.10	0.52
2:D:299:THR:O	2:D:302:ASP:HB2	2.10	0.52
1:B:203:VAL:HG12	1:B:203:VAL:O	2.07	0.52
2:C:203:GLN:O	2:C:204:VAL:C	2.45	0.52
1:B:153:LEU:C	1:B:155:LYS:N	2.61	0.52
2:D:162:THR:HA	2:D:179:GLU:HA	1.92	0.52
2:D:11:THR:HG23	2:D:68:LYS:NZ	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:64:ILE:HD13	2:C:89:ILE:HG12	1.92	0.52
2:D:201:PHE:CD1	2:D:281:LEU:HD23	2.45	0.52
2:C:362:ASP:C	2:C:363:VAL:HG22	2.30	0.52
2:D:150:ALA:O	2:D:154:GLY:N	2.43	0.52
2:G:396:THR:OG1	2:G:397:THR:N	2.41	0.52
2:C:308:LEU:CD1	2:C:330:PRO:HB2	2.40	0.52
2:C:270:THR:HG22	2:C:271:ARG:H	1.75	0.52
2:H:438:VAL:N	2:H:439:PRO:HD3	2.23	0.52
1:A:169:ASP:O	1:A:171:TYR:N	2.43	0.52
2:H:409:VAL:HG21	2:H:470:ILE:CD1	2.40	0.52
2:H:479:GLU:HA	2:H:482:GLN:HG3	1.91	0.52
2:H:143:ILE:CG2	2:H:144:ASN:N	2.73	0.51
1:E:75:LEU:O	1:E:79:GLU:HG3	2.10	0.51
2:H:494:ALA:HA	2:H:496:ARG:HH11	1.76	0.51
2:C:307:ILE:C	2:C:308:LEU:HD12	2.30	0.51
2:D:498:ARG:HB3	2:D:498:ARG:CZ	2.40	0.51
2:C:401:ASN:ND2	2:H:1:MET:HG3	2.25	0.51
2:H:79:ILE:HG22	2:H:80:GLU:CG	2.40	0.51
2:G:152:ALA:HB2	2:G:343:GLY:CA	2.41	0.51
2:C:129:LYS:CD	2:C:142:ILE:HD12	2.39	0.51
2:G:274:PHE:HA	2:G:277:LEU:HB2	1.92	0.51
2:D:192:GLY:HA2	2:D:288:PRO:CB	2.40	0.51
2:D:323:LYS:HE3	2:D:329:GLU:N	2.25	0.51
2:C:282:VAL:O	2:C:285:THR:HB	2.09	0.51
2:H:193:ASP:OD2	2:H:196:LEU:HD22	2.11	0.51
1:A:75:LEU:HG	1:B:75:LEU:HD21	1.92	0.51
2:H:12:THR:CB	2:H:170:GLY:H	2.23	0.51
2:G:155:LEU:HD22	2:G:155:LEU:N	2.25	0.51
2:C:1:MET:HG3	2:C:2:SER:N	2.24	0.51
2:G:306:VAL:CG1	2:G:307:ILE:N	2.72	0.51
2:D:173:PHE:C	2:D:174:ASP:OD1	2.48	0.51
2:D:116:VAL:CG1	2:D:128:THR:HG21	2.39	0.51
1:E:67:GLN:OE1	1:F:68:ILE:CD1	2.58	0.51
2:G:205:ILE:CG2	2:G:235:ALA:CB	2.85	0.51
2:H:290:ARG:O	2:H:294:GLN:HB2	2.11	0.51
1:A:163:ALA:O	1:A:166:LYS:HD2	2.09	0.51
1:E:94:ARG:HA	1:E:97:ARG:HB3	1.92	0.51
2:H:420:ASN:ND2	2:H:420:ASN:N	2.59	0.51
2:C:232:LYS:O	2:C:233:ASP:C	2.48	0.51
2:G:118:ALA:HB1	2:G:187:VAL:HG21	1.92	0.51
2:H:156:ASP:HA	2:H:180:LEU:CD1	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:THR:N	2:H:359:VAL:O	2.42	0.51
2:C:29:ASN:HB3	2:C:100:TYR:CE2	2.45	0.51
2:H:135:ALA:CB	2:H:137:LEU:HD12	2.37	0.51
1:E:81:ARG:O	1:E:84:ARG:HB3	2.09	0.51
2:G:458:LYS:HZ3	2:G:465:GLU:HB3	1.75	0.51
1:F:147:ARG:O	1:F:151:ASP:CB	2.58	0.51
2:C:390:SER:HB3	2:C:446:ASP:CG	2.30	0.51
2:G:483:ARG:NH1	2:G:486:LYS:HZ2	2.08	0.51
2:H:431:ILE:HG23	2:H:432:PRO:HD2	1.92	0.51
1:B:178:GLN:CG	1:B:213:GLN:HB3	2.41	0.51
2:C:119:TYR:HD2	2:C:190:THR:HG21	1.74	0.51
2:D:441:ILE:HG23	2:D:458:LYS:O	2.10	0.51
2:D:366:LEU:HD21	2:D:484:MET:SD	2.51	0.51
2:G:162:THR:HG22	2:G:179:GLU:CG	2.39	0.51
1:B:171:TYR:CE1	2:D:52:VAL:HG21	2.46	0.51
2:C:273:LYS:HE3	2:C:277:LEU:HD21	1.92	0.51
2:G:470:ILE:C	2:G:471:LYS:HD3	2.30	0.51
2:H:412:GLY:HA3	2:H:420:ASN:HB3	1.92	0.51
2:H:373:MET:HG2	2:H:398:ALA:CB	2.41	0.51
2:D:82:LYS:HD2	2:D:83:GLN:N	2.26	0.51
2:G:367:SER:HB3	2:G:379:LYS:HG2	1.92	0.51
2:D:44:ASN:C	2:D:46:GLU:H	2.11	0.51
2:D:230:ARG:HD2	2:D:252:LEU:HD21	1.91	0.51
1:A:117:PRO:O	1:A:120:ASP:HB2	2.11	0.51
2:G:383:ARG:HD2	2:G:384:ASN:CA	2.38	0.51
2:D:50:GLY:O	2:D:53:ALA:HB3	2.10	0.51
1:A:89:PHE:CB	1:B:89:PHE:CD1	2.91	0.51
2:H:104:TYR:HD1	2:H:104:TYR:O	1.94	0.51
2:C:166:TYR:CZ	2:C:173:PHE:HE1	2.27	0.51
2:C:431:ILE:HD13	2:C:441:ILE:HD11	1.92	0.51
2:G:285:THR:O	2:G:288:PRO:HD2	2.11	0.51
1:B:84:ARG:O	1:B:85:LEU:C	2.48	0.51
2:D:143:ILE:CG2	2:D:144:ASN:N	2.73	0.51
1:B:112:ALA:O	1:B:113:SER:C	2.49	0.51
2:D:492:ALA:C	2:D:494:ALA:N	2.62	0.51
1:A:133:GLU:OE2	1:B:133:GLU:OE1	2.29	0.51
2:G:492:ALA:C	2:G:493:GLU:HG2	2.31	0.51
2:C:124:GLN:O	2:C:125:ARG:C	2.48	0.51
2:H:79:ILE:HG22	2:H:80:GLU:HG3	1.92	0.51
2:D:214:LYS:HE2	2:D:220:ASP:OD1	2.11	0.51
2:D:4:ILE:HD13	2:D:351:ILE:HB	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:381:ILE:HG22	2:G:382:GLU:O	2.10	0.51
2:D:376:VAL:CG2	2:D:377:PHE:N	2.74	0.51
1:A:138:ILE:HD13	1:B:139:LEU:CD1	2.41	0.51
2:D:497:LYS:HD3	2:D:498:ARG:HA	1.92	0.51
2:C:258:ASN:CG	2:C:260:ASN:HB3	2.30	0.51
1:A:85:LEU:N	1:A:85:LEU:HD23	2.25	0.51
2:C:27:ILE:CD1	2:C:101:ALA:HB1	2.40	0.51
1:E:96:THR:HG23	1:F:100:MET:CE	2.41	0.51
2:D:168:LEU:O	2:D:310:GLY:HA3	2.10	0.51
2:D:168:LEU:HD11	2:D:197:GLY:HA2	1.93	0.51
1:A:92:PHE:CE1	1:A:96:THR:OG1	2.63	0.51
2:D:436:ARG:HB3	2:D:436:ARG:NH1	2.26	0.51
2:G:67:ILE:CG2	2:G:67:ILE:O	2.59	0.51
1:E:196:GLY:HA3	1:E:207:ALA:HB2	1.93	0.51
2:G:280:HIS:CE1	2:G:281:LEU:CD1	2.94	0.51
2:D:99:SER:O	2:D:102:GLU:HB2	2.11	0.51
1:A:123:GLU:HG2	1:A:195:LYS:HE2	1.94	0.51
2:D:55:ARG:HG3	2:D:55:ARG:NH1	2.26	0.51
1:B:190:VAL:HG12	1:B:191:GLU:HG2	1.92	0.51
1:A:75:LEU:HD21	1:B:75:LEU:HD22	1.93	0.51
2:D:494:ALA:HA	2:D:496:ARG:CD	2.41	0.51
2:D:504:LEU:O	2:D:504:LEU:HD13	2.11	0.51
2:D:274:PHE:O	2:D:278:SER:N	2.43	0.51
2:H:381:ILE:HD13	2:H:447:ILE:HD11	1.90	0.50
1:A:89:PHE:CD1	1:A:90:GLU:N	2.78	0.50
2:H:202:ASP:OD1	2:H:235:ALA:HB1	2.11	0.50
2:C:366:LEU:HD23	2:C:383:ARG:CG	2.35	0.50
2:G:92:ILE:HA	2:G:95:GLN:HB2	1.93	0.50
1:F:98:GLN:HA	1:F:101:GLU:CG	2.42	0.50
2:C:162:THR:HB	2:C:304:ASP:OD1	2.10	0.50
2:G:126:GLN:HG3	2:G:130:ASP:OD2	2.10	0.50
1:B:142:MET:HE1	2:C:254:PHE:CZ	2.46	0.50
1:A:149:LEU:HG	1:B:118:VAL:HG21	1.93	0.50
2:G:414:ARG:HH21	2:G:491:ASN:HB3	1.76	0.50
2:D:49:VAL:CG2	2:D:50:GLY:N	2.74	0.50
2:H:97:LEU:O	2:H:100:TYR:CD1	2.65	0.50
2:H:163:ILE:HG22	2:H:164:LEU:O	2.11	0.50
2:H:166:TYR:HB3	2:H:307:ILE:O	2.11	0.50
2:C:497:LYS:CA	2:C:500:GLU:OE2	2.59	0.50
2:C:257:ALA:HA	2:C:263:LEU:HD12	1.90	0.50
2:G:403:THR:HG23	2:G:404:THR:HG22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:ASN:ND2	2:C:260:ASN:HB3	2.27	0.50
1:B:163:ALA:O	1:B:164:VAL:C	2.48	0.50
2:D:70:HIS:CE1	2:D:75:TYR:HE2	2.28	0.50
2:D:27:ILE:HG23	2:D:28:PRO:HD2	1.93	0.50
2:D:52:VAL:O	2:D:52:VAL:HG22	2.11	0.50
2:C:409:VAL:CG1	2:C:470:ILE:CD1	2.77	0.50
2:C:431:ILE:CG2	2:C:432:PRO:HD2	2.40	0.50
1:A:162:GLU:HG2	1:A:166:LYS:HZ2	1.76	0.50
2:G:28:PRO:O	2:G:100:TYR:CE2	2.65	0.50
2:G:94:LEU:HD13	2:G:97:LEU:HD22	1.92	0.50
2:D:90:SER:HA	2:D:93:ILE:HD12	1.92	0.50
2:D:459:ASP:OD1	2:D:463:ASN:N	2.44	0.50
2:H:310:GLY:O	2:H:313:THR:HG22	2.11	0.50
2:D:409:VAL:CG2	2:D:409:VAL:O	2.58	0.50
2:C:372:THR:HB	2:H:358:VAL:O	2.10	0.50
2:C:29:ASN:HB2	2:C:30:PRO:HD2	1.93	0.50
2:G:387:ILE:O	2:G:447:ILE:HG22	2.11	0.50
2:D:120:PHE:CD2	2:D:124:GLN:CB	2.95	0.50
1:E:64:ALA:O	1:E:68:ILE:HG13	2.11	0.50
2:C:484:MET:HA	2:C:487:GLU:HB2	1.93	0.50
2:C:59:THR:HG22	2:C:59:THR:O	2.11	0.50
2:C:387:ILE:HB	2:C:388:PRO:HD3	1.94	0.50
2:C:37:PRO:O	2:C:50:GLY:HA2	2.10	0.50
2:C:43:LYS:NZ	2:C:60:ASN:HA	2.25	0.50
2:H:496:ARG:HD3	2:H:496:ARG:H	1.71	0.50
2:D:497:LYS:C	2:D:499:LYS:N	2.64	0.50
2:C:288:PRO:HA	2:C:291:GLN:HB2	1.94	0.50
2:G:118:ALA:HB1	2:G:187:VAL:HG11	1.91	0.50
2:H:405:VAL:HG11	2:H:441:ILE:CD1	2.42	0.50
2:D:367:SER:OG	2:D:413:GLU:OE1	2.27	0.50
2:H:180:LEU:HB2	2:H:185:PHE:CE1	2.47	0.50
2:C:130:ASP:O	2:C:131:ALA:C	2.49	0.50
2:D:67:ILE:HD13	2:D:89:ILE:HB	1.93	0.50
2:D:109:VAL:HG23	2:D:110:THR:N	2.25	0.50
1:A:111:LEU:O	1:A:112:ALA:C	2.48	0.50
2:C:196:LEU:HD12	2:C:197:GLY:H	1.68	0.50
1:A:78:MET:O	1:A:82:TYR:CD1	2.65	0.50
1:A:82:TYR:HA	1:B:82:TYR:HD2	1.76	0.50
2:D:494:ALA:O	2:D:496:ARG:HG2	2.11	0.50
1:E:85:LEU:HG	1:F:82:TYR:OH	2.11	0.50
2:D:458:LYS:HG2	2:D:465:GLU:HA	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:LEU:O	2:D:362:ASP:OD1	2.29	0.50
1:B:174:GLN:HA	2:D:55:ARG:HG2	1.94	0.50
2:H:203:GLN:OE1	2:H:206:ILE:HD12	2.12	0.50
1:A:75:LEU:O	1:A:78:MET:N	2.45	0.50
2:D:14:SER:O	2:D:36:THR:HG23	2.12	0.50
2:D:180:LEU:O	2:D:180:LEU:HG	2.08	0.50
2:C:205:ILE:HD11	2:C:274:PHE:CD2	2.47	0.50
2:H:502:ALA:O	2:H:504:LEU:N	2.44	0.50
2:D:426:PHE:CE1	2:D:427:GLN:O	2.63	0.50
2:C:395:PHE:CE2	2:C:443:VAL:HG11	2.47	0.50
2:H:361:LEU:HD21	2:H:387:ILE:CD1	2.40	0.50
2:D:67:ILE:HD11	2:D:89:ILE:HD13	1.94	0.50
2:H:17:ALA:N	2:H:341:ALA:HB1	2.27	0.50
2:H:481:ILE:O	2:H:483:ARG:N	2.45	0.50
2:D:347:GLN:O	2:D:351:ILE:HG13	2.11	0.50
2:C:100:TYR:O	2:C:103:ASP:N	2.45	0.50
2:C:416:MET:HE2	2:C:496:ARG:NH2	2.27	0.50
2:D:335:ASN:O	2:D:338:GLU:HG2	2.11	0.50
2:D:8:ASP:HA	2:D:115:THR:CG2	2.42	0.50
1:F:81:ARG:O	1:F:85:LEU:HD23	2.11	0.50
1:E:194:GLN:O	1:E:208:MET:N	2.44	0.50
1:A:201:ASP:OD1	1:A:201:ASP:C	2.50	0.50
2:G:153:TYR:CE1	2:G:334:VAL:HB	2.47	0.50
2:D:372:THR:HG21	2:D:378:THR:HG23	1.94	0.50
2:H:370:ILE:CG2	2:H:371:GLU:N	2.74	0.50
2:C:155:LEU:HD13	2:C:155:LEU:H	1.75	0.50
2:G:414:ARG:HE	2:G:491:ASN:HB3	1.78	0.49
2:G:334:VAL:HG22	2:G:335:ASN:N	2.27	0.49
2:D:192:GLY:N	2:D:288:PRO:HB3	2.26	0.49
2:D:309:VAL:O	2:D:313:THR:HG21	2.12	0.49
1:B:94:ARG:CZ	1:B:98:GLN:NE2	2.75	0.49
2:D:370:ILE:CD1	2:D:445:PHE:CZ	2.95	0.49
2:H:414:ARG:CZ	2:H:491:ASN:HD21	2.25	0.49
1:E:92:PHE:HE1	1:F:92:PHE:CE2	2.30	0.49
2:D:16:VAL:CG1	2:D:100:TYR:OH	2.60	0.49
1:A:198:LYS:HB2	1:A:203:VAL:HG22	1.94	0.49
2:G:308:LEU:CD1	2:G:330:PRO:HG3	2.41	0.49
2:D:145:GLU:HB2	2:D:146:PRO:HD3	1.94	0.49
2:C:426:PHE:CD1	2:C:426:PHE:C	2.85	0.49
2:C:269:LEU:C	2:C:269:LEU:HD12	2.33	0.49
1:F:61:LEU:CD2	1:F:61:LEU:H	2.24	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:258:ASN:OD1	2:C:260:ASN:HB3	2.12	0.49
2:G:11:THR:O	2:G:12:THR:CB	2.59	0.49
1:B:186:PRO:O	1:B:187:ASN:C	2.50	0.49
1:B:93:ARG:O	1:B:96:THR:OG1	2.22	0.49
2:C:468:ILE:CG2	2:C:469:THR:N	2.75	0.49
2:C:366:LEU:HA	2:C:383:ARG:HG2	1.95	0.49
2:G:472:SER:C	2:G:474:SER:H	2.16	0.49
2:D:484:MET:HA	2:D:487:GLU:HB2	1.95	0.49
2:D:270:THR:OG1	2:D:271:ARG:C	2.51	0.49
2:C:29:ASN:OD1	2:C:29:ASN:C	2.50	0.49
2:H:164:LEU:HB3	2:H:306:VAL:HG13	1.94	0.49
1:F:66:ALA:O	1:F:69:ALA:HB3	2.11	0.49
2:G:495:ASP:OD2	2:G:498:ARG:NH2	2.41	0.49
1:B:133:GLU:O	1:B:136:LYS:HD3	2.12	0.49
2:H:487:GLU:O	2:H:490:GLU:HG2	2.12	0.49
2:D:294:GLN:O	2:D:297:GLY:N	2.43	0.49
1:E:113:SER:CB	1:E:204:LEU:CB	2.91	0.49
2:D:407:ILE:HD12	2:D:426:PHE:HE2	1.70	0.49
1:B:121:ASN:N	1:B:121:ASN:OD1	2.45	0.49
2:D:251:SER:OG	2:D:253:PRO:CD	2.45	0.49
2:D:51:GLU:C	2:D:53:ALA:N	2.64	0.49
2:G:394:VAL:HG13	2:G:441:ILE:C	2.32	0.49
1:A:69:ALA:HA	1:A:72:GLU:OE2	2.12	0.49
2:D:43:LYS:NZ	2:D:59:THR:CG2	2.76	0.49
2:G:347:GLN:NE2	2:G:350:VAL:HG11	2.27	0.49
2:H:67:ILE:HG22	2:H:67:ILE:O	2.12	0.49
2:G:227:ALA:O	2:G:231:LEU:CD1	2.60	0.49
2:C:208:TYR:CE2	2:C:273:LYS:CE	2.96	0.49
2:C:238:ALA:O	2:C:242:LEU:HD22	2.12	0.49
2:C:277:LEU:HD23	2:C:277:LEU:N	2.27	0.49
1:A:103:ALA:O	1:A:107:ARG:CB	2.61	0.49
2:G:476:LEU:HB3	2:G:480:GLU:OE2	2.12	0.49
2:G:347:GLN:HE22	2:G:350:VAL:HG11	1.77	0.49
2:H:385:THR:HG22	2:H:386:THR:HG22	1.95	0.49
2:D:140:GLU:CB	2:D:351:ILE:HG21	2.41	0.49
2:C:13:ASN:HA	2:C:38:SER:H	1.76	0.49
1:E:65:LYS:O	1:E:69:ALA:HB2	2.11	0.49
2:G:70:HIS:CE1	2:G:75:TYR:CE1	3.01	0.49
1:A:64:ALA:HB2	1:B:64:ALA:HB1	1.95	0.49
2:C:18:VAL:HG23	2:C:19:LEU:H	1.76	0.49
2:H:133:ARG:HA	2:H:137:LEU:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:GLN:HA	1:F:70:GLU:HB2	1.93	0.49
2:D:339:VAL:HA	2:D:342:ILE:HD12	1.93	0.49
2:C:390:SER:O	2:H:482:GLN:OE1	2.31	0.49
1:A:185:GLU:O	1:A:212:SER:HB2	2.12	0.49
2:C:265:LEU:C	2:C:265:LEU:CD2	2.82	0.49
2:H:365:PRO:CB	2:H:481:ILE:HD13	2.43	0.49
2:G:164:LEU:HD23	2:G:177:ILE:N	2.27	0.49
2:D:110:THR:HG22	2:D:111:ARG:N	2.27	0.49
2:C:116:VAL:HB	2:C:117:PRO:HD2	1.95	0.49
1:B:116:LEU:CD1	1:B:197:TYR:CD2	2.92	0.49
2:H:207:ASP:O	2:H:211:ASN:HB2	2.12	0.49
2:C:403:THR:CG2	2:C:404:THR:HG22	2.38	0.49
2:G:120:PHE:HB3	2:G:124:GLN:HG3	1.95	0.49
2:C:167:ASP:HA	2:C:309:VAL:HB	1.94	0.49
2:H:347:GLN:O	2:H:350:VAL:N	2.45	0.49
2:D:366:LEU:HD21	2:D:412:GLY:HA2	1.94	0.49
2:H:385:THR:O	2:H:386:THR:HB	2.12	0.49
1:B:149:LEU:CD2	1:B:149:LEU:C	2.77	0.49
2:D:190:THR:HG22	2:D:191:ALA:N	2.28	0.49
1:B:92:PHE:O	1:B:93:ARG:C	2.49	0.49
2:C:325:GLU:OE1	2:C:325:GLU:CA	2.60	0.49
2:D:355:VAL:HG23	2:D:355:VAL:O	2.12	0.49
1:A:70:GLU:HB3	1:A:74:LYS:CE	2.35	0.49
2:G:206:ILE:HG23	2:G:231:LEU:CD2	2.38	0.49
2:H:12:THR:O	2:H:13:ASN:CG	2.52	0.49
2:C:315:ILE:O	2:C:318:VAL:HB	2.12	0.49
1:A:84:ARG:O	1:A:85:LEU:C	2.50	0.48
2:C:1:MET:HE3	2:C:111:ARG:HD2	1.95	0.48
2:G:308:LEU:HD11	2:G:319:GLN:CD	2.34	0.48
2:D:19:LEU:HA	2:D:24:VAL:HA	1.95	0.48
2:G:369:GLY:C	2:G:377:PHE:CE1	2.86	0.48
2:H:4:ILE:CG2	2:H:348:GLY:O	2.61	0.48
2:G:498:ARG:CZ	2:G:498:ARG:CB	2.91	0.48
2:G:91:ALA:O	2:G:95:GLN:HG3	2.13	0.48
2:D:483:ARG:O	2:D:486:LYS:CG	2.61	0.48
2:C:380:LEU:O	2:C:391:LYS:HD3	2.13	0.48
1:B:67:GLN:CA	1:B:67:GLN:NE2	2.76	0.48
1:E:70:GLU:O	1:E:73:ALA:HB3	2.13	0.48
2:C:44:ASN:C	2:C:46:GLU:H	2.16	0.48
2:G:361:LEU:CB	2:G:387:ILE:HD12	2.34	0.48
2:H:409:VAL:CG2	2:H:470:ILE:HD11	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:THR:H	2:D:68:LYS:HZ2	1.61	0.48
2:D:443:VAL:O	2:D:443:VAL:HG22	2.13	0.48
2:C:438:VAL:N	2:C:439:PRO:CD	2.76	0.48
2:C:143:ILE:HG22	2:C:144:ASN:N	2.28	0.48
2:G:409:VAL:CG1	2:G:424:GLY:H	2.23	0.48
2:G:372:THR:O	2:G:373:MET:C	2.52	0.48
2:D:141:ARG:HG3	2:D:142:ILE:H	1.78	0.48
1:B:165:GLY:HA2	1:B:189:VAL:O	2.13	0.48
2:D:325:GLU:C	2:D:326:LEU:CD1	2.80	0.48
2:G:495:ASP:CG	2:G:498:ARG:HH12	2.16	0.48
2:D:178:LEU:N	2:D:178:LEU:CD1	2.73	0.48
2:D:6:GLY:HA2	2:D:113:VAL:CG1	2.44	0.48
2:G:484:MET:O	2:G:487:GLU:N	2.46	0.48
2:G:164:LEU:HA	2:G:177:ILE:HA	1.94	0.48
2:D:18:VAL:CG2	2:D:19:LEU:N	2.75	0.48
2:G:380:LEU:HD12	2:G:445:PHE:HE2	1.67	0.48
2:G:210:VAL:HB	2:G:221:LEU:HB2	1.95	0.48
2:G:462:THR:CG2	2:G:464:LYS:CB	2.85	0.48
2:D:504:LEU:CD1	2:D:507:GLU:HB3	2.40	0.48
2:C:397:THR:HG23	2:C:436:ARG:HA	1.94	0.48
1:B:124:ARG:HB3	2:D:254:PHE:CD2	2.48	0.48
2:H:214:LYS:CE	2:H:220:ASP:HA	2.43	0.48
2:G:227:ALA:O	2:G:231:LEU:HD13	2.14	0.48
2:G:299:THR:HB	2:G:300:PRO:HD2	1.95	0.48
2:D:381:ILE:HD13	2:D:447:ILE:CD1	2.44	0.48
2:C:191:ALA:HB2	2:C:292:ALA:HB2	1.95	0.48
2:C:25:LYS:HA	2:C:25:LYS:HD2	1.63	0.48
1:F:93:ARG:O	1:F:94:ARG:C	2.52	0.48
2:C:131:ALA:O	2:C:134:ILE:HB	2.14	0.48
2:D:221:LEU:H	2:D:221:LEU:HD12	1.78	0.48
2:D:272:ALA:O	2:D:275:GLU:N	2.47	0.48
2:G:162:THR:HG22	2:G:179:GLU:CD	2.34	0.48
2:D:136:GLY:C	2:D:137:LEU:HD23	2.34	0.48
2:G:412:GLY:HA3	2:G:420:ASN:OD1	2.13	0.48
1:F:87:ALA:HA	2:G:386:THR:CB	2.43	0.48
2:D:50:GLY:O	2:D:53:ALA:N	2.37	0.48
2:C:366:LEU:CD2	2:C:367:SER:H	2.21	0.48
2:D:493:GLU:C	2:D:495:ASP:N	2.66	0.48
2:H:292:ALA:O	2:H:295:ASP:HB2	2.14	0.48
2:D:224:ASP:OD2	2:D:226:MET:CB	2.61	0.48
1:B:142:MET:HE3	1:B:142:MET:N	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:CB	1:B:85:LEU:HD12	2.44	0.48
2:D:107:GLU:HG2	2:D:107:GLU:O	2.13	0.48
2:H:492:ALA:C	2:H:494:ALA:N	2.67	0.48
2:C:89:ILE:O	2:C:92:ILE:N	2.47	0.48
2:H:143:ILE:CG2	2:H:144:ASN:H	2.26	0.48
2:C:27:ILE:HD13	2:C:101:ALA:CA	2.44	0.48
2:G:370:ILE:CG2	2:G:371:GLU:N	2.49	0.48
2:C:423:LEU:HB3	2:C:470:ILE:HG21	1.95	0.48
1:B:71:LEU:HD22	1:B:74:LYS:HZ1	1.79	0.48
2:H:119:TYR:CD2	2:H:190:THR:HG21	2.48	0.48
2:C:309:VAL:HG12	2:C:310:GLY:N	2.29	0.48
1:E:198:LYS:C	1:E:200:LYS:H	2.16	0.48
1:B:123:GLU:HB3	1:B:127:LYS:HD2	1.95	0.48
2:D:124:GLN:O	2:D:127:ALA:HB3	2.14	0.48
1:B:169:ASP:C	1:B:171:TYR:H	2.16	0.48
2:D:502:ALA:C	2:D:504:LEU:H	2.17	0.48
2:G:225:LYS:NZ	2:G:225:LYS:CB	2.77	0.48
2:H:401:ASN:CA	2:H:434:ALA:O	2.62	0.48
2:D:64:ILE:CG2	2:D:67:ILE:HG13	2.44	0.48
1:B:87:ALA:HB2	2:C:388:PRO:HB2	1.96	0.48
1:A:71:LEU:HA	1:A:74:LYS:HD2	1.96	0.48
2:H:407:ILE:HB	2:H:426:PHE:CE1	2.48	0.48
2:D:334:VAL:HB	2:D:339:VAL:HG22	1.96	0.48
2:H:503:GLU:O	2:H:506:ASN:ND2	2.47	0.48
2:C:380:LEU:HA	2:C:380:LEU:HD23	1.69	0.48
2:H:154:GLY:HA2	2:H:156:ASP:OD2	2.14	0.47
2:D:75:TYR:C	2:D:75:TYR:CD1	2.88	0.47
2:D:98:LYS:O	2:D:99:SER:C	2.52	0.47
2:G:370:ILE:HA	2:G:409:VAL:HA	1.95	0.47
2:H:414:ARG:HA	2:H:415:PRO:HD3	1.60	0.47
2:C:198:GLY:HA2	2:C:201:PHE:HD2	1.79	0.47
2:C:207:ASP:O	2:C:208:TYR:C	2.53	0.47
2:D:497:LYS:C	2:D:499:LYS:H	2.17	0.47
2:H:95:GLN:HG2	2:H:96:TYR:N	2.25	0.47
2:G:155:LEU:HB2	2:G:185:PHE:CZ	2.48	0.47
2:D:422:SER:OG	2:D:423:LEU:N	2.46	0.47
2:H:383:ARG:O	2:H:385:THR:N	2.46	0.47
2:D:242:LEU:O	2:D:271:ARG:NH1	2.48	0.47
2:C:143:ILE:CG2	2:C:144:ASN:N	2.76	0.47
2:D:309:VAL:O	2:D:313:THR:CG2	2.61	0.47
2:C:269:LEU:HD12	2:C:270:THR:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:TYR:O	1:F:85:LEU:CB	2.60	0.47
2:C:430:GLY:O	2:C:431:ILE:C	2.51	0.47
2:G:483:ARG:HH12	2:G:486:LYS:NZ	2.12	0.47
2:G:225:LYS:HB3	2:G:225:LYS:HZ3	1.79	0.47
2:H:161:GLN:O	2:H:179:GLU:HG2	2.13	0.47
2:H:368:LEU:HB2	2:H:445:PHE:HE2	1.77	0.47
2:G:364:THR:HB	2:G:385:THR:N	2.28	0.47
2:D:141:ARG:HG2	2:D:143:ILE:HG13	1.95	0.47
2:D:139:VAL:HG11	2:D:142:ILE:HG13	1.96	0.47
1:B:169:ASP:O	1:B:170:PRO:C	2.50	0.47
2:C:75:TYR:C	2:C:75:TYR:CD1	2.86	0.47
2:C:280:HIS:CD2	2:C:281:LEU:HD13	2.49	0.47
2:D:14:SER:O	2:D:36:THR:HG22	2.14	0.47
2:D:483:ARG:HH21	1:F:85:LEU:HD22	1.79	0.47
1:B:178:GLN:HG3	1:B:213:GLN:CB	2.44	0.47
2:G:285:THR:C	2:G:288:PRO:HD2	2.34	0.47
1:E:160:ALA:HA	1:E:197:TYR:CB	2.44	0.47
2:D:85:THR:O	2:D:86:PRO:C	2.51	0.47
2:D:270:THR:OG1	2:D:273:LYS:N	2.47	0.47
2:H:335:ASN:ND2	2:H:338:GLU:HG3	2.29	0.47
2:C:27:ILE:HG21	2:C:101:ALA:HA	1.96	0.47
2:C:423:LEU:HB3	2:C:470:ILE:HD13	1.95	0.47
2:D:308:LEU:HD12	2:D:308:LEU:HA	1.64	0.47
2:H:426:PHE:CB	2:H:468:ILE:CD1	2.85	0.47
2:C:498:ARG:C	2:C:500:GLU:H	2.17	0.47
2:C:274:PHE:C	2:C:274:PHE:CD1	2.87	0.47
2:C:64:ILE:HG22	2:C:67:ILE:CD1	2.35	0.47
1:A:115:LEU:C	1:A:117:PRO:HD2	2.35	0.47
2:D:303:ILE:HG22	2:D:304:ASP:N	2.29	0.47
2:G:403:THR:HG23	2:G:404:THR:CG2	2.45	0.47
2:H:204:VAL:HG23	2:H:277:LEU:HD13	1.96	0.47
2:C:177:ILE:C	2:C:178:LEU:HD12	2.34	0.47
2:G:105:LEU:HD23	2:G:107:GLU:HB3	1.95	0.47
2:C:58:ILE:O	2:C:58:ILE:HG22	2.14	0.47
2:D:64:ILE:HG22	2:D:67:ILE:HG13	1.96	0.47
2:D:98:LYS:CB	2:D:137:LEU:HD11	2.38	0.47
2:G:390:SER:HB2	2:G:445:PHE:O	2.15	0.47
1:B:167:PRO:O	1:B:168:PHE:HB3	2.13	0.47
1:F:68:ILE:HG22	1:F:72:GLU:OE2	2.15	0.47
1:E:77:GLU:O	1:E:78:MET:C	2.50	0.47
2:H:486:LYS:O	2:H:486:LYS:NZ	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:387:ILE:O	2:H:388:PRO:O	2.32	0.47
2:D:64:ILE:HG21	2:D:89:ILE:HD13	1.97	0.47
2:D:209:LEU:HD13	2:D:209:LEU:C	2.34	0.47
2:D:212:GLN:O	2:D:215:GLN:HB3	2.14	0.47
1:B:144:MET:HA	1:B:144:MET:HE3	1.94	0.47
1:B:144:MET:HG2	2:C:253:PRO:HB3	1.97	0.47
2:H:152:ALA:HB2	2:H:342:ILE:CG2	2.38	0.47
2:D:104:TYR:CD2	2:D:105:LEU:CD1	2.97	0.47
2:D:104:TYR:CD2	2:D:105:LEU:HD13	2.49	0.47
1:A:105:LYS:HB3	1:A:106:TYR:CE1	2.50	0.47
2:D:388:PRO:HG3	2:D:449:ALA:N	2.30	0.47
2:G:372:THR:CG2	2:G:373:MET:N	2.78	0.47
2:D:156:ASP:N	2:D:156:ASP:OD1	2.47	0.47
2:D:312:SER:O	2:D:315:ILE:CG1	2.63	0.47
2:D:315:ILE:CG2	2:D:316:PRO:HD2	2.44	0.47
2:C:70:HIS:CD2	2:C:75:TYR:CD2	3.03	0.47
2:C:462:THR:CB	2:C:464:LYS:H	2.18	0.47
1:F:158:VAL:CA	1:F:198:LYS:O	2.55	0.47
1:A:191:GLU:CG	1:A:210:LYS:HD2	2.38	0.47
2:C:416:MET:CE	2:C:497:LYS:CB	2.93	0.47
2:H:397:THR:HG21	2:H:439:PRO:HG2	1.96	0.47
2:G:497:LYS:C	2:G:499:LYS:N	2.68	0.47
1:B:153:LEU:HB3	1:B:158:VAL:CG1	2.44	0.47
2:H:460:LEU:HD13	2:H:460:LEU:HA	1.60	0.47
2:H:391:LYS:HG3	2:H:392:SER:N	2.30	0.47
1:A:134:GLN:HG2	1:A:134:GLN:O	2.15	0.47
2:D:236:GLU:O	2:D:239:LYS:HB3	2.15	0.47
1:E:134:GLN:C	1:E:136:LYS:H	2.18	0.47
2:C:294:GLN:O	2:C:294:GLN:HG2	2.14	0.47
1:B:108:ALA:O	1:B:109:GLN:C	2.53	0.47
2:G:17:ALA:HB1	2:G:25:LYS:O	2.15	0.47
2:G:57:ALA:HB1	2:G:63:THR:CB	2.45	0.47
2:H:445:PHE:CD1	2:H:455:VAL:HG22	2.50	0.47
2:D:204:VAL:HG22	2:D:277:LEU:CD1	2.40	0.47
2:H:17:ALA:H	2:H:341:ALA:HB1	1.79	0.47
2:C:27:ILE:HG12	2:C:104:TYR:CD2	2.44	0.47
2:C:29:ASN:ND2	2:C:36:THR:CG2	2.73	0.47
2:C:97:LEU:O	2:C:98:LYS:C	2.53	0.47
2:C:9:LEU:HA	2:C:14:SER:OG	2.15	0.47
2:G:381:ILE:HD11	2:G:447:ILE:CD1	2.43	0.47
1:A:135:ALA:CB	1:B:135:ALA:CB	2.87	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:166:TYR:HD1	2:C:166:TYR:C	2.19	0.47
2:C:285:THR:HG22	2:C:285:THR:O	2.15	0.47
2:C:308:LEU:HD11	2:C:330:PRO:HB2	1.97	0.47
2:H:12:THR:HG23	2:H:13:ASN:N	2.22	0.47
2:H:2:SER:OG	2:H:110:THR:CB	2.61	0.47
2:C:296:ALA:CB	2:C:298:LEU:HD22	2.41	0.47
2:C:390:SER:HB2	2:C:445:PHE:O	2.15	0.47
2:D:408:HIS:CE1	2:D:425:ARG:HH11	2.32	0.47
2:H:401:ASN:N	2:H:401:ASN:OD1	2.48	0.47
2:D:476:LEU:HB2	2:D:480:GLU:OE2	2.15	0.47
2:H:456:ARG:HA	2:H:467:SER:HB2	1.95	0.47
1:A:142:MET:O	1:A:144:MET:N	2.47	0.47
2:C:249:GLN:HA	2:C:267:MET:O	2.14	0.47
2:C:248:THR:OG1	2:C:249:GLN:N	2.48	0.47
2:G:163:ILE:O	2:G:177:ILE:HG23	2.15	0.47
2:G:240:LYS:O	2:G:243:SER:HB2	2.15	0.47
1:F:84:ARG:HA	2:G:388:PRO:HB2	1.97	0.47
2:D:129:LYS:HB2	2:D:142:ILE:HD12	1.94	0.47
2:C:198:GLY:O	2:C:201:PHE:CB	2.59	0.47
1:B:153:LEU:O	1:B:154:LYS:C	2.52	0.47
2:G:483:ARG:HH11	2:G:486:LYS:NZ	2.12	0.47
2:H:364:THR:O	2:H:365:PRO:C	2.50	0.47
2:G:164:LEU:HG	2:G:177:ILE:CG1	2.45	0.47
1:B:122:PHE:HA	1:B:146:TYR:CD2	2.42	0.47
1:F:87:ALA:HB2	2:G:388:PRO:HD2	1.97	0.47
1:B:97:ARG:CG	1:B:98:GLN:N	2.78	0.47
2:C:166:TYR:CD1	2:C:166:TYR:C	2.89	0.47
2:D:131:ALA:O	2:D:134:ILE:HB	2.15	0.47
2:H:407:ILE:HD12	2:H:426:PHE:CZ	2.50	0.47
2:C:366:LEU:HD23	2:C:366:LEU:HA	1.36	0.47
2:C:164:LEU:HD13	2:C:164:LEU:C	2.35	0.47
2:C:347:GLN:HE21	2:C:347:GLN:CA	2.27	0.47
2:C:459:ASP:OD1	2:C:461:GLY:N	2.39	0.47
2:D:366:LEU:O	2:D:368:LEU:CD2	2.63	0.46
2:C:438:VAL:N	2:C:439:PRO:HD2	2.31	0.46
1:B:142:MET:N	1:B:142:MET:CE	2.78	0.46
2:C:266:GLU:O	2:C:267:MET:CB	2.58	0.46
2:D:111:ARG:HD3	2:D:140:GLU:OE2	2.16	0.46
1:B:93:ARG:O	1:B:94:ARG:C	2.54	0.46
2:H:4:ILE:HD11	2:H:111:ARG:NH1	2.30	0.46
1:A:114:ASP:OD2	1:B:155:LYS:HE2	2.13	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:164:LEU:HD21	2:C:175:VAL:HG13	1.97	0.46
2:H:505:ARG:C	2:H:507:GLU:N	2.68	0.46
2:H:192:GLY:N	2:H:288:PRO:HB3	2.30	0.46
2:C:478:GLU:O	2:C:481:ILE:HB	2.15	0.46
2:C:254:PHE:CE1	2:C:264:HIS:CE1	2.96	0.46
2:H:15:CYS:SG	2:H:338:GLU:HB3	2.56	0.46
2:H:335:ASN:ND2	2:H:338:GLU:CG	2.78	0.46
2:H:366:LEU:HA	2:H:366:LEU:HD12	1.43	0.46
2:G:177:ILE:CD1	2:G:292:ALA:CB	2.91	0.46
2:G:289:VAL:O	2:G:292:ALA:HB3	2.15	0.46
2:G:304:ASP:O	2:G:305:LYS:HG2	2.16	0.46
1:A:95:ARG:CD	2:C:104:TYR:CE1	2.87	0.46
1:B:117:PRO:O	1:B:120:ASP:HB2	2.15	0.46
1:B:204:LEU:HD12	1:B:204:LEU:N	2.20	0.46
2:H:492:ALA:C	2:H:494:ALA:H	2.18	0.46
2:D:396:THR:OG1	2:D:439:PRO:HD2	2.15	0.46
2:C:121:ASN:O	2:C:125:ARG:HG2	2.15	0.46
2:G:163:ILE:CG2	2:G:164:LEU:N	2.78	0.46
2:G:273:LYS:O	2:G:277:LEU:HB2	2.15	0.46
2:D:3:LYS:HD2	2:D:3:LYS:H	1.80	0.46
2:C:116:VAL:O	2:C:145:GLU:N	2.37	0.46
1:B:168:PHE:HD2	1:B:173:HIS:HB2	1.80	0.46
1:A:89:PHE:CG	1:B:89:PHE:HD1	2.29	0.46
2:G:210:VAL:HG12	2:G:221:LEU:CD1	2.39	0.46
2:D:41:ALA:HB1	2:D:62:ASN:O	2.15	0.46
2:D:97:LEU:N	2:D:97:LEU:CD1	2.78	0.46
2:H:141:ARG:HH12	2:H:143:ILE:HD11	1.59	0.46
2:C:372:THR:OG1	2:C:373:MET:N	2.48	0.46
2:C:373:MET:SD	2:C:373:MET:C	2.93	0.46
2:H:387:ILE:HD13	2:H:387:ILE:HG21	1.67	0.46
2:C:2:SER:HB3	2:C:110:THR:HG22	1.98	0.46
1:B:173:HIS:HB3	1:B:209:VAL:HG21	1.97	0.46
2:D:164:LEU:HD13	2:D:165:VAL:CA	2.46	0.46
1:A:89:PHE:CE2	1:B:89:PHE:HA	2.51	0.46
2:H:27:ILE:HG12	2:H:104:TYR:HD2	1.81	0.46
2:D:380:LEU:O	2:D:381:ILE:HG13	2.15	0.46
2:C:399:ALA:HB3	2:H:355:VAL:HG11	1.97	0.46
1:E:140:GLN:C	1:E:142:MET:H	2.18	0.46
2:H:67:ILE:HD13	2:H:89:ILE:CG1	2.45	0.46
2:D:421:LYS:CE	2:D:480:GLU:OE2	2.63	0.46
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.57	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:386:THR:CG2	2:D:389:THR:HG22	2.45	0.46
2:H:5:ILE:HD12	2:H:109:VAL:HG11	1.97	0.46
2:G:459:ASP:HB3	2:G:462:THR:HB	1.97	0.46
2:H:117:PRO:HD2	2:H:120:PHE:CE1	2.51	0.46
1:A:172:LEU:N	1:A:172:LEU:CD2	2.75	0.46
2:C:380:LEU:HD12	2:C:445:PHE:HE1	1.79	0.46
2:H:134:ILE:C	2:H:136:GLY:H	2.19	0.46
2:G:166:TYR:CE1	2:G:318:VAL:HG11	2.50	0.46
2:G:277:LEU:O	2:G:280:HIS:CD2	2.69	0.46
2:C:166:TYR:CE2	2:C:322:ILE:HD11	2.50	0.46
2:G:400:ASP:OD1	2:G:400:ASP:N	2.49	0.46
1:F:65:LYS:CA	1:F:68:ILE:HD12	2.34	0.46
2:G:91:ALA:O	2:G:135:ALA:CB	2.64	0.46
2:D:493:GLU:C	2:D:495:ASP:H	2.18	0.46
2:D:503:GLU:O	2:D:505:ARG:N	2.48	0.46
1:A:131:ASP:OD1	1:B:134:GLN:NE2	2.48	0.46
2:D:29:ASN:O	2:D:31:GLU:N	2.49	0.46
2:H:118:ALA:CB	2:H:144:ASN:HD22	2.29	0.46
2:H:118:ALA:HB2	2:H:144:ASN:HB3	1.96	0.46
2:H:383:ARG:HG2	2:H:384:ASN:HD22	1.78	0.46
2:D:248:THR:OG1	2:D:249:GLN:N	2.47	0.46
2:H:339:VAL:HA	2:H:342:ILE:HG13	1.98	0.46
2:D:361:LEU:HA	2:D:361:LEU:HD23	1.33	0.46
2:C:409:VAL:CG1	2:C:409:VAL:O	2.63	0.46
1:B:179:ALA:HB2	1:B:210:LYS:HE2	1.97	0.46
2:H:397:THR:HB	2:H:439:PRO:HG2	1.96	0.46
2:G:496:ARG:HD2	2:G:497:LYS:N	2.30	0.46
2:C:87:GLN:HE21	2:C:87:GLN:HB2	1.59	0.46
2:D:64:ILE:HD13	2:D:89:ILE:CG1	2.45	0.46
2:D:280:HIS:NE2	2:D:281:LEU:CD1	2.78	0.46
1:A:95:ARG:HA	1:A:98:GLN:HE21	1.81	0.46
2:C:27:ILE:HD13	2:C:101:ALA:HB1	1.97	0.46
2:G:372:THR:HG22	2:G:373:MET:HB2	1.96	0.46
2:D:359:VAL:CG2	2:D:360:LEU:N	2.61	0.46
1:B:111:LEU:O	1:B:114:ASP:N	2.48	0.46
2:H:7:ILE:HD13	2:H:97:LEU:CD2	2.46	0.46
1:B:190:VAL:N	1:B:210:LYS:O	2.45	0.46
2:C:493:GLU:O	2:C:496:ARG:HG3	2.14	0.46
2:D:502:ALA:C	2:D:504:LEU:N	2.69	0.46
1:B:153:LEU:HD12	1:B:158:VAL:HG21	1.98	0.46
2:C:221:LEU:O	2:C:224:ASP:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:329:GLU:OE1	2:D:330:PRO:HD2	2.16	0.46
2:C:60:ASN:OD1	2:C:62:ASN:N	2.46	0.46
2:C:293:LEU:HA	2:C:293:LEU:HD23	1.51	0.46
2:H:388:PRO:HG2	2:H:388:PRO:O	2.15	0.46
2:D:201:PHE:O	2:D:204:VAL:HG12	2.16	0.46
2:D:230:ARG:HB3	2:D:252:LEU:HD21	1.96	0.46
2:D:173:PHE:CE1	2:D:175:VAL:CG1	2.99	0.46
2:D:290:ARG:O	2:D:293:LEU:N	2.49	0.46
2:D:38:SER:C	2:D:39:VAL:CG1	2.85	0.46
1:A:83:LEU:O	1:A:86:TYR:HB2	2.16	0.46
1:B:111:LEU:O	1:B:112:ALA:C	2.51	0.46
2:H:72:GLY:HA2	2:H:127:ALA:HB2	1.98	0.46
2:C:283:GLU:O	2:C:283:GLU:OE1	2.34	0.46
2:G:91:ALA:CB	2:G:134:ILE:HG22	2.45	0.46
1:A:162:GLU:H	1:A:162:GLU:CD	2.18	0.46
2:H:283:GLU:OE1	2:H:283:GLU:HA	2.15	0.46
2:H:118:ALA:HB2	2:H:144:ASN:HD22	1.80	0.45
2:C:395:PHE:CE2	2:C:443:VAL:CG1	2.99	0.45
2:D:251:SER:OG	2:D:252:LEU:N	2.47	0.45
1:A:86:TYR:HE2	1:A:90:GLU:OE2	1.98	0.45
2:H:16:VAL:CG1	2:H:100:TYR:OH	2.64	0.45
1:B:82:TYR:N	1:B:82:TYR:CD1	2.83	0.45
2:C:505:ARG:CG	2:C:505:ARG:HH11	2.28	0.45
2:G:459:ASP:HB3	2:G:462:THR:CB	2.46	0.45
2:C:205:ILE:CD1	2:C:274:PHE:CE2	2.92	0.45
2:H:170:GLY:O	2:H:198:GLY:N	2.43	0.45
2:D:490:GLU:HG2	1:F:81:ARG:NH2	2.31	0.45
2:C:240:LYS:O	2:C:241:GLU:C	2.54	0.45
2:H:292:ALA:HA	2:H:295:ASP:CG	2.36	0.45
2:H:464:LYS:NZ	2:H:464:LYS:CB	2.76	0.45
2:C:216:GLU:OE1	2:C:216:GLU:HA	2.16	0.45
2:H:432:PRO:HA	2:H:433:PRO:HD3	1.82	0.45
1:B:105:LYS:O	1:B:107:ARG:N	2.49	0.45
2:C:67:ILE:CD1	2:C:89:ILE:HD13	2.47	0.45
2:H:156:ASP:HA	2:H:180:LEU:CD2	2.46	0.45
2:H:181:GLY:O	2:H:183:GLY:N	2.49	0.45
1:A:193:LEU:HB3	2:C:226:MET:SD	2.56	0.45
2:G:414:ARG:HE	2:G:491:ASN:CB	2.29	0.45
2:H:109:VAL:CG2	2:H:111:ARG:O	2.62	0.45
2:C:60:ASN:ND2	2:C:62:ASN:O	2.50	0.45
1:A:75:LEU:HA	1:A:75:LEU:HD23	1.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:94:LEU:N	2:G:94:LEU:HD22	2.31	0.45
2:G:94:LEU:HA	2:G:97:LEU:HB2	1.97	0.45
2:H:62:ASN:CB	2:H:79:ILE:CG2	2.94	0.45
2:D:113:VAL:O	2:D:113:VAL:HG13	2.14	0.45
2:D:85:THR:OG1	2:D:87:GLN:NE2	2.49	0.45
1:B:85:LEU:HA	1:B:85:LEU:HD22	1.73	0.45
1:A:152:ALA:O	1:A:153:LEU:C	2.51	0.45
2:C:73:THR:HG23	2:C:75:TYR:HB3	1.98	0.45
2:C:416:MET:HE2	2:C:497:LYS:CB	2.46	0.45
2:D:499:LYS:O	2:D:502:ALA:HB3	2.16	0.45
2:H:192:GLY:O	2:H:288:PRO:CG	2.65	0.45
2:C:482:GLN:HA	2:C:485:ILE:HD12	1.98	0.45
2:H:181:GLY:C	2:H:183:GLY:H	2.20	0.45
2:D:269:LEU:CD1	2:D:270:THR:O	2.65	0.45
2:H:71:MET:O	2:H:124:GLN:CB	2.64	0.45
2:H:109:VAL:O	2:H:109:VAL:HG22	2.17	0.45
2:G:214:LYS:HZ2	2:G:221:LEU:H	1.62	0.45
2:D:60:ASN:C	2:D:62:ASN:N	2.70	0.45
2:C:52:VAL:HG22	2:C:52:VAL:O	2.17	0.45
2:C:20:GLU:O	2:C:21:GLY:O	2.35	0.45
2:G:291:GLN:O	2:G:295:ASP:CG	2.55	0.45
2:G:82:LYS:HB2	2:G:82:LYS:HE2	1.83	0.45
2:H:147:THR:O	2:H:151:LEU:N	2.50	0.45
2:D:67:ILE:HD13	2:D:89:ILE:CD1	2.47	0.45
2:C:227:ALA:O	2:C:231:LEU:HD12	2.17	0.45
1:B:119:LEU:HA	1:B:119:LEU:HD22	1.06	0.45
2:H:168:LEU:HD13	2:H:172:THR:O	2.17	0.45
1:B:75:LEU:O	1:B:76:SER:C	2.52	0.45
2:C:276:GLU:O	2:C:278:SER:N	2.50	0.45
1:A:143:GLU:O	1:A:147:ARG:HB2	2.16	0.45
1:B:67:GLN:HE21	1:B:67:GLN:N	2.14	0.45
1:E:97:ARG:HG3	1:E:98:GLN:OE1	2.15	0.45
2:C:64:ILE:CD1	2:C:89:ILE:HG12	2.47	0.45
2:C:67:ILE:HD13	2:C:89:ILE:CB	2.44	0.45
2:C:221:LEU:HD21	2:C:255:ILE:CG2	2.46	0.45
2:D:104:TYR:CE2	2:D:105:LEU:HD11	2.51	0.45
2:G:443:VAL:O	2:G:443:VAL:HG13	2.17	0.45
1:B:165:GLY:O	1:B:166:LYS:C	2.55	0.45
2:H:71:MET:HE2	2:H:128:THR:CG2	2.45	0.45
2:D:332:LYS:O	2:D:334:VAL:HG23	2.16	0.45
2:D:486:LYS:HB2	2:D:486:LYS:HE3	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:405:VAL:HA	2:H:356:LYS:O	2.17	0.45
1:B:193:LEU:HD21	2:D:226:MET:CG	2.43	0.45
1:A:81:ARG:NH2	2:C:355:VAL:HG22	2.31	0.45
2:D:245:VAL:HG23	2:D:246:THR:N	2.32	0.45
2:D:231:LEU:O	2:D:232:LYS:O	2.35	0.45
2:H:365:PRO:O	2:H:366:LEU:CD1	2.65	0.45
2:G:145:GLU:HB2	2:G:146:PRO:CD	2.34	0.45
2:D:386:THR:HG22	2:D:389:THR:CG2	2.47	0.45
2:D:388:PRO:HD3	2:D:449:ALA:HA	1.98	0.45
2:H:27:ILE:HG23	2:H:104:TYR:CD2	2.52	0.45
2:H:94:LEU:HD12	2:H:97:LEU:CB	2.47	0.45
2:G:438:VAL:N	2:G:439:PRO:HD2	2.32	0.45
2:G:121:ASN:OD1	2:G:121:ASN:N	2.50	0.45
2:H:208:TYR:CZ	2:H:273:LYS:HD2	2.51	0.45
2:G:347:GLN:OE1	2:G:350:VAL:HB	2.17	0.45
2:C:395:PHE:HE2	2:C:443:VAL:HG11	1.82	0.45
2:H:149:ALA:HB2	2:H:339:VAL:HG13	1.97	0.45
1:B:86:TYR:O	1:B:87:ALA:C	2.52	0.45
2:C:36:THR:HG22	2:C:37:PRO:HD2	1.99	0.45
2:C:8:ASP:HA	2:C:115:THR:CG2	2.44	0.45
2:D:377:PHE:HB3	2:D:415:PRO:O	2.17	0.45
1:B:111:LEU:HD13	1:B:111:LEU:C	2.37	0.45
2:D:160:ASP:HA	2:D:180:LEU:CD2	2.47	0.45
2:D:184:VAL:HG12	2:D:185:PHE:H	1.81	0.45
2:G:290:ARG:HA	2:G:293:LEU:HB2	1.99	0.45
1:E:176:VAL:CB	2:G:225:LYS:HD3	2.47	0.45
2:H:141:ARG:CZ	2:H:347:GLN:HE21	2.29	0.45
2:C:363:VAL:HA	2:C:386:THR:HA	1.99	0.45
2:C:16:VAL:CG1	2:C:100:TYR:OH	2.65	0.45
1:A:105:LYS:HD3	1:A:200:LYS:HZ3	1.78	0.45
2:G:377:PHE:CG	2:G:410:LEU:HD12	2.52	0.45
2:G:445:PHE:HD1	2:G:455:VAL:CG2	2.30	0.45
2:H:371:GLU:N	2:H:410:LEU:HD11	2.32	0.45
2:G:214:LYS:HG2	2:G:220:ASP:HA	1.99	0.45
2:C:496:ARG:O	2:C:499:LYS:CB	2.59	0.45
1:A:174:GLN:OE1	1:A:208:MET:HB3	2.16	0.45
2:H:484:MET:HE2	2:H:484:MET:HB2	1.69	0.45
2:H:405:VAL:HG11	2:H:441:ILE:HD11	1.99	0.45
2:D:476:LEU:CB	2:D:480:GLU:CD	2.84	0.45
2:D:221:LEU:C	2:D:223:LYS:H	2.19	0.45
2:G:164:LEU:CB	2:G:177:ILE:HG12	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:239:LYS:CA	2:G:242:LEU:HD22	2.46	0.45
2:C:116:VAL:HB	2:C:117:PRO:CD	2.47	0.45
2:G:361:LEU:CD2	2:G:387:ILE:CD1	2.87	0.45
2:C:408:HIS:NE2	2:C:410:LEU:HD21	2.32	0.45
1:A:127:LYS:HA	1:A:129:GLU:OE1	2.17	0.45
2:D:164:LEU:C	2:D:164:LEU:CD1	2.84	0.45
1:B:89:PHE:O	1:B:92:PHE:N	2.32	0.45
1:B:120:ASP:OD2	1:B:194:GLN:NE2	2.49	0.45
1:A:78:MET:SD	1:A:82:TYR:CE1	3.10	0.45
1:B:78:MET:O	1:B:81:ARG:N	2.50	0.45
2:H:468:ILE:HG22	2:H:469:THR:O	2.17	0.45
2:G:503:GLU:C	2:G:505:ARG:N	2.70	0.45
2:D:274:PHE:C	2:D:274:PHE:CD1	2.90	0.45
1:F:94:ARG:NH2	1:F:97:ARG:NH1	2.65	0.45
2:G:360:LEU:HA	2:G:360:LEU:HD22	1.86	0.45
2:D:71:MET:SD	2:D:86:PRO:CB	3.06	0.44
1:B:86:TYR:HD1	1:B:86:TYR:HA	1.55	0.44
1:A:201:ASP:OD1	1:A:202:ARG:N	2.50	0.44
1:B:189:VAL:HG22	1:B:209:VAL:HG11	1.98	0.44
1:B:189:VAL:N	1:B:211:VAL:HG23	2.31	0.44
1:A:89:PHE:CB	1:B:89:PHE:HD1	2.27	0.44
1:B:94:ARG:O	1:B:98:GLN:HG3	2.16	0.44
2:H:7:ILE:CD1	2:H:97:LEU:HD23	2.46	0.44
1:B:152:ALA:HA	1:B:155:LYS:HB2	1.98	0.44
2:G:77:VAL:HG13	2:G:79:ILE:HG13	1.99	0.44
2:H:374:GLY:N	2:H:375:GLY:CA	2.79	0.44
2:C:157:LYS:HE3	2:C:356:LYS:HZ3	1.82	0.44
2:D:239:LYS:O	2:D:240:LYS:C	2.55	0.44
1:A:150:VAL:O	1:A:154:LYS:HB2	2.17	0.44
2:H:151:LEU:HA	2:H:151:LEU:HD12	1.63	0.44
2:D:476:LEU:HD13	2:D:476:LEU:HA	1.73	0.44
2:C:443:VAL:HA	2:C:456:ARG:O	2.17	0.44
2:C:10:GLY:N	2:C:14:SER:OG	2.47	0.44
2:C:39:VAL:HG22	2:C:39:VAL:O	2.17	0.44
2:D:361:LEU:HD22	2:D:387:ILE:HG12	1.94	0.44
2:G:383:ARG:CD	2:G:384:ASN:H	2.25	0.44
2:G:372:THR:O	2:G:375:GLY:N	2.49	0.44
1:A:138:ILE:HG21	1:B:139:LEU:CD2	2.29	0.44
2:H:370:ILE:HD13	2:H:407:ILE:CG2	2.43	0.44
2:G:470:ILE:HA	2:G:471:LYS:NZ	2.32	0.44
2:C:153:TYR:CZ	2:C:334:VAL:HG12	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:HIS:N	2:C:217:HIS:ND1	2.65	0.44
2:H:155:LEU:HB3	2:H:158:GLU:OE1	2.17	0.44
2:G:238:ALA:O	2:G:242:LEU:HD13	2.17	0.44
2:G:370:ILE:CD1	2:G:445:PHE:HZ	2.29	0.44
2:D:146:PRO:O	2:D:147:THR:C	2.56	0.44
2:H:306:VAL:CG1	2:H:307:ILE:N	2.78	0.44
1:B:75:LEU:HA	1:B:75:LEU:HD22	1.69	0.44
1:F:148:SER:HA	1:F:151:ASP:CB	2.47	0.44
2:C:483:ARG:HA	2:C:483:ARG:HD2	1.68	0.44
2:D:465:GLU:O	2:D:467:SER:OG	2.35	0.44
2:H:180:LEU:HD11	2:H:183:GLY:O	2.17	0.44
2:C:265:LEU:C	2:C:265:LEU:HD23	2.38	0.44
2:C:362:ASP:O	2:C:363:VAL:HG22	2.17	0.44
2:H:481:ILE:C	2:H:483:ARG:H	2.20	0.44
2:C:414:ARG:HB2	2:C:420:ASN:HD21	1.83	0.44
2:D:381:ILE:CD1	2:D:447:ILE:HD11	2.48	0.44
2:D:29:ASN:HB2	2:D:30:PRO:CD	2.47	0.44
2:H:316:PRO:O	2:H:320:GLU:HB2	2.17	0.44
2:D:77:VAL:O	2:D:77:VAL:HG13	2.18	0.44
2:D:426:PHE:HZ	2:D:457:ALA:CB	2.31	0.44
2:H:361:LEU:CD1	2:H:387:ILE:HD12	2.43	0.44
2:D:18:VAL:HG11	2:D:27:ILE:HD11	1.99	0.44
2:G:368:LEU:HB2	2:G:381:ILE:HB	1.99	0.44
2:D:168:LEU:CD1	2:D:197:GLY:HA2	2.46	0.44
2:H:499:LYS:HG2	2:H:500:GLU:N	2.32	0.44
2:D:505:ARG:HG3	2:D:506:ASN:N	2.33	0.44
2:H:11:THR:N	2:H:68:LYS:HD3	2.33	0.44
2:C:250:ILE:HG22	2:C:252:LEU:HD22	2.00	0.44
1:F:91:ASN:CG	2:G:386:THR:OG1	2.56	0.44
1:B:169:ASP:H	1:B:173:HIS:CD2	2.34	0.44
2:D:38:SER:C	2:D:39:VAL:HG13	2.37	0.44
2:C:41:ALA:HB1	2:C:60:ASN:HD22	1.81	0.44
2:H:425:ARG:O	2:H:426:PHE:HB3	2.17	0.44
2:G:214:LYS:HE3	2:G:220:ASP:OD1	2.17	0.44
2:D:496:ARG:O	2:D:497:LYS:C	2.54	0.44
2:G:97:LEU:O	2:G:100:TYR:HD1	2.00	0.44
2:C:288:PRO:O	2:C:289:VAL:C	2.56	0.44
2:C:124:GLN:O	2:C:127:ALA:N	2.51	0.44
1:B:85:LEU:HD23	2:H:483:ARG:HH21	1.83	0.44
1:A:204:LEU:H	1:A:204:LEU:HD12	1.82	0.44
2:D:167:ASP:OD1	2:D:168:LEU:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:399:ALA:O	2:G:400:ASP:C	2.56	0.44
1:A:188:THR:O	1:A:211:VAL:HG23	2.17	0.44
2:H:379:LYS:O	2:H:380:LEU:HD23	2.18	0.44
2:G:234:ALA:O	2:G:237:LYS:HB3	2.17	0.44
2:D:361:LEU:CD1	2:D:387:ILE:CD1	2.95	0.44
2:D:192:GLY:CA	2:D:288:PRO:HB3	2.47	0.44
2:H:127:ALA:C	2:H:130:ASP:HB2	2.35	0.44
1:B:81:ARG:O	1:B:82:TYR:HD1	2.01	0.44
2:D:29:ASN:HA	2:D:100:TYR:CD1	2.53	0.44
2:C:157:LYS:HE3	2:C:356:LYS:NZ	2.32	0.44
2:C:194:ASN:O	2:C:195:HIS:CD2	2.70	0.44
2:H:379:LYS:HB2	2:H:379:LYS:HE2	1.72	0.44
2:H:458:LYS:HA	2:H:465:GLU:HB3	2.00	0.44
2:D:9:LEU:HA	2:D:9:LEU:HD12	1.77	0.44
2:C:395:PHE:HB3	2:H:358:VAL:HG23	2.00	0.44
1:A:119:LEU:CD1	1:A:197:TYR:CE2	3.01	0.44
2:C:119:TYR:O	2:C:120:PHE:C	2.56	0.44
1:E:104:GLU:HA	1:F:107:ARG:HH12	1.83	0.44
2:H:115:THR:OG1	2:H:145:GLU:HG2	2.16	0.43
2:C:88:GLU:O	2:C:91:ALA:HB3	2.18	0.43
2:D:217:HIS:CD2	2:D:263:LEU:HD21	2.53	0.43
2:G:179:GLU:HB2	2:G:188:LYS:NZ	2.33	0.43
2:D:387:ILE:HD13	2:D:387:ILE:HG21	1.58	0.43
2:G:334:VAL:HG13	2:G:336:PRO:N	2.32	0.43
2:D:196:LEU:HA	2:D:196:LEU:HD12	1.64	0.43
2:G:214:LYS:HZ2	2:G:221:LEU:N	2.16	0.43
2:D:479:GLU:O	2:D:482:GLN:N	2.51	0.43
2:C:270:THR:HG22	2:C:272:ALA:H	1.83	0.43
1:A:108:ALA:HB2	1:A:156:GLU:OE1	2.17	0.43
2:C:284:ARG:HB3	2:C:284:ARG:HE	1.32	0.43
2:H:368:LEU:HD22	2:H:411:GLN:HB2	1.98	0.43
2:D:4:ILE:HD13	2:D:351:ILE:CG2	2.48	0.43
2:C:118:ALA:HB2	2:C:146:PRO:HG2	2.00	0.43
1:A:196:GLY:CA	1:A:207:ALA:HB2	2.48	0.43
2:H:127:ALA:O	2:H:130:ASP:CB	2.50	0.43
2:D:160:ASP:HA	2:D:180:LEU:HD23	1.99	0.43
1:E:193:LEU:H	1:E:209:VAL:HA	1.83	0.43
2:C:368:LEU:HD23	2:C:368:LEU:HA	1.46	0.43
2:C:400:ASP:O	2:C:401:ASN:HB2	2.18	0.43
2:C:44:ASN:C	2:C:46:GLU:N	2.71	0.43
2:H:184:VAL:CG1	2:H:185:PHE:N	2.79	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:MET:HE2	2:D:266:GLU:CD	2.39	0.43
2:C:102:GLU:O	2:C:103:ASP:C	2.56	0.43
2:G:416:MET:HE3	2:G:417:ALA:N	2.10	0.43
1:B:94:ARG:HD2	1:B:98:GLN:HG3	2.00	0.43
2:D:371:GLU:HG3	2:D:371:GLU:O	2.18	0.43
1:A:177:MET:HE2	2:C:225:LYS:HZ3	1.82	0.43
2:C:339:VAL:CG1	2:C:340:VAL:N	2.80	0.43
2:G:41:ALA:HB2	2:G:62:ASN:O	2.18	0.43
2:C:182:ASP:O	2:C:183:GLY:C	2.57	0.43
2:C:47:ARG:HD3	2:C:92:ILE:HD13	2.00	0.43
2:C:396:THR:HG23	2:H:361:LEU:HB2	2.00	0.43
2:D:204:VAL:HG21	2:D:277:LEU:O	2.18	0.43
2:D:232:LYS:O	2:D:233:ASP:C	2.56	0.43
1:B:142:MET:CE	2:C:254:PHE:CZ	3.01	0.43
2:C:253:PRO:HB2	2:C:254:PHE:CD1	2.53	0.43
2:C:39:VAL:CG2	2:C:39:VAL:O	2.62	0.43
1:B:166:LYS:HG2	1:B:167:PRO:CD	2.48	0.43
2:C:43:LYS:HD2	2:C:43:LYS:HA	1.55	0.43
1:A:75:LEU:CD2	1:B:75:LEU:CD2	2.96	0.43
1:E:77:GLU:O	1:E:81:ARG:HG2	2.18	0.43
2:G:205:ILE:HD13	2:G:235:ALA:O	2.18	0.43
2:H:12:THR:HB	2:H:170:GLY:H	1.84	0.43
2:D:507:GLU:CA	2:D:507:GLU:OE1	2.62	0.43
1:B:67:GLN:HA	1:B:67:GLN:NE2	2.31	0.43
2:H:324:ARG:HG3	2:H:325:GLU:N	2.32	0.43
2:C:291:GLN:HA	2:C:291:GLN:OE1	2.19	0.43
2:D:83:GLN:HG3	2:D:83:GLN:O	2.17	0.43
2:G:484:MET:N	2:G:484:MET:SD	2.91	0.43
2:H:287:GLY:O	2:H:291:GLN:HB2	2.18	0.43
2:H:86:PRO:O	2:H:89:ILE:HB	2.18	0.43
2:D:89:ILE:O	2:D:92:ILE:N	2.51	0.43
2:G:162:THR:C	2:G:303:ILE:HG23	2.38	0.43
1:F:69:ALA:HA	1:F:72:GLU:OE1	2.19	0.43
1:A:75:LEU:CD2	1:B:75:LEU:HD22	2.48	0.43
1:E:63:ALA:HA	1:E:66:ALA:CB	2.48	0.43
1:E:75:LEU:O	1:E:78:MET:CB	2.63	0.43
2:C:207:ASP:O	2:C:210:VAL:N	2.52	0.43
1:A:171:TYR:HB3	1:A:172:LEU:HD23	2.00	0.43
2:C:164:LEU:HD21	2:C:175:VAL:CG1	2.49	0.43
2:G:144:ASN:HD21	2:G:147:THR:H	1.62	0.43
2:H:489:GLU:O	2:H:490:GLU:C	2.56	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:300:PRO:O	2:C:301:ALA:C	2.55	0.43
2:H:347:GLN:HA	2:H:350:VAL:HG23	2.01	0.43
2:D:208:TYR:HE2	2:D:273:LYS:HD3	1.83	0.43
2:D:204:VAL:CG2	2:D:277:LEU:HD13	2.42	0.43
2:C:1:MET:CG	2:C:2:SER:H	2.30	0.43
2:G:161:GLN:HG2	2:G:180:LEU:HB2	2.00	0.43
2:G:387:ILE:HG22	2:G:449:ALA:HA	2.00	0.43
2:D:290:ARG:CA	2:D:293:LEU:HG	2.45	0.43
2:D:318:VAL:O	2:D:319:GLN:C	2.57	0.43
1:A:78:MET:SD	1:A:82:TYR:CZ	3.11	0.43
2:C:495:ASP:CG	2:C:498:ARG:CZ	2.87	0.43
2:D:80:GLU:OE1	2:D:80:GLU:N	2.51	0.43
2:C:241:GLU:O	2:C:245:VAL:CG1	2.66	0.43
2:D:225:LYS:O	2:D:228:LEU:HB3	2.18	0.43
1:A:168:PHE:CE2	1:A:175:ALA:HB2	2.53	0.43
2:H:273:LYS:HD3	2:H:276:GLU:OE1	2.19	0.43
2:C:157:LYS:CE	2:C:356:LYS:HZ3	2.31	0.43
2:C:317:ALA:O	2:C:318:VAL:C	2.56	0.43
2:G:484:MET:CE	2:G:487:GLU:HB2	2.48	0.43
1:E:144:MET:O	1:E:148:SER:CB	2.66	0.43
2:H:113:VAL:CG2	2:H:141:ARG:HB3	2.49	0.43
1:A:84:ARG:HH22	2:C:354:GLU:N	2.16	0.43
2:C:361:LEU:O	2:C:387:ILE:HD12	2.19	0.43
2:C:97:LEU:HA	2:C:97:LEU:HD12	1.39	0.43
1:A:106:TYR:CD2	1:A:202:ARG:NH1	2.71	0.43
2:H:90:SER:O	2:H:94:LEU:HD22	2.19	0.43
1:E:72:GLU:O	1:E:75:LEU:HB2	2.18	0.43
2:H:88:GLU:HA	2:H:91:ALA:CB	2.45	0.43
2:G:293:LEU:HD22	2:G:300:PRO:N	2.34	0.43
2:C:298:LEU:HD12	2:C:298:LEU:HA	1.78	0.43
2:C:434:ALA:HB1	2:C:435:PRO:HD2	2.00	0.43
2:G:152:ALA:CA	2:G:346:ILE:HD12	2.32	0.43
2:G:346:ILE:O	2:G:350:VAL:HG23	2.19	0.43
2:H:143:ILE:HG22	2:H:144:ASN:H	1.82	0.43
2:C:369:GLY:HA3	2:C:378:THR:O	2.17	0.43
2:D:280:HIS:CD2	2:D:281:LEU:H	2.37	0.43
2:D:388:PRO:HB3	2:D:448:ASP:C	2.38	0.43
2:H:202:ASP:O	2:H:206:ILE:HD12	2.19	0.43
2:H:24:VAL:CG1	2:H:345:ALA:HB1	2.49	0.43
1:E:75:LEU:O	1:E:76:SER:C	2.57	0.43
1:F:74:LYS:O	1:F:78:MET:CB	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:497:LYS:O	2:C:500:GLU:OE2	2.37	0.43
2:C:245:VAL:CG2	2:C:246:THR:N	2.79	0.43
2:C:153:TYR:CE1	2:C:334:VAL:CB	3.02	0.43
2:G:155:LEU:HD13	2:G:155:LEU:HA	1.79	0.43
2:D:395:PHE:HA	2:D:395:PHE:HD1	1.64	0.43
2:C:128:THR:OG1	2:C:129:LYS:N	2.52	0.43
2:D:73:THR:C	2:D:75:TYR:H	2.20	0.43
2:D:203:GLN:O	2:D:204:VAL:C	2.57	0.43
1:A:84:ARG:NH2	2:C:354:GLU:N	2.67	0.43
2:G:274:PHE:CA	2:G:277:LEU:HB2	2.48	0.43
2:D:5:ILE:HD11	2:D:109:VAL:HG11	2.00	0.43
2:G:366:LEU:HD13	2:G:412:GLY:CA	2.48	0.43
2:G:370:ILE:CG2	2:G:408:HIS:O	2.60	0.43
2:G:206:ILE:HG12	2:G:231:LEU:HB3	2.01	0.43
2:C:483:ARG:O	2:C:487:GLU:OE1	2.36	0.43
2:C:92:ILE:O	2:C:95:GLN:HB2	2.19	0.43
2:D:267:MET:SD	2:D:268:THR:N	2.92	0.43
2:G:173:PHE:CZ	2:G:175:VAL:CG1	2.97	0.43
2:D:361:LEU:CD1	2:D:387:ILE:HG13	2.48	0.43
2:G:372:THR:HB	2:G:376:VAL:CG1	2.24	0.43
2:D:51:GLU:O	2:D:53:ALA:N	2.51	0.43
2:H:4:ILE:HG12	2:H:111:ARG:HB2	2.01	0.43
2:H:88:GLU:O	2:H:91:ALA:HB3	2.19	0.43
2:C:500:GLU:HA	2:C:503:GLU:CG	2.49	0.43
2:D:438:VAL:N	2:D:439:PRO:HD3	2.33	0.43
1:E:94:ARG:CA	1:E:97:ARG:HB3	2.49	0.43
2:G:107:GLU:O	2:G:107:GLU:HG2	2.19	0.43
2:H:272:ALA:HA	2:H:275:GLU:OE1	2.19	0.43
2:H:386:THR:CG2	2:H:387:ILE:O	2.55	0.42
2:D:107:GLU:O	2:D:108:PRO:C	2.57	0.42
2:C:18:VAL:HG12	2:C:27:ILE:CD1	2.49	0.42
2:G:153:TYR:OH	2:G:334:VAL:HG12	2.19	0.42
2:D:53:ALA:O	2:D:54:LYS:C	2.56	0.42
2:D:147:THR:O	2:D:151:LEU:HD13	2.19	0.42
2:D:79:ILE:HD12	2:D:84:TYR:CE2	2.51	0.42
2:H:403:THR:OG1	2:H:404:THR:N	2.52	0.42
2:C:68:LYS:HZ1	2:C:117:PRO:HG3	1.82	0.42
2:D:328:LYS:HG2	2:D:329:GLU:N	2.28	0.42
2:H:71:MET:HE3	2:H:128:THR:HG23	2.00	0.42
2:H:119:TYR:HD2	2:H:190:THR:HG21	1.84	0.42
2:D:495:ASP:O	2:D:497:LYS:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:TYR:CB	1:A:172:LEU:HD23	2.50	0.42
1:F:82:TYR:HA	1:F:82:TYR:HD1	1.78	0.42
2:G:486:LYS:HE3	2:G:490:GLU:OE2	2.19	0.42
1:B:193:LEU:HD23	1:B:193:LEU:O	2.18	0.42
2:C:138:GLU:OE2	2:C:140:GLU:OE1	2.37	0.42
2:C:162:THR:N	2:C:304:ASP:OD1	2.52	0.42
2:G:54:LYS:O	2:G:57:ALA:HB3	2.19	0.42
2:C:71:MET:SD	2:C:86:PRO:HB2	2.58	0.42
2:H:67:ILE:HD11	2:H:89:ILE:HG21	1.78	0.42
2:H:358:VAL:HG23	2:H:359:VAL:N	2.34	0.42
2:H:367:SER:OG	2:H:413:GLU:OE1	2.37	0.42
2:D:221:LEU:C	2:D:223:LYS:N	2.72	0.42
2:H:332:LYS:C	2:H:332:LYS:HD2	2.39	0.42
2:G:308:LEU:CD1	2:G:330:PRO:CB	2.96	0.42
1:F:75:LEU:HD13	1:F:76:SER:N	2.35	0.42
2:C:307:ILE:O	2:C:308:LEU:HD12	2.20	0.42
2:D:375:GLY:O	2:D:416:MET:HE3	2.18	0.42
2:D:16:VAL:HG11	2:D:100:TYR:OH	2.18	0.42
2:G:144:ASN:OD1	2:G:147:THR:CG2	2.68	0.42
2:H:392:SER:CB	2:H:444:THR:HB	2.48	0.42
1:A:198:LYS:CG	1:A:198:LYS:O	2.66	0.42
1:A:185:GLU:HB3	1:A:186:PRO:CD	2.50	0.42
1:A:208:MET:H	1:A:208:MET:HG2	1.60	0.42
2:D:246:THR:OG1	2:D:246:THR:O	2.36	0.42
1:F:165:GLY:HA2	1:F:189:VAL:H	1.84	0.42
2:D:270:THR:OG1	2:D:272:ALA:N	2.52	0.42
2:G:243:SER:CB	2:G:315:ILE:HA	2.50	0.42
1:B:71:LEU:O	1:B:72:GLU:C	2.57	0.42
2:H:370:ILE:CD1	2:H:407:ILE:HG23	2.43	0.42
2:H:12:THR:C	2:H:13:ASN:ND2	2.73	0.42
2:C:42:PHE:H	2:C:42:PHE:HD1	1.67	0.42
2:D:408:HIS:CD2	2:D:425:ARG:HD2	2.53	0.42
2:H:460:LEU:N	2:H:460:LEU:CD2	2.79	0.42
2:G:255:ILE:H	2:G:264:HIS:CB	2.33	0.42
2:G:477:SER:OG	2:G:478:GLU:N	2.51	0.42
2:C:466:GLN:HA	2:C:466:GLN:NE2	2.34	0.42
2:D:208:TYR:CE2	2:D:273:LYS:HD3	2.54	0.42
2:C:68:LYS:CE	2:C:117:PRO:HG3	2.49	0.42
1:B:119:LEU:HD22	1:B:122:PHE:HB2	2.01	0.42
1:A:120:ASP:OD2	1:A:205:ARG:NH2	2.51	0.42
2:G:369:GLY:CA	2:G:377:PHE:CE1	3.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ALA:CB	1:A:197:TYR:CE1	3.02	0.42
2:G:397:THR:CB	2:G:436:ARG:HA	2.49	0.42
2:C:330:PRO:O	2:C:330:PRO:HG2	2.19	0.42
2:D:7:ILE:HG22	2:D:8:ASP:N	2.35	0.42
1:B:153:LEU:HA	1:B:153:LEU:HD22	1.60	0.42
2:C:175:VAL:CG1	2:C:176:SER:N	2.82	0.42
2:C:380:LEU:O	2:C:391:LYS:CD	2.67	0.42
1:E:70:GLU:H	1:E:70:GLU:HG3	1.67	0.42
2:D:97:LEU:HD12	2:D:97:LEU:HA	1.67	0.42
2:C:110:THR:HG23	2:C:111:ARG:CG	2.26	0.42
1:B:116:LEU:HD22	1:B:197:TYR:CE2	2.54	0.42
2:H:18:VAL:O	2:H:24:VAL:HG13	2.19	0.42
2:G:210:VAL:HB	2:G:214:LYS:HZ3	1.83	0.42
1:A:169:ASP:C	1:A:171:TYR:N	2.71	0.42
1:A:174:GLN:O	1:A:208:MET:HA	2.19	0.42
2:D:89:ILE:C	2:D:91:ALA:N	2.71	0.42
1:B:128:ILE:HG22	1:B:128:ILE:O	2.20	0.42
2:D:213:PHE:HZ	2:D:263:LEU:HD13	1.83	0.42
2:C:221:LEU:O	2:C:222:SER:C	2.58	0.42
2:D:101:ALA:O	2:D:105:LEU:HD22	2.20	0.42
2:C:38:SER:C	2:C:39:VAL:CG1	2.86	0.42
1:A:123:GLU:OE1	1:A:195:LYS:HB2	2.19	0.42
2:D:39:VAL:CG2	2:D:53:ALA:HB3	2.50	0.42
1:A:92:PHE:HZ	1:B:92:PHE:CE1	2.36	0.42
1:A:118:VAL:HG12	1:A:119:LEU:N	2.34	0.42
1:B:114:ASP:O	1:B:117:PRO:HD2	2.20	0.42
2:H:71:MET:SD	2:H:87:GLN:HG3	2.60	0.42
1:E:76:SER:HA	1:E:79:GLU:CD	2.39	0.42
2:C:440:GLN:O	2:C:441:ILE:HG13	2.19	0.42
2:H:401:ASN:ND2	2:H:433:PRO:O	2.53	0.42
2:D:421:LYS:HE2	2:D:421:LYS:HB2	1.41	0.42
2:D:73:THR:O	2:D:75:TYR:N	2.53	0.42
2:G:173:PHE:HZ	2:G:175:VAL:HG13	1.78	0.42
2:D:18:VAL:HG22	2:D:19:LEU:N	2.34	0.42
2:D:3:LYS:N	2:D:3:LYS:HD2	2.35	0.42
1:A:120:ASP:HA	1:A:123:GLU:OE2	2.20	0.42
2:G:395:PHE:CD1	2:G:395:PHE:N	2.87	0.42
2:D:141:ARG:HG3	2:D:142:ILE:N	2.34	0.42
1:B:169:ASP:O	1:B:173:HIS:HD2	2.03	0.42
2:D:377:PHE:C	2:D:377:PHE:CD1	2.91	0.42
2:D:150:ALA:O	2:D:155:LEU:HD22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:400:ASP:CB	2:G:401:ASN:ND2	2.83	0.42
2:C:273:LYS:CE	2:C:277:LEU:HD21	2.50	0.42
1:F:85:LEU:HA	1:F:85:LEU:HD13	1.83	0.42
2:D:408:HIS:CE1	2:D:425:ARG:NH1	2.88	0.42
1:A:124:ARG:NH2	2:C:230:ARG:HD2	2.34	0.42
2:D:356:LYS:HD3	2:G:406:ASP:HB2	2.02	0.42
2:H:339:VAL:HA	2:H:342:ILE:CG1	2.50	0.42
2:C:394:VAL:CG2	2:H:363:VAL:HG11	2.46	0.42
2:G:164:LEU:HD23	2:G:177:ILE:HG13	2.02	0.42
2:C:145:GLU:HB2	2:C:146:PRO:CD	2.41	0.42
1:A:200:LYS:O	1:A:201:ASP:OD1	2.37	0.42
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.56	0.42
2:H:414:ARG:CZ	2:H:491:ASN:ND2	2.83	0.42
2:D:334:VAL:O	2:D:336:PRO:HD3	2.19	0.42
2:G:293:LEU:HD13	2:G:300:PRO:CG	2.41	0.42
2:H:505:ARG:O	2:H:507:GLU:C	2.57	0.42
2:C:471:LYS:NZ	2:C:471:LYS:H	2.15	0.42
2:D:77:VAL:CG1	2:D:77:VAL:O	2.66	0.42
2:H:380:LEU:HD23	2:H:380:LEU:HA	1.26	0.42
2:G:226:MET:HG2	2:G:226:MET:O	2.19	0.42
2:D:209:LEU:HD22	2:D:209:LEU:HA	1.72	0.42
2:D:233:ASP:O	2:D:234:ALA:C	2.58	0.42
2:G:370:ILE:CG1	2:G:445:PHE:HZ	2.33	0.42
2:H:377:PHE:CE1	2:H:378:THR:O	2.73	0.42
2:C:205:ILE:O	2:C:206:ILE:C	2.54	0.42
2:H:12:THR:HB	2:H:170:GLY:N	2.35	0.42
2:G:402:GLN:HG2	2:G:404:THR:O	2.20	0.42
2:D:10:GLY:HA2	2:D:68:LYS:NZ	2.34	0.42
2:H:305:LYS:HE2	2:H:328:LYS:HD3	2.02	0.42
2:C:64:ILE:HG22	2:C:65:ILE:N	2.34	0.41
2:H:8:ASP:O	2:H:14:SER:CB	2.67	0.41
2:D:210:VAL:CA	2:D:221:LEU:HD13	2.50	0.41
2:H:15:CYS:SG	2:H:341:ALA:HB3	2.60	0.41
1:B:85:LEU:O	1:B:86:TYR:C	2.58	0.41
2:G:308:LEU:HD21	2:G:319:GLN:CD	2.40	0.41
2:G:242:LEU:HD13	2:G:242:LEU:H	1.84	0.41
2:D:4:ILE:CD1	2:D:351:ILE:HB	2.50	0.41
1:A:200:LYS:O	1:A:202:ARG:N	2.47	0.41
2:D:121:ASN:CG	2:D:122:ASP:N	2.73	0.41
2:H:132:GLY:O	2:H:137:LEU:HB2	2.19	0.41
2:D:317:ALA:O	2:D:318:VAL:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:PHE:CE2	1:B:92:PHE:CZ	3.08	0.41
2:C:281:LEU:O	2:C:282:VAL:C	2.58	0.41
1:B:78:MET:O	1:B:79:GLU:C	2.59	0.41
2:C:498:ARG:C	2:C:500:GLU:N	2.73	0.41
2:C:204:VAL:HG21	2:C:277:LEU:O	2.20	0.41
2:H:281:LEU:CD1	2:H:284:ARG:NH1	2.81	0.41
2:H:397:THR:O	2:H:397:THR:HG23	2.20	0.41
2:D:6:GLY:CA	2:D:344:ALA:HB1	2.50	0.41
2:G:171:GLY:O	2:G:195:HIS:HA	2.19	0.41
2:D:423:LEU:HD13	2:D:470:ILE:HD13	2.01	0.41
2:G:163:ILE:HA	2:G:303:ILE:CG2	2.50	0.41
2:G:163:ILE:HA	2:G:303:ILE:HG23	2.01	0.41
1:B:119:LEU:HD21	1:B:149:LEU:HD22	2.02	0.41
1:B:135:ALA:O	1:B:138:ILE:HB	2.20	0.41
2:D:303:ILE:HG22	2:D:305:LYS:N	2.35	0.41
2:D:319:GLN:O	2:D:320:GLU:C	2.59	0.41
2:H:24:VAL:HG11	2:H:345:ALA:HB1	2.01	0.41
2:C:366:LEU:HA	2:C:383:ARG:HG3	2.02	0.41
2:H:116:VAL:CG1	2:H:117:PRO:CD	2.92	0.41
1:F:98:GLN:HA	1:F:101:GLU:HG3	2.02	0.41
2:C:151:LEU:HD22	2:C:347:GLN:HG2	1.99	0.41
2:H:479:GLU:CD	2:H:479:GLU:C	2.78	0.41
2:D:214:LYS:O	2:D:218:GLY:N	2.52	0.41
2:D:242:LEU:HD21	2:D:248:THR:HG22	2.02	0.41
2:D:230:ARG:CZ	2:D:252:LEU:HD11	2.48	0.41
1:A:192:GLU:CG	1:A:195:LYS:HA	2.50	0.41
2:H:231:LEU:O	2:H:235:ALA:CB	2.68	0.41
2:H:168:LEU:HD12	2:H:169:GLY:O	2.20	0.41
2:H:172:THR:C	2:H:196:LEU:O	2.58	0.41
1:E:81:ARG:O	1:E:84:ARG:N	2.53	0.41
2:G:358:VAL:HG23	2:G:359:VAL:N	2.35	0.41
2:C:164:LEU:O	2:C:306:VAL:HG13	2.20	0.41
1:B:133:GLU:HB2	1:B:134:GLN:H	1.69	0.41
2:C:399:ALA:CB	2:H:355:VAL:HG11	2.50	0.41
2:G:167:ASP:HB3	2:G:174:ASP:HB3	2.02	0.41
2:H:160:ASP:OD1	2:H:182:ASP:N	2.53	0.41
1:F:194:GLN:O	1:F:207:ALA:HB2	2.21	0.41
2:C:87:GLN:O	2:C:91:ALA:CB	2.66	0.41
1:E:80:HIS:O	1:E:81:ARG:C	2.58	0.41
2:G:499:LYS:HE2	2:G:500:GLU:OE1	2.21	0.41
2:D:348:GLY:O	2:D:349:GLY:C	2.58	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:186:GLU:HG3	2:H:186:GLU:O	2.20	0.41
2:D:476:LEU:HB3	2:D:480:GLU:HB3	2.02	0.41
2:D:476:LEU:O	2:D:480:GLU:HB3	2.21	0.41
2:C:42:PHE:N	2:C:42:PHE:HD1	2.14	0.41
2:D:420:ASN:HD22	2:D:420:ASN:N	2.17	0.41
2:H:457:ALA:O	2:H:465:GLU:HB2	2.20	0.41
2:H:381:ILE:HD11	2:H:445:PHE:CB	2.50	0.41
1:A:84:ARG:HH21	2:C:354:GLU:HB2	1.82	0.41
2:G:180:LEU:HG	2:G:182:ASP:H	1.86	0.41
1:A:145:VAL:O	1:A:148:SER:HB3	2.21	0.41
2:D:37:PRO:HG2	2:D:51:GLU:N	2.35	0.41
2:D:315:ILE:HG21	2:D:318:VAL:HG23	2.02	0.41
2:C:326:LEU:H	2:C:326:LEU:HD22	1.86	0.41
2:D:444:THR:O	2:D:445:PHE:CD1	2.66	0.41
2:G:358:VAL:HG23	2:G:359:VAL:H	1.85	0.41
1:A:190:VAL:N	1:A:210:LYS:O	2.47	0.41
2:C:500:GLU:CD	2:C:500:GLU:N	2.73	0.41
2:C:484:MET:HE2	2:C:484:MET:CA	2.46	0.41
2:G:10:GLY:CA	2:G:13:ASN:O	2.68	0.41
1:B:119:LEU:O	1:B:123:GLU:OE1	2.38	0.41
1:A:192:GLU:C	1:A:193:LEU:HD23	2.40	0.41
1:A:192:GLU:CD	1:A:195:LYS:HG2	2.41	0.41
2:G:426:PHE:CD1	2:G:468:ILE:HD12	2.53	0.41
2:D:358:VAL:HG22	2:G:372:THR:HA	2.02	0.41
1:F:83:LEU:O	2:G:388:PRO:HG2	2.21	0.41
2:D:329:GLU:HA	2:D:330:PRO:HD2	1.96	0.41
2:G:400:ASP:HB3	2:G:401:ASN:ND2	2.35	0.41
1:F:63:ALA:HA	1:F:66:ALA:CB	2.51	0.41
2:G:70:HIS:CD2	2:G:75:TYR:CD1	3.09	0.41
2:C:366:LEU:HD22	2:C:367:SER:N	2.28	0.41
2:H:210:VAL:O	2:H:214:LYS:CG	2.56	0.41
2:H:498:ARG:O	2:H:499:LYS:C	2.59	0.41
2:D:397:THR:HG23	2:D:436:ARG:CG	2.50	0.41
2:H:290:ARG:HA	2:H:293:LEU:HD11	2.02	0.41
2:G:225:LYS:O	2:G:229:GLN:HB2	2.21	0.41
2:G:6:GLY:O	2:G:16:VAL:HA	2.21	0.41
2:C:234:ALA:HA	2:C:237:LYS:HD3	2.02	0.41
2:D:366:LEU:CD2	2:D:412:GLY:HA2	2.51	0.41
1:B:125:ALA:HA	2:D:254:PHE:CZ	2.54	0.41
2:C:1:MET:CE	2:C:110:THR:HG21	2.51	0.41
2:C:97:LEU:HA	2:C:100:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:27:ILE:CD1	2:C:101:ALA:CB	2.98	0.41
2:G:381:ILE:HD11	2:G:447:ILE:HD11	1.94	0.41
2:G:385:THR:O	2:G:386:THR:C	2.59	0.41
2:D:50:GLY:O	2:D:53:ALA:CB	2.69	0.41
1:A:135:ALA:O	1:A:138:ILE:HB	2.21	0.41
1:F:60:GLU:CA	1:F:63:ALA:HB3	2.50	0.41
2:H:409:VAL:O	2:H:423:LEU:HB2	2.21	0.41
1:F:95:ARG:HG3	1:F:99:GLU:OE2	2.21	0.41
2:H:6:GLY:CA	2:H:344:ALA:HB1	2.50	0.41
1:B:83:LEU:HD22	1:B:83:LEU:HA	1.75	0.41
2:G:154:GLY:O	2:G:157:LYS:HE2	2.21	0.41
2:D:67:ILE:C	2:D:69:ARG:N	2.73	0.41
2:D:109:VAL:CG2	2:D:110:THR:N	2.77	0.41
2:C:144:ASN:O	2:C:146:PRO:N	2.54	0.41
2:C:9:LEU:HD13	2:C:94:LEU:HD11	2.03	0.41
1:B:149:LEU:HD23	1:B:150:VAL:N	2.35	0.41
1:A:205:ARG:HD3	1:A:205:ARG:O	2.21	0.41
1:A:192:GLU:OE2	1:A:195:LYS:CB	2.69	0.41
2:D:361:LEU:C	2:D:362:ASP:CG	2.79	0.41
1:F:80:HIS:HA	1:F:83:LEU:HG	2.03	0.41
1:F:91:ASN:OD1	2:G:386:THR:OG1	2.39	0.41
2:D:310:GLY:O	2:D:311:GLY:C	2.58	0.41
1:A:126:LEU:O	1:A:126:LEU:HD22	2.21	0.41
2:D:164:LEU:HD23	2:D:177:ILE:CG1	2.51	0.41
2:C:75:TYR:HE1	2:C:77:VAL:HB	1.86	0.41
2:C:75:TYR:CE1	2:C:77:VAL:HB	2.56	0.41
2:H:130:ASP:O	2:H:131:ALA:C	2.58	0.41
2:H:5:ILE:O	2:H:112:ALA:HB1	2.21	0.41
1:B:190:VAL:CG1	1:B:191:GLU:HG2	2.50	0.41
2:D:445:PHE:CD1	2:D:445:PHE:N	2.88	0.41
2:H:214:LYS:HE3	2:H:220:ASP:HA	2.03	0.41
2:C:225:LYS:HB3	2:C:225:LYS:HE3	1.75	0.41
2:G:228:LEU:HA	2:G:231:LEU:HD13	2.03	0.41
2:C:500:GLU:OE1	2:C:503:GLU:HG3	2.21	0.41
2:D:8:ASP:OD1	2:D:340:VAL:HG11	2.21	0.41
2:C:203:GLN:O	2:C:206:ILE:N	2.54	0.41
2:C:208:TYR:O	2:C:212:GLN:HG2	2.21	0.41
1:A:143:GLU:HB2	1:A:147:ARG:HH12	1.86	0.41
2:D:60:ASN:OD1	2:D:62:ASN:HB2	2.21	0.41
1:B:153:LEU:CD1	1:B:158:VAL:HG21	2.51	0.41
2:C:151:LEU:O	2:C:154:GLY:CA	2.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:347:GLN:HE21	2:C:347:GLN:C	2.24	0.41
2:C:431:ILE:CD1	2:C:441:ILE:HD11	2.50	0.41
2:G:169:GLY:N	2:G:172:THR:O	2.50	0.41
2:D:380:LEU:C	2:D:381:ILE:HG13	2.41	0.41
2:D:258:ASN:OD1	2:D:260:ASN:ND2	2.53	0.41
2:G:72:GLY:HA3	2:G:124:GLN:HB3	2.03	0.41
2:G:48:LEU:O	2:G:53:ALA:HB2	2.21	0.41
2:C:488:ALA:O	2:C:491:ASN:O	2.39	0.41
2:G:479:GLU:HA	2:G:482:GLN:NE2	2.35	0.41
2:C:395:PHE:HE2	2:C:443:VAL:CG1	2.34	0.41
2:D:267:MET:C	2:D:267:MET:SD	2.99	0.41
1:A:204:LEU:O	1:A:205:ARG:C	2.60	0.41
2:D:361:LEU:HD11	2:D:387:ILE:HD12	2.03	0.41
2:D:120:PHE:CD2	2:D:124:GLN:HB3	2.56	0.41
1:B:169:ASP:HB2	1:B:172:LEU:HG	2.02	0.41
2:H:377:PHE:CD1	2:H:378:THR:N	2.89	0.41
2:D:303:ILE:CG2	2:D:304:ASP:N	2.84	0.41
2:H:203:GLN:NE2	2:H:206:ILE:HB	2.36	0.41
2:H:202:ASP:OD2	2:H:235:ALA:HB3	2.21	0.41
2:H:238:ALA:O	2:H:242:LEU:N	2.54	0.41
2:G:459:ASP:HB3	2:G:462:THR:OG1	2.21	0.41
2:C:472:SER:O	2:C:473:SER:HB3	2.21	0.41
2:C:47:ARG:HD3	2:C:92:ILE:CD1	2.51	0.40
2:H:361:LEU:HD13	2:H:362:ASP:N	2.36	0.40
2:H:15:CYS:SG	2:H:338:GLU:HB2	2.61	0.40
2:D:361:LEU:HD22	2:D:387:ILE:HG13	1.99	0.40
2:D:372:THR:HB	2:D:378:THR:OG1	2.21	0.40
2:D:153:TYR:HD2	2:D:331:HIS:CD2	2.40	0.40
1:F:74:LYS:HG3	1:F:78:MET:HG2	2.03	0.40
2:D:31:GLU:C	2:D:32:GLY:O	2.59	0.40
2:D:407:ILE:HG22	2:D:409:VAL:CG1	2.51	0.40
2:D:476:LEU:HB3	2:D:480:GLU:CB	2.51	0.40
1:B:125:ALA:HB3	1:B:126:LEU:HD23	2.03	0.40
2:D:252:LEU:O	2:D:255:ILE:HD11	2.19	0.40
2:D:270:THR:H	2:D:270:THR:HG23	1.51	0.40
2:H:363:VAL:O	2:H:364:THR:CB	2.69	0.40
2:G:303:ILE:HG21	2:G:306:VAL:CG2	2.51	0.40
2:G:273:LYS:HA	2:G:276:GLU:HG2	2.03	0.40
2:C:104:TYR:CD1	2:C:104:TYR:C	2.94	0.40
2:C:116:VAL:O	2:C:145:GLU:HG3	2.22	0.40
2:D:121:ASN:OD1	2:D:124:GLN:N	2.41	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:16:VAL:HG13	2:H:100:TYR:OH	2.22	0.40
1:A:143:GLU:HB2	1:A:147:ARG:NH1	2.35	0.40
2:C:459:ASP:C	2:C:460:LEU:HD23	2.41	0.40
2:C:335:ASN:OD1	2:C:337:ASP:N	2.54	0.40
1:A:162:GLU:HG2	1:A:166:LYS:NZ	2.36	0.40
2:D:357:ASP:O	2:G:398:ALA:HB2	2.22	0.40
2:G:90:SER:O	2:G:94:LEU:HD23	2.21	0.40
2:H:355:VAL:O	2:H:355:VAL:HG12	2.21	0.40
1:A:187:ASN:O	1:A:187:ASN:ND2	2.54	0.40
2:H:146:PRO:HB2	2:H:178:LEU:HD11	2.03	0.40
2:H:383:ARG:O	2:H:384:ASN:C	2.58	0.40
2:D:75:TYR:CD1	2:D:76:LYS:N	2.89	0.40
2:H:332:LYS:C	2:H:334:VAL:H	2.25	0.40
2:C:362:ASP:O	2:C:363:VAL:CG1	2.63	0.40
2:G:332:LYS:C	2:G:334:VAL:H	2.25	0.40
2:D:51:GLU:O	2:D:52:VAL:C	2.60	0.40
2:G:438:VAL:N	2:G:439:PRO:CD	2.84	0.40
1:E:84:ARG:HG2	1:E:88:ASP:OD2	2.22	0.40
2:C:483:ARG:O	2:C:487:GLU:HB2	2.21	0.40
1:B:121:ASN:HA	1:B:124:ARG:CB	2.31	0.40
2:D:198:GLY:O	2:D:200:ASP:N	2.54	0.40
2:G:310:GLY:O	2:G:313:THR:HG22	2.20	0.40
2:H:5:ILE:CG2	2:H:16:VAL:HG23	2.52	0.40
2:D:80:GLU:OE1	2:D:80:GLU:CA	2.69	0.40
2:C:414:ARG:HB2	2:C:420:ASN:ND2	2.36	0.40
2:D:21:GLY:C	2:D:23:GLU:N	2.75	0.40
2:C:182:ASP:C	2:C:184:VAL:N	2.75	0.40
2:G:213:PHE:CE1	2:G:217:HIS:HD2	2.39	0.40
2:D:207:ASP:O	2:D:208:TYR:C	2.59	0.40
2:D:208:TYR:HD2	2:D:277:LEU:CD1	2.35	0.40
2:H:149:ALA:HB1	2:H:339:VAL:CG1	2.46	0.40
2:G:306:VAL:CG1	2:G:307:ILE:H	2.34	0.40
2:G:198:GLY:HA3	2:G:312:SER:OG	2.21	0.40
2:G:204:VAL:HG13	2:G:277:LEU:HD22	2.04	0.40
2:G:281:LEU:CA	2:G:284:ARG:HG3	2.38	0.40
1:A:199:LEU:O	1:A:200:LYS:O	2.39	0.40
1:A:200:LYS:C	1:A:202:ARG:H	2.23	0.40
2:G:369:GLY:C	2:G:370:ILE:HG13	2.41	0.40
2:G:390:SER:HB3	2:G:447:ILE:H	1.85	0.40
2:D:286:MET:O	2:D:289:VAL:N	2.54	0.40
1:B:173:HIS:N	1:B:173:HIS:CD2	2.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:PRO:CG	2:D:51:GLU:HG2	2.25	0.40
2:D:151:LEU:N	2:D:151:LEU:HD12	2.37	0.40
1:A:119:LEU:HD11	1:A:197:TYR:CE2	2.57	0.40
1:E:72:GLU:CA	1:E:75:LEU:HB2	2.51	0.40
1:E:69:ALA:O	1:E:72:GLU:OE1	2.39	0.40
2:C:460:LEU:N	2:C:460:LEU:HD23	2.37	0.40
2:C:334:VAL:HG22	2:C:335:ASN:N	2.37	0.40
2:D:43:LYS:HZ3	2:D:59:THR:HG21	1.86	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	154/213 (72%)	125 (81%)	26 (17%)	3 (2%)	10 54
1	B	152/213 (71%)	119 (78%)	27 (18%)	6 (4%)	4 38
1	E	127/213 (60%)	103 (81%)	22 (17%)	2 (2%)	12 57
1	F	124/213 (58%)	100 (81%)	22 (18%)	2 (2%)	12 57
2	C	507/509 (100%)	458 (90%)	47 (9%)	2 (0%)	39 79
2	D	507/509 (100%)	426 (84%)	72 (14%)	9 (2%)	11 55
2	G	498/509 (98%)	430 (86%)	62 (12%)	6 (1%)	16 62
2	H	497/509 (98%)	423 (85%)	63 (13%)	11 (2%)	8 51
All	All	2566/2888 (89%)	2184 (85%)	341 (13%)	41 (2%)	12 57

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	359	VAL
1	E	170	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	253	PRO
1	B	168	PHE
2	D	361	LEU
2	D	383	ARG
2	G	39	VAL
2	G	40	VAL
2	H	28	PRO
2	H	39	VAL
2	H	387	ILE
2	C	363	VAL
1	F	89	PHE
2	H	504	LEU
2	D	504	LEU
2	H	12	THR
1	B	64	ALA
2	D	226	MET
2	D	309	VAL
1	E	80	HIS
2	G	373	MET
2	H	383	ARG
1	A	75	LEU
1	A	187	ASN
1	B	93	ARG
1	B	106	TYR
1	B	122	PHE
2	D	307	ILE
2	G	492	ALA
1	A	164	VAL
2	D	439	PRO
2	H	346	ILE
2	H	485	ILE
1	B	158	VAL
1	F	164	VAL
2	G	37	PRO
2	G	252	LEU
2	D	318	VAL
2	H	26	VAL
2	C	359	VAL
2	H	32	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	128/174 (74%)	89 (70%)	39 (30%)	0 3
1	B	129/174 (74%)	88 (68%)	41 (32%)	0 3
1	E	35/174 (20%)	24 (69%)	11 (31%)	0 3
1	F	39/174 (22%)	26 (67%)	13 (33%)	0 2
2	C	416/418 (100%)	302 (73%)	114 (27%)	0 5
2	D	416/418 (100%)	305 (73%)	111 (27%)	0 5
2	G	316/418 (76%)	251 (79%)	65 (21%)	1 12
2	H	319/418 (76%)	221 (69%)	98 (31%)	0 3
All	All	1798/2368 (76%)	1306 (73%)	492 (27%)	0 5

All (492) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	60	GLU
1	A	72	GLU
1	A	75	LEU
1	A	78	MET
1	A	83	LEU
1	A	84	ARG
1	A	86	TYR
1	A	89	PHE
1	A	91	ASN
1	A	92	PHE
1	A	95	ARG
1	A	109	GLN
1	A	113	SER
1	A	114	ASP
1	A	119	LEU
1	A	126	LEU
1	A	131	ASP
1	A	132	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	133	GLU
1	A	134	GLN
1	A	140	GLN
1	A	142	MET
1	A	143	GLU
1	A	144	MET
1	A	147	ARG
1	A	153	LEU
1	A	159	GLU
1	A	166	LYS
1	A	168	PHE
1	A	172	LEU
1	A	176	VAL
1	A	182	GLU
1	A	187	ASN
1	A	191	GLU
1	A	198	LYS
1	A	205	ARG
1	A	208	MET
1	A	213	GLN
1	B	60	GLU
1	B	61	LEU
1	B	67	GLN
1	B	71	LEU
1	B	72	GLU
1	B	75	LEU
1	B	80	HIS
1	B	83	LEU
1	B	84	ARG
1	B	86	TYR
1	B	93	ARG
1	B	96	THR
1	B	97	ARG
1	B	101	GLU
1	B	109	GLN
1	B	115	LEU
1	B	119	LEU
1	B	121	ASN
1	B	124	ARG
1	B	126	LEU
1	B	129	GLU
1	B	133	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	LYS
1	B	144	MET
1	B	145	VAL
1	B	148	SER
1	B	150	VAL
1	B	153	LEU
1	B	159	GLU
1	B	168	PHE
1	B	169	ASP
1	B	172	LEU
1	B	176	VAL
1	B	187	ASN
1	B	189	VAL
1	B	190	VAL
1	B	199	LEU
1	B	201	ASP
1	B	202	ARG
1	B	204	LEU
1	B	209	VAL
2	C	3	LYS
2	C	11	THR
2	C	12	THR
2	C	13	ASN
2	C	16	VAL
2	C	18	VAL
2	C	19	LEU
2	C	23	GLU
2	C	34	ARG
2	C	36	THR
2	C	38	SER
2	C	39	VAL
2	C	42	PHE
2	C	49	VAL
2	C	62	ASN
2	C	66	SER
2	C	75	TYR
2	C	77	VAL
2	C	87	GLN
2	C	97	LEU
2	C	98	LYS
2	C	102	GLU
2	C	103	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	104	TYR
2	C	105	LEU
2	C	119	TYR
2	C	120	PHE
2	C	121	ASN
2	C	125	ARG
2	C	128	THR
2	C	133	ARG
2	C	141	ARG
2	C	144	ASN
2	C	155	LEU
2	C	156	ASP
2	C	164	LEU
2	C	165	VAL
2	C	166	TYR
2	C	168	LEU
2	C	172	THR
2	C	179	GLU
2	C	182	ASP
2	C	194	ASN
2	C	196	LEU
2	C	203	GLN
2	C	204	VAL
2	C	210	VAL
2	C	214	LYS
2	C	216	GLU
2	C	217	HIS
2	C	225	LYS
2	C	226	MET
2	C	229	GLN
2	C	231	LEU
2	C	237	LYS
2	C	242	LEU
2	C	245	VAL
2	C	252	LEU
2	C	254	PHE
2	C	259	GLU
2	C	269	LEU
2	C	271	ARG
2	C	281	LEU
2	C	282	VAL
2	C	283	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	291	GLN
2	C	293	LEU
2	C	298	LEU
2	C	323	LYS
2	C	324	ARG
2	C	325	GLU
2	C	326	LEU
2	C	334	VAL
2	C	338	GLU
2	C	347	GLN
2	C	355	VAL
2	C	361	LEU
2	C	362	ASP
2	C	363	VAL
2	C	366	LEU
2	C	372	THR
2	C	376	VAL
2	C	377	PHE
2	C	396	THR
2	C	400	ASP
2	C	403	THR
2	C	404	THR
2	C	405	VAL
2	C	409	VAL
2	C	416	MET
2	C	428	LEU
2	C	436	ARG
2	C	440	GLN
2	C	443	VAL
2	C	444	THR
2	C	446	ASP
2	C	453	VAL
2	C	455	VAL
2	C	456	ARG
2	C	460	LEU
2	C	466	GLN
2	C	467	SER
2	C	469	THR
2	C	471	LYS
2	C	480	GLU
2	C	483	ARG
2	C	484	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	487	GLU
2	C	490	GLU
2	C	496	ARG
2	C	497	LYS
2	C	500	GLU
2	C	504	LEU
2	C	505	ARG
2	D	1	MET
2	D	3	LYS
2	D	13	ASN
2	D	18	VAL
2	D	19	LEU
2	D	20	GLU
2	D	23	GLU
2	D	29	ASN
2	D	35	THR
2	D	40	VAL
2	D	42	PHE
2	D	44	ASN
2	D	46	GLU
2	D	49	VAL
2	D	56	GLN
2	D	63	THR
2	D	69	ARG
2	D	74	ASP
2	D	77	VAL
2	D	80	GLU
2	D	85	THR
2	D	87	GLN
2	D	94	LEU
2	D	105	LEU
2	D	109	VAL
2	D	120	PHE
2	D	121	ASN
2	D	130	ASP
2	D	144	ASN
2	D	151	LEU
2	D	153	TYR
2	D	155	LEU
2	D	157	LYS
2	D	160	ASP
2	D	164	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	165	VAL
2	D	166	TYR
2	D	168	LEU
2	D	172	THR
2	D	173	PHE
2	D	174	ASP
2	D	178	LEU
2	D	180	LEU
2	D	184	VAL
2	D	193	ASP
2	D	194	ASN
2	D	199	ASP
2	D	208	TYR
2	D	210	VAL
2	D	215	GLN
2	D	222	SER
2	D	225	LYS
2	D	231	LEU
2	D	245	VAL
2	D	246	THR
2	D	260	ASN
2	D	263	LEU
2	D	269	LEU
2	D	270	THR
2	D	274	PHE
2	D	277	LEU
2	D	280	HIS
2	D	286	MET
2	D	294	GLN
2	D	304	ASP
2	D	319	GLN
2	D	320	GLU
2	D	324	ARG
2	D	332	LYS
2	D	334	VAL
2	D	337	ASP
2	D	338	GLU
2	D	339	VAL
2	D	360	LEU
2	D	371	GLU
2	D	372	THR
2	D	376	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	380	LEU
2	D	389	THR
2	D	390	SER
2	D	395	PHE
2	D	410	LEU
2	D	416	MET
2	D	420	ASN
2	D	421	LYS
2	D	426	PHE
2	D	436	ARG
2	D	438	VAL
2	D	440	GLN
2	D	443	VAL
2	D	444	THR
2	D	446	ASP
2	D	450	ASN
2	D	453	VAL
2	D	456	ARG
2	D	459	ASP
2	D	464	LYS
2	D	465	GLU
2	D	467	SER
2	D	469	THR
2	D	472	SER
2	D	476	LEU
2	D	482	GLN
2	D	483	ARG
2	D	484	MET
2	D	487	GLU
2	D	489	GLU
2	D	491	ASN
2	D	495	ASP
2	D	497	LYS
2	D	504	LEU
1	E	61	LEU
1	E	65	LYS
1	E	70	GLU
1	E	72	GLU
1	E	75	LEU
1	E	79	GLU
1	E	83	LEU
1	E	84	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	89	PHE
1	E	92	PHE
1	E	97	ARG
1	F	61	LEU
1	F	67	GLN
1	F	70	GLU
1	F	74	LYS
1	F	75	LEU
1	F	81	ARG
1	F	82	TYR
1	F	83	LEU
1	F	85	LEU
1	F	86	TYR
1	F	90	GLU
1	F	94	ARG
1	F	96	THR
2	G	66	SER
2	G	77	VAL
2	G	82	LYS
2	G	87	GLN
2	G	100	TYR
2	G	105	LEU
2	G	121	ASN
2	G	147	THR
2	G	156	ASP
2	G	157	LYS
2	G	158	GLU
2	G	159	GLU
2	G	161	GLN
2	G	164	LEU
2	G	165	VAL
2	G	174	ASP
2	G	194	ASN
2	G	201	PHE
2	G	204	VAL
2	G	220	ASP
2	G	225	LYS
2	G	226	MET
2	G	242	LEU
2	G	246	THR
2	G	277	LEU
2	G	281	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	308	LEU
2	G	319	GLN
2	G	320	GLU
2	G	325	GLU
2	G	326	LEU
2	G	331	HIS
2	G	355	VAL
2	G	356	LYS
2	G	357	ASP
2	G	360	LEU
2	G	363	VAL
2	G	371	GLU
2	G	373	MET
2	G	378	THR
2	G	389	THR
2	G	393	GLN
2	G	395	PHE
2	G	396	THR
2	G	397	THR
2	G	400	ASP
2	G	401	ASN
2	G	403	THR
2	G	404	THR
2	G	408	HIS
2	G	414	ARG
2	G	422	SER
2	G	436	ARG
2	G	440	GLN
2	G	453	VAL
2	G	471	LYS
2	G	484	MET
2	G	489	GLU
2	G	491	ASN
2	G	493	GLU
2	G	497	LYS
2	G	498	ARG
2	G	500	GLU
2	G	505	ARG
2	G	507	GLU
2	H	1	MET
2	H	11	THR
2	H	15	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	16	VAL
2	H	18	VAL
2	H	19	LEU
2	H	23	GLU
2	H	73	THR
2	H	77	VAL
2	H	78	GLU
2	H	82	LYS
2	H	94	LEU
2	H	95	GLN
2	H	96	TYR
2	H	99	SER
2	H	100	TYR
2	H	104	TYR
2	H	105	LEU
2	H	109	VAL
2	H	111	ARG
2	H	113	VAL
2	H	116	VAL
2	H	119	TYR
2	H	121	ASN
2	H	122	ASP
2	H	124	GLN
2	H	125	ARG
2	H	128	THR
2	H	153	TYR
2	H	155	LEU
2	H	156	ASP
2	H	157	LYS
2	H	161	GLN
2	H	166	TYR
2	H	168	LEU
2	H	174	ASP
2	H	175	VAL
2	H	176	SER
2	H	185	PHE
2	H	193	ASP
2	H	194	ASN
2	H	195	HIS
2	H	203	GLN
2	H	285	THR
2	H	293	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	294	GLN
2	H	325	GLU
2	H	326	LEU
2	H	328	LYS
2	H	332	LYS
2	H	338	GLU
2	H	359	VAL
2	H	361	LEU
2	H	363	VAL
2	H	366	LEU
2	H	367	SER
2	H	368	LEU
2	H	376	VAL
2	H	378	THR
2	H	380	LEU
2	H	382	GLU
2	H	386	THR
2	H	389	THR
2	H	393	GLN
2	H	395	PHE
2	H	396	THR
2	H	401	ASN
2	H	403	THR
2	H	409	VAL
2	H	410	LEU
2	H	411	GLN
2	H	416	MET
2	H	420	ASN
2	H	425	ARG
2	H	436	ARG
2	H	443	VAL
2	H	444	THR
2	H	448	ASP
2	H	456	ARG
2	H	459	ASP
2	H	462	THR
2	H	464	LYS
2	H	465	GLU
2	H	469	THR
2	H	471	LYS
2	H	476	LEU
2	H	479	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	480	GLU
2	H	482	GLN
2	H	483	ARG
2	H	484	MET
2	H	486	LYS
2	H	496	ARG
2	H	497	LYS
2	H	498	ARG
2	H	503	GLU
2	H	504	LEU
2	H	506	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	98	GLN
1	A	109	GLN
1	A	121	ASN
1	A	178	GLN
1	A	213	GLN
1	B	67	GLN
1	B	98	GLN
1	B	173	HIS
1	B	178	GLN
1	B	187	ASN
2	C	13	ASN
2	C	70	HIS
2	C	87	GLN
2	C	161	GLN
2	C	195	HIS
2	C	212	GLN
2	C	249	GLN
2	C	264	HIS
2	C	347	GLN
2	C	401	ASN
2	C	466	GLN
2	D	29	ASN
2	D	62	ASN
2	D	161	GLN
2	D	260	ASN
2	D	280	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	319	GLN
2	D	408	HIS
2	D	420	ASN
2	D	466	GLN
2	D	491	ASN
1	E	80	HIS
2	G	70	HIS
2	G	124	GLN
2	G	203	GLN
2	G	215	GLN
2	G	217	HIS
2	G	280	HIS
2	G	319	GLN
2	G	384	ASN
2	G	393	GLN
2	G	401	ASN
2	G	411	GLN
2	G	491	ASN
2	H	87	GLN
2	H	95	GLN
2	H	144	ASN
2	H	195	HIS
2	H	203	GLN
2	H	212	GLN
2	H	347	GLN
2	H	384	ASN
2	H	420	ASN
2	H	450	ASN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	156/213 (73%)	-0.67	0 100 100	108, 165, 240, 281	0
1	B	154/213 (72%)	-0.62	0 100 100	108, 151, 213, 293	0
1	E	135/213 (63%)	0.27	9 (6%) 21 14	193, 261, 363, 476	0
1	F	130/213 (61%)	-0.01	0 100 100	185, 244, 324, 370	0
2	C	509/509 (100%)	-0.60	0 100 100	109, 152, 216, 283	0
2	D	509/509 (100%)	-0.61	0 100 100	109, 163, 217, 333	0
2	G	502/509 (98%)	0.01	34 (6%) 20 14	141, 283, 373, 481	0
2	H	501/509 (98%)	-0.21	14 (2%) 56 45	115, 237, 370, 516	0
All	All	2596/2888 (89%)	-0.34	57 (2%) 65 55	108, 193, 341, 516	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	205	ARG	10.6
1	E	206	PRO	10.0
2	H	225	LYS	6.1
2	G	320	GLU	6.1
2	H	245	VAL	5.4
1	E	207	ALA	4.4
2	H	207	ASP	4.3
1	E	175	ALA	4.2
2	H	202	ASP	4.1
2	G	55	ARG	4.0
2	G	50	GLY	3.9
2	G	192	GLY	3.7
2	G	54	LYS	3.5
2	G	14	SER	3.2
2	G	321	ALA	3.2
2	G	72	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	272	ALA	3.1
2	G	8	ASP	3.1
2	H	217	HIS	3.0
2	H	66	SER	3.0
2	G	74	ASP	3.0
2	G	197	GLY	2.9
2	G	190	THR	2.9
2	G	474	SER	2.9
2	G	319	GLN	2.7
2	G	216	GLU	2.7
2	G	6	GLY	2.7
2	G	51	GLU	2.7
2	H	314	ARG	2.7
2	G	53	ALA	2.6
2	H	226	MET	2.6
2	G	73	THR	2.6
1	E	137	SER	2.6
2	G	189	ALA	2.6
2	G	191	ALA	2.6
1	E	138	ILE	2.5
2	G	322	ILE	2.5
2	H	218	GLY	2.5
2	G	303	ILE	2.5
2	H	197	GLY	2.4
2	G	224	ASP	2.4
2	G	17	ALA	2.4
2	G	473	SER	2.3
2	G	332	LYS	2.3
2	G	63	THR	2.3
2	H	270	THR	2.3
2	G	331	HIS	2.3
2	G	57	ALA	2.3
2	G	329	GLU	2.3
2	G	472	SER	2.2
2	G	324	ARG	2.1
2	H	231	LEU	2.1
2	H	315	ILE	2.1
1	E	59	GLU	2.1
1	E	167	PRO	2.0
1	E	169	ASP	2.0
2	H	200	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.