Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:01 AM EDT

PDB ID	:	4GO3
Title	:	Crystal structure of PnpE from Pseudomonas sp. WBC-3
Authors	:	Su, J.; Zhang, C.; Liu, S.; Zhu, D.; Gu, L.
Deposited on	:	2012-08-18
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

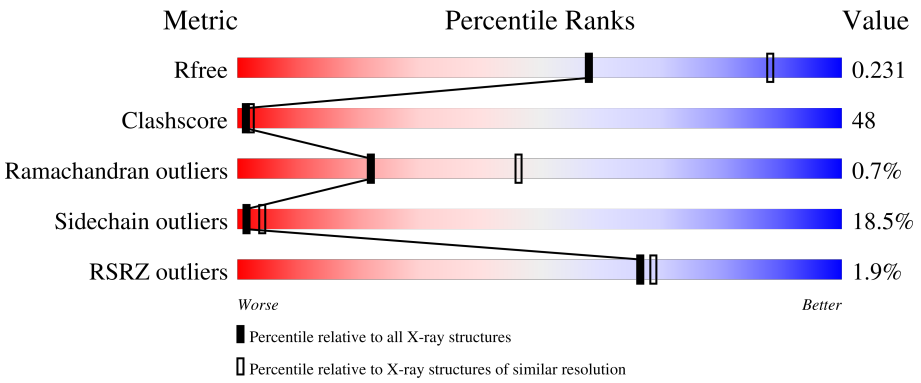
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	495	41% 47% 11% •
1	B	495	% 44% 42% 12% • •
1	C	495	44% 42% 12% •
1	D	495	% 44% 45% 10% •
1	E	495	2% 42% 44% 11% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	495	2% 36% 50% 12%
1	G	495	4% 36% 48% 13%
1	H	495	5% 44% 42% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29686 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 Putative gamma-hydroxymuconic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3685	2333	652	684	16	0	0	0
1	B	487	3692	2338	654	684	16	0	1	0
1	C	487	3691	2337	652	686	16	0	1	0
1	D	487	3685	2333	652	684	16	0	0	0
1	E	485	3665	2321	646	682	16	0	0	0
1	F	487	3685	2333	652	684	16	0	0	0
1	G	487	3685	2333	652	684	16	0	0	0
1	H	487	3685	2333	652	684	16	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	ASN	SER	engineered mutation	UNP C1I208
A	484	HIS	TYR	engineered mutation	UNP C1I208
A	488	LEU	-	expression tag	UNP C1I208
A	489	GLY	-	expression tag	UNP C1I208
A	490	HIS	-	expression tag	UNP C1I208
A	491	HIS	-	expression tag	UNP C1I208
A	492	HIS	-	expression tag	UNP C1I208
A	493	HIS	-	expression tag	UNP C1I208
A	494	HIS	-	expression tag	UNP C1I208
A	495	HIS	-	expression tag	UNP C1I208
B	426	ASN	SER	engineered mutation	UNP C1I208
B	484	HIS	TYR	engineered mutation	UNP C1I208
B	488	LEU	-	expression tag	UNP C1I208

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	489	GLY	-	expression tag	UNP C1I208
B	490	HIS	-	expression tag	UNP C1I208
B	491	HIS	-	expression tag	UNP C1I208
B	492	HIS	-	expression tag	UNP C1I208
B	493	HIS	-	expression tag	UNP C1I208
B	494	HIS	-	expression tag	UNP C1I208
B	495	HIS	-	expression tag	UNP C1I208
C	426	ASN	SER	engineered mutation	UNP C1I208
C	484	HIS	TYR	engineered mutation	UNP C1I208
C	488	LEU	-	expression tag	UNP C1I208
C	489	GLY	-	expression tag	UNP C1I208
C	490	HIS	-	expression tag	UNP C1I208
C	491	HIS	-	expression tag	UNP C1I208
C	492	HIS	-	expression tag	UNP C1I208
C	493	HIS	-	expression tag	UNP C1I208
C	494	HIS	-	expression tag	UNP C1I208
C	495	HIS	-	expression tag	UNP C1I208
D	426	ASN	SER	engineered mutation	UNP C1I208
D	484	HIS	TYR	engineered mutation	UNP C1I208
D	488	LEU	-	expression tag	UNP C1I208
D	489	GLY	-	expression tag	UNP C1I208
D	490	HIS	-	expression tag	UNP C1I208
D	491	HIS	-	expression tag	UNP C1I208
D	492	HIS	-	expression tag	UNP C1I208
D	493	HIS	-	expression tag	UNP C1I208
D	494	HIS	-	expression tag	UNP C1I208
D	495	HIS	-	expression tag	UNP C1I208
E	426	ASN	SER	engineered mutation	UNP C1I208
E	484	HIS	TYR	engineered mutation	UNP C1I208
E	488	LEU	-	expression tag	UNP C1I208
E	489	GLY	-	expression tag	UNP C1I208
E	490	HIS	-	expression tag	UNP C1I208
E	491	HIS	-	expression tag	UNP C1I208
E	492	HIS	-	expression tag	UNP C1I208
E	493	HIS	-	expression tag	UNP C1I208
E	494	HIS	-	expression tag	UNP C1I208
E	495	HIS	-	expression tag	UNP C1I208
F	426	ASN	SER	engineered mutation	UNP C1I208
F	484	HIS	TYR	engineered mutation	UNP C1I208
F	488	LEU	-	expression tag	UNP C1I208
F	489	GLY	-	expression tag	UNP C1I208
F	490	HIS	-	expression tag	UNP C1I208

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	491	HIS	-	expression tag	UNP C1I208
F	492	HIS	-	expression tag	UNP C1I208
F	493	HIS	-	expression tag	UNP C1I208
F	494	HIS	-	expression tag	UNP C1I208
F	495	HIS	-	expression tag	UNP C1I208
G	426	ASN	SER	engineered mutation	UNP C1I208
G	484	HIS	TYR	engineered mutation	UNP C1I208
G	488	LEU	-	expression tag	UNP C1I208
G	489	GLY	-	expression tag	UNP C1I208
G	490	HIS	-	expression tag	UNP C1I208
G	491	HIS	-	expression tag	UNP C1I208
G	492	HIS	-	expression tag	UNP C1I208
G	493	HIS	-	expression tag	UNP C1I208
G	494	HIS	-	expression tag	UNP C1I208
G	495	HIS	-	expression tag	UNP C1I208
H	426	ASN	SER	engineered mutation	UNP C1I208
H	484	HIS	TYR	engineered mutation	UNP C1I208
H	488	LEU	-	expression tag	UNP C1I208
H	489	GLY	-	expression tag	UNP C1I208
H	490	HIS	-	expression tag	UNP C1I208
H	491	HIS	-	expression tag	UNP C1I208
H	492	HIS	-	expression tag	UNP C1I208
H	493	HIS	-	expression tag	UNP C1I208
H	494	HIS	-	expression tag	UNP C1I208
H	495	HIS	-	expression tag	UNP C1I208

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	29	29	29	0	0
			Total	O		
2	B	29	29	29	0	0
			Total	O		
2	C	31	31	31	0	0
			Total	O		
2	D	24	24	24	0	0
			Total	O		
2	E	30	30	30	0	0
			Total	O		
2	F	34	34	34	0	0
			Total	O		
2	G	23	23	23	0	0

Continued on next page...

Continued from previous page...

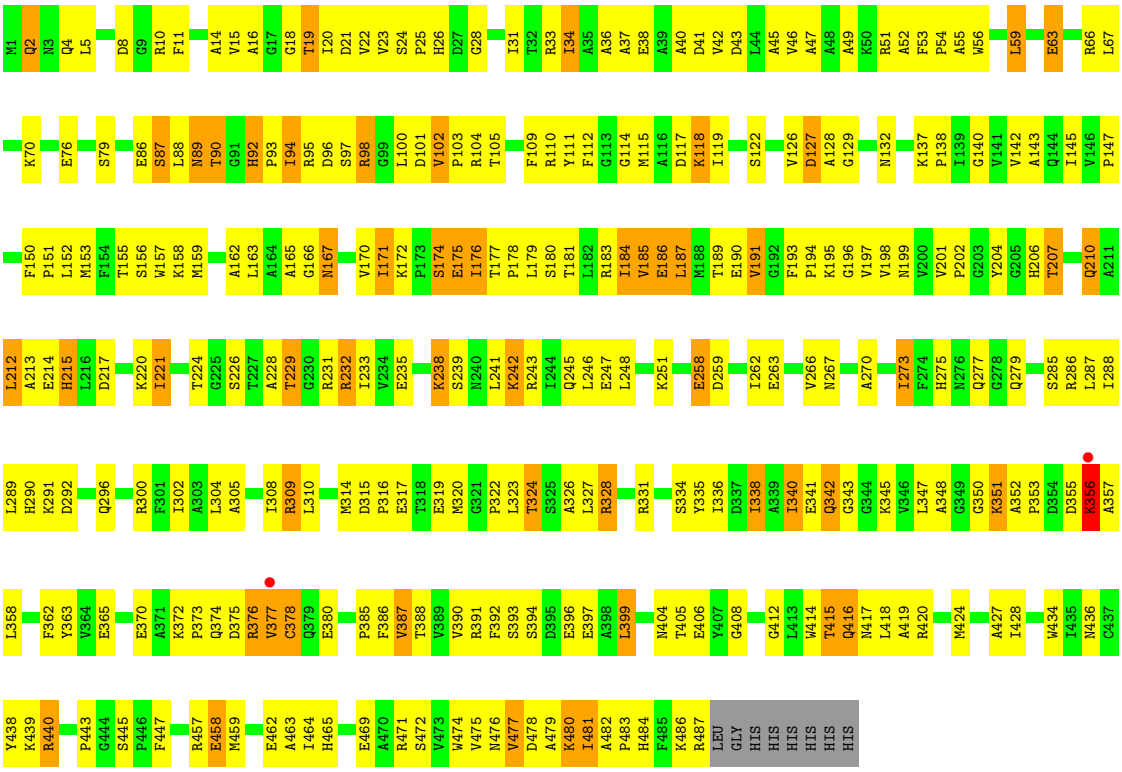
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	H	13	13	13	0	0

3 Residue-property plots (i)

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

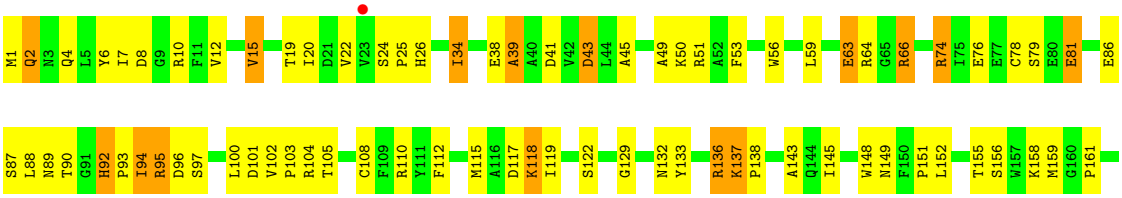
• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

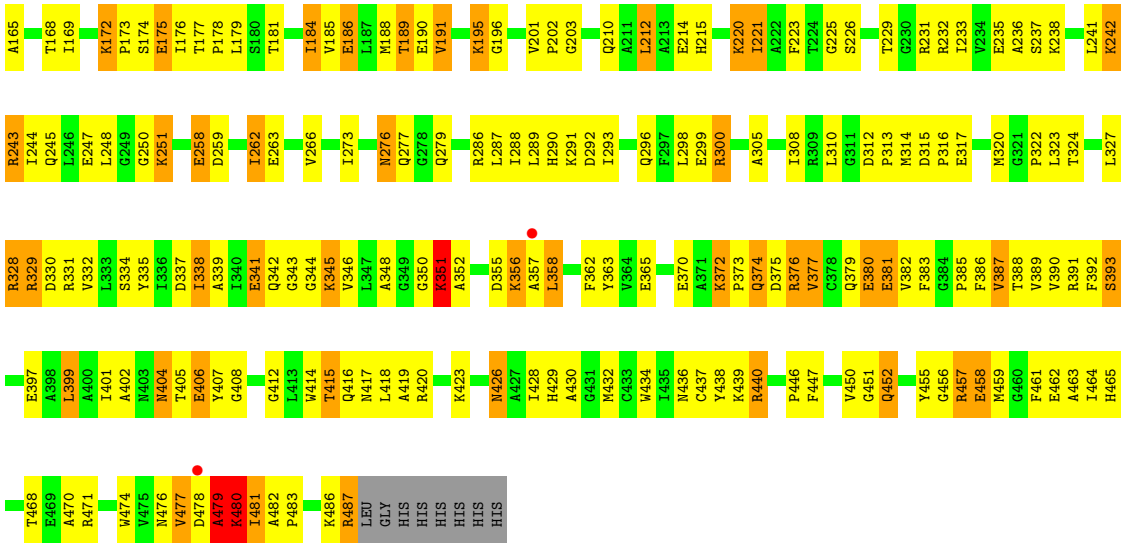
Chain A:



• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

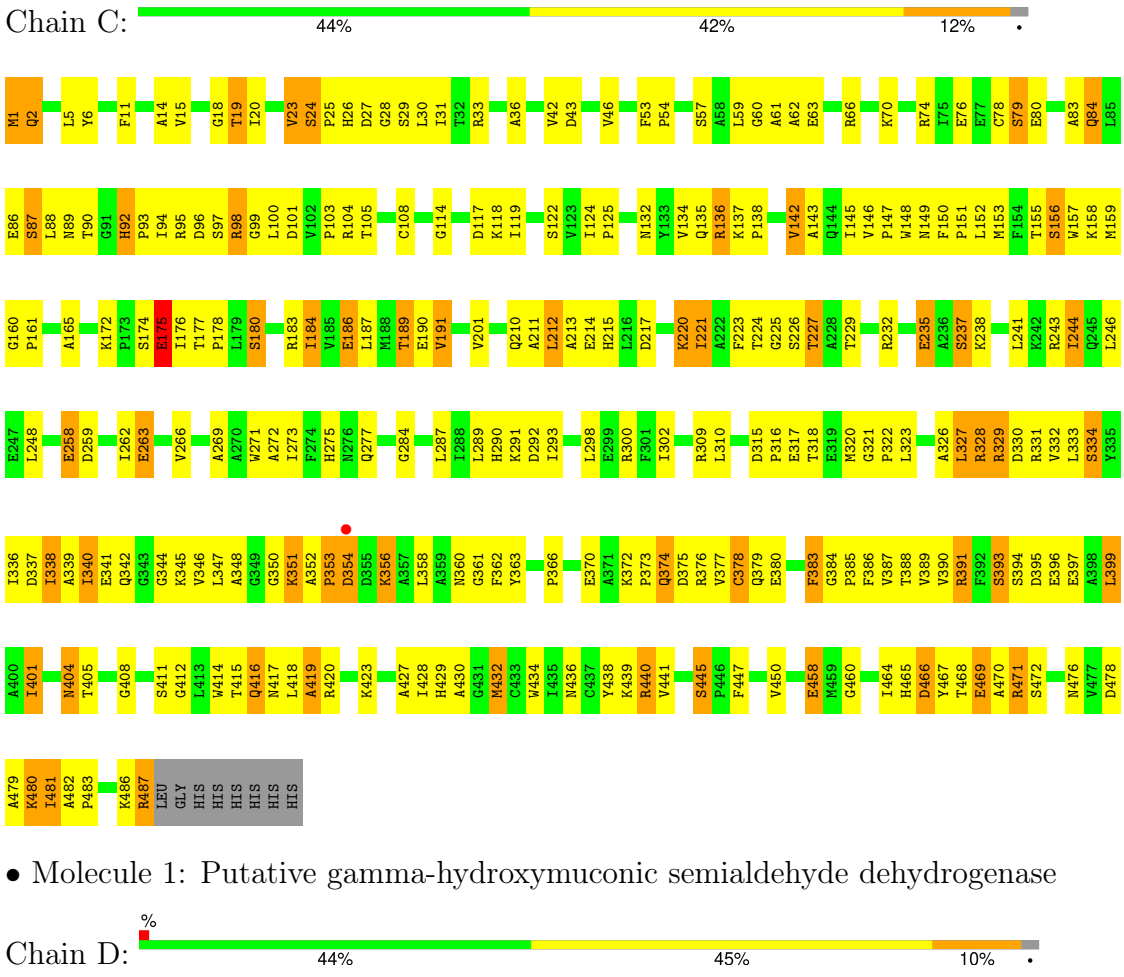
Chain B:





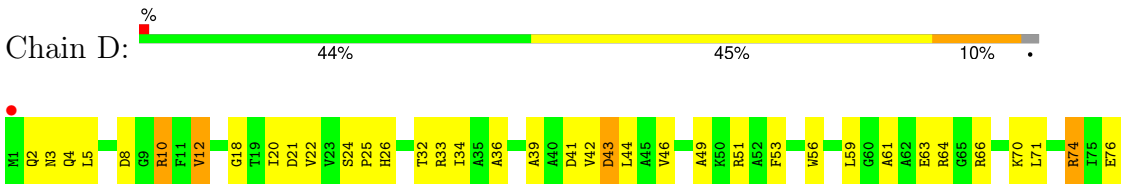
• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

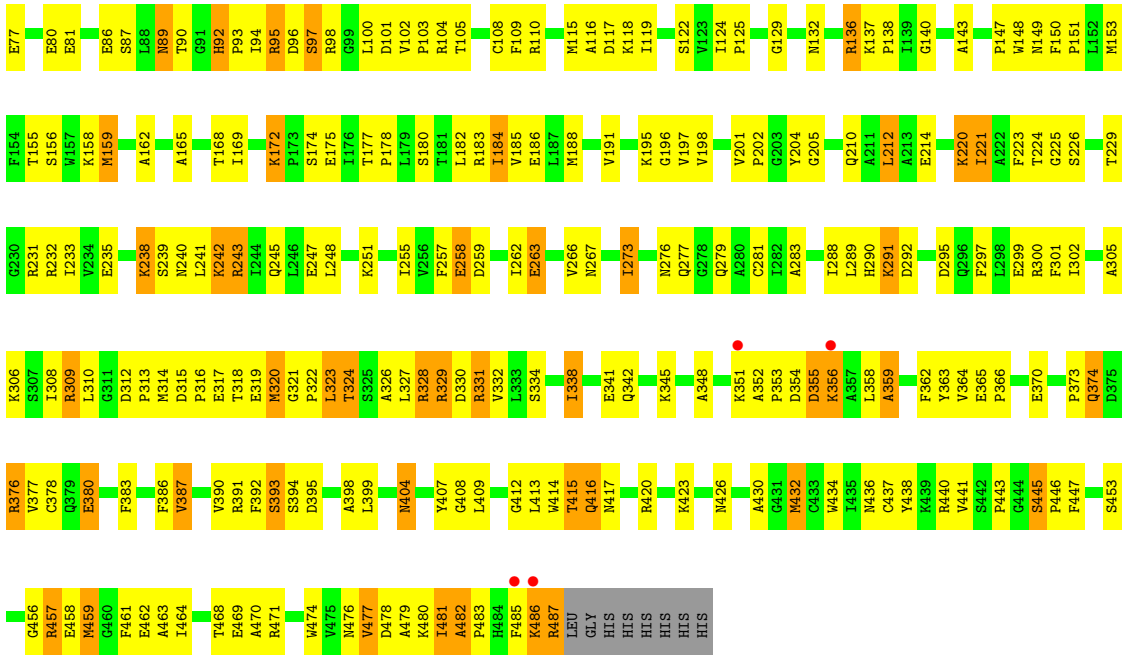
Chain C:



• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

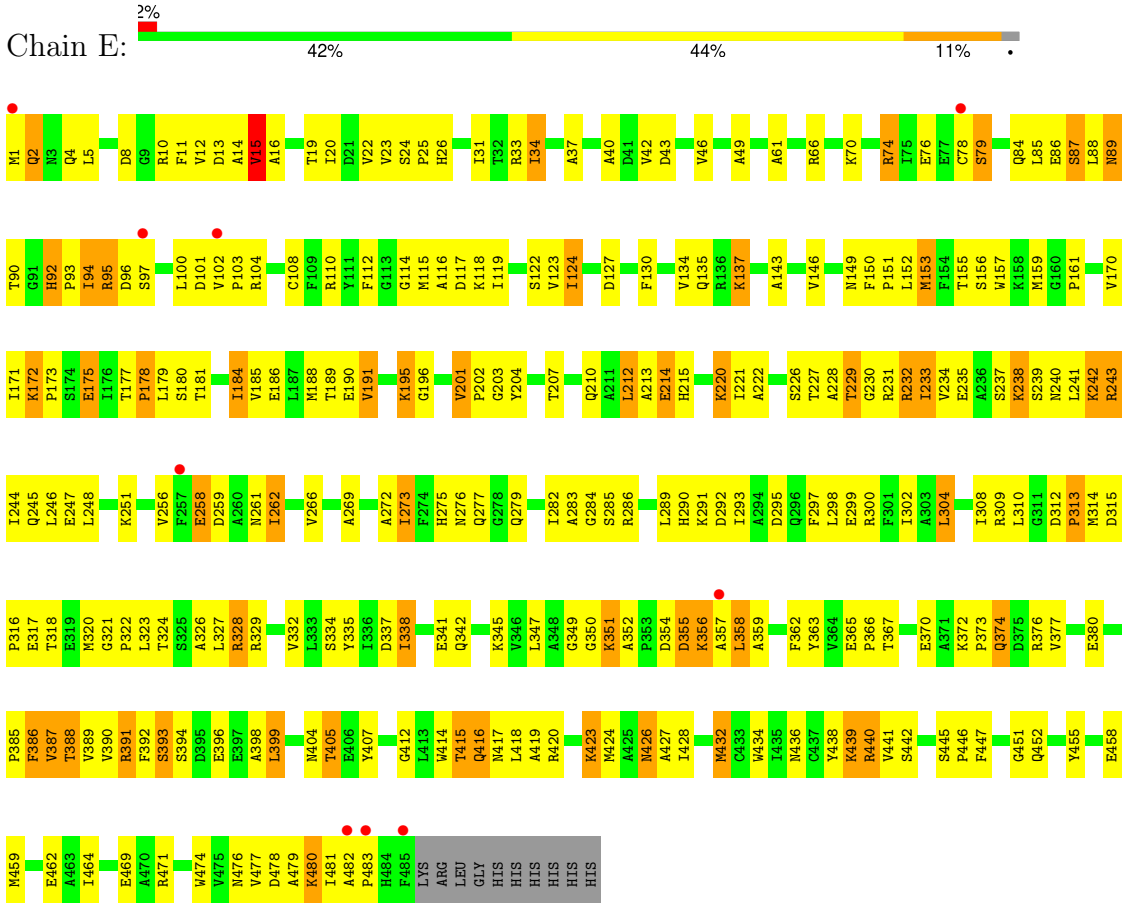
Chain D:





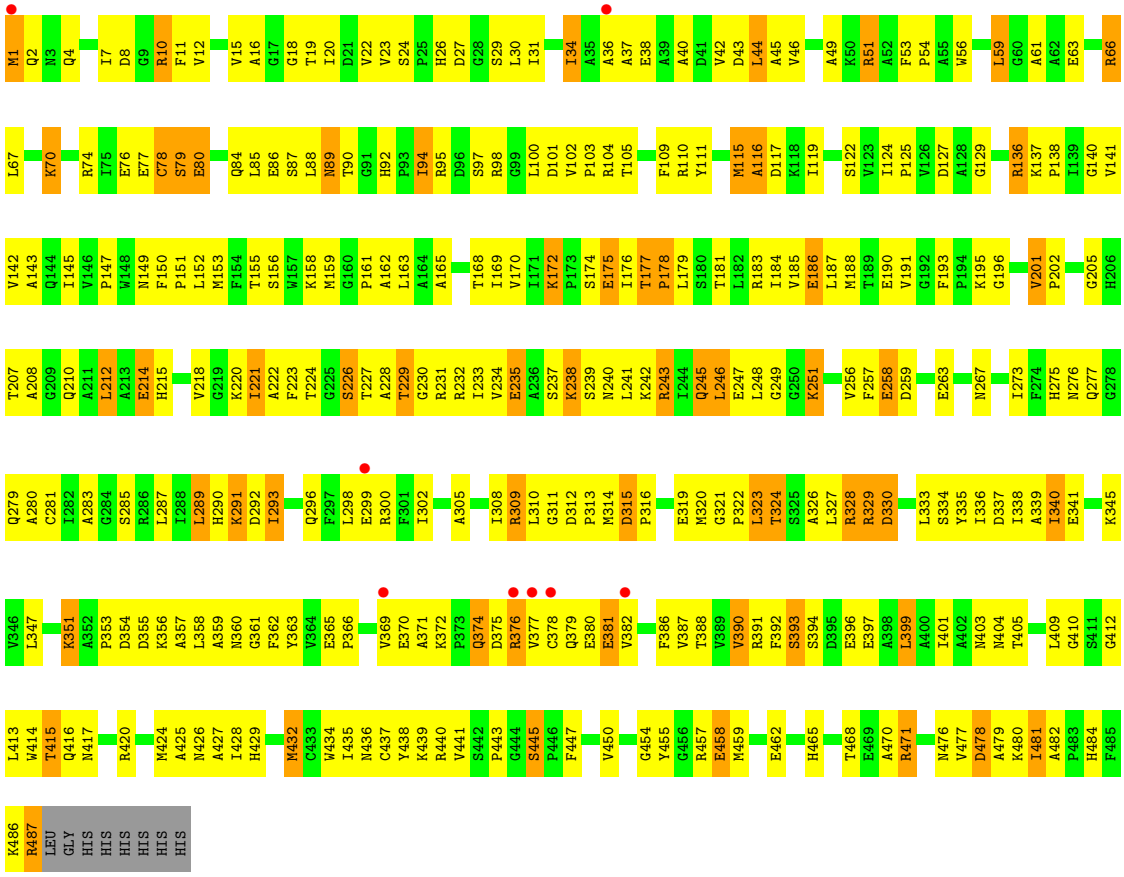
• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain E:



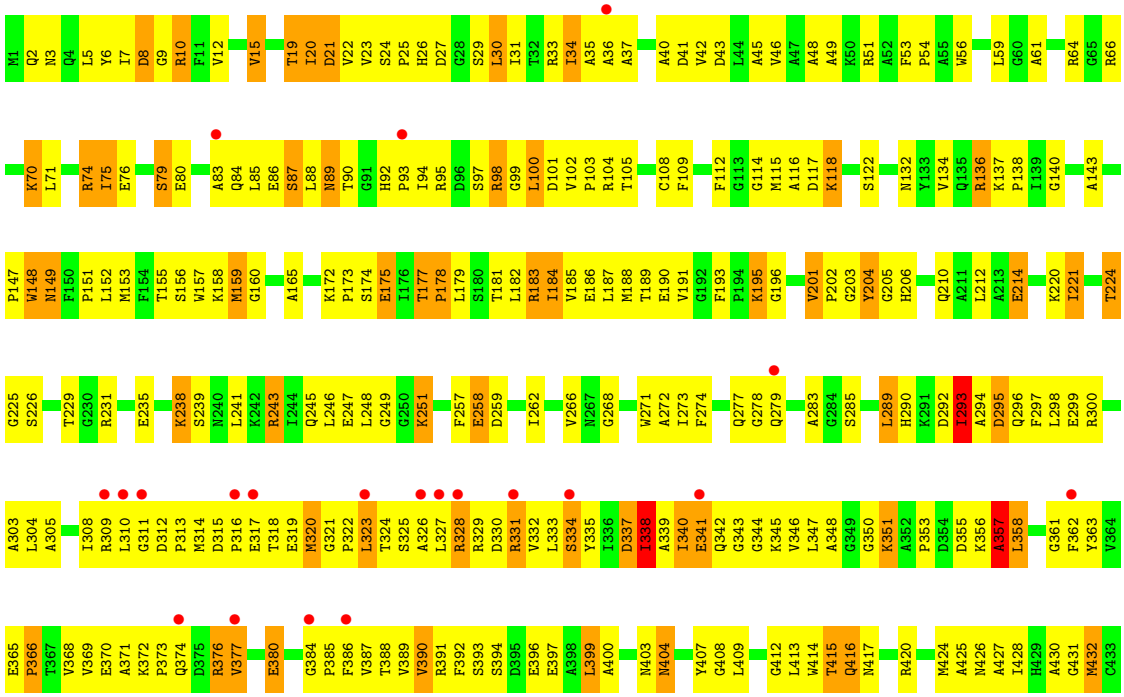
• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain F:



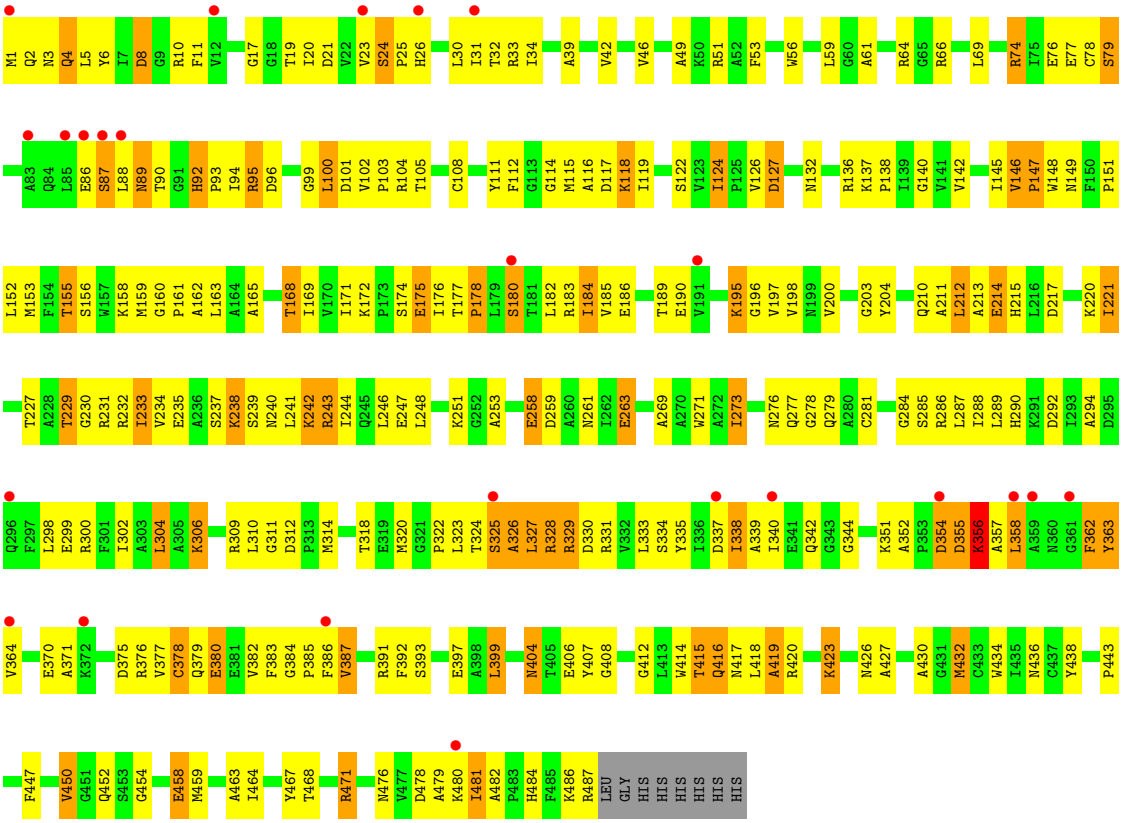
• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain G:



• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.53Å 144.25Å 138.29Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	41.68 – 2.70 50.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (41.68-2.70) 96.4 (50.03-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.223 , 0.237 0.218 , 0.231	Depositor DCC
R_{free} test set	4296 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	29686	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.97	2/3761 (0.1%)	0.68	1/5101 (0.0%)
1	B	0.95	1/3772 (0.0%)	0.72	4/5116 (0.1%)
1	C	1.01	2/3770 (0.1%)	0.70	0/5113
1	D	0.98	1/3761 (0.0%)	0.74	5/5101 (0.1%)
1	E	0.98	1/3741 (0.0%)	0.69	1/5076 (0.0%)
1	F	0.90	1/3761 (0.0%)	0.76	7/5101 (0.1%)
1	G	0.90	1/3761 (0.0%)	0.85	8/5101 (0.2%)
1	H	0.92	3/3761 (0.1%)	0.69	1/5101 (0.0%)
All	All	0.95	12/30088 (0.0%)	0.73	27/40810 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	G	0	1
All	All	0	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	CYS	CB-SG	-10.06	1.65	1.82
1	E	78	CYS	CB-SG	-10.06	1.65	1.82
1	H	78	CYS	CB-SG	-10.06	1.65	1.82
1	F	78	CYS	CB-SG	-10.05	1.65	1.82
1	D	378	CYS	CB-SG	-5.91	1.72	1.81
1	H	378	CYS	CB-SG	-5.28	1.73	1.81
1	A	378	CYS	CB-SG	-5.27	1.73	1.81
1	B	186	GLU	CD-OE2	-5.09	1.20	1.25
1	A	186	GLU	CD-OE2	-5.07	1.20	1.25
1	C	186	GLU	CD-OE2	-5.03	1.20	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	204	TYR	CD1-CE1	-5.01	1.31	1.39
1	G	204	TYR	CD1-CE1	-5.00	1.31	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	482	ALA	CB-CA-C	16.20	134.40	110.10
1	B	479	ALA	CB-CA-C	13.03	129.65	110.10
1	G	477	VAL	CB-CA-C	13.02	136.14	111.40
1	G	315	ASP	CB-CA-C	11.93	134.27	110.40
1	F	115	MET	CB-CA-C	-10.98	88.44	110.40
1	G	315	ASP	N-CA-C	-9.19	86.18	111.00
1	B	480	LYS	C-N-CA	8.99	144.19	121.70
1	G	357	ALA	CB-CA-C	8.88	123.42	110.10
1	F	462	GLU	CB-CA-C	-8.28	93.84	110.40
1	F	116	ALA	CB-CA-C	-8.07	98.00	110.10
1	H	326	ALA	CB-CA-C	-8.02	98.08	110.10
1	G	83	ALA	CB-CA-C	-7.88	98.28	110.10
1	D	355	ASP	CB-CA-C	7.35	125.11	110.40
1	B	39	ALA	CB-CA-C	-7.29	99.17	110.10
1	A	340	ILE	CB-CA-C	-6.76	98.08	111.60
1	E	15	VAL	CB-CA-C	-6.27	99.48	111.40
1	D	359	ALA	CB-CA-C	6.26	119.49	110.10
1	D	356	LYS	CB-CA-C	-6.24	97.91	110.40
1	F	462	GLU	N-CA-C	6.23	127.82	111.00
1	D	481	ILE	CB-CA-C	-6.05	99.49	111.60
1	F	315	ASP	N-CA-C	-5.58	95.93	111.00
1	B	480	LYS	CB-CA-C	5.50	121.40	110.40
1	G	224	THR	N-CA-C	-5.49	96.18	111.00
1	G	100	LEU	CB-CA-C	-5.33	100.07	110.20
1	F	246	LEU	CA-CB-CG	5.16	127.17	115.30
1	F	177	THR	C-N-CD	-5.16	109.25	120.60
1	G	295	ASP	CB-CA-C	-5.10	100.20	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	479	ALA	Peptide
1	B	480	LYS	Peptide
1	G	477	VAL	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	3685	0	3676	346	4
1	B	3692	0	3683	426	18
1	C	3691	0	3680	326	2
1	D	3685	0	3678	304	2
1	E	3665	0	3651	373	2
1	F	3685	0	3677	419	10
1	G	3685	0	3678	455	0
1	H	3685	0	3675	336	15
2	A	29	0	0	19	1
2	B	29	0	0	32	0
2	C	31	0	0	34	0
2	D	24	0	0	15	0
2	E	30	0	0	30	0
2	F	34	0	0	21	0
2	G	23	0	0	28	0
2	H	13	0	0	11	0
All	All	29686	0	29398	2820	27

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 48.

All (2820) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:263:GLU:CG	1:H:300:ARG:NH2	1.68	1.51
1:G:10:ARG:NH1	1:G:12:VAL:CG1	1.73	1.50
1:B:479:ALA:HB1	1:B:480:LYS:CB	1.44	1.47
1:B:479:ALA:HB1	1:B:480:LYS:CG	1.43	1.46
1:B:238:LYS:CE	1:F:235:GLU:HG2	1.50	1.41
1:A:159:MET:CE	1:A:198:VAL:HG11	1.47	1.41
1:B:238:LYS:NZ	1:F:235:GLU:HG2	1.31	1.37
1:H:49:ALA:HB1	1:H:168:THR:CG2	1.55	1.37
1:B:238:LYS:NZ	1:F:235:GLU:CG	1.87	1.36
1:A:159:MET:CE	1:A:198:VAL:CG1	2.01	1.36
1:E:74:ARG:NH2	1:E:190:GLU:OE1	1.56	1.35

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:329:ARG:CD	1:H:330:ASP:OD1	1.75	1.34
1:A:97:SER:O	1:A:102:VAL:CG2	1.77	1.33
1:A:376:ARG:HD3	1:A:380:GLU:OE2	1.21	1.31
1:A:235:GLU:HB3	1:C:238:LYS:CE	1.60	1.31
1:C:440:ARG:HA	2:C:530:HOH:O	1.33	1.27
1:A:94:ILE:O	1:A:98:ARG:HG3	1.33	1.26
1:H:263:GLU:HG3	1:H:300:ARG:NH2	1.31	1.25
1:E:376:ARG:HD2	1:E:380:GLU:OE2	1.32	1.25
1:E:291:LYS:HE2	1:E:393:SER:OG	1.09	1.25
1:B:238:LYS:HZ3	1:F:235:GLU:CG	1.42	1.24
1:H:229:THR:HG23	1:H:232:ARG:NH2	1.51	1.24
1:H:87:SER:OG	1:H:92:HIS:O	1.55	1.23
1:H:329:ARG:HD2	1:H:330:ASP:OD1	1.18	1.23
1:D:273:ILE:HD12	1:D:273:ILE:O	1.37	1.22
1:G:338:ILE:HD12	1:G:338:ILE:C	1.54	1.22
1:A:97:SER:O	1:A:102:VAL:HG23	1.06	1.22
1:F:273:ILE:HG12	1:F:387:VAL:CG2	1.69	1.22
1:F:326:ALA:O	1:F:330:ASP:OD1	1.57	1.22
1:F:181:THR:O	1:F:184:ILE:HG22	1.37	1.21
1:G:10:ARG:NH1	1:G:12:VAL:HG11	0.90	1.21
1:A:183:ARG:NH1	1:A:186:GLU:OE1	1.73	1.21
1:H:263:GLU:HG2	1:H:300:ARG:NH2	1.39	1.21
1:D:210:GLN:O	1:D:214:GLU:HG2	1.39	1.20
1:D:259:ASP:OD1	1:D:415:THR:CG2	1.88	1.20
1:E:231:ARG:NH2	1:H:239:SER:O	1.75	1.19
1:F:338:ILE:HD11	1:F:376:ARG:NE	1.57	1.19
1:B:479:ALA:CB	1:B:480:LYS:HB3	1.70	1.19
1:A:217:ASP:OD2	1:B:374:GLN:NE2	1.77	1.18
1:B:238:LYS:CE	1:F:235:GLU:CG	2.21	1.17
1:B:238:LYS:NZ	1:F:235:GLU:CD	1.98	1.17
1:G:347:LEU:HD11	1:G:370:GLU:HG3	1.25	1.16
1:E:273:ILE:O	1:E:273:ILE:HD12	1.46	1.16
1:F:377:VAL:CG1	1:F:388:THR:HG21	1.76	1.16
1:D:323:LEU:HD23	1:D:323:LEU:N	1.53	1.15
1:G:350:GLY:O	1:G:351:LYS:HG2	1.46	1.15
1:B:132:ASN:ND2	1:F:445:SER:OG	1.79	1.15
1:A:210:GLN:O	1:A:214:GLU:HG2	1.44	1.15
1:G:481:ILE:N	1:G:481:ILE:HD12	1.58	1.14
1:D:259:ASP:OD1	1:D:415:THR:HG22	0.98	1.14
1:G:251:LYS:HB2	1:G:407:TYR:CD1	1.81	1.14
1:E:291:LYS:CE	1:E:393:SER:OG	1.95	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:VAL:HG12	1:E:16:ALA:N	1.47	1.13
1:B:405:THR:CG2	1:B:407:TYR:H	1.59	1.13
1:C:408:GLY:O	1:C:430:ALA:HA	1.49	1.13
1:G:293:ILE:HD12	1:G:293:ILE:C	1.61	1.13
1:G:310:LEU:HD12	1:G:320:MET:HG2	1.19	1.12
1:H:49:ALA:HB1	1:H:168:THR:HG22	1.21	1.12
1:H:328:ARG:HH11	1:H:328:ARG:CG	1.59	1.12
1:A:86:GLU:O	1:A:90:THR:OG1	1.66	1.12
1:A:159:MET:HE1	1:A:198:VAL:CG1	1.66	1.12
1:A:221:ILE:HD12	1:A:233:ILE:HG23	1.28	1.12
1:B:351:LYS:HG3	1:B:352:ALA:H	1.09	1.12
1:B:426:ASN:O	1:F:137:LYS:NZ	1.82	1.12
1:B:405:THR:HG22	1:B:407:TYR:N	1.63	1.12
1:C:2:GLN:HA	1:C:2:GLN:HE21	1.06	1.12
1:A:376:ARG:CD	1:A:380:GLU:OE2	1.97	1.12
1:A:21:ASP:OD1	1:A:33:ARG:HD3	1.50	1.11
1:E:235:GLU:O	1:E:238:LYS:HD3	1.49	1.11
1:F:183:ARG:NH1	1:F:186:GLU:OE1	1.82	1.11
1:A:132:ASN:ND2	1:C:445:SER:OG	1.84	1.11
1:F:38:GLU:HA	1:F:207:THR:HG22	1.30	1.11
1:H:328:ARG:NH1	1:H:328:ARG:HG2	1.47	1.11
1:E:110:ARG:NH2	2:E:517:HOH:O	1.84	1.11
1:D:415:THR:HG21	1:D:420:ARG:HH11	1.12	1.10
1:C:2:GLN:HA	1:C:2:GLN:NE2	1.57	1.10
1:C:262:ILE:O	1:C:266:VAL:HG23	1.50	1.10
1:F:61:ALA:HB1	1:F:116:ALA:O	1.52	1.10
1:F:273:ILE:CG1	1:F:387:VAL:HG22	1.80	1.10
1:F:471:ARG:NH2	2:F:531:HOH:O	1.82	1.10
1:G:3:ASN:ND2	1:G:33:ARG:O	1.83	1.10
1:H:99:GLY:C	1:H:100:LEU:HD23	1.72	1.10
1:F:338:ILE:CD1	1:F:376:ARG:HE	1.65	1.10
1:G:357:ALA:C	1:G:358:LEU:HD12	1.72	1.10
1:H:338:ILE:O	1:H:338:ILE:HD13	1.50	1.10
1:H:329:ARG:HG3	1:H:329:ARG:HH11	0.99	1.09
1:G:363:TYR:N	2:G:519:HOH:O	1.84	1.09
1:D:115:MET:HE1	1:D:461:PHE:CE1	1.87	1.09
1:D:10:ARG:HG2	1:D:10:ARG:HH11	1.03	1.09
1:D:137:LYS:NZ	1:G:426:ASN:ND2	1.99	1.09
1:G:87:SER:HB2	1:G:94:ILE:CD1	1.82	1.09
1:B:479:ALA:CB	1:B:480:LYS:CB	2.30	1.08
1:F:38:GLU:HA	1:F:207:THR:CG2	1.81	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:464:ILE:O	1:H:468:THR:HG23	1.52	1.08
1:G:183:ARG:HD2	1:G:183:ARG:O	1.52	1.08
1:B:479:ALA:CB	1:B:480:LYS:CG	2.30	1.08
1:B:479:ALA:HB1	1:B:480:LYS:HB3	1.13	1.08
1:E:159:MET:HE1	1:E:171:ILE:HD13	1.25	1.08
1:G:338:ILE:HD12	1:G:338:ILE:O	1.53	1.08
1:F:234:VAL:O	1:F:237:SER:OG	1.67	1.08
1:A:484:HIS:O	1:C:95:ARG:NH2	1.87	1.07
1:H:8:ASP:OD2	1:H:51:ARG:NH2	1.86	1.07
1:E:239:SER:O	1:H:231:ARG:NH2	1.87	1.07
1:G:327:LEU:CD2	1:G:331:ARG:HD2	1.84	1.07
1:D:351:LYS:CG	1:D:352:ALA:H	1.68	1.07
1:G:251:LYS:HB2	1:G:407:TYR:HD1	0.91	1.07
1:B:100:LEU:O	1:B:104:ARG:HG3	1.55	1.06
1:F:210:GLN:O	1:F:214:GLU:HG3	1.56	1.06
1:G:335:TYR:O	1:G:339:ALA:HB2	1.55	1.06
1:F:210:GLN:O	1:F:214:GLU:CG	2.03	1.05
1:H:351:LYS:HG3	1:H:352:ALA:H	1.20	1.05
1:G:10:ARG:HH11	1:G:12:VAL:CG1	1.47	1.05
1:E:104:ARG:NE	1:E:153:MET:CE	2.20	1.05
1:A:235:GLU:CB	1:C:238:LYS:HE3	1.86	1.05
1:B:238:LYS:HZ2	1:F:235:GLU:CD	1.57	1.04
1:B:329:ARG:HH11	1:B:329:ARG:HG3	1.15	1.04
1:A:235:GLU:HB3	1:C:238:LYS:HE3	1.07	1.04
1:A:481:ILE:HG13	1:A:482:ALA:N	1.67	1.04
1:G:376:ARG:HH11	1:G:376:ARG:CG	1.70	1.04
1:C:302:ILE:CD1	1:C:347:LEU:HB3	1.87	1.04
1:G:201:VAL:O	1:G:201:VAL:HG13	1.57	1.04
1:G:376:ARG:HH11	1:G:376:ARG:HG3	0.90	1.04
1:A:43:ASP:OD1	1:B:374:GLN:HG2	1.54	1.04
1:A:159:MET:HE3	1:A:198:VAL:CG1	1.83	1.04
1:A:462:GLU:OE1	1:C:136:ARG:NH2	1.89	1.04
1:A:42:VAL:O	1:A:46:VAL:HG23	1.56	1.03
1:H:481:ILE:HD12	1:H:482:ALA:H	1.23	1.03
1:A:221:ILE:CD1	1:A:233:ILE:CG2	2.36	1.03
1:A:159:MET:CE	1:A:198:VAL:HG13	1.85	1.03
1:B:136:ARG:NH2	2:B:514:HOH:O	1.89	1.03
1:F:443:PRO:HA	1:F:459:MET:CE	1.88	1.02
1:F:481:ILE:HD12	1:F:482:ALA:H	1.22	1.02
1:G:25:PRO:HD2	2:G:512:HOH:O	1.59	1.02
1:A:55:ALA:C	2:A:525:HOH:O	1.95	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:ILE:HD11	1:C:347:LEU:HB3	1.39	1.02
1:A:158:LYS:HD3	1:A:458:GLU:OE2	1.60	1.02
1:A:258:GLU:HB3	1:A:290:HIS:CD2	1.93	1.02
1:D:309:ARG:HG2	1:D:309:ARG:NH1	1.59	1.02
1:F:94:ILE:O	1:F:98:ARG:HG3	1.58	1.02
1:B:401:ILE:O	1:B:404:ASN:HB3	1.60	1.02
1:H:281:CYS:SG	2:H:503:HOH:O	2.17	1.02
1:A:232:ARG:HA	1:A:235:GLU:CG	1.89	1.01
1:D:132:ASN:ND2	1:G:445:SER:OG	1.92	1.01
1:D:351:LYS:HG3	1:D:352:ALA:H	1.21	1.01
1:E:15:VAL:CG1	1:E:16:ALA:N	2.16	1.01
1:F:338:ILE:HD11	1:F:376:ARG:HE	0.86	1.01
1:G:90:THR:O	1:G:324:THR:HG22	1.59	1.01
1:G:376:ARG:HG3	1:G:376:ARG:NH1	1.64	1.01
1:F:377:VAL:HG12	1:F:388:THR:HG21	1.39	1.01
1:A:232:ARG:CA	1:A:235:GLU:HG2	1.90	1.01
1:G:481:ILE:H	1:G:481:ILE:CD1	1.69	1.01
1:D:137:LYS:HZ1	1:G:426:ASN:ND2	1.54	1.01
1:G:151:PRO:CG	1:G:177:THR:OG1	2.08	1.01
1:G:10:ARG:HH12	1:G:12:VAL:CG1	1.53	1.00
1:H:259:ASP:OD1	1:H:415:THR:HG22	1.58	1.00
1:C:432:MET:CE	1:C:447:PHE:CD1	2.44	1.00
1:H:49:ALA:CB	1:H:168:THR:CG2	2.39	1.00
1:G:322:PRO:HG3	1:G:363:TYR:CZ	1.96	1.00
1:B:152:LEU:CD1	1:B:184:ILE:CD1	2.39	1.00
1:C:302:ILE:HD11	1:C:347:LEU:CB	1.91	1.00
1:F:86:GLU:O	1:F:90:THR:OG1	1.80	1.00
1:B:439:LYS:NZ	2:B:501:HOH:O	1.93	0.99
1:B:479:ALA:HB1	1:B:480:LYS:HG2	1.41	0.99
1:H:273:ILE:HD13	1:H:285:SER:HA	1.41	0.99
1:B:2:GLN:HE21	1:B:2:GLN:HA	1.24	0.99
1:F:339:ALA:HB2	1:F:377:VAL:HG21	1.39	0.99
1:B:238:LYS:HE2	1:F:235:GLU:HG2	1.39	0.99
1:D:309:ARG:HH11	1:D:309:ARG:CG	1.74	0.99
1:G:373:PRO:HG2	1:G:374:GLN:OE1	1.60	0.99
1:G:362:PHE:C	2:G:519:HOH:O	2.01	0.98
1:A:221:ILE:HD12	1:A:233:ILE:CG2	1.92	0.98
1:F:210:GLN:NE2	2:F:527:HOH:O	1.97	0.98
1:G:293:ILE:C	1:G:293:ILE:CD1	2.30	0.98
1:A:232:ARG:HA	1:A:235:GLU:HG2	0.99	0.98
1:A:251:LYS:NZ	2:A:524:HOH:O	1.95	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ILE:HD13	1:G:314:MET:CE	1.94	0.98
1:G:309:ARG:NH1	1:G:317:GLU:HB3	1.77	0.98
1:C:26:HIS:O	1:C:361:GLY:HA3	1.62	0.98
1:G:358:LEU:HD12	1:G:358:LEU:N	1.78	0.98
1:D:188:MET:HE1	1:D:198:VAL:HG11	1.45	0.98
1:D:309:ARG:HG2	1:D:309:ARG:HH11	0.82	0.98
1:F:415:THR:HG21	1:F:420:ARG:HD2	1.43	0.98
1:A:94:ILE:O	1:A:98:ARG:CG	2.11	0.98
1:E:42:VAL:HG13	1:E:212:LEU:HD13	1.44	0.98
1:D:8:ASP:OD2	1:D:51:ARG:NH2	1.95	0.97
1:F:115:MET:O	1:F:115:MET:HG3	1.64	0.97
1:B:405:THR:HG22	1:B:407:TYR:H	0.81	0.97
1:D:328:ARG:HH11	1:D:383:PHE:HB3	1.28	0.97
1:A:100:LEU:O	1:A:104:ARG:HG3	1.65	0.97
1:G:481:ILE:HD12	1:G:481:ILE:H	0.81	0.97
1:H:102:VAL:HG22	1:H:152:LEU:HD21	1.45	0.97
1:B:74:ARG:NH2	2:B:525:HOH:O	1.97	0.97
1:C:6:TYR:OH	1:C:189:THR:HG21	1.63	0.97
1:G:373:PRO:HD2	1:G:374:GLN:OE1	1.63	0.97
1:B:238:LYS:CD	1:F:235:GLU:HG3	1.93	0.97
1:B:238:LYS:HD3	1:F:235:GLU:HG3	1.47	0.97
1:E:226:SER:OG	1:E:229:THR:HG22	1.64	0.97
1:F:26:HIS:O	1:F:361:GLY:HA3	1.65	0.97
1:C:375:ASP:OD2	2:C:507:HOH:O	1.83	0.97
1:G:408:GLY:O	1:G:430:ALA:HA	1.65	0.97
1:G:322:PRO:HB3	2:G:519:HOH:O	1.65	0.96
1:A:47:ALA:HB2	1:B:374:GLN:HB2	1.44	0.96
1:A:159:MET:HE3	1:A:198:VAL:HG13	1.43	0.96
1:C:153:MET:O	1:C:156:SER:OG	1.84	0.96
1:C:23:VAL:HG12	1:C:29:SER:O	1.64	0.96
1:H:328:ARG:HH11	1:H:328:ARG:HG2	0.81	0.96
1:D:309:ARG:HD3	1:D:319:GLU:OE1	1.62	0.96
1:D:329:ARG:NH2	1:D:330:ASP:OD1	1.99	0.96
1:H:240:ASN:OD1	2:H:506:HOH:O	1.84	0.96
1:B:95:ARG:NH2	1:F:484:HIS:O	1.99	0.96
1:E:478:ASP:N	2:E:514:HOH:O	1.97	0.96
1:A:132:ASN:ND2	1:C:445:SER:HG	1.59	0.96
1:C:190:GLU:OE2	2:C:516:HOH:O	1.84	0.96
1:E:476:ASN:O	2:E:508:HOH:O	1.82	0.96
1:F:481:ILE:HD12	1:F:482:ALA:N	1.80	0.96
1:B:381:GLU:OE1	2:B:527:HOH:O	1.81	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ARG:NH2	1:G:484:HIS:O	1.99	0.95
1:E:479:ALA:O	1:E:480:LYS:HD3	1.66	0.95
1:F:201:VAL:O	1:F:201:VAL:HG12	1.65	0.95
1:G:273:ILE:HD13	1:G:285:SER:HA	1.47	0.95
1:D:93:PRO:O	1:D:96:ASP:HB2	1.64	0.95
1:E:97:SER:HA	1:E:101:ASP:HB2	1.46	0.95
1:F:26:HIS:O	1:F:361:GLY:CA	2.13	0.95
1:G:322:PRO:HG3	1:G:363:TYR:CE1	2.00	0.95
1:G:278:GLY:HA3	1:G:384:GLY:O	1.65	0.95
1:G:37:ALA:CB	1:G:201:VAL:HG22	1.97	0.95
1:B:137:LYS:HG3	1:B:471:ARG:HG3	1.49	0.95
1:B:22:VAL:CG2	1:B:34:ILE:CG2	2.44	0.95
1:D:426:ASN:OD1	1:G:137:LYS:NZ	1.99	0.94
1:B:152:LEU:HD11	1:B:184:ILE:HD11	1.48	0.94
1:C:2:GLN:NE2	2:C:521:HOH:O	1.99	0.94
1:F:335:TYR:OH	1:F:380:GLU:OE1	1.84	0.94
1:G:94:ILE:HD13	1:G:314:MET:HE2	1.48	0.94
1:C:480:LYS:O	1:C:480:LYS:HD3	1.67	0.94
1:C:415:THR:HG22	1:C:416:GLN:H	1.28	0.94
1:A:471:ARG:NH1	1:C:428:ILE:O	2.00	0.94
1:B:479:ALA:CB	1:B:480:LYS:HG2	1.93	0.94
1:A:226:SER:OG	1:A:229:THR:HG22	1.65	0.94
1:G:241:LEU:O	2:G:504:HOH:O	1.85	0.94
1:A:22:VAL:CG2	1:A:34:ILE:CG2	2.46	0.93
1:E:258:GLU:OE1	2:E:516:HOH:O	1.84	0.93
1:G:87:SER:CB	1:G:94:ILE:CD1	2.46	0.93
1:G:358:LEU:N	1:G:358:LEU:CD1	2.30	0.93
1:B:334:SER:O	1:B:338:ILE:HG22	1.68	0.93
1:D:10:ARG:HH11	1:D:10:ARG:CG	1.82	0.93
1:G:415:THR:HG21	1:G:420:ARG:HD2	1.46	0.93
1:F:117:ASP:OD2	2:F:524:HOH:O	1.85	0.93
1:D:257:PHE:HB2	1:D:415:THR:HG23	1.51	0.93
1:F:273:ILE:HG21	1:F:387:VAL:HG21	1.50	0.93
1:D:323:LEU:N	1:D:323:LEU:CD2	2.30	0.93
1:C:24:SER:OG	2:C:512:HOH:O	1.85	0.93
1:A:232:ARG:CB	1:A:235:GLU:OE2	2.16	0.93
1:E:351:LYS:HE2	1:E:352:ALA:O	1.69	0.93
1:G:363:TYR:CA	2:G:519:HOH:O	2.10	0.93
1:E:351:LYS:O	1:E:365:GLU:HG3	1.69	0.93
1:B:22:VAL:HG21	1:B:34:ILE:HG21	1.50	0.92
1:F:429:HIS:O	2:F:516:HOH:O	1.87	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:LYS:CG	1:D:352:ALA:N	2.30	0.92
1:C:432:MET:HE1	1:C:447:PHE:CD1	2.03	0.92
1:F:326:ALA:HB2	1:F:362:PHE:CZ	2.05	0.92
1:F:94:ILE:O	1:F:94:ILE:HG13	1.68	0.92
1:F:377:VAL:CG1	1:F:388:THR:CG2	2.48	0.92
1:E:159:MET:HE1	1:E:171:ILE:CD1	2.00	0.92
1:F:326:ALA:HB2	1:F:362:PHE:CE1	2.05	0.92
1:F:404:ASN:O	1:F:405:THR:HG22	1.69	0.92
1:F:458:GLU:OE1	2:F:511:HOH:O	1.88	0.92
1:B:226:SER:OG	1:B:229:THR:HG22	1.70	0.92
1:E:259:ASP:OD1	1:E:415:THR:HG22	1.70	0.92
1:H:127:ASP:OD1	2:H:509:HOH:O	1.86	0.91
1:H:229:THR:HG23	1:H:232:ARG:HH22	1.25	0.91
1:A:481:ILE:HG13	1:A:482:ALA:H	1.27	0.91
1:A:221:ILE:CD1	1:A:233:ILE:HG21	1.97	0.91
1:H:229:THR:CG2	1:H:232:ARG:NH2	2.33	0.91
1:C:2:GLN:HE21	1:C:2:GLN:CA	1.81	0.91
1:D:259:ASP:CG	1:D:415:THR:HG22	1.89	0.91
1:E:479:ALA:O	1:E:480:LYS:HE2	1.71	0.91
1:D:226:SER:OG	1:D:229:THR:HG22	1.71	0.91
1:E:201:VAL:O	1:E:201:VAL:HG12	1.68	0.91
1:G:226:SER:OG	1:G:229:THR:HG22	1.71	0.91
1:H:329:ARG:HG3	1:H:329:ARG:NH1	1.69	0.91
1:D:462:GLU:OE1	1:G:136:ARG:NH2	2.04	0.91
1:B:273:ILE:HG12	1:B:387:VAL:HG22	1.53	0.91
1:B:329:ARG:HG3	1:B:329:ARG:NH1	1.77	0.91
1:B:101:ASP:OD1	2:B:511:HOH:O	1.87	0.90
1:F:23:VAL:HG12	1:F:24:SER:O	1.71	0.90
1:G:457:ARG:HG2	1:G:457:ARG:HH11	1.36	0.90
1:E:104:ARG:CZ	1:E:153:MET:HE1	2.01	0.90
1:E:386:PHE:O	1:E:386:PHE:HD1	1.54	0.90
1:E:477:VAL:C	2:E:514:HOH:O	2.07	0.90
1:C:23:VAL:CG1	1:C:29:SER:O	2.19	0.90
1:D:323:LEU:HD23	1:D:323:LEU:H	1.30	0.90
1:G:289:LEU:HD11	1:G:389:VAL:HG13	1.54	0.90
1:B:22:VAL:HG21	1:B:34:ILE:CG2	2.02	0.90
1:D:356:LYS:HA	1:D:359:ALA:HB2	1.54	0.90
1:G:293:ILE:HD12	1:G:294:ALA:N	1.85	0.90
1:A:55:ALA:O	2:A:525:HOH:O	1.83	0.90
1:E:152:LEU:CD1	1:E:184:ILE:CD1	2.49	0.90
1:B:136:ARG:NE	2:B:514:HOH:O	1.96	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLU:HB3	1:C:238:LYS:HE2	1.52	0.90
1:C:26:HIS:O	1:C:361:GLY:CA	2.19	0.90
1:E:404:ASN:O	1:E:405:THR:HG22	1.72	0.90
1:G:97:SER:HA	1:G:101:ASP:HB2	1.51	0.90
1:C:482:ALA:O	2:C:529:HOH:O	1.88	0.90
1:F:351:LYS:O	1:F:365:GLU:HG3	1.71	0.90
1:G:338:ILE:C	1:G:338:ILE:CD1	2.30	0.90
1:C:432:MET:HE3	1:C:447:PHE:CD1	2.06	0.89
1:C:439:LYS:O	2:C:530:HOH:O	1.90	0.89
1:B:41:ASP:OD2	2:B:522:HOH:O	1.89	0.89
1:B:63:GLU:OE1	1:B:66:ARG:NH1	2.05	0.89
1:C:259:ASP:OD1	1:C:415:THR:HG23	1.72	0.89
1:C:315:ASP:OD1	1:C:316:PRO:HD2	1.72	0.89
1:E:15:VAL:HG12	1:E:16:ALA:H	1.30	0.89
1:G:373:PRO:CD	1:G:374:GLN:OE1	2.19	0.89
1:C:220:LYS:HE3	1:C:466:ASP:O	1.73	0.89
1:D:2:GLN:NE2	2:D:506:HOH:O	2.04	0.89
1:G:327:LEU:HD21	1:G:331:ARG:HD2	1.54	0.89
1:G:373:PRO:CG	1:G:374:GLN:OE1	2.20	0.89
1:F:329:ARG:NH1	2:F:510:HOH:O	1.99	0.89
1:G:210:GLN:HG2	2:G:517:HOH:O	1.71	0.89
1:B:101:ASP:O	1:B:105:THR:OG1	1.91	0.89
1:C:432:MET:HE1	1:C:447:PHE:CE1	2.08	0.88
1:E:377:VAL:HG21	1:E:386:PHE:CZ	2.08	0.88
1:G:22:VAL:HG23	1:G:34:ILE:HG23	1.55	0.88
1:C:440:ARG:CA	2:C:530:HOH:O	2.02	0.88
1:D:115:MET:CE	1:D:461:PHE:CE1	2.55	0.88
1:B:357:ALA:HB2	1:G:12:VAL:HG12	1.53	0.88
1:H:329:ARG:HH11	1:H:329:ARG:CG	1.86	0.88
1:B:238:LYS:HB2	1:F:231:ARG:HG2	1.55	0.88
1:E:210:GLN:O	1:E:214:GLU:HG2	1.73	0.88
1:E:104:ARG:NE	1:E:153:MET:HE3	1.87	0.88
1:A:213:ALA:O	1:A:242:LYS:HE2	1.74	0.88
1:H:148:TRP:CD1	1:H:176:ILE:HD12	2.09	0.88
1:E:42:VAL:CG1	1:E:212:LEU:HD13	2.02	0.88
1:G:363:TYR:CG	2:G:519:HOH:O	2.25	0.88
1:H:99:GLY:O	1:H:100:LEU:HD23	1.72	0.88
1:A:259:ASP:OD1	1:A:415:THR:HG22	1.74	0.88
1:F:415:THR:HG21	1:F:420:ARG:CD	2.04	0.88
1:B:479:ALA:HB1	1:B:480:LYS:CD	2.03	0.88
1:B:479:ALA:HA	1:B:480:LYS:HB3	1.55	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:338:ILE:CD1	1:F:376:ARG:NE	2.29	0.88
1:G:148:TRP:HB3	1:G:177:THR:CG2	2.03	0.88
1:B:351:LYS:HG3	1:B:352:ALA:N	1.87	0.87
1:E:159:MET:CE	1:E:171:ILE:HD13	2.04	0.87
1:H:273:ILE:HG12	1:H:387:VAL:HG22	1.54	0.87
1:B:415:THR:HG21	1:B:420:ARG:HD2	1.57	0.87
1:H:108:CYS:HB3	1:H:156:SER:HB2	1.54	0.87
1:D:10:ARG:HG2	1:D:10:ARG:NH1	1.86	0.87
1:B:329:ARG:HD2	1:B:330:ASP:N	1.89	0.87
1:A:22:VAL:HG23	1:A:34:ILE:CG2	2.04	0.87
1:A:377:VAL:HG13	1:A:388:THR:HG21	1.54	0.87
1:D:20:ILE:HG21	1:D:175:GLU:HB3	1.55	0.86
1:F:443:PRO:HA	1:F:459:MET:HE2	1.54	0.86
1:B:351:LYS:CG	1:B:352:ALA:H	1.88	0.86
1:D:351:LYS:O	1:D:365:GLU:HG3	1.75	0.86
1:A:8:ASP:OD2	1:A:51:ARG:NH2	2.06	0.86
1:B:115:MET:CE	1:B:461:PHE:CE1	2.59	0.86
1:D:457:ARG:HG2	1:D:457:ARG:HH11	1.39	0.86
1:H:351:LYS:HG3	1:H:352:ALA:N	1.90	0.86
1:C:142:VAL:HG22	1:C:220:LYS:HB3	1.56	0.86
1:D:36:ALA:O	2:D:524:HOH:O	1.91	0.86
1:C:2:GLN:NE2	1:C:2:GLN:CA	2.36	0.86
1:C:23:VAL:N	2:C:520:HOH:O	1.96	0.86
1:G:335:TYR:O	1:G:339:ALA:CB	2.24	0.86
1:C:24:SER:CB	2:C:512:HOH:O	2.22	0.86
1:A:56:TRP:HA	2:A:525:HOH:O	1.74	0.85
1:A:310:LEU:CD2	1:A:353:PRO:HG2	2.06	0.85
1:C:467:TYR:OH	2:C:508:HOH:O	1.90	0.85
1:E:370:GLU:OE2	2:E:518:HOH:O	1.94	0.85
1:E:377:VAL:CG2	1:E:386:PHE:CZ	2.58	0.85
1:B:417:ASN:HD22	1:B:420:ARG:HB2	1.41	0.85
1:B:479:ALA:CB	1:B:480:LYS:CE	2.54	0.85
1:E:87:SER:OG	1:E:92:HIS:O	1.94	0.85
1:G:138:PRO:HG3	1:G:165:ALA:O	1.75	0.85
1:A:415:THR:HG21	1:A:420:ARG:HD2	1.57	0.85
1:E:292:ASP:OD2	2:E:529:HOH:O	1.93	0.85
1:H:86:GLU:OE1	1:H:151:PRO:HD2	1.77	0.85
1:G:249:GLY:O	1:G:453:SER:OG	1.94	0.85
1:A:232:ARG:HB3	1:A:235:GLU:OE2	1.76	0.85
1:B:416:GLN:NE2	2:B:503:HOH:O	1.98	0.85
1:E:415:THR:HG21	1:E:420:ARG:HD2	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:SER:OG	1:C:92:HIS:O	1.94	0.85
1:E:318:THR:O	2:E:512:HOH:O	1.94	0.85
1:E:396:GLU:OE1	2:E:520:HOH:O	1.94	0.85
1:F:51:ARG:O	2:F:528:HOH:O	1.94	0.85
1:A:47:ALA:HB2	1:B:374:GLN:CB	2.05	0.84
1:D:10:ARG:NE	2:D:504:HOH:O	2.11	0.84
1:H:49:ALA:HB1	1:H:168:THR:HG21	1.58	0.84
1:D:86:GLU:O	1:D:90:THR:OG1	1.94	0.84
1:A:221:ILE:HD13	1:A:233:ILE:HG21	1.57	0.84
1:A:404:ASN:O	1:A:405:THR:CG2	2.25	0.84
1:C:379:GLN:NE2	1:C:404:ASN:OD1	2.10	0.84
1:G:310:LEU:CD2	1:G:353:PRO:HG3	2.06	0.84
1:G:327:LEU:CD2	1:G:331:ARG:CD	2.55	0.84
1:B:334:SER:O	1:B:338:ILE:CG2	2.24	0.84
1:G:87:SER:OG	1:G:92:HIS:O	1.96	0.84
1:B:81:GLU:OE1	2:B:518:HOH:O	1.93	0.84
1:E:152:LEU:HD11	1:E:184:ILE:HD11	1.58	0.84
1:H:355:ASP:OD1	1:H:357:ALA:HB3	1.77	0.84
1:D:80:GLU:OE1	1:D:98:ARG:NH2	2.11	0.84
1:F:124:ILE:O	2:F:514:HOH:O	1.95	0.84
1:H:355:ASP:C	1:H:357:ALA:H	1.77	0.84
1:D:458:GLU:O	1:D:459:MET:HB2	1.76	0.84
1:H:377:VAL:HG21	1:H:386:PHE:CZ	2.13	0.84
1:A:41:ASP:OD1	2:A:511:HOH:O	1.93	0.84
1:B:238:LYS:CD	1:F:235:GLU:CG	2.52	0.84
1:C:326:ALA:HB2	1:C:362:PHE:CE1	2.12	0.84
1:D:481:ILE:HG22	1:D:482:ALA:N	1.93	0.84
1:E:320:MET:CE	1:E:366:PRO:HG3	2.08	0.84
1:F:443:PRO:HA	1:F:459:MET:HE3	1.60	0.84
1:G:100:LEU:O	1:G:104:ARG:HG3	1.78	0.84
1:H:26:HIS:ND1	1:H:363:TYR:OH	1.95	0.84
1:H:237:SER:O	2:H:506:HOH:O	1.96	0.84
1:H:408:GLY:O	1:H:430:ALA:HA	1.76	0.83
1:H:415:THR:HG21	1:H:420:ARG:HD2	1.57	0.83
1:B:132:ASN:ND2	1:F:445:SER:HG	1.71	0.83
1:A:4:GLN:OE1	2:A:518:HOH:O	1.96	0.83
1:A:273:ILE:HG13	1:A:273:ILE:O	1.76	0.83
1:C:318:THR:CG2	1:C:320:MET:O	2.26	0.83
1:G:22:VAL:HG21	1:G:34:ILE:CG2	2.09	0.83
1:A:404:ASN:O	1:A:405:THR:HG22	1.77	0.83
1:B:244:ILE:N	2:B:524:HOH:O	1.87	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LEU:HD22	1:B:289:LEU:HD21	1.60	0.83
1:D:8:ASP:OD1	1:D:195:LYS:HG3	1.77	0.83
1:E:22:VAL:CG2	1:E:34:ILE:CG2	2.57	0.83
1:E:227:THR:HG23	1:H:241:LEU:HD11	1.61	0.83
1:A:129:GLY:HA3	1:A:479:ALA:HB3	1.60	0.83
1:C:397:GLU:O	1:C:401:ILE:HG13	1.77	0.83
1:D:235:GLU:O	1:D:238:LYS:HG2	1.79	0.83
1:E:386:PHE:O	1:E:386:PHE:CD1	2.30	0.83
1:B:479:ALA:CA	1:B:480:LYS:HB3	2.08	0.83
1:E:248:LEU:HD12	1:H:241:LEU:HD13	1.59	0.83
1:A:213:ALA:O	1:A:242:LYS:CE	2.27	0.82
1:B:479:ALA:HB2	1:B:480:LYS:NZ	1.93	0.82
1:C:290:HIS:HD2	1:C:292:ASP:H	1.22	0.82
1:G:87:SER:CB	1:G:94:ILE:HD12	2.09	0.82
1:G:151:PRO:HG2	1:G:177:THR:OG1	1.79	0.82
1:B:76:GLU:CD	1:B:110:ARG:NH1	2.33	0.82
1:B:100:LEU:O	1:B:104:ARG:CG	2.28	0.82
1:G:22:VAL:CG2	1:G:34:ILE:CG2	2.57	0.82
1:H:481:ILE:HD12	1:H:482:ALA:N	1.92	0.82
1:C:417:ASN:ND2	1:C:420:ARG:H	1.76	0.82
1:F:257:PHE:HB2	1:F:415:THR:HG23	1.58	0.82
1:B:22:VAL:CG2	1:B:34:ILE:HG21	2.08	0.82
1:D:415:THR:HG21	1:D:420:ARG:NH1	1.93	0.82
1:F:371:ALA:O	2:F:517:HOH:O	1.98	0.82
1:B:137:LYS:NZ	1:F:426:ASN:OD1	2.12	0.82
1:H:102:VAL:HG22	1:H:152:LEU:CD2	2.10	0.82
1:A:20:ILE:HG13	1:A:36:ALA:HB2	1.61	0.82
1:F:259:ASP:O	1:F:416:GLN:HG3	1.79	0.82
1:G:289:LEU:CD1	1:G:389:VAL:HG13	2.07	0.82
1:C:229:THR:OG1	1:C:232:ARG:NH2	2.13	0.82
1:G:340:ILE:HG22	1:G:341:GLU:N	1.95	0.82
1:B:376:ARG:NH1	1:B:380:GLU:OE1	2.13	0.81
1:F:336:ILE:O	1:F:340:ILE:HG12	1.80	0.81
1:H:158:LYS:HD3	1:H:458:GLU:OE2	1.80	0.81
1:C:57:SER:O	2:C:523:HOH:O	1.98	0.81
1:D:302:ILE:O	1:D:306:LYS:HG3	1.80	0.81
1:F:258:GLU:HG3	1:F:290:HIS:CG	2.16	0.81
1:H:138:PRO:HG3	1:H:165:ALA:O	1.79	0.81
1:A:43:ASP:OD1	1:B:374:GLN:CG	2.28	0.81
1:A:47:ALA:CB	1:B:374:GLN:HB2	2.10	0.81
1:D:334:SER:O	1:D:338:ILE:HG23	1.81	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:MET:HB2	2:E:510:HOH:O	1.79	0.81
1:D:184:ILE:O	1:D:188:MET:HG3	1.80	0.81
1:F:355:ASP:OD1	2:F:518:HOH:O	1.99	0.81
1:G:445:SER:O	2:G:507:HOH:O	1.98	0.81
1:A:221:ILE:CD1	1:A:233:ILE:HG23	1.99	0.81
1:B:259:ASP:OD1	1:B:415:THR:HG22	1.81	0.81
1:F:101:ASP:OD1	2:F:503:HOH:O	1.98	0.81
1:F:417:ASN:HD22	1:F:420:ARG:H	1.27	0.81
1:G:148:TRP:CB	1:G:177:THR:CG2	2.59	0.81
1:D:328:ARG:O	1:D:332:VAL:HG23	1.81	0.81
1:G:476:ASN:OD1	1:G:479:ALA:HB3	1.81	0.81
1:B:136:ARG:CZ	2:B:514:HOH:O	2.19	0.80
1:B:238:LYS:HZ3	1:F:235:GLU:CD	1.70	0.80
1:F:291:LYS:HE2	1:F:393:SER:HB3	1.63	0.80
1:C:175:GLU:OE2	2:C:522:HOH:O	1.98	0.80
1:C:480:LYS:O	1:C:480:LYS:CD	2.29	0.80
1:E:159:MET:CE	1:E:171:ILE:CD1	2.59	0.80
1:C:93:PRO:O	1:C:96:ASP:HB2	1.81	0.80
1:D:2:GLN:HE21	1:D:2:GLN:HA	1.44	0.80
1:C:210:GLN:O	1:C:214:GLU:HG2	1.81	0.80
1:E:376:ARG:CD	1:E:380:GLU:OE2	2.22	0.80
1:G:201:VAL:O	1:G:201:VAL:CG1	2.30	0.80
1:A:273:ILE:HG21	1:A:387:VAL:CG2	2.11	0.80
1:B:20:ILE:HD13	1:B:175:GLU:HB3	1.61	0.80
1:F:152:LEU:O	1:F:155:THR:OG1	1.99	0.80
1:E:153:MET:CB	2:E:510:HOH:O	2.27	0.80
1:B:2:GLN:HE21	1:B:2:GLN:CA	1.92	0.80
1:D:328:ARG:HA	1:D:328:ARG:HE	1.47	0.80
1:B:335:TYR:HA	1:B:338:ILE:HG23	1.62	0.80
1:F:221:ILE:O	1:F:221:ILE:CG2	2.30	0.80
1:G:475:VAL:HG12	1:G:477:VAL:HG12	1.63	0.80
1:D:273:ILE:HG21	1:D:387:VAL:HG22	1.64	0.80
1:F:53:PHE:CE1	1:F:140:GLY:HA2	2.17	0.80
1:G:259:ASP:O	1:G:416:GLN:NE2	2.16	0.80
1:F:27:ASP:OD1	1:F:29:SER:CB	2.30	0.79
1:A:52:ALA:O	2:A:529:HOH:O	2.00	0.79
1:A:152:LEU:CD1	1:A:184:ILE:CD1	2.59	0.79
1:A:210:GLN:O	1:A:214:GLU:CG	2.30	0.79
1:A:338:ILE:HD13	1:A:376:ARG:HH21	1.48	0.79
1:B:152:LEU:HD12	1:B:184:ILE:CD1	2.12	0.79
1:B:337:ASP:O	1:B:341:GLU:HG2	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:SER:OG	1:E:229:THR:CG2	2.30	0.79
1:H:327:LEU:O	1:H:331:ARG:HG3	1.83	0.79
1:E:201:VAL:O	1:E:201:VAL:CG1	2.29	0.79
1:G:338:ILE:O	1:G:338:ILE:CD1	2.30	0.79
1:H:338:ILE:O	1:H:338:ILE:CD1	2.30	0.79
1:E:22:VAL:HG21	1:E:34:ILE:HG21	1.63	0.79
1:B:115:MET:HE1	1:B:461:PHE:CE1	2.17	0.79
1:F:94:ILE:HG12	1:F:98:ARG:NH1	1.97	0.79
1:D:338:ILE:HD11	1:D:376:ARG:HB3	1.65	0.79
1:F:377:VAL:HG11	1:F:388:THR:HG21	1.63	0.79
1:A:355:ASP:O	1:A:357:ALA:N	2.16	0.79
1:B:6:TYR:OH	1:B:189:THR:HG21	1.82	0.79
1:D:115:MET:HE2	1:D:461:PHE:CD1	2.17	0.79
1:B:2:GLN:HA	1:B:2:GLN:NE2	1.97	0.79
1:D:2:GLN:NE2	1:D:2:GLN:HA	1.97	0.79
1:F:377:VAL:HG11	1:F:388:THR:CG2	2.13	0.79
1:A:33:ARG:NH2	1:F:8:ASP:OD2	2.16	0.79
1:B:74:ARG:NH1	1:B:78:CYS:SG	2.56	0.79
1:D:291:LYS:HE2	1:D:393:SER:HB2	1.65	0.79
1:E:235:GLU:O	1:E:238:LYS:CD	2.30	0.79
1:E:291:LYS:HE2	1:E:393:SER:HG	1.47	0.79
1:F:404:ASN:O	1:F:405:THR:CG2	2.30	0.79
1:F:459:MET:N	2:F:506:HOH:O	2.15	0.79
1:H:99:GLY:O	1:H:100:LEU:CD2	2.30	0.79
1:H:333:LEU:HD22	1:H:351:LYS:HE2	1.63	0.79
1:A:56:TRP:CA	2:A:525:HOH:O	2.29	0.78
1:H:25:PRO:HA	1:H:362:PHE:CE2	2.18	0.78
1:F:429:HIS:HB3	2:F:516:HOH:O	1.83	0.78
1:G:53:PHE:CE1	1:G:140:GLY:HA2	2.17	0.78
1:D:204:TYR:O	2:D:517:HOH:O	2.02	0.78
1:E:479:ALA:O	1:E:480:LYS:CD	2.30	0.78
1:F:227:THR:CG2	1:F:231:ARG:NH1	2.45	0.78
1:G:350:GLY:O	1:G:351:LYS:CG	2.30	0.78
1:H:20:ILE:HD13	1:H:175:GLU:HB3	1.63	0.78
1:B:76:GLU:OE2	1:B:110:ARG:NH1	2.15	0.78
1:F:38:GLU:HG2	1:F:207:THR:HG21	1.65	0.78
1:F:259:ASP:OD1	1:F:415:THR:HG22	1.82	0.78
1:B:428:ILE:O	1:F:471:ARG:NH1	2.16	0.78
1:D:351:LYS:HG2	1:D:352:ALA:N	1.97	0.78
1:F:410:GLY:O	2:F:519:HOH:O	2.02	0.78
1:A:152:LEU:HD11	1:A:184:ILE:HD11	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:GLU:CB	2:B:518:HOH:O	2.31	0.78
1:E:479:ALA:O	1:E:480:LYS:CE	2.30	0.78
1:F:201:VAL:O	1:F:201:VAL:CG1	2.29	0.78
1:F:356:LYS:HA	1:F:359:ALA:HB2	1.66	0.78
1:A:232:ARG:HB2	1:A:235:GLU:OE2	1.82	0.78
1:F:273:ILE:HG12	1:F:387:VAL:HG22	0.85	0.78
1:G:338:ILE:HD12	1:G:339:ALA:N	1.98	0.78
2:A:515:HOH:O	1:B:374:GLN:HG3	1.81	0.78
1:B:312:ASP:OD1	1:B:313:PRO:HD2	1.83	0.78
1:F:210:GLN:O	1:F:214:GLU:HG2	1.82	0.78
1:G:76:GLU:O	1:G:79:SER:HB3	1.83	0.78
1:G:372:LYS:HB3	1:G:373:PRO:HD2	1.65	0.78
1:A:34:ILE:HD11	1:A:202:PRO:HB2	1.66	0.78
1:C:119:ILE:HD11	1:C:464:ILE:HD12	1.66	0.78
1:F:477:VAL:HG23	1:F:478:ASP:HB2	1.64	0.78
1:F:273:ILE:CG1	1:F:387:VAL:CG2	2.52	0.78
1:C:275:HIS:NE2	2:C:524:HOH:O	2.00	0.77
1:E:248:LEU:HD11	1:H:241:LEU:HD22	1.65	0.77
1:F:335:TYR:CE2	1:F:376:ARG:CZ	2.66	0.77
1:G:221:ILE:CG2	1:G:221:ILE:O	2.31	0.77
1:B:172:LYS:NZ	1:B:203:GLY:O	2.17	0.77
1:B:238:LYS:HZ3	1:F:235:GLU:HG2	0.94	0.77
1:G:74:ARG:HG3	1:G:187:LEU:HD22	1.65	0.77
1:G:95:ARG:NH1	1:G:319:GLU:HG2	1.99	0.77
1:E:377:VAL:HG21	1:E:386:PHE:HZ	1.48	0.77
1:G:369:VAL:O	1:G:369:VAL:HG12	1.83	0.77
1:B:94:ILE:O	1:B:94:ILE:HG13	1.83	0.77
1:F:227:THR:HA	1:F:248:LEU:HD13	1.67	0.77
1:A:159:MET:HE1	1:A:198:VAL:HG11	0.77	0.77
1:D:257:PHE:CB	1:D:415:THR:HG23	2.15	0.77
1:F:22:VAL:HG21	1:F:34:ILE:CG2	2.15	0.77
1:G:310:LEU:HD12	1:G:320:MET:CG	2.09	0.77
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.66	0.77
1:A:241:LEU:HD13	1:C:248:LEU:CD1	2.14	0.77
1:B:115:MET:HE3	1:B:461:PHE:CE1	2.20	0.77
1:B:451:GLY:O	2:B:502:HOH:O	2.01	0.77
1:E:22:VAL:CG2	1:E:34:ILE:HG21	2.14	0.77
1:C:480:LYS:O	1:C:480:LYS:CG	2.30	0.77
1:D:204:TYR:C	2:D:517:HOH:O	2.23	0.77
1:F:2:GLN:HA	1:F:2:GLN:NE2	1.97	0.77
1:C:70:LYS:HD2	1:C:191:VAL:HG22	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:302:ILE:O	1:H:306:LYS:HG3	1.85	0.77
1:C:302:ILE:HD13	1:C:347:LEU:HB3	1.67	0.76
1:D:185:VAL:HG23	1:D:188:MET:HE2	1.66	0.76
1:F:235:GLU:O	1:F:238:LYS:HD3	1.84	0.76
1:B:152:LEU:CD1	1:B:184:ILE:HD11	2.05	0.76
1:H:333:LEU:CD2	1:H:351:LYS:HE2	2.14	0.76
1:B:235:GLU:HG2	1:F:238:LYS:CE	2.16	0.76
1:B:328:ARG:NH1	1:B:331:ARG:HE	1.82	0.76
1:F:37:ALA:CB	1:F:201:VAL:HG13	2.15	0.76
1:G:326:ALA:N	1:G:362:PHE:CE2	2.53	0.76
1:H:124:ILE:HB	1:H:132:ASN:ND2	2.01	0.76
1:A:292:ASP:O	1:A:296:GLN:NE2	2.19	0.76
1:B:345:LYS:CD	1:B:345:LYS:N	2.49	0.76
1:H:90:THR:HG21	1:H:92:HIS:CE1	2.21	0.76
1:E:102:VAL:HB	1:E:103:PRO:HD3	1.67	0.76
1:A:235:GLU:CB	1:C:238:LYS:CE	2.50	0.76
1:A:37:ALA:O	2:A:519:HOH:O	2.03	0.76
1:C:408:GLY:O	1:C:430:ALA:CA	2.32	0.76
1:E:104:ARG:CZ	1:E:153:MET:CE	2.61	0.76
1:D:355:ASP:O	1:D:356:LYS:HB2	1.85	0.75
1:E:258:GLU:HG3	1:E:290:HIS:CD2	2.21	0.75
1:F:221:ILE:O	1:F:221:ILE:HG23	1.85	0.75
1:G:15:VAL:HG11	1:G:40:ALA:HB3	1.68	0.75
1:G:21:ASP:HB3	1:G:30:LEU:CD1	2.15	0.75
1:A:184:ILE:O	1:A:187:LEU:HB2	1.87	0.75
1:B:87:SER:OG	1:B:97:SER:OG	2.05	0.75
1:G:51:ARG:O	2:G:520:HOH:O	2.04	0.75
1:H:49:ALA:CA	1:H:168:THR:HG21	2.16	0.75
1:B:132:ASN:HD21	1:F:445:SER:HG	1.25	0.75
1:C:215:HIS:HD2	1:C:217:ASP:H	1.32	0.75
1:D:481:ILE:HG22	1:D:482:ALA:H	1.49	0.75
1:A:22:VAL:CG2	1:A:34:ILE:HG21	2.15	0.75
1:A:22:VAL:HG21	1:A:34:ILE:CG2	2.15	0.75
1:E:22:VAL:HG23	1:E:34:ILE:CG2	2.15	0.75
1:G:22:VAL:CG2	1:G:34:ILE:HG23	2.16	0.75
1:G:335:TYR:OH	2:G:523:HOH:O	1.81	0.75
1:G:394:SER:HB2	1:G:396:GLU:OE2	1.87	0.75
1:A:228:ALA:O	1:A:232:ARG:NE	2.19	0.75
1:E:262:ILE:O	1:E:266:VAL:HG23	1.86	0.75
1:F:281:CYS:HB3	1:F:409:LEU:CD2	2.17	0.75
1:G:326:ALA:HB2	1:G:362:PHE:CZ	2.22	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:SER:O	1:A:338:ILE:HG23	1.85	0.75
1:D:10:ARG:CD	2:D:504:HOH:O	2.35	0.75
1:G:80:GLU:OE1	1:G:84:GLN:NE2	2.19	0.75
1:H:215:HIS:HD2	1:H:217:ASP:H	1.34	0.75
1:H:328:ARG:NE	1:H:383:PHE:HB3	2.01	0.75
1:A:34:ILE:CD1	1:A:202:PRO:HB2	2.17	0.75
1:E:329:ARG:NH1	2:E:505:HOH:O	2.16	0.75
1:F:22:VAL:HG21	1:F:34:ILE:HG21	1.68	0.75
1:G:53:PHE:HB3	1:G:54:PRO:HD3	1.67	0.75
1:A:143:ALA:HB1	1:A:212:LEU:HG	1.69	0.75
1:C:404:ASN:O	1:C:405:THR:HG23	1.87	0.75
1:B:258:GLU:HG2	1:B:290:HIS:CD2	2.21	0.74
1:C:321:GLY:O	2:C:511:HOH:O	2.05	0.74
1:C:370:GLU:OE2	1:C:391:ARG:HD2	1.87	0.74
1:D:376:ARG:NH1	1:D:380:GLU:OE2	2.14	0.74
1:E:277:GLN:NE2	1:E:321:GLY:H	1.85	0.74
1:E:451:GLY:O	2:E:501:HOH:O	2.05	0.74
1:F:415:THR:CG2	1:F:420:ARG:HH11	1.99	0.74
1:C:63[A]:GLU:OE1	1:C:66:ARG:NE	2.19	0.74
1:H:163:LEU:CD2	1:H:169:ILE:HD12	2.17	0.74
1:A:138:PRO:HG3	1:A:165:ALA:O	1.87	0.74
1:A:273:ILE:HG21	1:A:387:VAL:HG22	1.69	0.74
1:B:133:TYR:OH	2:B:521:HOH:O	2.05	0.74
1:G:293:ILE:CD1	1:G:293:ILE:O	2.35	0.74
1:B:337:ASP:OD2	2:B:517:HOH:O	2.05	0.74
1:D:376:ARG:CD	1:D:380:GLU:OE2	2.36	0.74
1:E:210:GLN:O	1:E:214:GLU:CG	2.36	0.74
1:G:231:ARG:O	1:G:235:GLU:HG3	1.88	0.74
1:A:457:ARG:NH1	1:C:470:ALA:O	2.21	0.74
1:B:22:VAL:HG23	1:B:34:ILE:CG2	2.16	0.74
1:D:457:ARG:NE	2:D:513:HOH:O	1.92	0.74
1:F:27:ASP:OD1	1:F:29:SER:HB3	1.86	0.74
1:F:115:MET:O	1:F:119:ILE:HG13	1.88	0.74
1:B:328:ARG:HH12	1:B:331:ARG:HE	1.36	0.74
1:G:357:ALA:CA	1:G:358:LEU:HD12	2.17	0.74
1:H:329:ARG:HD3	1:H:330:ASP:OD1	1.85	0.74
1:B:320:MET:HE3	1:B:385:PRO:HG3	1.68	0.73
1:C:334:SER:O	1:C:338:ILE:HG23	1.87	0.73
1:B:344:GLY:C	1:B:345:LYS:HD3	2.09	0.73
1:B:457:ARG:NH2	1:F:470:ALA:O	2.20	0.73
1:G:148:TRP:O	1:G:151:PRO:HD3	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:327:LEU:HD23	1:G:327:LEU:O	1.88	0.73
1:B:379:GLN:OE1	2:B:506:HOH:O	2.05	0.73
1:A:475:VAL:HG12	1:A:477:VAL:HG12	1.70	0.73
1:B:479:ALA:HB3	1:B:480:LYS:HE2	1.68	0.73
1:D:137:LYS:NZ	1:G:426:ASN:HD21	1.86	0.73
1:H:355:ASP:C	1:H:357:ALA:N	2.39	0.73
1:B:342:GLN:OE1	1:B:376:ARG:HB2	1.88	0.73
1:D:273:ILE:O	1:D:273:ILE:CD1	2.30	0.73
1:D:458:GLU:O	1:D:459:MET:CB	2.36	0.73
1:F:246:LEU:O	1:F:454:GLY:HA3	1.87	0.73
1:C:210:GLN:O	1:C:214:GLU:CG	2.36	0.73
1:C:327:LEU:CD2	1:C:331:ARG:NH1	2.52	0.73
1:G:148:TRP:HB3	1:G:177:THR:HG22	1.69	0.73
1:E:22:VAL:HG21	1:E:34:ILE:CG2	2.19	0.73
1:G:87:SER:OG	1:G:94:ILE:HD12	1.89	0.73
1:H:49:ALA:C	1:H:168:THR:HG21	2.08	0.73
1:A:56:TRP:N	2:A:525:HOH:O	2.14	0.72
1:G:148:TRP:CB	1:G:177:THR:HG21	2.19	0.72
1:G:151:PRO:HG3	1:G:177:THR:OG1	1.88	0.72
1:H:175:GLU:CD	1:H:175:GLU:H	1.91	0.72
1:H:333:LEU:HD22	1:H:351:LYS:CE	2.19	0.72
1:C:351:LYS:HG3	1:C:352:ALA:H	1.53	0.72
1:E:266:VAL:HG22	1:E:297:PHE:CE1	2.25	0.72
1:E:320:MET:HE3	1:E:366:PRO:HG3	1.70	0.72
1:F:338:ILE:CD1	1:F:376:ARG:CD	2.67	0.72
1:G:37:ALA:HB1	1:G:201:VAL:HG22	1.70	0.72
1:H:152:LEU:HD11	1:H:184:ILE:HD11	1.71	0.72
1:B:320:MET:CE	1:B:385:PRO:HB3	2.19	0.72
1:B:481:ILE:HB	2:B:515:HOH:O	1.88	0.72
1:C:158:LYS:HD3	1:C:458:GLU:OE2	1.88	0.72
1:G:305:ALA:HA	1:G:308:ILE:HD12	1.69	0.72
1:B:90:THR:HG22	1:B:177:THR:HG21	1.69	0.72
1:B:231:ARG:O	1:B:235:GLU:HG3	1.89	0.72
1:G:457:ARG:HG2	1:G:457:ARG:NH1	2.04	0.72
1:A:220:LYS:HZ1	1:A:245:GLN:HB2	1.52	0.72
1:H:377:VAL:CG2	1:H:386:PHE:CE1	2.72	0.72
1:A:328:ARG:HA	1:A:328:ARG:HH11	1.54	0.72
1:A:424:MET:O	1:A:428:ILE:HG13	1.89	0.72
1:E:213:ALA:HA	1:E:221:ILE:HD12	1.71	0.72
1:B:22:VAL:HG23	1:B:34:ILE:HG23	1.71	0.72
1:G:22:VAL:HG21	1:G:34:ILE:HG21	1.69	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASP:C	1:A:357:ALA:H	1.92	0.72
1:A:377:VAL:O	2:A:524:HOH:O	2.07	0.72
1:E:266:VAL:HG22	1:E:297:PHE:CD1	2.25	0.72
1:H:56:TRP:CH2	1:H:64:ARG:HG2	2.25	0.72
1:C:190:GLU:CD	2:C:516:HOH:O	2.23	0.72
1:C:327:LEU:HD22	1:C:331:ARG:NH1	2.04	0.72
1:C:353:PRO:HG2	1:C:358:LEU:HD23	1.69	0.72
1:D:148:TRP:CZ3	1:D:324:THR:OG1	2.42	0.72
1:F:22:VAL:CG2	1:F:34:ILE:CG2	2.68	0.72
1:F:61:ALA:CB	1:F:116:ALA:O	2.36	0.72
1:G:172:LYS:HG2	1:G:172:LYS:O	1.89	0.72
1:A:21:ASP:OD1	1:A:33:ARG:CD	2.34	0.72
1:C:337:ASP:O	1:C:341:GLU:HG3	1.90	0.72
1:C:340:ILE:HG22	1:C:341:GLU:N	2.05	0.72
1:E:97:SER:O	1:E:102:VAL:HG23	1.90	0.72
1:E:117:ASP:OD2	2:E:502:HOH:O	2.06	0.72
1:F:335:TYR:CD2	1:F:376:ARG:NH2	2.58	0.72
1:E:152:LEU:CD1	1:E:184:ILE:HD11	2.15	0.71
1:E:273:ILE:HG13	1:E:387:VAL:HG22	1.71	0.71
1:A:152:LEU:CD1	1:A:184:ILE:HD11	2.18	0.71
1:B:56:TRP:CH2	1:B:64:ARG:HG2	2.25	0.71
1:C:108:CYS:HB3	1:C:156:SER:HB2	1.73	0.71
1:D:210:GLN:O	1:D:214:GLU:CG	2.29	0.71
1:E:386:PHE:CD1	1:E:386:PHE:C	2.63	0.71
1:F:394:SER:OG	1:F:397:GLU:HB2	1.90	0.71
1:C:373:PRO:HG3	1:C:390:VAL:HG11	1.70	0.71
1:H:393:SER:OG	1:H:397:GLU:OE1	2.06	0.71
1:F:2:GLN:HA	1:F:2:GLN:HE21	1.55	0.71
1:H:163:LEU:HD21	1:H:169:ILE:HD12	1.72	0.71
1:B:377:VAL:HG13	1:B:388:THR:HG21	1.73	0.71
1:D:143:ALA:HB1	1:D:212:LEU:HG	1.70	0.71
1:G:273:ILE:HG13	1:G:273:ILE:O	1.91	0.71
1:C:417:ASN:HD22	1:C:420:ARG:H	1.38	0.71
1:H:210:GLN:O	1:H:214:GLU:HG3	1.90	0.71
1:E:277:GLN:HG3	1:E:320:MET:CG	2.20	0.71
1:G:5:LEU:HD21	1:G:35:ALA:O	1.91	0.71
1:A:2:GLN:HA	1:A:2:GLN:HE21	1.56	0.71
1:F:290:HIS:CD2	1:F:292:ASP:H	2.09	0.71
1:F:375:ASP:O	1:F:378:CYS:HB2	1.89	0.71
1:B:243:ARG:HB3	2:B:524:HOH:O	1.90	0.71
1:E:242:LYS:O	2:E:507:HOH:O	2.08	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:ALA:HB1	1:F:116:ALA:C	2.12	0.71
1:C:190:GLU:OE1	2:C:516:HOH:O	2.08	0.71
1:C:290:HIS:CD2	1:C:292:ASP:H	2.07	0.71
1:E:20:ILE:HD13	1:E:175:GLU:HB3	1.73	0.71
1:E:221:ILE:HG23	1:E:221:ILE:O	1.91	0.71
1:B:88:LEU:HA	1:B:314:MET:HE3	1.71	0.70
1:D:310:LEU:HD23	1:D:353:PRO:HG2	1.73	0.70
1:E:290:HIS:HE1	1:E:393:SER:O	1.74	0.70
1:F:227:THR:HG22	1:F:231:ARG:NH1	2.06	0.70
1:H:90:THR:CG2	1:H:92:HIS:CE1	2.74	0.70
1:D:486:LYS:O	1:D:487:ARG:C	2.30	0.70
1:E:354:ASP:C	1:E:355:ASP:OD2	2.30	0.70
1:A:377:VAL:HG21	1:A:386:PHE:CZ	2.27	0.70
1:A:477:VAL:CG2	1:A:478:ASP:N	2.54	0.70
1:E:404:ASN:O	1:E:405:THR:CG2	2.38	0.70
1:F:415:THR:HG21	1:F:420:ARG:HH11	1.53	0.70
1:B:320:MET:CE	1:B:385:PRO:CG	2.70	0.70
1:B:417:ASN:HD22	1:B:420:ARG:CB	2.04	0.70
1:F:259:ASP:OD1	1:F:420:ARG:NH1	2.24	0.70
1:H:355:ASP:O	1:H:357:ALA:N	2.24	0.70
1:D:21:ASP:OD1	1:D:33:ARG:HD3	1.92	0.70
1:G:334:SER:O	1:G:338:ILE:HG23	1.91	0.70
1:B:345:LYS:HE2	1:C:404:ASN:HA	1.73	0.70
1:C:263:GLU:HG3	1:C:300:ARG:NH2	2.06	0.70
1:D:2:GLN:HE21	1:D:2:GLN:CA	2.00	0.70
1:D:404:ASN:O	1:D:404:ASN:CG	2.29	0.70
1:F:287:LEU:HD22	1:F:289:LEU:HD21	1.72	0.70
1:G:396:GLU:CD	1:G:396:GLU:H	1.95	0.70
1:H:277:GLN:HG3	1:H:320:MET:HG3	1.73	0.70
1:D:328:ARG:HE	1:D:328:ARG:CA	1.94	0.70
1:F:281:CYS:HB3	1:F:409:LEU:HD23	1.73	0.70
1:G:24:SER:OG	2:G:512:HOH:O	2.10	0.70
1:G:155:THR:O	1:G:159:MET:HG3	1.92	0.70
1:G:344:GLY:O	2:G:505:HOH:O	2.10	0.70
1:A:92:HIS:HD2	1:A:101:ASP:OD2	1.75	0.69
1:C:310:LEU:HD12	1:C:320:MET:HB3	1.72	0.69
1:D:115:MET:CE	1:D:461:PHE:CD1	2.75	0.69
1:E:20:ILE:HG21	1:E:175:GLU:HB3	1.74	0.69
1:E:31:ILE:CD1	1:E:88:LEU:HG	2.22	0.69
1:G:23:VAL:CG1	1:G:24:SER:N	2.54	0.69
1:H:213:ALA:O	1:H:242:LYS:HE2	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG23	1:A:34:ILE:HG23	1.71	0.69
1:B:344:GLY:C	1:B:345:LYS:CD	2.60	0.69
1:D:477:VAL:HG22	1:D:478:ASP:N	2.07	0.69
1:F:74:ARG:NH1	1:F:78:CYS:SG	2.65	0.69
1:F:275:HIS:ND1	1:F:439:LYS:NZ	2.39	0.69
1:A:241:LEU:HD13	1:C:248:LEU:HD11	1.74	0.69
1:B:335:TYR:CA	1:B:338:ILE:HG23	2.21	0.69
1:C:415:THR:HG22	1:C:416:GLN:N	2.05	0.69
1:F:38:GLU:CA	1:F:207:THR:CG2	2.65	0.69
1:H:251:LYS:HB2	1:H:407:TYR:CD1	2.28	0.69
1:A:310:LEU:CD2	1:A:353:PRO:CG	2.70	0.69
1:C:259:ASP:OD1	1:C:415:THR:CG2	2.39	0.69
1:D:309:ARG:CD	1:D:319:GLU:OE1	2.39	0.69
1:H:30:LEU:HD21	1:H:33:ARG:HE	1.58	0.69
1:B:250:GLY:O	1:B:381:GLU:HG3	1.93	0.69
1:E:93:PRO:O	1:E:96:ASP:HB2	1.92	0.69
1:E:337:ASP:OD1	2:E:523:HOH:O	2.09	0.69
1:A:377:VAL:CG1	1:A:388:THR:HG21	2.23	0.69
1:B:328:ARG:O	1:B:332:VAL:HG23	1.92	0.69
1:B:328:ARG:NH2	1:B:383:PHE:H	1.91	0.69
1:B:329:ARG:HH11	1:B:329:ARG:CG	1.94	0.69
1:C:291:LYS:HE3	1:C:393:SER:OG	1.92	0.69
1:D:328:ARG:HH11	1:D:383:PHE:CB	2.03	0.69
1:E:251:LYS:HB2	1:E:407:TYR:CD1	2.26	0.69
1:E:377:VAL:HG22	1:E:386:PHE:CZ	2.27	0.69
1:E:423:LYS:HD3	2:E:526:HOH:O	1.92	0.69
1:F:129:GLY:O	1:F:477:VAL:HG22	1.93	0.69
1:F:404:ASN:C	1:F:405:THR:CG2	2.60	0.69
1:B:320:MET:HE3	1:B:385:PRO:CG	2.23	0.69
1:C:404:ASN:O	1:C:404:ASN:CG	2.29	0.69
1:E:22:VAL:HG23	1:E:34:ILE:HG23	1.75	0.69
1:G:304:LEU:HA	2:G:513:HOH:O	1.91	0.69
1:H:152:LEU:CD1	1:H:184:ILE:HD11	2.22	0.69
1:H:329:ARG:HD2	1:H:330:ASP:N	2.07	0.69
1:H:351:LYS:CG	1:H:352:ALA:H	2.02	0.69
1:E:370:GLU:OE1	1:E:391:ARG:NH1	2.25	0.69
1:G:87:SER:CB	1:G:94:ILE:HD13	2.23	0.69
1:A:417:ASN:ND2	1:A:420:ARG:H	1.90	0.68
1:D:4:GLN:OE1	2:D:506:HOH:O	2.11	0.68
1:D:196:GLY:N	2:D:523:HOH:O	2.00	0.68
1:E:273:ILE:HG21	1:E:387:VAL:HG21	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD12	1:B:320:MET:HG2	1.76	0.68
1:G:19:THR:CG2	1:G:20:ILE:N	2.56	0.68
1:G:458:GLU:C	1:G:459:MET:HG2	2.14	0.68
1:E:273:ILE:CG1	1:E:387:VAL:HG22	2.22	0.68
1:F:94:ILE:HD11	1:F:98:ARG:CZ	2.24	0.68
1:G:259:ASP:OD1	1:G:415:THR:HG22	1.93	0.68
1:H:415:THR:CG2	1:H:420:ARG:HH11	2.05	0.68
1:A:377:VAL:HG13	1:A:388:THR:CG2	2.23	0.68
1:F:43:ASP:O	2:F:522:HOH:O	2.11	0.68
1:H:56:TRP:CZ2	1:H:64:ARG:HG2	2.28	0.68
1:A:38:GLU:O	1:A:42:VAL:HG13	1.92	0.68
1:A:320:MET:HE3	1:A:385:PRO:HG3	1.75	0.68
1:C:487:ARG:HB3	2:C:505:HOH:O	1.93	0.68
1:E:152:LEU:HD12	1:E:184:ILE:CD1	2.23	0.68
1:A:417:ASN:HD22	1:A:420:ARG:H	1.41	0.68
1:B:320:MET:CE	1:B:385:PRO:CB	2.71	0.68
1:B:479:ALA:CB	1:B:480:LYS:NZ	2.55	0.68
1:E:273:ILE:HG21	1:E:387:VAL:CG2	2.24	0.68
1:G:6:TYR:OH	1:G:189:THR:CG2	2.42	0.68
1:G:485:PHE:O	1:G:487:ARG:N	2.27	0.68
1:C:397:GLU:O	1:C:401:ILE:CG1	2.42	0.68
1:E:417:ASN:ND2	1:E:420:ARG:H	1.90	0.68
1:G:363:TYR:HA	2:G:519:HOH:O	1.87	0.68
1:H:417:ASN:ND2	1:H:420:ARG:H	1.91	0.68
1:B:481:ILE:HG23	1:B:482:ALA:N	2.08	0.68
1:H:136:ARG:HG3	1:H:468:THR:OG1	1.94	0.68
1:D:273:ILE:HG21	1:D:387:VAL:CG2	2.24	0.68
1:E:104:ARG:HE	1:E:153:MET:HE3	1.59	0.68
1:F:177:THR:N	1:F:178:PRO:HD3	2.08	0.68
1:B:415:THR:HB	1:B:417:ASN:H	1.59	0.67
1:H:124:ILE:HB	1:H:132:ASN:HD22	1.59	0.67
1:A:310:LEU:HD21	1:A:363:TYR:HB3	1.76	0.67
1:B:185:VAL:O	1:B:189:THR:HG22	1.94	0.67
1:B:235:GLU:HG2	1:F:238:LYS:HE3	1.76	0.67
1:C:76:GLU:O	1:C:79:SER:HB3	1.93	0.67
1:D:87:SER:OG	1:D:97:SER:OG	2.11	0.67
1:H:329:ARG:NH1	1:H:329:ARG:CG	2.51	0.67
1:B:243:ARG:CB	2:B:524:HOH:O	2.41	0.67
1:E:345:LYS:HD3	1:E:347:LEU:HD23	1.77	0.67
1:F:63:GLU:OE1	1:F:66:ARG:HD2	1.94	0.67
1:H:6:TYR:OH	1:H:189:THR:HG21	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:LEU:O	1:H:155:THR:OG1	2.12	0.67
1:B:317:GLU:OE1	1:G:193:PHE:O	2.13	0.67
1:D:259:ASP:O	1:D:416:GLN:CG	2.42	0.67
1:G:357:ALA:HB3	1:G:358:LEU:CD1	2.24	0.67
1:F:432:MET:CE	1:F:447:PHE:CD1	2.77	0.67
1:A:22:VAL:HG21	1:A:34:ILE:HG21	1.73	0.67
1:E:417:ASN:HD22	1:E:420:ARG:H	1.41	0.67
1:F:338:ILE:HD11	1:F:376:ARG:CD	2.22	0.67
1:C:18:GLY:HA3	2:C:515:HOH:O	1.94	0.67
1:C:25:PRO:HA	1:C:362:PHE:CE2	2.30	0.67
1:E:2:GLN:HA	1:E:2:GLN:HE21	1.59	0.67
1:F:97:SER:HA	1:F:101:ASP:HB2	1.77	0.67
1:A:20:ILE:HD12	1:A:175:GLU:HB3	1.76	0.67
1:A:129:GLY:HA3	1:A:479:ALA:CB	2.24	0.67
1:A:277:GLN:HE21	1:A:320:MET:HG3	1.59	0.67
1:C:441:VAL:N	2:C:530:HOH:O	2.28	0.67
1:E:231:ARG:HH21	1:H:239:SER:C	1.93	0.67
1:F:23:VAL:C	1:F:31:ILE:HD11	2.16	0.67
1:F:335:TYR:CE2	1:F:376:ARG:NH2	2.62	0.67
1:G:277:GLN:HG2	1:G:321:GLY:O	1.95	0.67
1:H:124:ILE:HD13	1:H:124:ILE:N	2.08	0.67
1:F:323:LEU:N	1:F:323:LEU:HD23	2.08	0.67
1:G:220:LYS:HG3	1:G:221:ILE:N	2.10	0.67
1:B:241:LEU:HD13	1:F:248:LEU:HD12	1.77	0.66
1:C:438:TYR:HD2	1:C:439:LYS:HG3	1.59	0.66
1:D:76:GLU:OE1	1:D:110:ARG:NH1	2.28	0.66
1:E:358:LEU:N	1:E:358:LEU:CD1	2.58	0.66
1:H:371:ALA:HB1	1:H:375:ASP:OD2	1.96	0.66
1:B:148:TRP:CH2	1:B:328:ARG:HG3	2.30	0.66
1:D:137:LYS:NZ	1:G:426:ASN:HD22	1.89	0.66
1:D:309:ARG:HD3	1:D:309:ARG:H	1.58	0.66
1:D:415:THR:CG2	1:D:420:ARG:HH11	2.01	0.66
1:F:458:GLU:O	1:F:459:MET:HB2	1.95	0.66
1:C:417:ASN:HD22	1:C:420:ARG:CB	2.08	0.66
1:C:476:ASN:OD1	1:C:479:ALA:HB3	1.96	0.66
1:E:462:GLU:OE2	1:H:136:ARG:NH1	2.29	0.66
1:G:424:MET:O	1:G:428:ILE:HG13	1.96	0.66
1:E:377:VAL:CG2	1:E:386:PHE:HZ	2.04	0.66
1:E:426:ASN:HD22	1:H:137:LYS:HE2	1.60	0.66
1:G:447:PHE:C	1:G:447:PHE:CD2	2.68	0.66
1:H:287:LEU:HD22	1:H:289:LEU:HD21	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LYS:NZ	1:B:377:VAL:O	2.28	0.66
1:B:323:LEU:CD1	1:B:332:VAL:HG21	2.24	0.66
1:B:345:LYS:HB2	1:B:370:GLU:HB3	1.77	0.66
1:B:405:THR:HG21	1:B:407:TYR:HB2	1.78	0.66
1:C:432:MET:HE3	1:C:447:PHE:HD1	1.56	0.66
1:E:34:ILE:O	1:E:34:ILE:HG13	1.91	0.66
1:F:143:ALA:HB1	1:F:212:LEU:HG	1.76	0.66
1:A:114:GLY:O	1:A:118:LYS:NZ	2.22	0.66
1:C:25:PRO:HA	1:C:362:PHE:CD2	2.30	0.66
1:E:175:GLU:CD	1:E:175:GLU:H	1.96	0.66
1:E:295:ASP:O	1:E:299:GLU:HB2	1.96	0.66
1:F:1:MET:CG	1:F:1:MET:O	2.44	0.66
1:D:312:ASP:OD1	1:D:313:PRO:HD2	1.96	0.66
1:D:485:PHE:HE2	1:G:308:ILE:HD11	1.59	0.66
1:E:462:GLU:CD	1:H:136:ARG:HH12	1.99	0.66
1:F:2:GLN:HE21	1:F:2:GLN:CA	2.06	0.66
1:G:340:ILE:O	1:G:342:GLN:N	2.29	0.66
1:H:92:HIS:HD2	1:H:101:ASP:OD2	1.78	0.66
1:B:210:GLN:NE2	1:B:214:GLU:OE2	2.29	0.66
1:C:340:ILE:CG2	1:C:341:GLU:N	2.59	0.66
1:E:258:GLU:CG	1:E:290:HIS:CD2	2.79	0.66
1:G:358:LEU:HB3	1:G:363:TYR:CE2	2.31	0.66
1:C:94:ILE:HG12	1:C:98:ARG:HD2	1.78	0.65
1:G:175:GLU:HG3	1:G:203:GLY:O	1.96	0.65
1:G:458:GLU:O	1:G:459:MET:CB	2.43	0.65
1:B:137:LYS:CG	1:B:471:ARG:HG3	2.24	0.65
1:B:468:THR:OG1	2:B:514:HOH:O	2.14	0.65
1:E:442:SER:OG	2:H:509:HOH:O	2.14	0.65
1:F:210:GLN:OE1	1:F:210:GLN:N	2.30	0.65
1:G:158:LYS:HE2	1:G:458:GLU:OE2	1.95	0.65
1:A:15:VAL:HG13	1:A:16:ALA:N	2.12	0.65
1:B:320:MET:HE3	1:B:385:PRO:HB3	1.77	0.65
1:D:158:LYS:HD3	1:D:458:GLU:OE2	1.95	0.65
1:D:457:ARG:HG2	1:D:457:ARG:NH1	2.07	0.65
1:E:221:ILE:O	1:E:221:ILE:CG2	2.44	0.65
1:E:262:ILE:HD11	1:E:293:ILE:HB	1.78	0.65
1:B:89:ASN:O	1:B:89:ASN:ND2	2.30	0.65
1:B:190:GLU:OE1	2:B:525:HOH:O	2.14	0.65
1:A:100:LEU:O	1:A:104:ARG:CG	2.42	0.65
1:A:157:TRP:O	2:A:501:HOH:O	2.13	0.65
1:A:226:SER:OG	1:A:229:THR:CG2	2.41	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ALA:O	2:C:515:HOH:O	2.15	0.65
1:G:94:ILE:HD13	1:G:314:MET:HE1	1.75	0.65
1:B:88:LEU:N	1:B:314:MET:HE1	2.12	0.65
1:B:115:MET:HE1	1:B:461:PHE:CD1	2.32	0.65
1:B:288:ILE:HG22	1:B:392:PHE:CD2	2.31	0.65
1:B:429[A]:HIS:CE1	1:B:450:VAL:HG11	2.32	0.65
1:D:4:GLN:HB3	1:D:12:VAL:O	1.97	0.65
1:D:188:MET:CE	1:D:198:VAL:HG21	2.27	0.65
1:H:26:HIS:HD1	1:H:363:TYR:HH	0.67	0.65
1:B:329:ARG:HD2	1:B:329:ARG:C	2.17	0.65
1:B:474:TRP:HB2	1:F:434:TRP:HA	1.79	0.65
1:D:188:MET:HE1	1:D:198:VAL:CG1	2.26	0.65
1:F:290:HIS:HD2	1:F:292:ASP:H	1.45	0.65
1:F:432:MET:HE1	1:F:447:PHE:CD1	2.31	0.65
1:A:228:ALA:O	1:A:232:ARG:CZ	2.45	0.65
1:B:263:GLU:HG3	1:B:300:ARG:NH2	2.12	0.65
1:C:80:GLU:OE1	1:C:84:GLN:NE2	2.30	0.65
1:C:201:VAL:O	1:C:201:VAL:CG1	2.45	0.65
1:D:183:ARG:NH1	1:D:186:GLU:OE1	2.30	0.65
1:E:42:VAL:HG13	1:E:212:LEU:CD1	2.24	0.65
1:E:94:ILE:HA	1:E:97:SER:OG	1.96	0.65
1:G:310:LEU:CD1	1:G:320:MET:HG2	2.12	0.65
1:A:201:VAL:O	1:A:201:VAL:CG1	2.45	0.65
1:F:18:GLY:HA3	2:F:504:HOH:O	1.96	0.65
1:F:221:ILE:HB	1:F:242:LYS:HD3	1.77	0.65
1:H:25:PRO:HB2	1:H:322:PRO:HG2	1.78	0.65
1:C:480:LYS:O	1:C:480:LYS:HG2	1.94	0.65
1:E:104:ARG:HD2	1:E:153:MET:HE2	1.79	0.65
1:G:87:SER:HB2	1:G:94:ILE:HD12	1.68	0.65
1:B:201:VAL:O	1:B:201:VAL:CG1	2.45	0.64
1:C:20:ILE:HD13	1:C:175:GLU:HB3	1.79	0.64
1:D:201:VAL:O	1:D:201:VAL:CG1	2.45	0.64
1:D:404:ASN:O	1:D:404:ASN:ND2	2.30	0.64
1:H:251:LYS:HD3	1:H:380:GLU:O	1.97	0.64
1:B:137:LYS:CE	1:F:426:ASN:OD1	2.45	0.64
1:B:328:ARG:NH1	1:B:331:ARG:NE	2.45	0.64
1:B:479:ALA:CB	1:B:480:LYS:HE2	2.25	0.64
1:C:302:ILE:HD11	1:C:347:LEU:HB2	1.78	0.64
1:E:355:ASP:OD2	1:E:355:ASP:N	2.30	0.64
1:F:89:ASN:O	1:F:89:ASN:ND2	2.29	0.64
1:G:273:ILE:HD13	1:G:285:SER:CA	2.24	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:GLY:C	1:H:100:LEU:CD2	2.59	0.64
1:A:273:ILE:HD13	1:A:285:SER:HA	1.79	0.64
1:A:342:GLN:O	1:A:342:GLN:NE2	2.30	0.64
1:A:112:PHE:HA	1:A:115:MET:HB3	1.77	0.64
1:B:405:THR:CG2	1:B:406:GLU:N	2.60	0.64
1:C:117:ASP:OD1	1:C:118:LYS:NZ	2.30	0.64
1:D:238:LYS:HD3	1:G:235:GLU:HG2	1.78	0.64
1:E:172:LYS:NZ	1:E:173:PRO:O	2.30	0.64
1:E:345:LYS:HD3	1:E:347:LEU:CD2	2.27	0.64
1:E:396:GLU:OE1	1:E:396:GLU:N	2.30	0.64
1:F:74:ARG:HG3	1:F:187:LEU:HD22	1.80	0.64
1:F:339:ALA:HB2	1:F:377:VAL:CG2	2.24	0.64
1:H:89:ASN:ND2	1:H:89:ASN:O	2.30	0.64
1:H:183:ARG:NH1	1:H:186:GLU:OE1	2.30	0.64
1:A:342:GLN:NE2	1:A:375:ASP:OD1	2.31	0.64
1:B:238:LYS:HD3	1:F:231:ARG:O	1.97	0.64
1:E:358:LEU:N	1:E:358:LEU:HD12	2.13	0.64
1:G:356:LYS:O	1:G:358:LEU:N	2.30	0.64
1:C:152:LEU:CD1	1:C:184:ILE:CD1	2.75	0.64
1:D:277:GLN:NE2	1:D:321:GLY:H	1.94	0.64
1:F:330:ASP:OD1	1:F:330:ASP:N	2.30	0.64
1:A:220:LYS:NZ	1:A:245:GLN:HB2	2.13	0.64
1:A:355:ASP:C	1:A:357:ALA:N	2.46	0.64
1:B:88:LEU:CA	1:B:314:MET:HE3	2.27	0.64
1:B:479:ALA:CB	1:B:480:LYS:CD	2.71	0.64
1:E:117:ASP:OD1	1:E:117:ASP:N	2.30	0.64
1:F:311:GLY:O	1:F:313:PRO:HD3	1.98	0.64
1:H:302:ILE:O	1:H:306:LYS:CG	2.46	0.64
1:B:235:GLU:HG2	1:F:238:LYS:CD	2.27	0.64
1:D:39:ALA:O	1:D:43:ASP:OD1	2.15	0.64
1:E:417:ASN:HD22	1:E:420:ARG:HB2	1.63	0.64
1:E:477:VAL:HG23	1:E:478:ASP:HB2	1.78	0.64
1:G:94:ILE:O	1:G:98:ARG:HG3	1.98	0.64
1:A:417:ASN:HD22	1:A:420:ARG:HB2	1.63	0.64
1:C:315:ASP:OD1	1:C:316:PRO:CD	2.45	0.64
1:E:220:LYS:HG3	1:E:221:ILE:N	2.12	0.64
1:A:89:ASN:O	1:A:89:ASN:ND2	2.30	0.64
1:A:338:ILE:HD13	1:A:376:ARG:NH2	2.13	0.64
1:E:251:LYS:HG3	1:E:286:ARG:HD3	1.79	0.64
1:G:404:ASN:CG	1:G:404:ASN:O	2.36	0.64
1:B:320:MET:HE1	1:B:385:PRO:CB	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:GLU:O	1:E:90:THR:OG1	2.13	0.63
1:F:43:ASP:OD1	1:F:215:HIS:NE2	2.32	0.63
1:G:94:ILE:O	1:G:98:ARG:CG	2.46	0.63
1:H:39:ALA:O	1:H:42:VAL:HG22	1.97	0.63
1:A:76:GLU:OE2	1:A:110:ARG:NH1	2.31	0.63
1:C:287:LEU:HD22	1:C:289:LEU:HD21	1.80	0.63
1:F:404:ASN:C	1:F:405:THR:HG23	2.17	0.63
1:G:310:LEU:CD2	1:G:353:PRO:CG	2.75	0.63
1:G:464:ILE:O	1:G:468:THR:OG1	2.14	0.63
1:H:406:GLU:OE1	1:H:406:GLU:HA	1.97	0.63
1:D:71:LEU:O	1:D:71:LEU:HD12	1.98	0.63
1:F:34:ILE:O	1:F:34:ILE:HG13	1.91	0.63
1:C:175:GLU:OE1	1:C:175:GLU:N	2.30	0.63
1:G:8:ASP:OD1	1:G:48:ALA:HB1	1.99	0.63
1:H:377:VAL:HG21	1:H:386:PHE:HZ	1.58	0.63
1:C:25:PRO:HB2	1:C:322:PRO:HG2	1.79	0.63
1:C:338:ILE:HD11	1:C:376:ARG:HB2	1.80	0.63
1:F:458:GLU:O	1:F:459:MET:CB	2.46	0.63
1:A:231:ARG:O	1:C:238:LYS:HE2	1.97	0.63
1:C:23:VAL:HG13	1:C:29:SER:O	1.98	0.63
1:D:374:GLN:N	1:D:374:GLN:OE1	2.30	0.63
1:F:220:LYS:HE2	1:F:245:GLN:HG3	1.79	0.63
1:F:320:MET:CE	1:F:366:PRO:HG3	2.29	0.63
1:G:86:GLU:O	1:G:90:THR:OG1	2.09	0.63
1:B:148:TRP:HH2	1:B:328:ARG:HG3	1.62	0.63
1:E:104:ARG:CD	1:E:153:MET:CE	2.77	0.63
1:E:334:SER:O	1:E:338:ILE:HG23	1.99	0.63
1:F:18:GLY:O	1:F:36:ALA:N	2.25	0.63
1:F:94:ILE:HG22	1:F:313:PRO:O	1.99	0.63
1:F:227:THR:HG22	1:F:231:ARG:HH11	1.63	0.63
1:G:92:HIS:O	1:G:93:PRO:C	2.35	0.63
1:G:94:ILE:CD1	1:G:314:MET:HE1	2.29	0.63
1:G:327:LEU:HD22	1:G:331:ARG:CD	2.28	0.63
1:H:90:THR:CG2	1:H:92:HIS:ND1	2.62	0.63
1:B:245:GLN:HB3	2:B:519:HOH:O	1.98	0.63
1:D:408:GLY:N	1:D:453:SER:OG	2.31	0.63
1:F:23:VAL:C	1:F:31:ILE:CD1	2.67	0.63
1:F:396:GLU:OE1	1:F:396:GLU:N	2.30	0.63
1:G:408:GLY:O	1:G:430:ALA:CA	2.45	0.63
1:H:273:ILE:O	1:H:273:ILE:HG13	1.99	0.63
1:H:304:LEU:HD12	1:H:304:LEU:O	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:OD2	1:A:127:ASP:N	2.30	0.63
1:B:76:GLU:CD	1:B:110:ARG:HH11	2.00	0.63
1:D:61:ALA:HB1	1:D:116:ALA:O	1.99	0.63
1:E:231:ARG:NE	1:H:238:LYS:O	2.30	0.63
1:E:259:ASP:OD1	1:E:415:THR:CG2	2.46	0.63
1:H:90:THR:O	1:H:324:THR:HG22	1.99	0.63
1:H:377:VAL:CG2	1:H:386:PHE:CZ	2.82	0.63
1:B:56:TRP:CZ2	1:B:64:ARG:HG2	2.33	0.62
1:B:479:ALA:HB3	1:B:480:LYS:HG2	1.80	0.62
1:D:376:ARG:HD2	1:D:380:GLU:OE2	1.99	0.62
2:E:525:HOH:O	1:H:426:ASN:HB2	1.99	0.62
1:F:162:ALA:HB3	1:F:169:ILE:HD11	1.81	0.62
1:G:6:TYR:OH	1:G:189:THR:HG21	1.99	0.62
1:G:87:SER:HB3	1:G:314:MET:CE	2.29	0.62
1:G:476:ASN:OD1	1:G:479:ALA:CB	2.46	0.62
1:C:213:ALA:HA	1:C:221:ILE:HG13	1.81	0.62
1:D:188:MET:CE	1:D:198:VAL:HG11	2.26	0.62
1:D:376:ARG:HD3	1:D:380:GLU:OE2	1.99	0.62
1:D:481:ILE:CG2	1:D:482:ALA:N	2.62	0.62
1:H:329:ARG:NE	1:H:330:ASP:OD1	2.33	0.62
1:D:485:PHE:CE2	1:G:308:ILE:HD11	2.34	0.62
1:G:108:CYS:HB3	1:G:156:SER:HB2	1.81	0.62
1:A:15:VAL:HG11	1:A:40:ALA:CB	2.29	0.62
1:A:480:LYS:N	2:A:528:HOH:O	2.30	0.62
1:B:401:ILE:O	1:B:404:ASN:CB	2.41	0.62
1:F:409:LEU:O	1:F:432:MET:HG2	1.99	0.62
1:G:173:PRO:HG3	1:G:181:THR:HG21	1.81	0.62
1:D:185:VAL:HA	1:D:188:MET:HG3	1.80	0.62
1:E:153:MET:O	1:E:156:SER:OG	2.18	0.62
1:A:406:GLU:OE1	1:A:406:GLU:HA	1.97	0.62
1:B:486:LYS:O	1:B:487:ARG:C	2.38	0.62
1:C:42:VAL:O	1:C:46:VAL:HG23	1.99	0.62
1:D:53:PHE:CZ	1:D:140:GLY:HA2	2.34	0.62
1:F:227:THR:HG21	1:F:231:ARG:HH12	1.64	0.62
1:H:335:TYR:CG	1:H:382:VAL:HG22	2.33	0.62
1:D:100:LEU:O	1:D:104:ARG:HG3	2.00	0.62
1:G:20:ILE:HD11	1:G:204:TYR:CE2	2.35	0.62
1:B:248:LEU:HD11	1:F:241:LEU:HD22	1.80	0.62
1:B:477:VAL:HG22	1:B:478:ASP:N	2.14	0.62
1:E:282:ILE:HG21	1:E:432:MET:HE3	1.79	0.62
1:E:342:GLN:HE22	1:E:376:ARG:H	1.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:THR:O	1:H:159:MET:HB2	1.99	0.62
1:B:88:LEU:N	1:B:314:MET:CE	2.63	0.62
1:B:323:LEU:HD11	1:B:332:VAL:HG21	1.82	0.62
1:C:237:SER:CB	1:C:244:ILE:HD11	2.30	0.62
1:C:356:LYS:HG2	1:C:356:LYS:O	1.97	0.62
1:F:424:MET:O	1:F:428:ILE:HG13	2.00	0.62
1:G:31:ILE:CD1	1:G:88:LEU:HG	2.30	0.62
1:G:85:LEU:O	1:G:85:LEU:HD12	2.00	0.62
1:A:273:ILE:HG21	1:A:387:VAL:HG21	1.79	0.62
1:B:235:GLU:HG2	1:F:238:LYS:HD2	1.82	0.62
1:C:119:ILE:CD1	1:C:464:ILE:HD12	2.30	0.62
1:D:414:TRP:CE3	1:D:436:ASN:HA	2.35	0.62
1:G:293:ILE:HD12	1:G:293:ILE:O	1.94	0.62
1:G:309:ARG:NH1	1:G:317:GLU:CB	2.60	0.62
1:B:273:ILE:HG21	1:B:387:VAL:CG2	2.30	0.61
1:B:481:ILE:CB	2:B:515:HOH:O	2.46	0.61
1:D:239:SER:O	1:G:231:ARG:NH2	2.30	0.61
1:F:8:ASP:OD2	1:F:51:ARG:NH2	2.33	0.61
1:F:27:ASP:OD1	1:F:29:SER:N	2.29	0.61
1:A:310:LEU:HD21	1:A:353:PRO:HG2	1.83	0.61
1:F:326:ALA:CB	1:F:362:PHE:CE1	2.83	0.61
1:A:262:ILE:O	1:A:266:VAL:HG23	2.00	0.61
1:E:157:TRP:CZ2	1:E:441:VAL:HG11	2.35	0.61
1:B:358:LEU:N	1:B:358:LEU:CD1	2.62	0.61
1:B:450:VAL:CG1	1:B:451:GLY:N	2.63	0.61
1:G:87:SER:HB2	1:G:94:ILE:HD11	1.80	0.61
1:H:49:ALA:O	1:H:168:THR:HG21	2.01	0.61
1:A:59:LEU:HG	1:A:63:GLU:HB3	1.81	0.61
1:B:298:LEU:HD11	1:B:389:VAL:HG11	1.82	0.61
1:D:462:GLU:OE2	1:G:465:HIS:NE2	2.16	0.61
1:H:417:ASN:HD22	1:H:420:ARG:CB	2.14	0.61
1:B:158:LYS:HD3	1:B:458:GLU:OE2	2.00	0.61
1:B:481:ILE:N	2:B:515:HOH:O	2.33	0.61
1:C:354:ASP:C	1:C:354:ASP:OD2	2.37	0.61
1:B:81:GLU:HB2	2:B:518:HOH:O	1.95	0.61
1:F:100:LEU:O	1:F:104:ARG:HG3	2.01	0.61
1:F:417:ASN:ND2	1:F:420:ARG:H	1.98	0.61
1:G:136:ARG:HH21	1:G:470:ALA:HB2	1.65	0.61
1:H:142:VAL:HG11	1:H:467:TYR:HE2	1.66	0.61
1:B:152:LEU:CD1	1:B:184:ILE:HD12	2.27	0.61
1:D:61:ALA:HB1	1:D:116:ALA:C	2.20	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:GLN:HG3	1:E:320:MET:HG3	1.81	0.61
1:F:22:VAL:CG2	1:F:34:ILE:HG21	2.30	0.61
1:F:230:GLY:O	1:F:234:VAL:HG23	2.01	0.61
1:G:148:TRP:CA	1:G:177:THR:HG21	2.30	0.61
1:B:185:VAL:O	1:B:189:THR:CG2	2.49	0.61
1:F:381:GLU:CG	1:F:381:GLU:O	2.48	0.61
1:H:49:ALA:CB	1:H:168:THR:HG21	2.18	0.61
1:B:152:LEU:HD12	1:B:184:ILE:HD13	1.82	0.61
1:E:273:ILE:HD12	1:E:273:ILE:C	2.17	0.61
1:G:310:LEU:HD23	1:G:353:PRO:CG	2.31	0.61
1:H:61:ALA:HB1	1:H:116:ALA:O	1.98	0.61
1:H:259:ASP:OD1	1:H:415:THR:CG2	2.42	0.61
1:A:477:VAL:HG22	1:A:478:ASP:N	2.15	0.60
1:B:137:LYS:HE2	1:F:426:ASN:OD1	2.00	0.60
1:E:261:ASN:C	1:E:261:ASN:OD1	2.39	0.60
1:F:310:LEU:HD21	1:F:363:TYR:HB3	1.81	0.60
1:A:25:PRO:HB2	1:A:322:PRO:HG2	1.82	0.60
1:A:213:ALA:O	1:A:242:LYS:HE3	2.01	0.60
1:A:481:ILE:CG1	1:A:482:ALA:H	2.09	0.60
1:C:18:GLY:CA	2:C:515:HOH:O	2.48	0.60
1:C:287:LEU:HD12	1:C:387:VAL:HG21	1.81	0.60
1:D:370:GLU:OE2	1:D:391:ARG:NH1	2.34	0.60
1:D:481:ILE:CG2	1:D:482:ALA:H	2.13	0.60
1:E:290:HIS:CE1	1:E:393:SER:O	2.53	0.60
1:A:228:ALA:O	1:A:232:ARG:NH2	2.34	0.60
1:C:63[A]:GLU:OE1	1:C:66:ARG:CZ	2.48	0.60
1:E:248:LEU:CD1	1:H:241:LEU:HD22	2.30	0.60
1:G:21:ASP:HB3	1:G:30:LEU:HD12	1.79	0.60
1:G:257:PHE:HZ	1:G:424:MET:CE	2.14	0.60
1:G:325:SER:C	1:G:362:PHE:CD2	2.74	0.60
1:H:337:ASP:HA	1:H:340:ILE:HD12	1.83	0.60
1:H:417:ASN:HD22	1:H:420:ARG:H	1.46	0.60
1:A:309:ARG:N	1:A:319:GLU:OE1	2.22	0.60
1:F:351:LYS:O	1:F:365:GLU:CG	2.48	0.60
1:G:221:ILE:O	1:G:221:ILE:HG23	2.00	0.60
1:C:332:VAL:O	1:C:332:VAL:HG12	2.01	0.60
1:D:53:PHE:CE1	1:D:140:GLY:HA2	2.36	0.60
1:D:137:LYS:HZ3	1:G:426:ASN:ND2	1.94	0.60
1:D:485:PHE:CE2	1:G:308:ILE:CD1	2.84	0.60
1:B:34:ILE:HG13	1:B:34:ILE:O	1.92	0.60
1:D:273:ILE:HD12	1:D:273:ILE:C	2.10	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ASN:OD1	1:E:177:THR:HA	2.02	0.60
1:G:143:ALA:HB1	1:G:212:LEU:HG	1.83	0.60
1:G:157:TRP:CD2	1:G:459:MET:HE2	2.37	0.60
1:H:328:ARG:HE	1:H:383:PHE:HB3	1.63	0.60
1:A:15:VAL:HG11	1:A:40:ALA:HB3	1.83	0.60
1:G:380:GLU:HG2	2:G:523:HOH:O	2.00	0.60
1:D:262:ILE:HG23	1:D:297:PHE:HD1	1.67	0.60
1:E:31:ILE:HD13	1:E:88:LEU:HG	1.83	0.60
1:E:43:ASP:OD1	1:E:215:HIS:NE2	2.35	0.60
1:D:231:ARG:HG2	1:G:238:LYS:HB2	1.84	0.60
1:D:310:LEU:HD23	1:D:353:PRO:CG	2.32	0.60
1:E:392:PHE:CD1	1:E:394:SER:O	2.54	0.60
1:A:93:PRO:O	1:A:96:ASP:HB2	2.01	0.60
1:C:2:GLN:HG3	1:C:11:PHE:CZ	2.37	0.60
1:C:23:VAL:HG11	1:C:28:GLY:O	2.02	0.60
1:E:227:THR:HA	1:E:248:LEU:HB3	1.83	0.60
1:G:26:HIS:CB	2:G:512:HOH:O	2.50	0.60
1:G:221:ILE:O	1:G:221:ILE:HG22	2.02	0.60
1:G:323:LEU:N	1:G:323:LEU:HD23	2.16	0.60
1:G:329:ARG:NH1	1:G:330:ASP:OD1	2.30	0.60
1:H:90:THR:HG22	1:H:92:HIS:ND1	2.16	0.60
1:D:201:VAL:O	1:D:201:VAL:HG12	2.01	0.59
1:E:184:ILE:O	1:E:188:MET:HG3	2.02	0.59
1:F:310:LEU:CD2	1:F:353:PRO:HG3	2.32	0.59
1:F:357:ALA:O	1:F:358:LEU:HD12	2.02	0.59
1:G:257:PHE:HZ	1:G:424:MET:HE2	1.67	0.59
1:G:335:TYR:O	1:G:339:ALA:N	2.34	0.59
1:F:38:GLU:HA	1:F:207:THR:HG21	1.83	0.59
1:D:263:GLU:O	1:D:267:ASN:ND2	2.34	0.59
1:D:477:VAL:CG2	1:D:478:ASP:N	2.66	0.59
1:F:298:LEU:O	1:F:302:ILE:HD12	2.02	0.59
1:C:138:PRO:HG3	1:C:165:ALA:O	2.02	0.59
1:E:283:ALA:O	2:E:527:HOH:O	2.15	0.59
1:A:167:ASN:ND2	1:A:167:ASN:H	2.01	0.59
1:B:38:GLU:O	1:B:41:ASP:N	2.32	0.59
1:D:20:ILE:HD13	1:D:175:GLU:HB3	1.85	0.59
1:E:143:ALA:HB1	1:E:212:LEU:HG	1.84	0.59
1:E:479:ALA:C	1:E:480:LYS:HE2	2.22	0.59
1:G:458:GLU:O	1:G:459:MET:HB2	2.01	0.59
1:H:261:ASN:C	1:H:261:ASN:OD1	2.39	0.59
1:B:201:VAL:O	1:B:201:VAL:HG12	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ARG:NH2	1:C:330:ASP:OD1	2.30	0.59
1:E:399:LEU:HD11	1:E:427:ALA:HB1	1.84	0.59
1:G:347:LEU:HD11	1:G:370:GLU:CG	2.18	0.59
1:H:21:ASP:HB3	1:H:30:LEU:CD1	2.32	0.59
1:A:102:VAL:CB	1:A:103:PRO:HD3	2.31	0.59
1:B:243:ARG:CA	2:B:524:HOH:O	2.50	0.59
1:B:320:MET:HE3	1:B:385:PRO:CB	2.32	0.59
1:D:220:LYS:NZ	2:D:501:HOH:O	2.07	0.59
1:D:309:ARG:HD3	1:D:309:ARG:N	2.17	0.59
1:E:76:GLU:O	1:E:79:SER:HB3	2.02	0.59
1:E:195:LYS:O	1:E:195:LYS:HG2	2.00	0.59
1:G:99:GLY:O	1:G:103:PRO:HG2	2.02	0.59
1:G:335:TYR:CZ	2:G:523:HOH:O	2.47	0.59
1:B:102:VAL:HB	1:B:103:PRO:HD3	1.85	0.59
1:E:417:ASN:HD22	1:E:420:ARG:CB	2.16	0.59
1:G:94:ILE:CD1	1:G:314:MET:CE	2.76	0.59
1:H:269:ALA:O	1:H:273:ILE:HG22	2.03	0.59
1:A:251:LYS:CE	2:A:524:HOH:O	2.45	0.59
1:E:74:ARG:CZ	1:E:190:GLU:OE1	2.44	0.59
1:F:40:ALA:O	1:F:44:LEU:HD12	2.03	0.59
1:F:486:LYS:O	1:F:487:ARG:C	2.39	0.59
1:G:340:ILE:C	1:G:342:GLN:N	2.56	0.59
1:A:87:SER:OG	1:A:92:HIS:O	2.10	0.58
1:B:479:ALA:HB2	1:B:480:LYS:HZ3	1.67	0.58
1:C:137:LYS:HG3	1:C:471:ARG:HG3	1.83	0.58
1:G:380:GLU:CG	2:G:523:HOH:O	2.51	0.58
1:H:30:LEU:HD21	1:H:33:ARG:NE	2.17	0.58
1:A:201:VAL:O	1:A:201:VAL:HG12	2.01	0.58
1:D:417:ASN:HD22	1:D:420:ARG:H	1.48	0.58
1:E:31:ILE:HD11	1:E:88:LEU:HG	1.86	0.58
1:E:42:VAL:O	1:E:46:VAL:HG23	2.03	0.58
1:E:153:MET:HG3	2:E:510:HOH:O	2.03	0.58
1:F:94:ILE:O	1:F:94:ILE:CG1	2.48	0.58
1:F:437:CYS:SG	1:F:440:ARG:HG3	2.43	0.58
1:H:76:GLU:O	1:H:79:SER:HB3	2.02	0.58
1:H:288:ILE:HG22	1:H:392:PHE:CD2	2.39	0.58
1:E:277:GLN:HG3	1:E:320:MET:HG2	1.83	0.58
1:G:6:TYR:CD2	1:G:185:VAL:HG21	2.39	0.58
1:G:56:TRP:CH2	1:G:64:ARG:HG2	2.39	0.58
1:H:183:ARG:O	1:H:183:ARG:HD2	2.03	0.58
1:A:162:ALA:O	1:A:167:ASN:ND2	2.30	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LYS:O	1:A:239:SER:C	2.42	0.58
1:C:186:GLU:O	1:C:190:GLU:HG3	2.03	0.58
1:D:137:LYS:HG3	1:D:471:ARG:HG3	1.83	0.58
1:D:374:GLN:CD	1:D:374:GLN:H	2.05	0.58
1:E:74:ARG:NH2	1:E:190:GLU:CD	2.50	0.58
1:G:23:VAL:HG13	1:G:24:SER:N	2.17	0.58
1:G:92:HIS:C	1:G:93:PRO:O	2.40	0.58
1:A:23:VAL:HG12	1:A:24:SER:N	2.17	0.58
1:A:305:ALA:HA	1:A:308:ILE:HD12	1.85	0.58
1:B:273:ILE:CG1	1:B:387:VAL:HG22	2.32	0.58
1:F:149:ASN:ND2	1:F:150:PHE:CD1	2.71	0.58
1:G:31:ILE:HD13	1:G:88:LEU:HG	1.85	0.58
1:G:459:MET:N	1:G:463:ALA:HB2	2.18	0.58
1:H:8:ASP:OD1	2:H:507:HOH:O	2.17	0.58
1:C:201:VAL:O	1:C:201:VAL:HG12	2.01	0.58
1:C:339:ALA:O	1:C:344:GLY:HA3	2.03	0.58
1:C:415:THR:CG2	1:C:416:GLN:H	2.09	0.58
1:D:5:LEU:HB2	1:D:12:VAL:HG12	1.84	0.58
1:C:151:PRO:HG2	1:C:177:THR:HB	1.86	0.58
1:D:277:GLN:HE21	1:D:320:MET:HG2	1.69	0.58
1:D:326:ALA:HB2	1:D:362:PHE:CE1	2.39	0.58
1:E:155:THR:HG22	1:E:181:THR:HG23	1.85	0.58
1:E:175:GLU:HG2	1:E:204:TYR:CD1	2.39	0.58
1:G:97:SER:CA	1:G:101:ASP:HB2	2.32	0.58
1:G:293:ILE:O	1:G:293:ILE:HD13	2.04	0.58
1:H:100:LEU:HD23	1:H:100:LEU:N	2.09	0.58
1:A:417:ASN:HD22	1:A:420:ARG:CB	2.16	0.58
1:C:19:THR:HG23	1:C:20:ILE:N	2.17	0.58
1:C:20:ILE:HG21	1:C:175:GLU:HB3	1.86	0.58
1:C:143:ALA:HB1	1:C:212:LEU:HG	1.84	0.58
1:F:313:PRO:HB2	1:F:314:MET:HE1	1.84	0.58
1:E:137:LYS:NZ	1:H:426:ASN:OD1	2.34	0.58
1:E:392:PHE:CE1	1:E:394:SER:O	2.57	0.58
1:G:148:TRP:CD1	1:G:148:TRP:N	2.72	0.58
1:G:323:LEU:O	1:G:362:PHE:HB2	2.04	0.58
1:G:357:ALA:HB3	1:G:358:LEU:HD11	1.86	0.58
1:E:87:SER:HB3	1:E:314:MET:CE	2.33	0.58
1:H:74:ARG:NE	1:H:77:GLU:OE1	2.37	0.58
1:A:309:ARG:HD3	1:A:309:ARG:C	2.24	0.57
1:A:477:VAL:HG23	1:A:478:ASP:HB2	1.85	0.57
1:B:258:GLU:HG2	1:B:290:HIS:NE2	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:MET:CE	1:B:385:PRO:HG3	2.34	0.57
1:F:145:ILE:HB	1:F:223:PHE:HD1	1.68	0.57
1:G:356:LYS:O	1:G:357:ALA:C	2.40	0.57
1:B:159:MET:HG2	1:B:169:ILE:HD13	1.86	0.57
1:B:186:GLU:HA	1:B:189:THR:HG23	1.86	0.57
1:C:259:ASP:OD2	1:C:415:THR:HG22	2.04	0.57
1:D:445:SER:HB2	1:G:132:ASN:ND2	2.19	0.57
1:E:452:GLN:HG2	1:H:240:ASN:O	2.03	0.57
1:F:70:LYS:HB3	1:F:191:VAL:CG1	2.33	0.57
1:F:163:LEU:HG	1:F:169:ILE:HD12	1.86	0.57
1:F:338:ILE:HD13	1:F:376:ARG:HD3	1.85	0.57
1:G:136:ARG:HG3	1:G:468:THR:HB	1.86	0.57
1:G:356:LYS:C	1:G:358:LEU:N	2.57	0.57
1:H:153:MET:O	1:H:156:SER:OG	2.22	0.57
1:B:25:PRO:HB2	1:B:322:PRO:HG2	1.85	0.57
1:B:312:ASP:OD1	1:B:313:PRO:CD	2.51	0.57
1:B:90:THR:HG22	1:B:177:THR:CG2	2.34	0.57
1:C:384:GLY:O	1:C:386:PHE:N	2.36	0.57
1:E:124:ILE:HD13	1:E:124:ILE:N	2.19	0.57
1:E:175:GLU:HG3	1:E:203:GLY:O	2.05	0.57
1:F:257:PHE:CB	1:F:415:THR:HG23	2.30	0.57
1:G:94:ILE:HD12	1:G:97:SER:HG	1.69	0.57
1:B:288:ILE:HG22	1:B:392:PHE:HD2	1.69	0.57
1:E:275:HIS:ND1	1:E:439:LYS:NZ	2.52	0.57
1:G:335:TYR:CE2	2:G:523:HOH:O	2.57	0.57
1:H:322:PRO:HB3	1:H:363:TYR:CD2	2.40	0.57
1:A:241:LEU:CD1	1:C:248:LEU:CD1	2.81	0.57
1:G:70:LYS:NZ	1:G:191:VAL:O	2.38	0.57
1:G:238:LYS:O	1:G:239:SER:C	2.42	0.57
1:G:351:LYS:O	1:G:365:GLU:HB2	2.05	0.57
1:G:369:VAL:O	1:G:369:VAL:CG1	2.53	0.57
1:A:335:TYR:OH	1:A:380:GLU:OE1	2.17	0.57
1:B:350:GLY:O	1:B:351:LYS:HB2	2.04	0.57
1:E:277:GLN:OE1	2:E:509:HOH:O	2.18	0.57
1:G:149:ASN:N	1:G:149:ASN:OD1	2.33	0.57
1:H:230:GLY:O	1:H:234:VAL:HG23	2.04	0.57
1:B:117:ASP:OD1	1:B:118:LYS:NZ	2.36	0.57
1:C:269:ALA:O	1:C:273:ILE:HG22	2.03	0.57
1:E:159:MET:HE1	1:E:171:ILE:HG21	1.86	0.57
1:G:10:ARG:NH1	1:G:12:VAL:HG13	2.07	0.57
1:H:377:VAL:HG22	1:H:386:PHE:CE1	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ARG:HD2	1:F:455:TYR:HB3	1.87	0.57
1:B:417:ASN:ND2	1:B:420:ARG:H	2.03	0.57
1:C:318:THR:HG22	1:C:320:MET:O	2.04	0.57
1:D:117:ASP:OD1	1:D:117:ASP:N	2.30	0.57
1:E:101:ASP:O	2:E:510:HOH:O	2.18	0.57
1:E:320:MET:HE1	1:E:366:PRO:HG3	1.86	0.57
1:G:151:PRO:CB	1:G:177:THR:OG1	2.53	0.57
1:H:152:LEU:CD1	1:H:184:ILE:CD1	2.82	0.57
1:A:117:ASP:OD1	1:A:117:ASP:N	2.33	0.57
1:A:376:ARG:HD2	1:A:380:GLU:OE2	2.02	0.57
1:C:346:VAL:CG1	1:C:348:ALA:O	2.53	0.57
1:C:486:LYS:O	1:C:487:ARG:C	2.42	0.57
1:D:105:THR:OG1	1:D:153:MET:HA	2.04	0.57
1:G:326:ALA:HB2	1:G:362:PHE:CE1	2.40	0.57
1:A:23:VAL:CG1	1:A:24:SER:N	2.68	0.56
1:A:320:MET:HE3	1:A:385:PRO:CG	2.35	0.56
1:B:262:ILE:O	1:B:266:VAL:HG23	2.05	0.56
1:E:426:ASN:ND2	1:H:137:LYS:HE2	2.20	0.56
1:B:15:VAL:HG12	1:B:41:ASP:CG	2.25	0.56
1:B:220:LYS:HE3	1:B:245:GLN:HB2	1.86	0.56
1:B:351:LYS:CG	1:B:352:ALA:N	2.53	0.56
1:D:188:MET:HE3	1:D:198:VAL:HB	1.88	0.56
1:E:356:LYS:HG3	1:E:356:LYS:O	2.04	0.56
1:F:386:PHE:O	1:F:387:VAL:HG22	2.05	0.56
1:A:404:ASN:O	1:A:405:THR:HG23	2.02	0.56
1:B:377:VAL:HG13	1:B:388:THR:CG2	2.35	0.56
1:B:483:PRO:HB3	1:F:267:ASN:OD1	2.06	0.56
1:E:177:THR:N	1:E:178:PRO:HD3	2.20	0.56
1:G:157:TRP:CE2	1:G:459:MET:CE	2.88	0.56
1:G:447:PHE:C	1:G:447:PHE:HD2	2.09	0.56
1:H:358:LEU:HB3	1:H:363:TYR:CD2	2.40	0.56
1:H:358:LEU:HD13	1:H:358:LEU:N	2.21	0.56
1:B:277:GLN:HG3	1:B:320:MET:HG3	1.87	0.56
1:B:335:TYR:HA	1:B:338:ILE:CG2	2.32	0.56
1:C:24:SER:CA	2:C:512:HOH:O	2.50	0.56
1:G:415:THR:HG21	1:G:420:ARG:CD	2.27	0.56
1:H:417:ASN:HD22	1:H:420:ARG:HB2	1.71	0.56
1:A:152:LEU:HD12	1:A:184:ILE:HD13	1.87	0.56
1:D:10:ARG:CG	1:D:10:ARG:NH1	2.49	0.56
1:D:162:ALA:HB3	1:D:169:ILE:HD11	1.88	0.56
1:E:87:SER:HB3	1:E:314:MET:HE1	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:HIS:N	2:G:512:HOH:O	1.89	0.56
1:G:235:GLU:O	1:G:238:LYS:HG2	2.05	0.56
1:B:290:HIS:CD2	1:B:292:ASP:H	2.24	0.56
1:C:434:TRP:CD1	1:C:440:ARG:HB2	2.40	0.56
1:C:246:LEU:HB3	1:C:248:LEU:HD21	1.87	0.56
1:F:94:ILE:HD11	1:F:98:ARG:NH2	2.21	0.56
1:H:142:VAL:HG22	1:H:220:LYS:HB3	1.88	0.56
1:H:377:VAL:HG22	1:H:386:PHE:HE1	1.69	0.56
1:E:155:THR:CG2	1:E:181:THR:HG23	2.35	0.56
1:F:441:VAL:HG13	2:F:515:HOH:O	2.04	0.56
1:H:186:GLU:O	1:H:190:GLU:HG3	2.05	0.56
1:A:394:SER:OG	1:A:397:GLU:HB2	2.06	0.56
1:C:302:ILE:CD1	1:C:347:LEU:CB	2.63	0.56
1:D:310:LEU:HD12	1:D:320:MET:HB3	1.88	0.56
1:E:5:LEU:HD11	1:E:37:ALA:HB2	1.88	0.56
1:E:273:ILE:O	1:E:273:ILE:CD1	2.38	0.56
1:E:289:LEU:HD13	1:E:297:PHE:HD2	1.71	0.56
1:A:290:HIS:CD2	1:A:292:ASP:HB2	2.41	0.56
1:D:328:ARG:HA	1:D:328:ARG:NE	2.17	0.56
1:E:159:MET:HE2	1:E:171:ILE:CD1	2.36	0.56
1:H:86:GLU:HG3	1:H:86:GLU:O	2.06	0.56
1:H:379:GLN:NE2	1:H:404:ASN:OD1	2.39	0.56
1:A:481:ILE:CG1	1:A:482:ALA:N	2.54	0.55
1:E:108:CYS:HB3	1:E:156:SER:HB2	1.88	0.55
1:G:175:GLU:CG	1:G:203:GLY:O	2.54	0.55
1:G:327:LEU:HD23	1:G:331:ARG:HD2	1.85	0.55
1:H:335:TYR:O	1:H:338:ILE:HG22	2.06	0.55
1:A:23:VAL:HG12	1:A:24:SER:O	2.07	0.55
1:A:310:LEU:HD22	1:A:353:PRO:HG3	1.87	0.55
1:D:377:VAL:O	1:D:377:VAL:HG13	2.06	0.55
1:F:177:THR:N	1:F:178:PRO:CD	2.70	0.55
1:G:177:THR:N	1:G:178:PRO:HD3	2.20	0.55
1:G:340:ILE:C	1:G:342:GLN:H	2.09	0.55
1:H:221:ILE:HD12	1:H:233:ILE:HG23	1.89	0.55
1:C:27:ASP:OD1	1:C:28:GLY:N	2.40	0.55
1:E:291:LYS:CE	1:E:393:SER:HG	2.11	0.55
1:F:336:ILE:O	1:F:340:ILE:CG1	2.50	0.55
1:G:290:HIS:CD2	1:G:292:ASP:H	2.24	0.55
1:A:445:SER:CB	1:C:132:ASN:HD21	2.19	0.55
1:C:60:GLY:O	1:C:61:ALA:C	2.45	0.55
1:G:20:ILE:HD12	1:G:36:ALA:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD12	1:A:184:ILE:CD1	2.35	0.55
1:B:235:GLU:CG	1:F:238:LYS:HD2	2.36	0.55
1:G:394:SER:OG	1:G:397:GLU:HB2	2.05	0.55
1:G:458:GLU:O	1:G:459:MET:HG2	2.06	0.55
1:H:253:ALA:HB2	1:H:286:ARG:NH2	2.21	0.55
1:E:312:ASP:O	1:E:314:MET:N	2.40	0.55
1:F:338:ILE:HD13	1:F:376:ARG:CD	2.35	0.55
1:B:337:ASP:O	1:B:341:GLU:CG	2.52	0.55
1:C:372:LYS:C	1:C:374:GLN:H	2.09	0.55
1:F:53:PHE:HB3	1:F:54:PRO:HD3	1.88	0.55
1:F:273:ILE:CG2	1:F:387:VAL:HG21	2.32	0.55
1:G:469:GLU:OE1	1:G:471:ARG:NE	2.33	0.55
2:A:515:HOH:O	1:B:374:GLN:N	2.39	0.55
1:D:188:MET:HE3	1:D:198:VAL:HG21	1.88	0.55
1:E:23:VAL:CG1	1:E:24:SER:N	2.70	0.55
1:G:413:LEU:HD11	1:G:435:ILE:HG12	1.88	0.55
1:H:370:GLU:OE1	1:H:391:ARG:NH1	2.40	0.55
1:A:177:THR:N	1:A:178:PRO:HD3	2.22	0.55
1:A:438:TYR:HD2	1:A:439:LYS:HG3	1.72	0.55
1:C:323:LEU:CD1	1:C:332:VAL:HG21	2.37	0.55
1:G:376:ARG:HD2	1:G:376:ARG:N	2.22	0.55
1:H:242:LYS:HG2	2:H:506:HOH:O	2.07	0.55
1:B:479:ALA:CA	1:B:480:LYS:CB	2.72	0.55
1:D:21:ASP:OD1	1:D:33:ARG:CD	2.55	0.55
1:D:485:PHE:HE2	1:G:308:ILE:CD1	2.20	0.55
1:F:231:ARG:O	1:F:235:GLU:HG3	2.07	0.55
1:A:328:ARG:NH1	1:A:331:ARG:HD3	2.22	0.54
1:A:355:ASP:O	1:A:356:LYS:C	2.45	0.54
1:D:305:ALA:HA	1:D:308:ILE:HD12	1.90	0.54
1:D:314:MET:O	1:D:316:PRO:HD3	2.07	0.54
1:E:374:GLN:NE2	1:E:374:GLN:H	2.03	0.54
1:F:235:GLU:O	1:F:238:LYS:CD	2.54	0.54
1:G:37:ALA:HB2	1:G:201:VAL:HG22	1.84	0.54
1:G:289:LEU:HD12	1:G:390:VAL:O	2.07	0.54
1:H:49:ALA:CA	1:H:168:THR:CG2	2.80	0.54
1:H:86:GLU:OE2	1:H:180:SER:OG	2.18	0.54
1:D:151:PRO:O	2:D:507:HOH:O	2.18	0.54
1:E:337:ASP:CG	2:E:523:HOH:O	2.46	0.54
1:F:15:VAL:CG1	1:F:16:ALA:N	2.70	0.54
1:F:15:VAL:HG13	1:F:16:ALA:N	2.20	0.54
1:G:97:SER:HA	1:G:101:ASP:CB	2.30	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:376:ARG:HD2	1:H:380:GLU:OE2	2.07	0.54
1:A:215:HIS:HD2	1:A:217:ASP:H	1.54	0.54
1:C:147:PRO:HD3	1:C:224:THR:HB	1.88	0.54
1:E:42:VAL:HG22	1:E:201:VAL:HG11	1.89	0.54
1:E:66:ARG:HG2	2:E:511:HOH:O	2.07	0.54
1:F:386:PHE:C	1:F:387:VAL:CG2	2.76	0.54
1:A:477:VAL:CG2	1:A:478:ASP:HB2	2.36	0.54
1:E:19:THR:HG21	1:E:33:ARG:HD3	1.89	0.54
1:E:95:ARG:NH2	1:H:484:HIS:O	2.41	0.54
1:E:123:VAL:C	1:E:124:ILE:HD13	2.28	0.54
1:E:185:VAL:HA	1:E:188:MET:HG3	1.87	0.54
1:G:15:VAL:HG11	1:G:40:ALA:CB	2.35	0.54
2:A:515:HOH:O	1:B:373:PRO:HD2	2.06	0.54
1:C:370:GLU:CD	1:C:391:ARG:HH11	2.11	0.54
1:D:417:ASN:ND2	1:D:420:ARG:H	2.06	0.54
1:F:258:GLU:CG	1:F:290:HIS:CE1	2.91	0.54
1:F:377:VAL:HG13	1:F:386:PHE:HE1	1.72	0.54
1:G:22:VAL:CG2	1:G:34:ILE:HG21	2.32	0.54
1:G:326:ALA:N	1:G:362:PHE:CD2	2.75	0.54
1:H:290:HIS:CD2	1:H:292:ASP:H	2.26	0.54
1:B:305:ALA:HA	1:B:308:ILE:HD12	1.90	0.54
1:B:334:SER:O	1:B:337:ASP:HB2	2.08	0.54
1:B:344:GLY:C	1:B:345:LYS:HD2	2.27	0.54
1:D:25:PRO:HB2	1:D:322:PRO:HG2	1.88	0.54
1:D:168:THR:HG22	1:D:197:VAL:HA	1.90	0.54
1:D:188:MET:HE3	1:D:198:VAL:CG2	2.38	0.54
1:E:256:VAL:HG12	1:E:293:ILE:HD13	1.89	0.54
1:F:386:PHE:C	1:F:387:VAL:HG23	2.28	0.54
1:G:340:ILE:O	1:G:343:GLY:N	2.36	0.54
1:A:147:PRO:HG3	1:A:224:THR:HG22	1.90	0.54
1:A:174:SER:C	1:A:176:ILE:H	2.11	0.54
1:E:104:ARG:CD	1:E:153:MET:HE2	2.37	0.54
1:G:220:LYS:HD3	1:G:243:ARG:HB2	1.90	0.54
1:A:415:THR:CG2	1:A:420:ARG:HH11	2.21	0.54
1:A:475:VAL:HG12	1:A:475:VAL:O	2.08	0.54
1:B:345:LYS:N	1:B:345:LYS:HD3	2.19	0.54
1:C:152:LEU:CD1	1:C:184:ILE:HD11	2.38	0.54
1:F:22:VAL:HG23	1:F:34:ILE:HG23	1.88	0.54
1:G:147:PRO:CG	1:G:224:THR:HG22	2.38	0.54
1:G:363:TYR:CD2	2:G:519:HOH:O	2.51	0.54
1:H:42:VAL:HB	1:H:212:LEU:HD13	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ILE:HG21	1:C:350:GLY:O	2.08	0.54
1:C:417:ASN:HD22	1:C:420:ARG:HB2	1.72	0.54
1:D:175:GLU:H	1:D:175:GLU:CD	2.10	0.54
1:E:291:LYS:HE2	1:E:393:SER:CB	2.25	0.54
1:G:19:THR:HA	1:G:34:ILE:O	2.08	0.54
1:G:151:PRO:O	1:G:155:THR:HG23	2.08	0.54
1:A:434:TRP:CD1	1:A:440:ARG:HB2	2.42	0.54
1:A:475:VAL:CG1	1:A:477:VAL:HG12	2.37	0.54
1:B:112:PHE:CZ	1:B:161:PRO:HG3	2.43	0.54
1:B:358:LEU:N	1:B:358:LEU:HD13	2.23	0.54
1:C:183:ARG:NH1	1:C:186:GLU:OE1	2.41	0.54
1:C:320:MET:CE	1:C:385:PRO:HG3	2.38	0.54
1:D:258:GLU:HG2	1:D:290:HIS:CD2	2.43	0.54
1:F:142:VAL:HG22	1:F:220:LYS:HB3	1.90	0.54
1:F:172:LYS:O	1:F:172:LYS:CG	2.55	0.54
1:F:412:GLY:HA3	1:F:438:TYR:CE1	2.43	0.54
1:A:93:PRO:O	1:A:96:ASP:N	2.36	0.53
1:A:215:HIS:O	1:A:242:LYS:NZ	2.40	0.53
1:B:334:SER:O	1:B:338:ILE:HG23	2.07	0.53
1:E:292:ASP:CG	2:E:529:HOH:O	2.42	0.53
1:F:372:LYS:O	1:F:378:CYS:SG	2.63	0.53
1:A:18:GLY:O	1:A:36:ALA:N	2.36	0.53
1:B:316:PRO:HG2	1:G:190:GLU:HG2	1.90	0.53
1:B:415:THR:CG2	1:B:420:ARG:HH11	2.21	0.53
1:C:27:ASP:O	1:C:360:ASN:HB3	2.08	0.53
1:E:415:THR:CG2	1:E:420:ARG:HH11	2.21	0.53
1:E:447:PHE:C	1:E:447:PHE:CD2	2.82	0.53
1:F:70:LYS:HB3	1:F:191:VAL:HG13	1.90	0.53
1:F:172:LYS:O	1:F:172:LYS:HG2	2.08	0.53
1:F:257:PHE:HB2	1:F:415:THR:CG2	2.33	0.53
1:G:303:ALA:C	2:G:513:HOH:O	2.46	0.53
1:H:273:ILE:CD1	1:H:285:SER:HA	2.27	0.53
1:D:412:GLY:HA2	1:D:434:TRP:O	2.08	0.53
1:D:415:THR:HB	1:D:417:ASN:H	1.74	0.53
1:E:241:LEU:HD11	1:H:227:THR:HG23	1.89	0.53
1:E:338:ILE:HD11	1:E:376:ARG:HB2	1.89	0.53
1:F:258:GLU:HG3	1:F:290:HIS:CD2	2.42	0.53
1:G:327:LEU:HD22	1:G:331:ARG:HD3	1.89	0.53
1:G:357:ALA:CB	1:G:358:LEU:HD12	2.38	0.53
1:H:376:ARG:C	1:H:378:CYS:H	2.11	0.53
1:B:81:GLU:CG	2:B:518:HOH:O	2.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ASP:O	1:D:416:GLN:HG3	2.07	0.53
1:F:20:ILE:HD13	1:F:175:GLU:HB3	1.91	0.53
1:F:335:TYR:CD1	1:F:382:VAL:HG13	2.44	0.53
1:G:152:LEU:CD1	1:G:184:ILE:CD1	2.86	0.53
1:G:357:ALA:CB	1:G:358:LEU:CD1	2.86	0.53
1:H:159:MET:CE	1:H:171:ILE:HD13	2.39	0.53
1:H:210:GLN:O	1:H:214:GLU:CG	2.56	0.53
1:H:233:ILE:O	1:H:233:ILE:HG22	2.07	0.53
1:B:235:GLU:O	1:B:238:LYS:HG2	2.09	0.53
1:B:273:ILE:HG21	1:B:387:VAL:HG21	1.89	0.53
1:B:338:ILE:HA	1:B:341:GLU:HG3	1.90	0.53
1:E:404:ASN:C	1:E:405:THR:CG2	2.76	0.53
1:H:102:VAL:CG2	1:H:152:LEU:CD2	2.84	0.53
1:H:288:ILE:HG22	1:H:392:PHE:HD2	1.73	0.53
1:A:86:GLU:OE1	1:A:151:PRO:HD2	2.09	0.53
1:E:266:VAL:CG2	1:E:297:PHE:CD1	2.91	0.53
1:F:80:GLU:OE2	1:F:80:GLU:HA	2.06	0.53
1:F:228:ALA:O	1:F:232:ARG:HG3	2.09	0.53
1:G:182:LEU:O	1:G:185:VAL:HG12	2.08	0.53
1:H:108:CYS:CB	1:H:156:SER:HB2	2.31	0.53
1:A:259:ASP:O	1:A:416:GLN:HG2	2.09	0.53
1:A:399:LEU:HD11	1:A:427:ALA:HB1	1.91	0.53
1:D:392:PHE:CE1	1:D:398:ALA:HB2	2.44	0.53
1:E:152:LEU:HD12	1:E:184:ILE:HD13	1.90	0.53
1:E:159:MET:CE	1:E:171:ILE:HD12	2.37	0.53
1:E:424:MET:O	1:E:428:ILE:HG13	2.09	0.53
1:F:1:MET:O	1:F:1:MET:HG3	2.09	0.53
1:F:386:PHE:O	1:F:387:VAL:CG2	2.57	0.53
1:F:443:PRO:CA	1:F:459:MET:HE2	2.35	0.53
1:G:289:LEU:HD12	1:G:289:LEU:H	1.73	0.53
1:G:310:LEU:HA	1:G:320:MET:O	2.08	0.53
1:H:277:GLN:HG3	1:H:320:MET:CG	2.38	0.53
1:H:458:GLU:O	1:H:459:MET:HB2	2.09	0.53
1:A:474:TRP:HB2	1:C:434:TRP:HA	1.91	0.53
1:C:1:MET:O	1:C:1:MET:HG2	2.06	0.53
1:D:290:HIS:CD2	1:D:292:ASP:H	2.27	0.53
1:D:328:ARG:CA	1:D:328:ARG:NE	2.67	0.53
1:D:338:ILE:HD11	1:D:376:ARG:CB	2.38	0.53
1:E:61:ALA:HB1	1:E:116:ALA:C	2.28	0.53
1:E:262:ILE:CD1	1:E:293:ILE:HB	2.39	0.53
1:F:186:GLU:O	1:F:190:GLU:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:ASN:OD1	1:F:240:ASN:N	2.41	0.53
1:G:179:LEU:N	1:G:179:LEU:HD23	2.24	0.53
1:G:358:LEU:N	1:G:358:LEU:HD13	2.23	0.53
1:A:221:ILE:HD13	1:A:233:ILE:CG2	2.23	0.53
1:A:412:GLY:HA2	1:A:434:TRP:O	2.09	0.53
1:B:88:LEU:CA	1:B:314:MET:CE	2.87	0.53
1:F:256:VAL:HG12	1:F:293:ILE:HD11	1.90	0.53
1:F:277:GLN:HG3	1:F:320:MET:HG2	1.91	0.53
1:G:396:GLU:CD	1:G:396:GLU:N	2.62	0.53
1:B:310:LEU:CD1	1:B:320:MET:HG2	2.38	0.53
1:C:174:SER:C	1:C:176:ILE:N	2.60	0.53
1:C:310:LEU:HD11	2:C:511:HOH:O	2.09	0.53
1:C:399:LEU:HD11	1:C:427:ALA:HB1	1.91	0.53
1:E:308:ILE:HG21	1:E:320:MET:HE3	1.91	0.53
1:F:258:GLU:HG2	1:F:290:HIS:CE1	2.44	0.53
1:F:399:LEU:HD11	1:F:427:ALA:HB1	1.91	0.53
1:G:10:ARG:HH11	1:G:12:VAL:HG12	1.61	0.53
1:G:348:ALA:HB3	1:G:368:VAL:HG23	1.90	0.53
1:A:22:VAL:CG2	1:A:34:ILE:HG22	2.39	0.52
1:A:86:GLU:O	1:A:86:GLU:HG3	2.08	0.52
1:A:147:PRO:CG	1:A:224:THR:HG22	2.40	0.52
1:A:482:ALA:O	1:A:483:PRO:C	2.47	0.52
1:B:296:GLN:O	1:B:300:ARG:HG3	2.09	0.52
1:C:262:ILE:O	1:C:266:VAL:CG2	2.41	0.52
1:E:228:ALA:HB1	1:E:232:ARG:NH2	2.23	0.52
1:E:298:LEU:HD21	1:E:389:VAL:HG21	1.91	0.52
1:E:469:GLU:OE2	1:H:450:VAL:HG22	2.09	0.52
1:F:22:VAL:HG23	1:F:34:ILE:CG2	2.38	0.52
1:G:87:SER:HB3	1:G:314:MET:HE3	1.89	0.52
1:H:339:ALA:O	1:H:344:GLY:N	2.42	0.52
1:A:167:ASN:H	1:A:167:ASN:HD22	1.57	0.52
1:A:217:ASP:CG	1:B:374:GLN:HE22	2.11	0.52
1:C:155:THR:O	1:C:159:MET:HB2	2.09	0.52
1:F:102:VAL:HB	1:F:103:PRO:HD3	1.90	0.52
1:F:277:GLN:NE2	1:F:321:GLY:H	2.07	0.52
1:A:2:GLN:HA	1:A:2:GLN:NE2	2.23	0.52
1:B:235:GLU:CG	1:F:238:LYS:HE3	2.38	0.52
1:C:226:SER:O	1:C:227:THR:C	2.47	0.52
1:E:97:SER:CA	1:E:101:ASP:HB2	2.31	0.52
1:E:289:LEU:HD13	1:E:297:PHE:CD2	2.44	0.52
1:H:221:ILE:HG23	1:H:221:ILE:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:C	1:A:378:CYS:H	2.12	0.52
1:B:214:GLU:HG3	1:B:236:ALA:HB1	1.91	0.52
1:B:477:VAL:CG2	1:B:478:ASP:N	2.72	0.52
1:C:86:GLU:HG3	1:C:86:GLU:O	2.08	0.52
1:D:221:ILE:HG23	1:D:221:ILE:O	2.09	0.52
1:E:93:PRO:CD	1:E:277:GLN:HE22	2.23	0.52
1:E:96:ASP:O	1:E:100:LEU:HB2	2.09	0.52
1:G:20:ILE:HD11	1:G:204:TYR:CZ	2.44	0.52
1:G:434:TRP:HB3	1:G:437:CYS:SG	2.49	0.52
1:G:458:GLU:O	1:G:459:MET:CG	2.57	0.52
1:G:475:VAL:CG1	1:G:477:VAL:HG12	2.37	0.52
1:B:221:ILE:HG23	1:B:221:ILE:O	2.09	0.52
1:D:184:ILE:O	1:D:188:MET:CG	2.57	0.52
1:F:185:VAL:HA	1:F:188:MET:HB2	1.92	0.52
1:G:87:SER:CB	1:G:314:MET:CE	2.87	0.52
1:A:310:LEU:HD22	1:A:353:PRO:CG	2.39	0.52
1:B:92:HIS:CE1	1:B:276:ASN:HD21	2.27	0.52
1:B:470:ALA:HB3	1:F:457:ARG:HE	1.75	0.52
1:C:221:ILE:O	1:C:221:ILE:CG2	2.58	0.52
1:E:25:PRO:HB2	1:E:322:PRO:HG2	1.90	0.52
1:E:412:GLY:HA2	1:E:434:TRP:O	2.09	0.52
1:C:151:PRO:CG	1:C:177:THR:HB	2.40	0.52
1:C:386:PHE:C	1:C:386:PHE:CD1	2.82	0.52
1:D:188:MET:HE3	1:D:198:VAL:CB	2.40	0.52
1:F:322:PRO:HG3	1:F:363:TYR:CZ	2.44	0.52
1:G:373:PRO:HG2	1:G:374:GLN:H	1.75	0.52
1:A:476:ASN:ND2	1:A:480:LYS:HE3	2.24	0.52
1:B:8:ASP:OD1	1:B:195:LYS:HG3	2.09	0.52
1:C:105:THR:OG1	1:C:153:MET:HA	2.09	0.52
1:C:263:GLU:CG	1:C:300:ARG:NH2	2.73	0.52
1:D:188:MET:CE	1:D:198:VAL:CB	2.87	0.52
1:D:351:LYS:HG3	1:D:352:ALA:N	2.03	0.52
1:E:86:GLU:OE1	1:E:151:PRO:HD2	2.09	0.52
1:E:478:ASP:CA	2:E:514:HOH:O	2.50	0.52
1:F:26:HIS:O	1:F:361:GLY:N	2.42	0.52
1:G:95:ARG:HH12	1:G:319:GLU:HG2	1.73	0.52
1:H:124:ILE:N	1:H:124:ILE:CD1	2.73	0.52
1:H:304:LEU:HD12	1:H:304:LEU:C	2.28	0.52
1:A:377:VAL:CG1	1:A:388:THR:CG2	2.86	0.52
1:C:404:ASN:O	1:C:405:THR:CG2	2.57	0.52
1:C:415:THR:HG22	1:C:417:ASN:H	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:MET:CG	1:D:153:MET:O	2.57	0.52
1:D:182:LEU:O	1:D:185:VAL:HG12	2.10	0.52
1:H:92:HIS:CD2	1:H:101:ASP:OD2	2.62	0.52
1:B:151:PRO:HG2	1:B:177:THR:HB	1.92	0.52
1:B:315:ASP:O	1:B:317:GLU:N	2.42	0.52
1:C:31:ILE:HD13	1:C:88:LEU:HG	1.90	0.52
1:D:445:SER:HB2	1:G:132:ASN:HD21	1.74	0.52
1:H:399:LEU:HD11	1:H:427:ALA:HB1	1.91	0.52
1:A:155:THR:HG22	1:A:181:THR:HG23	1.91	0.51
1:B:357:ALA:CB	1:G:12:VAL:HG12	2.34	0.51
1:B:404:ASN:CG	1:B:404:ASN:O	2.48	0.51
1:D:223:PHE:CZ	1:D:229:THR:HG23	2.45	0.51
1:E:61:ALA:HB1	1:E:116:ALA:O	2.09	0.51
1:G:19:THR:HG23	1:G:20:ILE:N	2.24	0.51
1:H:90:THR:HG22	1:H:92:HIS:CE1	2.45	0.51
1:H:412:GLY:HA2	1:H:434:TRP:O	2.09	0.51
1:C:152:LEU:HD12	1:C:184:ILE:CD1	2.40	0.51
1:C:411:SER:OG	1:C:432:MET:O	2.28	0.51
1:E:86:GLU:O	1:E:86:GLU:HG3	2.08	0.51
1:G:94:ILE:O	1:G:98:ARG:HG2	2.11	0.51
1:G:173:PRO:CG	1:G:181:THR:HG21	2.39	0.51
1:B:291:LYS:HG3	1:B:392:PHE:O	2.11	0.51
1:B:376:ARG:O	1:B:380:GLU:HB2	2.11	0.51
1:C:53:PHE:HB3	1:C:54:PRO:HD3	1.92	0.51
1:F:432:MET:HE2	1:F:447:PHE:CD1	2.45	0.51
1:G:137:LYS:O	1:G:468:THR:HG22	2.10	0.51
1:G:330:ASP:O	1:G:334:SER:OG	2.28	0.51
1:H:404:ASN:CG	1:H:404:ASN:O	2.48	0.51
1:A:267:ASN:ND2	1:C:483:PRO:HG3	2.25	0.51
1:B:223:PHE:CZ	1:B:229:THR:HG23	2.45	0.51
1:C:27:ASP:OD1	1:C:27:ASP:C	2.46	0.51
1:F:296:GLN:HE21	1:F:300:ARG:NH1	2.07	0.51
1:G:262:ILE:O	1:G:266:VAL:HG23	2.11	0.51
1:H:323:LEU:HD21	1:H:385:PRO:HD3	1.92	0.51
1:A:404:ASN:C	1:A:405:THR:CG2	2.78	0.51
1:C:174:SER:C	1:C:176:ILE:H	2.14	0.51
1:D:240:ASN:O	1:D:241:LEU:HB2	2.09	0.51
1:E:104:ARG:NH2	1:E:153:MET:HE1	2.24	0.51
1:E:170:VAL:HG11	1:E:212:LEU:HD11	1.92	0.51
1:E:322:PRO:HG3	1:E:363:TYR:CZ	2.46	0.51
1:E:338:ILE:CD1	1:E:376:ARG:HB2	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:229:THR:HA	1:F:232:ARG:HG3	1.93	0.51
1:A:396:GLU:OE1	1:A:396:GLU:N	2.30	0.51
1:B:344:GLY:O	1:B:345:LYS:HD2	2.11	0.51
1:C:191:VAL:HG13	1:C:191:VAL:O	2.11	0.51
1:D:32:THR:HG23	1:D:33:ARG:N	2.25	0.51
1:E:5:LEU:CD1	1:E:37:ALA:HB2	2.40	0.51
1:F:377:VAL:CG1	1:F:377:VAL:O	2.55	0.51
1:G:89:ASN:OD1	1:G:177:THR:HA	2.11	0.51
1:G:328:ARG:O	1:G:332:VAL:HG23	2.10	0.51
1:A:53:PHE:CE1	1:A:140:GLY:HA2	2.46	0.51
1:B:245:GLN:NE2	1:B:457:ARG:O	2.43	0.51
1:B:259:ASP:OD1	1:B:415:THR:CG2	2.55	0.51
1:D:26:HIS:ND1	1:D:363:TYR:OH	2.25	0.51
1:E:26:HIS:ND1	1:E:363:TYR:OH	2.25	0.51
1:F:329:ARG:HD2	2:F:510:HOH:O	2.09	0.51
1:G:172:LYS:O	1:G:172:LYS:CG	2.59	0.51
1:H:119:ILE:HG12	1:H:464:ILE:HG21	1.92	0.51
1:H:352:ALA:HA	1:H:364:VAL:HA	1.92	0.51
1:A:320:MET:CE	1:A:385:PRO:CG	2.88	0.51
1:C:210:GLN:O	1:C:214:GLU:HG3	2.09	0.51
1:E:455:TYR:HB3	1:H:243:ARG:HD2	1.91	0.51
1:F:357:ALA:C	1:F:358:LEU:HD12	2.30	0.51
1:G:102:VAL:HB	1:G:103:PRO:HD3	1.91	0.51
1:B:251:LYS:HG3	1:B:286:ARG:HD3	1.93	0.51
1:C:100:LEU:O	1:C:104:ARG:HG3	2.11	0.51
1:C:332:VAL:O	1:C:332:VAL:CG1	2.59	0.51
1:C:376:ARG:NH1	2:C:506:HOH:O	2.40	0.51
1:D:20:ILE:HG13	1:D:36:ALA:HB2	1.92	0.51
1:E:392:PHE:CE1	1:E:398:ALA:HB2	2.45	0.51
1:F:88:LEU:HA	1:F:314:MET:HE3	1.92	0.51
1:F:403:ASN:O	1:F:405:THR:N	2.42	0.51
1:G:298:LEU:HD21	1:G:389:VAL:HG21	1.92	0.51
1:H:4:GLN:HG3	1:H:11:PHE:HB3	1.93	0.51
1:A:25:PRO:HA	1:A:362:PHE:CE2	2.45	0.51
1:B:4:GLN:HB3	1:B:12:VAL:O	2.11	0.51
1:C:119:ILE:HG12	1:C:464:ILE:HG21	1.91	0.51
1:C:354:ASP:OD2	1:C:354:ASP:O	2.29	0.51
1:C:372:LYS:C	1:C:374:GLN:N	2.65	0.51
1:D:328:ARG:NH1	1:D:383:PHE:HB3	2.11	0.51
1:G:273:ILE:HD12	1:G:283:ALA:HB1	1.93	0.51
1:G:274:PHE:HB3	1:G:320:MET:HE1	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:464:ILE:O	1:H:468:THR:CG2	2.43	0.51
1:A:259:ASP:OD1	1:A:415:THR:CG2	2.55	0.50
1:B:74:ARG:HG2	1:B:191:VAL:HG23	1.92	0.50
1:B:87:SER:OG	1:B:92:HIS:O	2.30	0.50
1:B:412:GLY:HA2	1:B:434:TRP:O	2.11	0.50
1:C:92:HIS:HD2	1:C:101:ASP:OD2	1.94	0.50
1:C:323:LEU:HD11	1:C:332:VAL:HG21	1.91	0.50
1:C:327:LEU:CD2	1:C:331:ARG:HH12	2.22	0.50
1:C:432:MET:CE	1:C:447:PHE:HD1	2.10	0.50
1:C:460:GLY:HA3	2:C:502:HOH:O	2.11	0.50
1:D:446:PRO:HD2	1:G:134:VAL:HG21	1.93	0.50
1:D:481:ILE:HD12	1:G:440:ARG:HH12	1.76	0.50
1:D:485:PHE:CE2	1:G:308:ILE:HG12	2.45	0.50
1:E:241:LEU:HD13	1:H:248:LEU:HD12	1.93	0.50
1:G:356:LYS:C	1:G:358:LEU:H	2.14	0.50
1:A:322:PRO:HG3	1:A:363:TYR:CZ	2.46	0.50
1:A:404:ASN:C	1:A:405:THR:HG23	2.31	0.50
1:B:455:TYR:HB3	1:F:243:ARG:HD2	1.93	0.50
1:C:14:ALA:HB2	1:C:36:ALA:O	2.11	0.50
1:D:25:PRO:HA	1:D:362:PHE:CE2	2.47	0.50
1:D:137:LYS:HZ1	1:G:426:ASN:HD22	1.45	0.50
1:G:210:GLN:O	1:G:214:GLU:HG2	2.12	0.50
1:G:377:VAL:HG21	1:G:386:PHE:CZ	2.47	0.50
1:G:425:ALA:HB2	1:G:435:ILE:HD11	1.93	0.50
1:C:415:THR:HG21	1:C:420:ARG:HD2	1.93	0.50
1:E:20:ILE:HG21	1:E:175:GLU:CB	2.40	0.50
1:F:53:PHE:CZ	1:F:140:GLY:HA2	2.45	0.50
1:F:249:GLY:HA2	1:F:281:CYS:SG	2.51	0.50
1:G:15:VAL:HG12	1:G:41:ASP:OD1	2.11	0.50
1:H:246:LEU:O	1:H:454:GLY:HA3	2.12	0.50
1:H:415:THR:HG21	1:H:420:ARG:HH11	1.76	0.50
1:C:322:PRO:HG3	1:C:363:TYR:CZ	2.46	0.50
1:D:377:VAL:O	1:D:377:VAL:CG1	2.59	0.50
1:E:87:SER:CB	1:E:314:MET:HE1	2.41	0.50
1:F:258:GLU:HG3	1:F:290:HIS:ND1	2.26	0.50
1:F:335:TYR:HE2	1:F:376:ARG:CZ	2.23	0.50
1:G:152:LEU:CD1	1:G:184:ILE:HD11	2.41	0.50
1:G:313:PRO:HG3	1:G:322:PRO:CD	2.41	0.50
1:H:182:LEU:O	1:H:185:VAL:HG12	2.11	0.50
1:H:326:ALA:O	1:H:330:ASP:CG	2.50	0.50
1:A:342:GLN:CD	1:A:375:ASP:OD1	2.50	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:OD1	1:B:478:ASP:O	2.30	0.50
1:E:240:ASN:O	1:H:452:GLN:HG2	2.11	0.50
1:F:205:GLY:O	1:F:210:GLN:OE1	2.30	0.50
1:B:100:LEU:C	1:B:104:ARG:HG3	2.27	0.50
1:B:221:ILE:HD12	1:B:233:ILE:HG23	1.92	0.50
1:B:408:GLY:O	1:B:430:ALA:HA	2.12	0.50
1:B:486:LYS:O	1:B:487:ARG:O	2.30	0.50
1:C:320:MET:HE3	1:C:385:PRO:HG3	1.94	0.50
1:C:412:GLY:HA2	1:C:434:TRP:O	2.11	0.50
1:C:414:TRP:CE3	1:C:436:ASN:HA	2.47	0.50
1:E:137:LYS:HG3	1:E:471:ARG:HG3	1.92	0.50
1:E:291:LYS:NZ	1:E:393:SER:OG	2.43	0.50
1:F:67:LEU:HB3	1:F:193:PHE:CE1	2.47	0.50
1:G:309:ARG:CZ	1:G:317:GLU:HB3	2.39	0.50
1:G:311:GLY:O	1:G:363:TYR:OH	2.24	0.50
1:B:238:LYS:CD	1:F:231:ARG:O	2.58	0.50
1:B:351:LYS:O	1:B:365:GLU:HG3	2.11	0.50
1:C:14:ALA:CB	2:C:515:HOH:O	2.58	0.50
1:C:404:ASN:OD1	1:C:404:ASN:O	2.29	0.50
1:D:92:HIS:HD2	1:D:101:ASP:OD2	1.94	0.50
1:D:115:MET:HE1	1:D:461:PHE:HE1	1.67	0.50
1:D:119:ILE:HG12	1:D:464:ILE:HG21	1.93	0.50
1:E:302:ILE:HD11	1:E:347:LEU:CD1	2.42	0.50
1:G:92:HIS:O	1:G:93:PRO:O	2.30	0.50
1:H:357:ALA:C	1:H:358:LEU:HD13	2.32	0.50
1:C:27:ASP:OD1	1:C:29:SER:OG	2.30	0.50
1:C:80:GLU:OE1	1:C:84:GLN:OE1	2.30	0.50
1:D:42:VAL:HG13	1:D:212:LEU:HD13	1.94	0.50
1:E:89:ASN:ND2	1:E:89:ASN:O	2.45	0.50
1:F:15:VAL:HG11	1:F:40:ALA:HB3	1.94	0.50
1:F:229:THR:O	1:F:233:ILE:HG12	2.11	0.50
1:A:20:ILE:CD1	1:A:175:GLU:HB3	2.41	0.50
1:B:251:LYS:CG	1:B:286:ARG:HD3	2.42	0.50
1:E:351:LYS:CE	1:E:352:ALA:O	2.51	0.50
1:G:89:ASN:O	1:G:89:ASN:ND2	2.45	0.50
1:G:148:TRP:CA	1:G:177:THR:CG2	2.89	0.50
1:G:344:GLY:N	2:G:515:HOH:O	2.44	0.50
1:H:240:ASN:OD1	1:H:242:LYS:NZ	2.42	0.50
1:H:294:ALA:O	1:H:298:LEU:HG	2.12	0.50
1:B:258:GLU:CG	1:B:290:HIS:CD2	2.91	0.49
1:C:340:ILE:HG22	1:C:341:GLU:H	1.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:VAL:HB	1:D:103:PRO:HD3	1.94	0.49
1:F:158:LYS:O	1:F:161:PRO:HD2	2.12	0.49
1:F:447:PHE:C	1:F:447:PHE:CD2	2.85	0.49
1:G:19:THR:HG22	1:G:20:ILE:N	2.27	0.49
1:H:108:CYS:HB3	1:H:156:SER:CB	2.34	0.49
1:A:174:SER:C	1:A:176:ILE:N	2.63	0.49
1:B:479:ALA:HB2	1:B:480:LYS:HZ2	1.73	0.49
1:C:152:LEU:HD11	1:C:184:ILE:HD11	1.94	0.49
1:C:302:ILE:HD11	1:C:347:LEU:CD1	2.42	0.49
1:C:315:ASP:C	1:C:317:GLU:H	2.13	0.49
1:D:469:GLU:CD	1:G:450:VAL:HG22	2.33	0.49
1:E:248:LEU:CD1	1:H:241:LEU:HD13	2.36	0.49
1:E:315:ASP:OD2	1:E:317:GLU:HB2	2.11	0.49
1:F:27:ASP:OD1	1:F:29:SER:OG	2.30	0.49
1:F:141:VAL:HG22	1:F:168:THR:OG1	2.11	0.49
1:F:251:LYS:CD	1:F:285:SER:OG	2.60	0.49
1:H:312:ASP:O	1:H:318:THR:OG1	2.17	0.49
1:H:329:ARG:CD	1:H:330:ASP:N	2.75	0.49
1:A:302:ILE:HD13	1:A:347:LEU:HB3	1.95	0.49
1:B:129:GLY:O	1:B:477:VAL:HG13	2.12	0.49
1:D:80:GLU:HA	1:D:80:GLU:OE2	2.11	0.49
1:D:329:ARG:HG2	1:D:364:VAL:CG2	2.43	0.49
1:E:149:ASN:HB2	1:E:279:GLN:O	2.12	0.49
1:E:323:LEU:HD13	1:E:328:ARG:HG3	1.95	0.49
1:E:349:GLY:N	2:E:503:HOH:O	1.87	0.49
1:F:76:GLU:O	1:F:79:SER:HB3	2.13	0.49
1:A:273:ILE:HD11	1:A:386:PHE:O	2.12	0.49
1:A:373:PRO:HG3	1:A:390:VAL:HG11	1.94	0.49
1:A:377:VAL:HG13	1:A:377:VAL:O	2.11	0.49
1:B:2:GLN:CA	1:B:2:GLN:NE2	2.61	0.49
1:B:320:MET:HE1	1:B:385:PRO:CG	2.41	0.49
1:B:450:VAL:HG12	1:B:451:GLY:N	2.26	0.49
1:C:18:GLY:N	2:C:515:HOH:O	2.46	0.49
1:C:310:LEU:CD2	1:C:353:PRO:HG3	2.43	0.49
1:C:481:ILE:O	1:C:483:PRO:HD3	2.13	0.49
1:D:18:GLY:HA2	1:E:33:ARG:NH2	2.27	0.49
1:D:289:LEU:O	1:D:391:ARG:HA	2.12	0.49
1:E:373:PRO:HG3	1:E:390:VAL:HG11	1.95	0.49
1:F:42:VAL:O	1:F:46:VAL:HG23	2.12	0.49
1:F:280:ALA:HB3	1:F:283:ALA:HB2	1.94	0.49
1:F:337:ASP:HA	1:F:340:ILE:HG13	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:ARG:O	1:H:95:ARG:HG2	2.12	0.49
1:H:323:LEU:O	1:H:362:PHE:HD2	1.95	0.49
1:B:373:PRO:HG3	1:B:390:VAL:HG11	1.94	0.49
1:D:56:TRP:CE2	1:D:64:ARG:HD3	2.48	0.49
1:D:315:ASP:O	1:D:318:THR:HB	2.12	0.49
1:E:146:VAL:HG22	1:E:173:PRO:HA	1.95	0.49
1:F:37:ALA:HB1	1:F:201:VAL:HG13	1.91	0.49
1:F:76:GLU:CD	1:F:110:ARG:HH12	2.16	0.49
1:F:458:GLU:CG	2:F:506:HOH:O	2.60	0.49
1:B:376:ARG:HH11	1:B:380:GLU:CD	2.15	0.49
1:D:89:ASN:O	1:D:89:ASN:ND2	2.45	0.49
1:D:241:LEU:HD22	1:G:248:LEU:CD1	2.42	0.49
1:E:23:VAL:HG12	1:E:24:SER:N	2.27	0.49
1:E:447:PHE:HD2	1:E:447:PHE:O	1.95	0.49
1:F:320:MET:HE1	1:F:366:PRO:HG3	1.93	0.49
1:G:100:LEU:O	1:G:104:ARG:CG	2.54	0.49
1:H:145:ILE:HG23	1:H:172:LYS:HE3	1.94	0.49
1:B:429[A]:HIS:CE1	1:B:450:VAL:CG1	2.96	0.49
1:C:59:LEU:O	1:C:59:LEU:HG	2.12	0.49
1:C:394:SER:O	1:C:395:ASP:C	2.49	0.49
1:F:23:VAL:O	1:F:31:ILE:HD11	2.11	0.49
1:F:313:PRO:HG3	1:F:322:PRO:HD3	1.93	0.49
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.94	0.49
1:A:89:ASN:ND2	1:A:89:ASN:C	2.66	0.49
1:B:402:ALA:C	1:B:404:ASN:H	2.15	0.49
1:C:19:THR:CG2	1:C:20:ILE:N	2.76	0.49
1:G:412:GLY:HA2	1:G:434:TRP:O	2.13	0.49
1:H:261:ASN:OD1	1:H:261:ASN:O	2.30	0.49
1:A:114:GLY:O	1:A:118:LYS:HG3	2.11	0.49
1:A:478:ASP:O	1:A:478:ASP:OD1	2.30	0.49
1:B:343:GLY:O	1:B:345:LYS:HD3	2.12	0.49
1:B:357:ALA:HB2	1:G:12:VAL:CG1	2.36	0.49
1:C:277:GLN:HE21	1:C:320:MET:HG3	1.76	0.49
1:D:220:LYS:HA	1:D:243:ARG:O	2.13	0.49
1:F:370:GLU:HG3	2:F:517:HOH:O	2.13	0.49
1:G:347:LEU:CD1	1:G:370:GLU:HG3	2.18	0.49
1:H:117:ASP:OD1	1:H:117:ASP:N	2.44	0.49
1:D:373:PRO:HG3	1:D:390:VAL:HG11	1.94	0.49
1:F:10:ARG:HD3	1:F:11:PHE:O	2.12	0.49
1:H:273:ILE:HD11	1:H:386:PHE:O	2.12	0.49
1:H:458:GLU:O	1:H:459:MET:CB	2.61	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:O	1:A:365:GLU:HG3	2.13	0.48
1:C:333:LEU:HD23	1:C:336:ILE:HD12	1.94	0.48
1:C:372:LYS:O	1:C:374:GLN:N	2.46	0.48
1:D:138:PRO:HG3	1:D:165:ALA:O	2.12	0.48
1:E:350:GLY:N	1:E:367:THR:HG23	2.28	0.48
1:F:330:ASP:CG	2:F:510:HOH:O	2.51	0.48
1:A:210:GLN:NE2	1:A:214:GLU:OE2	2.46	0.48
1:C:221:ILE:HG22	1:C:244:ILE:HG23	1.95	0.48
1:E:235:GLU:O	1:E:238:LYS:CE	2.60	0.48
1:E:312:ASP:C	1:E:312:ASP:OD1	2.51	0.48
1:F:258:GLU:CD	1:F:258:GLU:H	2.16	0.48
1:H:114:GLY:O	1:H:118:LYS:HG3	2.13	0.48
1:C:74:ARG:NH2	2:C:516:HOH:O	2.47	0.48
1:C:370:GLU:OE1	1:C:391:ARG:NH1	2.47	0.48
1:D:149:ASN:HB2	1:D:279:GLN:O	2.13	0.48
1:E:84:GLN:HG3	1:E:94:ILE:HD11	1.95	0.48
1:F:227:THR:HG21	1:F:231:ARG:NH1	2.22	0.48
1:H:112:PHE:HA	1:H:115:MET:HB3	1.95	0.48
1:H:377:VAL:HG22	1:H:377:VAL:O	2.14	0.48
1:H:379:GLN:NE2	1:H:404:ASN:O	2.46	0.48
1:A:137:LYS:HG3	1:A:471:ARG:HG3	1.95	0.48
1:B:223:PHE:HZ	1:B:229:THR:HG23	1.79	0.48
1:B:248:LEU:CD1	1:F:241:LEU:HD13	2.44	0.48
1:B:355:ASP:O	1:B:357:ALA:N	2.47	0.48
1:B:404:ASN:O	1:B:404:ASN:OD1	2.30	0.48
1:D:155:THR:O	1:D:159:MET:HG3	2.14	0.48
1:D:328:ARG:NH1	1:D:383:PHE:CB	2.73	0.48
1:E:350:GLY:O	1:E:351:LYS:HB3	2.13	0.48
1:E:414:TRP:CE3	1:E:436:ASN:HA	2.49	0.48
1:G:195:LYS:HG2	1:G:195:LYS:O	2.14	0.48
1:G:337:ASP:C	1:G:339:ALA:N	2.65	0.48
1:H:2:GLN:HG3	1:H:11:PHE:CZ	2.49	0.48
1:H:195:LYS:O	2:H:510:HOH:O	2.19	0.48
1:A:105:THR:OG1	1:A:153:MET:HA	2.12	0.48
1:B:243:ARG:HD2	1:F:455:TYR:CB	2.43	0.48
1:D:309:ARG:NH1	1:D:309:ARG:CG	2.45	0.48
1:E:434:TRP:CD1	1:E:440:ARG:HB2	2.49	0.48
1:F:27:ASP:O	1:F:360:ASN:HB3	2.13	0.48
1:F:38:GLU:CB	1:F:207:THR:CG2	2.92	0.48
1:F:150:PHE:N	1:F:151:PRO:HD3	2.28	0.48
1:A:251:LYS:HG3	1:A:286:ARG:CD	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:SER:HB2	1:C:132:ASN:ND2	2.29	0.48
1:B:289:LEU:O	1:B:391:ARG:HA	2.14	0.48
1:B:405:THR:CG2	1:B:407:TYR:HD1	2.26	0.48
1:C:83:ALA:HA	1:C:97:SER:HB3	1.96	0.48
1:D:376:ARG:HD3	1:E:376:ARG:HD3	1.95	0.48
1:G:399:LEU:HD11	1:G:427:ALA:HB1	1.96	0.48
1:H:342:GLN:HE22	1:H:376:ARG:H	1.60	0.48
1:B:229:THR:O	1:B:232:ARG:HB2	2.14	0.48
1:B:414:TRP:CE3	1:B:436:ASN:HA	2.49	0.48
1:C:87:SER:OG	1:C:97:SER:OG	2.31	0.48
1:C:315:ASP:OD1	1:C:317:GLU:HB2	2.13	0.48
1:D:302:ILE:HG23	1:D:348:ALA:HB2	1.96	0.48
1:E:185:VAL:HG23	1:E:188:MET:HE3	1.96	0.48
1:E:338:ILE:HD11	1:E:376:ARG:CB	2.44	0.48
1:F:7:ILE:HG23	1:F:45:ALA:HA	1.94	0.48
1:F:443:PRO:CA	1:F:459:MET:HE3	2.38	0.48
1:G:293:ILE:HD13	1:G:297:PHE:HB2	1.96	0.48
1:G:310:LEU:HD13	1:G:366:PRO:HD3	1.96	0.48
1:H:195:LYS:HA	2:H:504:HOH:O	2.13	0.48
1:H:414:TRP:CE3	1:H:436:ASN:HA	2.49	0.48
1:A:414:TRP:CE3	1:A:436:ASN:HA	2.49	0.48
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.57	0.48
1:B:143:ALA:HB1	1:B:212:LEU:HG	1.96	0.48
1:C:293:ILE:C	1:C:293:ILE:HD12	2.34	0.48
1:D:34:ILE:HD13	1:D:178:PRO:HG3	1.95	0.48
1:E:153:MET:CG	2:E:510:HOH:O	2.54	0.48
1:F:337:ASP:O	1:F:341:GLU:HG2	2.14	0.48
1:H:10:ARG:HH22	1:H:195:LYS:HE3	1.79	0.48
1:H:99:GLY:O	1:H:100:LEU:HD22	2.13	0.48
1:B:263:GLU:HG3	1:B:300:ARG:HH22	1.78	0.48
1:C:117:ASP:OD1	2:C:519:HOH:O	2.20	0.48
1:F:412:GLY:HA2	1:F:434:TRP:O	2.14	0.48
1:F:414:TRP:CE3	1:F:436:ASN:HA	2.49	0.48
1:G:485:PHE:C	1:G:487:ARG:N	2.68	0.48
1:H:42:VAL:HG21	1:H:211:ALA:HB1	1.95	0.48
1:H:93:PRO:O	1:H:96:ASP:HB2	2.14	0.48
1:A:15:VAL:CG1	1:A:16:ALA:N	2.76	0.47
1:B:115:MET:O	1:B:115:MET:HG3	2.12	0.47
1:B:262:ILE:HD11	1:B:293:ILE:HB	1.96	0.47
1:B:452:GLN:HG2	1:F:241:LEU:HD12	1.95	0.47
1:C:289:LEU:HD12	1:C:389:VAL:CG1	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ILE:O	1:C:342:GLN:HG3	2.14	0.47
1:F:109:PHE:CZ	1:F:156:SER:HA	2.49	0.47
1:F:185:VAL:O	1:F:188:MET:HB2	2.14	0.47
1:H:251:LYS:CB	1:H:407:TYR:CD1	2.97	0.47
1:H:330:ASP:O	1:H:334:SER:OG	2.29	0.47
1:B:315:ASP:C	1:B:317:GLU:N	2.67	0.47
1:C:411:SER:O	1:C:434:TRP:CE3	2.67	0.47
1:E:230:GLY:O	1:E:233:ILE:HB	2.13	0.47
1:G:15:VAL:HG12	1:G:41:ASP:CG	2.34	0.47
1:G:245:GLN:HG3	1:G:456:GLY:HA3	1.96	0.47
1:A:273:ILE:HG12	1:A:387:VAL:HG22	1.96	0.47
1:A:351:LYS:HG2	1:A:352:ALA:H	1.78	0.47
1:B:273:ILE:HG21	1:B:387:VAL:HG22	1.96	0.47
1:D:223:PHE:HZ	1:D:229:THR:HG23	1.79	0.47
1:E:19:THR:HG23	1:E:33:ARG:HB3	1.96	0.47
1:E:127:ASP:HB2	1:E:130:PHE:CD1	2.50	0.47
1:E:235:GLU:O	1:E:238:LYS:HE2	2.14	0.47
1:F:94:ILE:CD1	1:F:98:ARG:CZ	2.91	0.47
1:F:309:ARG:HG3	1:F:319:GLU:HG3	1.95	0.47
1:F:377:VAL:CG1	1:F:386:PHE:HE1	2.26	0.47
1:F:381:GLU:O	1:F:381:GLU:HG2	2.13	0.47
1:G:76:GLU:O	1:G:79:SER:CB	2.59	0.47
1:G:278:GLY:HA3	1:G:384:GLY:C	2.32	0.47
1:H:42:VAL:O	1:H:46:VAL:HG23	2.14	0.47
1:A:155:THR:CG2	1:A:181:THR:HG23	2.44	0.47
1:A:248:LEU:HD11	1:C:241:LEU:HD22	1.96	0.47
1:B:465:HIS:CE1	1:F:465:HIS:CE1	3.03	0.47
1:C:223:PHE:CZ	1:C:229:THR:HG22	2.50	0.47
1:C:323:LEU:HD21	1:C:385:PRO:HD3	1.96	0.47
1:D:41:ASP:HA	1:D:44:LEU:HD12	1.96	0.47
1:D:93:PRO:O	1:D:96:ASP:CB	2.51	0.47
1:D:276:ASN:O	1:D:277:GLN:HB2	2.14	0.47
1:E:159:MET:HE2	1:E:171:ILE:HD12	1.96	0.47
1:F:159:MET:HG2	1:F:169:ILE:HD13	1.94	0.47
1:F:374:GLN:H	1:F:374:GLN:HG3	1.49	0.47
1:G:277:GLN:CG	1:G:321:GLY:O	2.60	0.47
1:H:408:GLY:O	1:H:430:ALA:CA	2.57	0.47
1:B:231:ARG:HB3	1:F:238:LYS:HB2	1.96	0.47
1:B:316:PRO:HG2	1:G:190:GLU:CG	2.44	0.47
1:B:429[A]:HIS:NE2	1:B:450:VAL:CG1	2.77	0.47
1:G:25:PRO:O	1:G:361:GLY:CA	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:95:ARG:HH11	1:G:319:GLU:HA	1.79	0.47
1:G:459:MET:H	1:G:463:ALA:HB2	1.79	0.47
1:A:19:THR:HG23	1:A:20:ILE:N	2.29	0.47
1:B:25:PRO:HA	1:B:362:PHE:CE2	2.48	0.47
1:D:374:GLN:N	1:D:374:GLN:CD	2.68	0.47
1:E:248:LEU:CD1	1:H:241:LEU:CD2	2.92	0.47
1:F:208:ALA:O	1:F:212:LEU:HB2	2.15	0.47
1:H:126:VAL:O	1:H:127:ASP:C	2.53	0.47
1:A:38:GLU:O	1:A:42:VAL:CG1	2.60	0.47
1:A:191:VAL:O	1:A:191:VAL:HG13	2.14	0.47
1:A:439:LYS:HB3	1:A:439:LYS:HE3	1.58	0.47
1:A:462:GLU:CD	1:C:136:ARG:NH2	2.65	0.47
1:B:92:HIS:NE2	1:B:149:ASN:O	2.47	0.47
1:B:220:LYS:HG3	1:B:221:ILE:N	2.30	0.47
1:B:238:LYS:HE2	1:F:235:GLU:CG	2.15	0.47
1:D:109:PHE:CZ	1:D:156:SER:HA	2.50	0.47
1:D:408:GLY:O	1:D:430:ALA:HA	2.15	0.47
1:D:443:PRO:HA	1:D:459:MET:SD	2.54	0.47
1:E:40:ALA:O	1:E:43:ASP:HB2	2.15	0.47
1:E:114:GLY:O	1:E:118:LYS:NZ	2.30	0.47
1:E:157:TRP:HZ2	1:E:441:VAL:HG11	1.77	0.47
1:F:89:ASN:C	1:F:89:ASN:HD22	2.04	0.47
1:F:335:TYR:CD2	1:F:376:ARG:CZ	2.98	0.47
1:G:84:GLN:HA	1:G:94:ILE:HD11	1.95	0.47
1:G:206:HIS:O	2:G:517:HOH:O	2.20	0.47
1:G:403:ASN:HD21	1:G:428:ILE:HA	1.79	0.47
1:H:160:GLY:N	1:H:161:PRO:HD2	2.29	0.47
1:H:289:LEU:O	1:H:391:ARG:HA	2.14	0.47
1:A:90:THR:O	1:A:324:THR:HB	2.15	0.47
1:A:195:LYS:NZ	2:A:512:HOH:O	2.44	0.47
1:B:455:TYR:CB	1:F:243:ARG:HD2	2.44	0.47
1:C:149:ASN:OD1	1:C:149:ASN:N	2.39	0.47
1:E:328:ARG:O	1:E:332:VAL:HG23	2.14	0.47
1:F:149:ASN:ND2	1:F:150:PHE:HD1	2.11	0.47
1:F:310:LEU:HD22	1:F:353:PRO:HG3	1.97	0.47
1:G:108:CYS:HB3	1:G:156:SER:CB	2.44	0.47
1:H:327:LEU:HD23	1:H:327:LEU:HA	1.68	0.47
1:B:351:LYS:HB2	1:B:351:LYS:HE3	1.36	0.47
1:D:56:TRP:CH2	1:D:64:ARG:HG2	2.50	0.47
1:D:229:THR:HA	1:D:232:ARG:NH1	2.30	0.47
1:E:11:PHE:HE2	1:E:186:GLU:HG3	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:LEU:HB2	1:H:314:MET:HE1	1.96	0.47
1:A:194:PRO:HD2	1:A:197:VAL:HG21	1.97	0.47
1:B:241:LEU:HD22	1:F:246:LEU:CD1	2.45	0.47
1:B:248:LEU:CD1	1:F:241:LEU:HD22	2.44	0.47
2:B:502:HOH:O	1:F:241:LEU:O	2.21	0.47
1:D:245:GLN:HG3	1:D:456:GLY:HA3	1.97	0.47
1:D:486:LYS:O	1:D:487:ARG:O	2.33	0.47
1:F:38:GLU:CG	1:F:207:THR:HG21	2.40	0.47
1:F:86:GLU:OE2	1:F:152:LEU:HB2	2.13	0.47
1:F:369:VAL:O	1:F:388:THR:HA	2.14	0.47
1:G:409:LEU:O	1:G:432:MET:HE2	2.15	0.47
1:H:10:ARG:NH2	1:H:195:LYS:HE3	2.31	0.47
1:H:174:SER:OG	1:H:177:THR:OG1	2.33	0.47
1:A:263:GLU:HG3	1:A:300:ARG:NH2	2.30	0.46
1:A:376:ARG:C	1:A:378:CYS:N	2.67	0.46
1:B:235:GLU:OE2	1:F:238:LYS:HE3	2.15	0.46
1:B:446:PRO:HB3	1:B:457:ARG:HG3	1.97	0.46
1:F:79:SER:HB2	1:F:102:VAL:HG11	1.96	0.46
1:F:90:THR:O	1:F:324:THR:HB	2.15	0.46
1:F:111:TYR:CG	1:F:443:PRO:HB2	2.49	0.46
1:F:222:ALA:HA	1:F:245:GLN:HB2	1.95	0.46
1:G:314:MET:O	1:G:316:PRO:HD3	2.15	0.46
1:H:238:LYS:HE2	1:H:238:LYS:HB2	1.64	0.46
1:A:109:PHE:CZ	1:A:156:SER:HA	2.50	0.46
1:A:342:GLN:OE1	1:A:375:ASP:OD1	2.33	0.46
1:C:429:HIS:CE1	1:C:450:VAL:HG13	2.51	0.46
1:D:136:ARG:HA	1:D:136:ARG:HD2	1.66	0.46
1:G:148:TRP:HA	1:G:177:THR:HG21	1.97	0.46
1:G:251:LYS:HA	1:G:251:LYS:HD2	1.57	0.46
1:H:227:THR:O	1:H:231:ARG:HG3	2.15	0.46
1:A:22:VAL:HG21	1:A:34:ILE:HG22	1.94	0.46
1:A:270:ALA:HB2	1:A:304:LEU:HD23	1.98	0.46
1:A:289:LEU:O	1:A:391:ARG:HA	2.14	0.46
1:B:415:THR:HG21	1:B:420:ARG:HH11	1.80	0.46
1:C:328:ARG:O	1:C:332:VAL:HG23	2.15	0.46
1:E:314:MET:CE	1:E:314:MET:HA	2.45	0.46
1:F:11:PHE:O	1:F:12:VAL:CG1	2.64	0.46
1:F:256:VAL:HG12	1:F:293:ILE:CD1	2.44	0.46
1:G:380:GLU:CB	2:G:523:HOH:O	2.64	0.46
1:H:137:LYS:HG3	1:H:471:ARG:HG3	1.97	0.46
1:H:233:ILE:O	1:H:233:ILE:CG2	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ILE:HG23	1:A:172:LYS:HE3	1.97	0.46
1:A:246:LEU:HD13	1:C:241:LEU:HD22	1.97	0.46
1:B:26:HIS:HD1	1:B:363:TYR:HH	0.55	0.46
1:B:53:PHE:HA	1:B:168:THR:CG2	2.46	0.46
1:C:338:ILE:HD11	1:C:376:ARG:CB	2.43	0.46
1:C:351:LYS:CG	1:C:352:ALA:H	2.24	0.46
1:C:447:PHE:C	1:C:447:PHE:CD2	2.88	0.46
1:D:320:MET:CE	1:D:366:PRO:HG3	2.46	0.46
1:E:100:LEU:O	1:E:101:ASP:C	2.52	0.46
1:E:289:LEU:O	1:E:391:ARG:HA	2.16	0.46
1:E:415:THR:HG21	1:E:420:ARG:HH11	1.81	0.46
1:F:11:PHE:C	1:F:12:VAL:HG13	2.35	0.46
1:F:23:VAL:CG1	1:F:24:SER:O	2.54	0.46
1:G:87:SER:OG	1:G:97:SER:OG	2.31	0.46
1:G:94:ILE:HG23	1:G:98:ARG:NE	2.30	0.46
1:G:148:TRP:HA	1:G:177:THR:CG2	2.45	0.46
1:G:289:LEU:O	1:G:391:ARG:HA	2.15	0.46
1:H:231:ARG:O	1:H:235:GLU:HG3	2.15	0.46
1:H:376:ARG:HD3	1:H:376:ARG:HA	1.79	0.46
1:A:287:LEU:HD22	1:A:289:LEU:HD21	1.97	0.46
1:A:486:LYS:O	1:A:487:ARG:HB2	2.14	0.46
1:B:89:ASN:OD1	1:B:177:THR:HA	2.15	0.46
1:B:235:GLU:CD	1:F:238:LYS:HE3	2.36	0.46
1:D:185:VAL:HG23	1:D:188:MET:CE	2.40	0.46
1:D:188:MET:CE	1:D:198:VAL:CG2	2.94	0.46
1:F:218:VAL:O	1:F:242:LYS:HE3	2.15	0.46
1:F:356:LYS:HA	1:F:359:ALA:CB	2.42	0.46
1:G:157:TRP:CE2	1:G:459:MET:HE1	2.50	0.46
1:H:136:ARG:HG3	1:H:468:THR:CB	2.45	0.46
1:D:251:LYS:HB2	1:D:407:TYR:CD1	2.51	0.46
1:E:95:ARG:HD3	1:E:318:THR:O	2.16	0.46
1:F:138:PRO:HG3	1:F:165:ALA:O	2.16	0.46
1:F:390:VAL:HG11	1:F:401:ILE:HD13	1.97	0.46
1:G:337:ASP:O	1:G:339:ALA:N	2.49	0.46
1:H:23:VAL:CG1	1:H:24:SER:N	2.78	0.46
1:B:15:VAL:HG12	1:B:41:ASP:OD1	2.16	0.46
1:C:329:ARG:O	1:C:330:ASP:C	2.54	0.46
1:E:258:GLU:HG3	1:E:290:HIS:CG	2.51	0.46
1:F:61:ALA:O	1:F:116:ALA:HB1	2.16	0.46
1:G:34:ILE:HD12	1:G:202:PRO:HB2	1.98	0.46
1:H:136:ARG:NE	1:H:468:THR:OG1	2.39	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:THR:HG21	1:A:420:ARG:HH11	1.80	0.46
1:B:251:LYS:HE3	2:B:526:HOH:O	2.16	0.46
1:B:470:ALA:HB3	1:F:457:ARG:NE	2.30	0.46
1:D:220:LYS:HE2	1:D:243:ARG:HB2	1.98	0.46
1:D:295:ASP:OD1	1:D:391:ARG:NH2	2.49	0.46
1:E:289:LEU:CD1	1:E:297:PHE:CD2	2.99	0.46
1:E:335:TYR:HE2	1:E:380:GLU:OE1	1.99	0.46
1:E:480:LYS:HD3	1:E:480:LYS:HA	1.60	0.46
1:G:27:ASP:OD1	1:G:29:SER:HB2	2.16	0.46
1:G:112:PHE:HA	1:G:115:MET:HB3	1.98	0.46
1:G:357:ALA:CA	1:G:358:LEU:CD1	2.91	0.46
1:A:5:LEU:O	1:A:11:PHE:HA	2.15	0.46
1:B:290:HIS:CD2	1:B:292:ASP:HB2	2.51	0.46
1:B:328:ARG:NH1	1:B:331:ARG:CD	2.79	0.46
1:B:417:ASN:HB3	1:B:420:ARG:HB3	1.96	0.46
1:C:151:PRO:HG2	1:C:177:THR:CB	2.45	0.46
1:E:152:LEU:CD1	1:E:184:ILE:HD12	2.40	0.46
1:E:310:LEU:HD12	1:E:320:MET:HB3	1.97	0.46
1:F:34:ILE:CD1	1:F:202:PRO:HB2	2.45	0.46
1:F:94:ILE:HG12	1:F:98:ARG:CZ	2.46	0.46
1:G:409:LEU:O	1:G:432:MET:CE	2.63	0.46
1:A:31:ILE:HD13	1:A:88:LEU:HG	1.98	0.46
1:D:474:TRP:CG	1:G:434:TRP:CD1	3.04	0.46
1:E:85:LEU:HD11	1:E:179:LEU:HB3	1.98	0.46
1:E:304:LEU:HD12	1:E:304:LEU:C	2.36	0.46
1:G:400:ALA:O	1:G:404:ASN:HB3	2.16	0.46
1:A:279:GLN:HE21	1:A:279:GLN:HB2	1.58	0.45
1:C:289:LEU:HD12	1:C:389:VAL:HG13	1.99	0.45
1:C:440:ARG:HA	1:C:440:ARG:HD2	1.42	0.45
1:D:459:MET:N	1:D:463:ALA:HB2	2.32	0.45
1:F:226:SER:OG	1:F:229:THR:CG2	2.64	0.45
1:F:310:LEU:CD2	1:F:353:PRO:CG	2.94	0.45
1:G:56:TRP:CZ2	1:G:64:ARG:HG2	2.52	0.45
1:H:276:ASN:O	1:H:277:GLN:HB2	2.15	0.45
1:A:336:ILE:HG21	1:A:350:GLY:O	2.16	0.45
1:A:394:SER:HB2	1:A:396:GLU:OE1	2.16	0.45
1:B:86:GLU:O	1:B:90:THR:OG1	2.29	0.45
1:B:405:THR:CG2	1:B:407:TYR:HB2	2.45	0.45
1:C:145:ILE:HD12	1:C:221:ILE:HD11	1.98	0.45
1:D:188:MET:CE	1:D:198:VAL:HB	2.46	0.45
1:D:312:ASP:OD1	1:D:313:PRO:CD	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:305:ALA:HA	1:F:308:ILE:HD12	1.98	0.45
1:G:6:TYR:OH	1:G:189:THR:HG22	2.13	0.45
1:G:392:PHE:HB2	1:G:397:GLU:HB3	1.97	0.45
1:H:105:THR:OG1	1:H:153:MET:HA	2.16	0.45
1:B:258:GLU:HG3	1:B:290:HIS:CG	2.50	0.45
1:E:153:MET:CA	2:E:510:HOH:O	2.63	0.45
1:E:234:VAL:CG2	1:E:246:LEU:HD11	2.46	0.45
1:H:149:ASN:OD1	1:H:149:ASN:N	2.42	0.45
1:H:162:ALA:HB3	1:H:169:ILE:HD11	1.97	0.45
1:H:241:LEU:N	2:H:506:HOH:O	2.48	0.45
1:H:459:MET:N	1:H:463:ALA:HB2	2.31	0.45
1:A:2:GLN:HB3	1:A:11:PHE:CE1	2.51	0.45
1:B:87:SER:HB3	1:B:314:MET:HE2	1.97	0.45
1:E:14:ALA:O	1:E:15:VAL:C	2.54	0.45
1:E:92:HIS:HD2	1:E:101:ASP:OD2	1.99	0.45
1:E:122:SER:O	1:E:134:VAL:N	2.43	0.45
1:E:370:GLU:CD	1:E:391:ARG:NH1	2.70	0.45
1:B:315:ASP:C	1:B:317:GLU:H	2.19	0.45
1:D:242:LYS:HZ2	1:D:242:LYS:HG2	1.63	0.45
1:F:20:ILE:HG21	1:F:175:GLU:HB3	1.98	0.45
1:F:136:ARG:HA	1:F:136:ARG:HD2	1.62	0.45
1:F:239:SER:OG	1:F:240:ASN:OD1	2.35	0.45
1:F:251:LYS:HD3	1:F:285:SER:OG	2.17	0.45
1:G:6:TYR:OH	1:G:9:GLY:HA2	2.16	0.45
1:G:310:LEU:HD23	1:G:353:PRO:HG2	1.98	0.45
1:G:310:LEU:HD23	1:G:353:PRO:HG3	1.85	0.45
1:H:90:THR:HG21	1:H:92:HIS:ND1	2.31	0.45
1:B:335:TYR:C	1:B:338:ILE:HG23	2.36	0.45
1:B:458:GLU:O	1:B:459:MET:HB2	2.16	0.45
1:F:88:LEU:CA	1:F:314:MET:HE3	2.47	0.45
1:F:415:THR:HG21	1:F:420:ARG:HD3	1.95	0.45
1:G:95:ARG:HD3	1:G:318:THR:O	2.17	0.45
1:A:251:LYS:HG3	1:A:286:ARG:HD3	1.98	0.45
1:A:372:LYS:HD3	1:A:372:LYS:HA	1.79	0.45
1:B:43:ASP:HA	1:B:215:HIS:HE2	1.81	0.45
1:B:405:THR:CG2	1:B:407:TYR:N	2.44	0.45
1:C:211:ALA:O	1:C:215:HIS:HB2	2.17	0.45
1:E:220:LYS:HA	1:E:243:ARG:O	2.16	0.45
1:F:56:TRP:O	1:F:59:LEU:HB2	2.16	0.45
1:F:70:LYS:HB3	1:F:191:VAL:HG11	1.99	0.45
1:F:415:THR:HG22	1:F:420:ARG:HH11	1.77	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:147:PRO:HG2	1:G:224:THR:HG22	1.98	0.45
1:H:339:ALA:O	1:H:344:GLY:HA3	2.17	0.45
1:A:49:ALA:HA	1:A:196:GLY:O	2.16	0.45
1:A:184:ILE:HG22	1:A:185:VAL:N	2.31	0.45
1:A:459:MET:N	1:A:463:ALA:HB2	2.32	0.45
1:B:329:ARG:NH1	1:B:329:ARG:CG	2.56	0.45
1:C:25:PRO:HD2	2:C:512:HOH:O	2.16	0.45
1:F:159:MET:O	1:F:163:LEU:HB2	2.17	0.45
1:F:413:LEU:C	1:F:413:LEU:HD12	2.37	0.45
1:G:109:PHE:CZ	1:G:156:SER:HA	2.51	0.45
1:H:177:THR:N	1:H:178:PRO:HD3	2.31	0.45
1:H:335:TYR:CD2	1:H:382:VAL:HG22	2.51	0.45
1:A:92:HIS:CD2	1:A:101:ASP:OD2	2.62	0.45
1:A:370:GLU:OE1	1:A:391:ARG:NH1	2.49	0.45
1:B:377:VAL:HG21	1:B:386:PHE:CZ	2.52	0.45
1:E:112:PHE:CZ	1:E:161:PRO:HG3	2.52	0.45
1:F:76:GLU:OE1	1:F:110:ARG:NH1	2.50	0.45
1:G:31:ILE:HD11	1:G:88:LEU:HG	1.98	0.45
1:G:86:GLU:O	1:G:86:GLU:HG3	2.15	0.45
1:G:205:GLY:O	1:G:210:GLN:N	2.50	0.45
1:G:377:VAL:HG22	1:G:386:PHE:CE1	2.52	0.45
1:H:3:ASN:HB2	1:H:34:ILE:HG22	1.99	0.45
1:H:112:PHE:CE2	1:H:161:PRO:HD3	2.52	0.45
1:H:306:LYS:HE3	1:H:306:LYS:HB3	1.31	0.45
1:A:326:ALA:HB2	1:A:362:PHE:CE1	2.52	0.45
1:B:7:ILE:HG23	1:B:45:ALA:HA	1.99	0.45
1:B:405:THR:HG23	1:B:406:GLU:N	2.31	0.45
1:B:459:MET:N	1:B:463:ALA:HB2	2.31	0.45
1:C:376:ARG:C	1:C:378:CYS:H	2.21	0.45
1:C:386:PHE:O	1:C:386:PHE:HD1	2.00	0.45
1:C:460:GLY:CA	2:C:502:HOH:O	2.64	0.45
1:C:469:GLU:OE2	2:C:513:HOH:O	2.20	0.45
1:E:49:ALA:HA	1:E:196:GLY:O	2.17	0.45
1:E:248:LEU:HD11	1:H:241:LEU:CD2	2.42	0.45
1:E:277:GLN:HE21	1:E:321:GLY:H	1.61	0.45
1:F:18:GLY:O	1:F:36:ALA:HB3	2.17	0.45
1:F:86:GLU:OE1	1:F:90:THR:HG21	2.16	0.45
1:G:313:PRO:HG3	1:G:322:PRO:HD2	1.98	0.45
1:H:20:ILE:HD13	1:H:175:GLU:CB	2.42	0.45
1:H:273:ILE:HG21	1:H:387:VAL:CG2	2.47	0.45
1:A:201:VAL:N	1:A:202:PRO:HD3	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ASN:HD22	1:C:420:ARG:N	2.10	0.44
1:D:49:ALA:HA	1:D:196:GLY:O	2.18	0.44
1:E:328:ARG:HE	1:E:328:ARG:HB2	1.54	0.44
1:F:85:LEU:HD11	1:F:179:LEU:HB2	1.98	0.44
1:F:273:ILE:HG12	1:F:386:PHE:O	2.17	0.44
1:G:2:GLN:NE2	1:G:2:GLN:HA	2.33	0.44
1:G:105:THR:OG1	1:G:153:MET:HA	2.17	0.44
1:H:258:GLU:H	1:H:258:GLU:HG3	1.15	0.44
1:H:258:GLU:HG2	1:H:290:HIS:CD2	2.52	0.44
1:A:150:PHE:O	1:A:151:PRO:C	2.55	0.44
1:B:279:GLN:HE21	1:B:279:GLN:HB2	1.58	0.44
1:C:124:ILE:HA	1:C:125:PRO:HD3	1.88	0.44
1:C:134:VAL:HA	1:C:472:SER:HA	1.99	0.44
1:C:329:ARG:O	1:C:332:VAL:N	2.50	0.44
1:D:150:PHE:O	1:D:151:PRO:C	2.55	0.44
1:D:259:ASP:O	1:D:416:GLN:HG2	2.14	0.44
1:D:356:LYS:HA	1:D:359:ALA:CB	2.35	0.44
1:F:105:THR:OG1	1:F:153:MET:HA	2.17	0.44
1:G:195:LYS:O	1:G:195:LYS:CG	2.65	0.44
1:G:338:ILE:HD12	1:G:339:ALA:CA	2.47	0.44
1:H:86:GLU:OE2	1:H:180:SER:CB	2.65	0.44
1:D:119:ILE:HD11	1:D:464:ILE:HD12	1.99	0.44
1:D:147:PRO:HG3	1:D:224:THR:O	2.16	0.44
1:E:337:ASP:O	1:E:341:GLU:HG3	2.16	0.44
1:G:49:ALA:HA	1:G:196:GLY:O	2.18	0.44
1:G:71:LEU:HD22	1:G:188:MET:HG3	1.99	0.44
1:A:235:GLU:HB2	1:C:235:GLU:OE2	2.18	0.44
1:A:258:GLU:OE2	1:A:420:ARG:NH1	2.50	0.44
1:A:465:HIS:CE1	1:C:465:HIS:CE1	3.05	0.44
1:A:477:VAL:HG23	1:A:478:ASP:N	2.32	0.44
1:C:60:GLY:O	1:C:62:ALA:N	2.51	0.44
1:D:201:VAL:N	1:D:202:PRO:HD3	2.33	0.44
1:D:281:CYS:HB3	1:D:409:LEU:CD2	2.47	0.44
1:D:288:ILE:HG22	1:D:392:PHE:CD2	2.52	0.44
1:E:326:ALA:HB2	1:E:362:PHE:CE1	2.52	0.44
1:F:328:ARG:O	1:F:329:ARG:C	2.55	0.44
1:G:59:LEU:HD12	1:G:59:LEU:HA	1.56	0.44
1:G:71:LEU:O	1:G:75:ILE:HG13	2.17	0.44
1:G:328:ARG:O	1:G:328:ARG:HD3	2.17	0.44
1:G:446:PRO:HB3	1:G:457:ARG:HD2	1.99	0.44
1:H:358:LEU:N	1:H:358:LEU:CD1	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:SER:O	1:A:102:VAL:HG22	1.98	0.44
1:A:259:ASP:O	1:A:416:GLN:CG	2.65	0.44
1:B:391:ARG:HD3	2:B:513:HOH:O	2.16	0.44
1:C:429:HIS:CE1	1:C:450:VAL:CG1	3.01	0.44
1:E:151:PRO:CG	1:E:177:THR:HB	2.47	0.44
1:E:251:LYS:HB2	1:E:407:TYR:HD1	1.80	0.44
1:G:85:LEU:HD11	1:G:179:LEU:HB2	1.99	0.44
1:H:10:ARG:CG	1:H:10:ARG:HH11	2.30	0.44
1:A:204:TYR:HB3	1:A:206:HIS:CE1	2.53	0.44
1:A:235:GLU:CB	1:C:238:LYS:HE2	2.32	0.44
1:A:340:ILE:HG22	1:A:341:GLU:N	2.28	0.44
1:B:179:LEU:HA	1:B:179:LEU:HD23	1.56	0.44
1:C:156:SER:HG	1:C:157:TRP:H	1.66	0.44
1:D:137:LYS:HB3	1:D:138:PRO:HD2	2.00	0.44
1:D:241:LEU:HD22	1:G:248:LEU:HD11	1.98	0.44
1:D:331:ARG:HE	1:D:331:ARG:HB2	1.41	0.44
1:D:377:VAL:HG13	1:D:386:PHE:HE1	1.83	0.44
1:D:480:LYS:O	1:D:480:LYS:HG2	2.17	0.44
1:E:185:VAL:O	1:E:188:MET:HB2	2.17	0.44
1:F:220:LYS:HE2	1:F:245:GLN:CG	2.47	0.44
1:H:26:HIS:HA	1:H:363:TYR:CE2	2.53	0.44
1:H:49:ALA:HA	1:H:196:GLY:O	2.18	0.44
1:H:163:LEU:HG	1:H:169:ILE:CD1	2.47	0.44
1:A:14:ALA:O	1:A:15:VAL:C	2.55	0.44
1:B:372:LYS:O	1:B:375:ASP:HB2	2.18	0.44
1:B:412:GLY:HA3	1:B:438:TYR:CE1	2.53	0.44
1:C:415:THR:CG2	1:C:417:ASN:H	2.30	0.44
1:D:56:TRP:O	1:D:59:LEU:HB2	2.18	0.44
1:D:412:GLY:HA3	1:D:438:TYR:CE1	2.53	0.44
1:E:365:GLU:O	1:E:367:THR:OG1	2.30	0.44
1:F:24:SER:N	1:F:31:ILE:HD11	2.32	0.44
1:F:376:ARG:C	1:F:378:CYS:H	2.20	0.44
1:F:392:PHE:CD1	1:F:392:PHE:C	2.91	0.44
1:G:440:ARG:HE	1:G:440:ARG:HB3	1.64	0.44
1:H:31:ILE:O	1:H:32:THR:HB	2.18	0.44
1:H:329:ARG:HD2	1:H:330:ASP:H	1.80	0.44
1:B:201:VAL:N	1:B:202:PRO:HD3	2.33	0.44
1:B:323:LEU:HD12	1:B:329:ARG:HA	1.99	0.44
1:C:333:LEU:HD22	1:C:351:LYS:HE3	1.99	0.44
1:E:237:SER:OG	1:E:244:ILE:HD11	2.18	0.44
1:E:258:GLU:CD	2:E:516:HOH:O	2.40	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:PHE:CD2	1:E:447:PHE:O	2.71	0.44
1:F:94:ILE:CG1	1:F:98:ARG:CZ	2.96	0.44
1:F:333:LEU:HA	1:F:333:LEU:HD23	1.72	0.44
1:H:221:ILE:HD11	1:H:233:ILE:CD1	2.48	0.44
1:A:23:VAL:CG1	1:A:28:GLY:HA2	2.48	0.44
1:B:34:ILE:CD1	1:B:202:PRO:HB2	2.47	0.44
1:B:237:SER:HA	1:B:242:LYS:HD2	1.99	0.44
1:B:329:ARG:C	1:B:329:ARG:CD	2.82	0.44
1:B:399:LEU:O	1:B:399:LEU:HD22	2.18	0.44
1:B:418:LEU:O	1:B:419:ALA:C	2.56	0.44
1:C:124:ILE:HB	1:C:132:ASN:HD22	1.83	0.44
1:C:272:ALA:HA	1:C:439:LYS:HD3	1.99	0.44
1:C:291:LYS:HE3	1:C:393:SER:HG	1.81	0.44
1:C:298:LEU:HD21	1:C:389:VAL:HG21	1.99	0.44
1:D:20:ILE:HG21	1:D:175:GLU:CB	2.35	0.44
1:D:178:PRO:O	1:D:182:LEU:HG	2.18	0.44
1:D:188:MET:CE	1:D:198:VAL:CG1	2.93	0.44
1:E:312:ASP:HA	1:E:313:PRO:HD3	1.91	0.44
1:F:1:MET:O	1:F:1:MET:HG2	2.18	0.44
1:F:150:PHE:CZ	1:F:276:ASN:ND2	2.85	0.44
1:F:256:VAL:CG1	1:F:293:ILE:HD11	2.48	0.44
1:G:327:LEU:CD2	1:G:327:LEU:O	2.62	0.44
1:H:273:ILE:HB	1:H:284:GLY:O	2.18	0.44
1:H:310:LEU:HA	1:H:320:MET:O	2.18	0.44
1:A:171:ILE:HG13	1:A:172:LYS:N	2.32	0.43
1:A:472:SER:O	1:C:432:MET:HA	2.18	0.43
1:B:185:VAL:HA	1:B:188:MET:HB2	2.00	0.43
1:B:248:LEU:HD12	1:F:241:LEU:HD13	2.01	0.43
1:B:335:TYR:CD1	1:B:382:VAL:HG13	2.53	0.43
1:C:100:LEU:HA	1:C:100:LEU:HD23	1.63	0.43
1:E:323:LEU:HD21	1:E:385:PRO:HD3	2.00	0.43
1:F:425:ALA:HB2	1:F:435:ILE:HD11	2.00	0.43
1:F:476:ASN:OD1	1:F:479:ALA:HB3	2.18	0.43
1:G:21:ASP:HB3	1:G:30:LEU:HD11	1.99	0.43
1:G:274:PHE:HB3	1:G:320:MET:CE	2.48	0.43
1:H:30:LEU:CD2	1:H:33:ARG:HE	2.27	0.43
1:A:412:GLY:HA3	1:A:438:TYR:CE1	2.53	0.43
1:B:112:PHE:HA	1:B:115:MET:HB3	2.00	0.43
1:B:119:ILE:HG12	1:B:464:ILE:HG21	2.00	0.43
1:D:255:ILE:O	1:D:414:TRP:HD1	2.01	0.43
1:D:432:MET:HA	1:G:472:SER:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:PHE:O	1:E:151:PRO:C	2.55	0.43
1:E:335:TYR:CE2	1:E:380:GLU:OE1	2.71	0.43
1:F:49:ALA:HA	1:F:196:GLY:O	2.18	0.43
1:F:181:THR:C	1:F:184:ILE:HG22	2.24	0.43
1:G:85:LEU:HD11	1:G:179:LEU:CB	2.47	0.43
1:G:159:MET:O	1:G:160:GLY:C	2.56	0.43
1:H:102:VAL:HB	1:H:103:PRO:HD3	2.00	0.43
1:A:231:ARG:HB2	1:A:232:ARG:HH21	1.83	0.43
1:B:339:ALA:HA	2:B:520:HOH:O	2.18	0.43
1:B:417:ASN:HD22	1:B:420:ARG:H	1.63	0.43
1:C:237:SER:O	1:C:238:LYS:C	2.55	0.43
1:D:266:VAL:HG13	1:D:301:PHE:HD2	1.83	0.43
1:E:12:VAL:O	1:E:12:VAL:HG23	2.18	0.43
1:E:241:LEU:CD1	1:H:227:THR:HG23	2.49	0.43
1:E:248:LEU:CD1	1:H:241:LEU:CD1	2.95	0.43
1:E:256:VAL:HG12	1:E:293:ILE:CD1	2.48	0.43
1:E:370:GLU:CD	1:E:391:ARG:HH11	2.22	0.43
1:A:119:ILE:HG12	1:A:464:ILE:HG21	2.00	0.43
1:A:242:LYS:O	2:A:516:HOH:O	2.21	0.43
1:A:273:ILE:CD1	1:A:386:PHE:O	2.66	0.43
1:C:14:ALA:CB	1:C:36:ALA:O	2.66	0.43
1:C:258:GLU:H	1:C:258:GLU:HG3	1.34	0.43
1:D:330:ASP:O	1:E:232:ARG:NH2	2.51	0.43
1:D:394:SER:O	1:D:395:ASP:C	2.56	0.43
1:E:412:GLY:HA3	1:E:438:TYR:CE1	2.53	0.43
1:F:46:VAL:HA	1:F:170:VAL:HG21	1.99	0.43
1:F:59:LEU:HD13	1:F:63:GLU:HB3	1.99	0.43
1:F:330:ASP:O	1:F:334:SER:OG	2.30	0.43
1:F:429:HIS:CE1	1:F:450:VAL:CG1	3.01	0.43
1:G:61:ALA:HB1	1:G:116:ALA:O	2.19	0.43
1:G:74:ARG:O	1:G:75:ILE:C	2.56	0.43
1:G:246:LEU:O	1:G:454:GLY:HA3	2.18	0.43
1:G:333:LEU:O	1:G:334:SER:C	2.56	0.43
1:G:371:ALA:O	1:G:390:VAL:HG23	2.18	0.43
1:H:279:GLN:HE21	1:H:279:GLN:HB2	1.64	0.43
1:A:418:LEU:O	1:A:419:ALA:C	2.56	0.43
1:B:434:TRP:HB3	1:B:437:CYS:SG	2.59	0.43
1:C:98:ARG:O	1:C:103:PRO:HD3	2.18	0.43
1:C:374:GLN:H	1:C:374:GLN:HG2	1.15	0.43
1:C:412:GLY:HA3	1:C:438:TYR:CE1	2.53	0.43
1:E:222:ALA:HA	1:E:245:GLN:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:LEU:HD12	1:H:241:LEU:CD1	2.39	0.43
1:G:7:ILE:HG23	1:G:45:ALA:HA	1.99	0.43
1:G:366:PRO:HA	1:G:385:PRO:HB2	2.00	0.43
1:H:10:ARG:HH11	1:H:10:ARG:HG2	1.82	0.43
1:H:412:GLY:HA3	1:H:438:TYR:CE1	2.53	0.43
1:A:15:VAL:HG13	1:A:16:ALA:H	1.79	0.43
1:A:128:ALA:O	1:A:479:ALA:HB3	2.19	0.43
1:B:25:PRO:HB2	1:B:322:PRO:CG	2.49	0.43
1:B:49:ALA:HA	1:B:196:GLY:O	2.18	0.43
1:B:310:LEU:HA	1:B:320:MET:O	2.18	0.43
1:C:108:CYS:CB	1:C:156:SER:HB2	2.45	0.43
1:C:220:LYS:HD2	1:C:243:ARG:HB2	2.00	0.43
1:E:19:THR:CG2	1:E:20:ILE:N	2.82	0.43
1:E:201:VAL:N	1:E:202:PRO:HD3	2.34	0.43
1:E:445:SER:HA	1:E:446:PRO:HD3	1.93	0.43
1:G:320:MET:CG	1:G:320:MET:O	2.66	0.43
1:H:211:ALA:O	1:H:215:HIS:HB2	2.19	0.43
1:A:163:LEU:O	1:A:166:GLY:N	2.49	0.43
1:B:174:SER:C	1:B:176:ILE:H	2.21	0.43
1:B:417:ASN:ND2	1:B:420:ARG:HB2	2.21	0.43
1:C:59:LEU:O	1:C:59:LEU:CG	2.67	0.43
1:C:80:GLU:OE1	1:C:84:GLN:CD	2.57	0.43
1:E:70:LYS:HE3	1:E:191:VAL:O	2.19	0.43
1:E:258:GLU:HG2	1:E:290:HIS:CD2	2.53	0.43
1:F:11:PHE:CZ	1:F:186:GLU:HG3	2.54	0.43
1:H:196:GLY:N	2:H:504:HOH:O	2.04	0.43
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.74	0.43
1:B:92:HIS:HD2	1:B:101:ASP:OD2	2.00	0.43
1:B:221:ILE:CD1	1:B:233:ILE:HG23	2.49	0.43
1:B:355:ASP:C	1:B:357:ALA:N	2.72	0.43
1:C:86:GLU:OE1	1:C:151:PRO:HD2	2.18	0.43
1:C:99:GLY:O	1:C:100:LEU:HD23	2.18	0.43
1:C:150:PHE:N	1:C:151:PRO:HD3	2.34	0.43
1:D:312:ASP:HA	1:D:313:PRO:HD3	1.89	0.43
1:D:474:TRP:HB2	1:G:434:TRP:CD1	2.54	0.43
1:E:226:SER:HG	1:E:229:THR:HG22	1.79	0.43
1:G:377:VAL:HG22	1:G:386:PHE:HE1	1.83	0.43
1:G:377:VAL:CG2	1:G:386:PHE:CE1	3.01	0.43
1:A:155:THR:O	1:A:159:MET:HB2	2.19	0.43
1:B:108:CYS:HB3	1:B:156:SER:HB2	2.01	0.43
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASP:CG	1:B:415:THR:HG22	2.37	0.43
1:C:74:ARG:HG3	1:C:187:LEU:HD22	2.01	0.43
1:C:223:PHE:CZ	1:C:229:THR:CG2	3.01	0.43
1:D:89:ASN:OD1	1:D:177:THR:HA	2.19	0.43
1:D:188:MET:HE1	1:D:198:VAL:HG21	2.01	0.43
1:D:457:ARG:NH1	1:D:457:ARG:CG	2.75	0.43
1:E:34:ILE:CD1	1:E:202:PRO:HB2	2.49	0.43
1:E:93:PRO:HD3	1:E:277:GLN:HE22	1.83	0.43
1:E:259:ASP:O	1:E:416:GLN:CG	2.67	0.43
1:F:147:PRO:HD3	1:F:224:THR:HB	2.01	0.43
1:F:376:ARG:HG2	1:F:377:VAL:N	2.34	0.43
1:G:257:PHE:HB2	1:G:415:THR:HG23	2.01	0.43
1:G:404:ASN:O	1:G:404:ASN:OD1	2.37	0.43
1:H:100:LEU:O	1:H:104:ARG:HG3	2.19	0.43
1:H:102:VAL:N	1:H:103:PRO:CD	2.82	0.43
1:H:171:ILE:HG23	1:H:200:VAL:HG13	2.01	0.43
1:H:432:MET:HE1	1:H:447:PHE:CD1	2.54	0.43
1:A:59:LEU:HD12	1:A:59:LEU:HA	1.56	0.43
1:A:67:LEU:HD13	1:A:193:PHE:HA	1.99	0.43
1:D:143:ALA:O	1:D:221:ILE:HA	2.18	0.43
1:E:137:LYS:HE3	1:H:426:ASN:OD1	2.18	0.43
1:E:151:PRO:HG3	1:E:177:THR:OG1	2.18	0.43
1:E:302:ILE:CD1	1:E:347:LEU:HB3	2.49	0.43
1:E:377:VAL:HG22	1:E:386:PHE:CE1	2.54	0.43
1:F:221:ILE:O	1:F:221:ILE:HG22	2.16	0.43
1:G:268:GLY:O	1:G:272:ALA:N	2.51	0.43
1:H:159:MET:HE1	1:H:171:ILE:HD13	2.01	0.43
1:A:323:LEU:HD21	1:A:385:PRO:HD3	2.00	0.42
1:B:440:ARG:HA	1:B:440:ARG:HD2	1.50	0.42
1:D:22:VAL:CG2	1:D:34:ILE:HG23	2.49	0.42
1:D:441:VAL:HG13	2:D:505:HOH:O	2.20	0.42
1:F:315:ASP:OD1	1:F:316:PRO:HD2	2.19	0.42
1:F:326:ALA:HA	1:F:362:PHE:CD1	2.54	0.42
1:H:94:ILE:C	1:H:96:ASP:N	2.73	0.42
1:H:146:VAL:HA	1:H:147:PRO:HD3	1.81	0.42
1:H:486:LYS:O	1:H:487:ARG:HB2	2.19	0.42
1:A:288:ILE:HG22	1:A:392:PHE:CD2	2.54	0.42
1:B:251:LYS:HG3	1:B:286:ARG:CD	2.49	0.42
1:B:405:THR:HG22	1:B:406:GLU:N	2.28	0.42
1:B:405:THR:HG23	1:B:407:TYR:HD1	1.83	0.42
1:C:160:GLY:N	1:C:161:PRO:CD	2.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:ILE:HG12	1:E:464:ILE:HG21	2.01	0.42
1:E:251:LYS:HA	1:E:251:LYS:HD2	1.70	0.42
1:E:259:ASP:CG	1:E:415:THR:HG22	2.37	0.42
1:E:372:LYS:HA	1:E:372:LYS:HD2	1.76	0.42
1:F:23:VAL:O	1:F:31:ILE:CD1	2.67	0.42
1:F:443:PRO:CA	1:F:459:MET:CE	2.78	0.42
1:B:155:THR:HB	1:B:159:MET:CE	2.48	0.42
1:B:357:ALA:HB3	1:B:358:LEU:HD13	2.01	0.42
1:D:42:VAL:HG22	1:D:201:VAL:HG11	2.01	0.42
1:D:437:CYS:HB2	1:D:440:ARG:HD3	2.01	0.42
1:E:102:VAL:CB	1:E:103:PRO:HD3	2.44	0.42
1:E:272:ALA:O	1:E:284:GLY:N	2.43	0.42
1:F:279:GLN:OE1	1:F:324:THR:HG23	2.19	0.42
1:F:376:ARG:CG	1:F:377:VAL:N	2.79	0.42
1:G:226:SER:HG	1:G:229:THR:HG22	1.82	0.42
1:G:340:ILE:O	1:G:341:GLU:C	2.56	0.42
1:H:42:VAL:HG21	1:H:211:ALA:CB	2.49	0.42
1:H:376:ARG:C	1:H:378:CYS:N	2.72	0.42
1:H:418:LEU:O	1:H:419:ALA:C	2.56	0.42
1:A:89:ASN:OD1	1:A:177:THR:HA	2.19	0.42
1:A:119:ILE:HD11	1:A:464:ILE:HD12	2.01	0.42
1:B:258:GLU:CG	1:B:290:HIS:CG	3.02	0.42
1:B:338:ILE:HD11	1:B:376:ARG:CB	2.49	0.42
1:D:151:PRO:HG3	1:D:177:THR:OG1	2.20	0.42
1:D:474:TRP:HB2	1:G:434:TRP:HA	2.02	0.42
1:E:119:ILE:HD11	1:E:464:ILE:HD12	2.01	0.42
1:E:477:VAL:CG2	1:E:478:ASP:N	2.82	0.42
1:G:87:SER:HB2	1:G:94:ILE:HD13	1.79	0.42
1:G:293:ILE:HD12	1:G:294:ALA:CA	2.47	0.42
1:G:412:GLY:HA3	1:G:438:TYR:CE1	2.53	0.42
1:A:302:ILE:HG23	1:A:348:ALA:HB2	2.01	0.42
1:A:309:ARG:HB2	1:A:319:GLU:OE1	2.18	0.42
1:C:89:ASN:O	1:C:89:ASN:ND2	2.53	0.42
1:C:273:ILE:HB	1:C:284:GLY:O	2.20	0.42
1:C:373:PRO:HB3	1:C:401:ILE:HG23	2.01	0.42
1:C:374:GLN:O	1:C:375:ASP:C	2.58	0.42
1:E:4:GLN:NE2	1:E:13:ASP:OD1	2.46	0.42
1:E:315:ASP:OD1	1:E:316:PRO:HD2	2.19	0.42
1:E:350:GLY:CA	1:E:367:THR:HG23	2.50	0.42
1:G:84:GLN:HA	1:G:314:MET:HE1	2.01	0.42
1:H:159:MET:HE2	1:H:171:ILE:HD13	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:O	1:A:351:LYS:HB2	2.19	0.42
1:C:31:ILE:CD1	1:C:88:LEU:HG	2.50	0.42
1:C:94:ILE:O	1:C:98:ARG:HD2	2.19	0.42
1:D:56:TRP:CE3	1:D:59:LEU:HD22	2.54	0.42
1:F:92:HIS:HD2	1:F:101:ASP:OD2	2.02	0.42
1:G:117:ASP:OD1	1:G:118:LYS:NZ	2.39	0.42
1:G:327:LEU:HD21	1:G:331:ARG:CD	2.32	0.42
1:G:358:LEU:HB3	1:G:363:TYR:CD2	2.53	0.42
1:A:199:ASN:N	1:A:199:ASN:ND2	2.67	0.42
1:B:323:LEU:HD21	1:B:385:PRO:HD3	2.00	0.42
1:B:374:GLN:O	1:B:375:ASP:C	2.58	0.42
1:C:151:PRO:CG	1:C:177:THR:CB	2.97	0.42
1:E:418:LEU:O	1:E:419:ALA:C	2.57	0.42
1:F:37:ALA:HB3	1:F:201:VAL:HG13	1.98	0.42
1:G:258:GLU:HG3	1:G:290:HIS:CG	2.54	0.42
1:A:102:VAL:HB	1:A:103:PRO:CD	2.43	0.42
1:A:314:MET:O	1:A:316:PRO:HD3	2.19	0.42
1:B:138:PRO:HG3	1:B:165:ALA:O	2.20	0.42
1:B:290:HIS:HD2	1:B:292:ASP:HB2	1.83	0.42
1:B:457:ARG:HD2	1:B:457:ARG:HA	1.88	0.42
1:D:95:ARG:NH1	1:D:319:GLU:HA	2.35	0.42
1:D:129:GLY:HA3	1:D:479:ALA:HB2	2.01	0.42
1:D:240:ASN:OD1	1:D:240:ASN:N	2.46	0.42
1:F:289:LEU:O	1:F:391:ARG:HA	2.20	0.42
1:G:10:ARG:HH12	1:G:12:VAL:HG11	0.59	0.42
1:A:45:ALA:HB1	1:A:170:VAL:HG13	2.01	0.42
1:B:242:LYS:HE3	1:B:242:LYS:HB3	1.33	0.42
1:C:376:ARG:O	1:C:379:GLN:N	2.48	0.42
1:E:355:ASP:O	1:E:359:ALA:N	2.50	0.42
1:E:482:ALA:HA	1:E:483:PRO:HD2	1.77	0.42
1:F:22:VAL:HG11	1:F:179:LEU:HD11	2.02	0.42
1:F:376:ARG:C	1:F:378:CYS:N	2.73	0.42
1:G:186:GLU:O	1:G:189:THR:N	2.51	0.42
1:G:417:ASN:HB3	1:G:420:ARG:HB3	2.01	0.42
1:H:5:LEU:O	1:H:11:PHE:HA	2.20	0.42
1:H:197:VAL:HG12	1:H:198:VAL:HG23	2.02	0.42
1:H:221:ILE:CD1	1:H:233:ILE:HD12	2.50	0.42
1:A:315:ASP:C	1:A:317:GLU:H	2.23	0.42
1:B:93:PRO:O	1:B:96:ASP:HB2	2.20	0.42
1:B:329:ARG:HD2	1:B:330:ASP:CA	2.50	0.42
1:B:346:VAL:HG13	1:B:348:ALA:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:ASN:O	1:D:34:ILE:HA	2.20	0.42
1:F:312:ASP:HA	1:F:313:PRO:HD2	1.81	0.42
1:F:313:PRO:HB2	1:F:314:MET:CE	2.50	0.42
1:F:340:ILE:HG12	1:F:340:ILE:H	1.62	0.42
1:G:90:THR:O	1:G:324:THR:CG2	2.49	0.42
1:G:451:GLY:O	2:G:503:HOH:O	2.21	0.42
1:H:447:PHE:CD2	1:H:447:PHE:C	2.93	0.42
1:A:343:GLY:O	1:A:345:LYS:HE3	2.20	0.41
1:B:458:GLU:O	1:B:459:MET:CB	2.68	0.41
1:C:146:VAL:HA	1:C:147:PRO:HD3	1.86	0.41
1:C:215:HIS:CD2	1:C:217:ASP:H	2.23	0.41
1:E:214:GLU:O	1:E:215:HIS:C	2.56	0.41
1:G:102:VAL:CB	1:G:103:PRO:HD3	2.50	0.41
1:H:111:TYR:CG	1:H:443:PRO:HB2	2.55	0.41
1:A:26:HIS:HD1	1:A:363:TYR:HH	0.54	0.41
1:B:8:ASP:OD2	1:B:51:ARG:NH2	2.53	0.41
1:C:148:TRP:CH2	1:C:383:PHE:HD2	2.38	0.41
1:C:394:SER:C	1:C:396:GLU:N	2.72	0.41
1:D:172:LYS:HZ2	1:D:172:LYS:HG2	1.62	0.41
1:D:262:ILE:O	1:D:263:GLU:C	2.58	0.41
1:G:34:ILE:CD1	1:G:202:PRO:HB2	2.50	0.41
1:G:148:TRP:HH2	1:G:328:ARG:CG	2.33	0.41
1:G:177:THR:OG1	1:G:177:THR:O	2.38	0.41
1:H:338:ILE:CD1	1:H:338:ILE:C	2.87	0.41
1:B:119:ILE:HD11	1:B:464:ILE:HD12	2.01	0.41
1:B:129:GLY:HA2	1:B:478:ASP:HB3	2.02	0.41
1:B:452:GLN:HG3	1:F:240:ASN:O	2.20	0.41
1:C:2:GLN:HG3	1:C:11:PHE:CE2	2.55	0.41
1:C:289:LEU:CD1	1:C:389:VAL:HG13	2.50	0.41
1:E:25:PRO:HA	1:E:362:PHE:CE2	2.55	0.41
1:F:61:ALA:CB	1:F:117:ASP:HA	2.50	0.41
1:G:6:TYR:CZ	1:G:9:GLY:HA2	2.55	0.41
1:G:114:GLY:O	1:G:118:LYS:HG3	2.20	0.41
1:G:172:LYS:HE2	1:G:204:TYR:O	2.19	0.41
1:H:476:ASN:OD1	1:H:479:ALA:HB3	2.20	0.41
1:A:15:VAL:CG1	1:A:40:ALA:HB3	2.51	0.41
1:A:38:GLU:HA	1:A:207:THR:HB	2.01	0.41
1:A:151:PRO:CG	1:A:177:THR:HB	2.50	0.41
1:A:440:ARG:HA	1:A:440:ARG:HD2	1.43	0.41
1:A:447:PHE:CD2	1:A:447:PHE:C	2.93	0.41
1:B:88:LEU:HA	1:B:314:MET:CE	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ASN:CB	1:F:436:ASN:O	2.68	0.41
1:C:152:LEU:HB2	1:C:180:SER:OG	2.20	0.41
1:C:476:ASN:ND2	1:C:481:ILE:HD11	2.35	0.41
1:D:476:ASN:HB2	1:G:437:CYS:HB3	2.02	0.41
1:D:482:ALA:HA	1:D:483:PRO:HD2	1.64	0.41
1:E:213:ALA:HB2	1:E:221:ILE:CD1	2.51	0.41
1:H:100:LEU:O	1:H:101:ASP:C	2.58	0.41
1:H:221:ILE:HD11	1:H:233:ILE:HD12	2.03	0.41
1:H:330:ASP:OD1	1:H:330:ASP:N	2.52	0.41
1:A:310:LEU:HD23	1:A:353:PRO:HG2	1.96	0.41
1:A:392:PHE:HB2	1:A:397:GLU:HB3	2.02	0.41
1:B:221:ILE:O	1:B:221:ILE:CG2	2.68	0.41
1:B:345:LYS:HZ3	1:B:345:LYS:HG3	1.70	0.41
1:B:438:TYR:O	1:B:439:LYS:HB2	2.19	0.41
1:D:74:ARG:HD3	1:D:77:GLU:OE1	2.21	0.41
1:E:428:ILE:O	1:H:471:ARG:NH1	2.53	0.41
1:F:74:ARG:NH2	1:F:190:GLU:OE1	2.53	0.41
1:F:124:ILE:HG22	1:F:125:PRO:HD2	2.03	0.41
1:G:340:ILE:HD11	1:G:346:VAL:CG2	2.51	0.41
1:H:235:GLU:O	1:H:238:LYS:HG3	2.21	0.41
1:H:325:SER:OG	1:H:328:ARG:HB2	2.20	0.41
1:A:56:TRP:O	1:A:59:LEU:HB2	2.20	0.41
1:A:111:TYR:CG	1:A:443:PRO:HB2	2.56	0.41
1:B:177:THR:N	1:B:178:PRO:HD3	2.35	0.41
1:B:405:THR:HG23	1:B:406:GLU:H	1.85	0.41
1:B:447:PHE:CD2	1:B:447:PHE:C	2.93	0.41
1:F:124:ILE:HA	1:F:125:PRO:HD3	1.73	0.41
1:F:315:ASP:HA	1:F:316:PRO:HD3	1.85	0.41
1:G:53:PHE:CD1	1:G:140:GLY:HA2	2.53	0.41
1:G:279:GLN:HE21	1:G:279:GLN:HB2	1.52	0.41
1:H:311:GLY:O	1:H:312:ASP:C	2.59	0.41
1:H:416:GLN:H	1:H:416:GLN:HG2	1.60	0.41
1:A:377:VAL:CG2	1:A:386:PHE:CE1	3.03	0.41
1:B:145:ILE:HG12	1:B:172:LYS:HD3	2.03	0.41
1:B:152:LEU:HD11	1:B:184:ILE:CD1	2.17	0.41
1:B:434:TRP:CD1	1:B:440:ARG:HB2	2.55	0.41
1:D:108:CYS:HB3	1:D:156:SER:HB2	2.03	0.41
1:F:234:VAL:O	1:F:237:SER:N	2.51	0.41
1:F:336:ILE:HG12	1:F:386:PHE:CE2	2.55	0.41
1:G:157:TRP:NE1	1:G:459:MET:HE1	2.35	0.41
1:C:53:PHE:N	1:C:54:PRO:CD	2.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:GLY:O	1:C:118:LYS:HG3	2.21	0.41
1:C:418:LEU:O	1:C:419:ALA:C	2.58	0.41
1:D:22:VAL:HG21	1:D:34:ILE:CG2	2.50	0.41
1:D:341:GLU:OE2	2:D:522:HOH:O	2.20	0.41
1:D:470:ALA:HB3	1:G:457:ARG:NE	2.36	0.41
1:F:23:VAL:HG12	1:F:24:SER:C	2.38	0.41
1:F:191:VAL:CG1	1:F:191:VAL:O	2.66	0.41
1:G:295:ASP:C	1:G:297:PHE:N	2.73	0.41
1:H:326:ALA:C	1:H:328:ARG:N	2.74	0.41
1:A:70:LYS:HB3	1:A:191:VAL:HG22	2.03	0.41
1:A:238:LYS:H	1:A:238:LYS:HG3	1.64	0.41
1:A:290:HIS:HD2	1:A:292:ASP:HB2	1.85	0.41
1:B:66:ARG:HH11	1:B:66:ARG:CG	2.34	0.41
1:B:173:PRO:HG3	1:B:181:THR:HG21	2.03	0.41
1:C:225:GLY:O	1:C:248:LEU:HA	2.21	0.41
1:D:18:GLY:HA3	2:D:524:HOH:O	2.20	0.41
1:D:42:VAL:O	1:D:46:VAL:HG23	2.21	0.41
1:D:221:ILE:O	1:D:221:ILE:CG2	2.68	0.41
1:D:273:ILE:HD13	1:D:283:ALA:HB1	2.02	0.41
1:E:15:VAL:HG12	1:E:16:ALA:CA	2.40	0.41
1:E:137:LYS:CE	1:H:426:ASN:OD1	2.68	0.41
1:E:185:VAL:HA	1:E:188:MET:HE2	2.03	0.41
1:E:275:HIS:CG	1:E:276:ASN:N	2.89	0.41
1:E:314:MET:O	1:E:316:PRO:HD3	2.21	0.41
1:F:18:GLY:C	1:F:36:ALA:HB3	2.40	0.41
1:F:61:ALA:HB1	1:F:117:ASP:HA	2.03	0.41
1:F:302:ILE:HD11	1:F:347:LEU:HD13	2.03	0.41
1:G:23:VAL:HG12	1:G:24:SER:N	2.29	0.41
1:G:25:PRO:O	1:G:361:GLY:HA2	2.21	0.41
1:G:152:LEU:HD12	1:G:184:ILE:CD1	2.50	0.41
1:G:312:ASP:HA	1:G:313:PRO:HD3	1.84	0.41
1:G:365:GLU:O	1:G:366:PRO:C	2.57	0.41
1:G:464:ILE:HD13	1:G:464:ILE:HA	1.87	0.41
1:H:69:LEU:HD23	1:H:69:LEU:HA	1.91	0.41
1:H:94:ILE:C	1:H:96:ASP:H	2.23	0.41
1:H:159:MET:HE1	1:H:171:ILE:HG21	2.03	0.41
1:H:221:ILE:O	1:H:221:ILE:CG2	2.68	0.41
1:A:20:ILE:HD13	1:A:204:TYR:CE1	2.56	0.41
1:A:126:VAL:HG11	1:A:474:TRP:CH2	2.56	0.41
1:A:445:SER:CB	1:C:132:ASN:ND2	2.82	0.41
1:B:174:SER:C	1:B:176:ILE:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:GLY:O	1:B:457:ARG:HD3	2.21	0.41
1:B:462:GLU:OE2	1:F:136:ARG:NH1	2.54	0.41
1:C:137:LYS:O	1:C:468:THR:HA	2.21	0.41
1:C:352:ALA:C	1:C:353:PRO:O	2.59	0.41
1:D:124:ILE:HA	1:D:125:PRO:HD3	1.95	0.41
1:D:225:GLY:O	1:D:248:LEU:HA	2.21	0.41
1:D:447:PHE:CD2	1:D:447:PHE:C	2.93	0.41
1:E:285:SER:O	1:E:388:THR:HG23	2.21	0.41
1:E:357:ALA:HB3	1:E:358:LEU:CD1	2.51	0.41
1:G:42:VAL:O	1:G:46:VAL:HG23	2.21	0.41
1:G:431:GLY:C	1:G:432:MET:HG3	2.40	0.41
1:H:172:LYS:NZ	1:H:203:GLY:O	2.53	0.41
1:B:20:ILE:HG21	1:B:175:GLU:HB3	2.03	0.40
1:D:177:THR:N	1:D:178:PRO:HD3	2.36	0.40
1:D:338:ILE:CD1	1:D:376:ARG:CB	2.99	0.40
1:F:124:ILE:CG2	1:F:125:PRO:HD2	2.52	0.40
1:H:185:VAL:HG11	1:H:200:VAL:HG21	2.04	0.40
1:A:53:PHE:N	1:A:54:PRO:CD	2.84	0.40
1:A:142:VAL:O	1:A:142:VAL:HG12	2.21	0.40
1:B:24:SER:HA	1:B:25:PRO:HD3	1.86	0.40
1:B:152:LEU:HD13	1:B:184:ILE:HD12	2.00	0.40
1:C:315:ASP:C	1:C:317:GLU:N	2.75	0.40
1:D:205:GLY:C	2:D:517:HOH:O	2.58	0.40
1:E:151:PRO:HG2	1:E:177:THR:HB	2.03	0.40
1:E:238:LYS:HB2	1:H:231:ARG:HB3	2.03	0.40
1:E:474:TRP:HB2	1:H:434:TRP:HD1	1.86	0.40
1:G:304:LEU:N	2:G:513:HOH:O	2.54	0.40
1:H:53:PHE:CE1	1:H:140:GLY:HA2	2.56	0.40
1:H:92:HIS:O	1:H:93:PRO:C	2.59	0.40
1:A:258:GLU:CD	1:A:258:GLU:H	2.24	0.40
1:A:275:HIS:ND1	1:A:439:LYS:NZ	2.70	0.40
1:B:355:ASP:O	1:B:358:LEU:N	2.50	0.40
1:C:323:LEU:N	1:C:323:LEU:HD23	2.37	0.40
1:D:153:MET:O	1:D:153:MET:HG2	2.21	0.40
1:E:24:SER:HA	1:E:25:PRO:HD3	1.88	0.40
1:E:238:LYS:O	1:H:231:ARG:NE	2.33	0.40
1:G:34:ILE:O	1:G:34:ILE:HG13	2.17	0.40
1:G:362:PHE:N	1:G:362:PHE:CD1	2.88	0.40
1:B:76:GLU:OE1	1:B:110:ARG:NH1	2.36	0.40
1:B:225:GLY:O	1:B:248:LEU:HA	2.21	0.40
1:C:5:LEU:O	1:C:11:PHE:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:PRO:CD	2:C:512:HOH:O	2.69	0.40
1:C:310:LEU:HD23	1:C:353:PRO:HG3	2.03	0.40
1:C:376:ARG:C	1:C:378:CYS:N	2.75	0.40
1:D:469:GLU:OE1	1:G:450:VAL:HG22	2.22	0.40
1:E:269:ALA:O	1:E:273:ILE:HG22	2.22	0.40
1:E:312:ASP:OD1	1:E:313:PRO:HD2	2.21	0.40
1:E:314:MET:HA	1:E:314:MET:HE2	2.03	0.40
1:G:94:ILE:HD12	1:G:94:ILE:HA	1.95	0.40
1:G:225:GLY:O	1:G:248:LEU:HA	2.21	0.40
1:G:373:PRO:CG	1:G:374:GLN:H	2.34	0.40
1:H:24:SER:HA	1:H:25:PRO:HD2	1.91	0.40
1:H:142:VAL:HG11	1:H:467:TYR:CE2	2.50	0.40
1:A:476:ASN:HD21	1:A:480:LYS:HE3	1.86	0.40
1:B:15:VAL:HG13	2:B:522:HOH:O	2.21	0.40
1:B:148:TRP:HB3	1:B:174:SER:OG	2.22	0.40
1:D:94:ILE:HA	1:D:97:SER:OG	2.21	0.40
1:E:115:MET:O	1:E:119:ILE:HG13	2.21	0.40
1:F:188:MET:O	1:F:193:PHE:HB2	2.21	0.40
1:G:414:TRP:CE3	1:G:436:ASN:HA	2.57	0.40
1:H:273:ILE:HG21	1:H:387:VAL:HG21	2.04	0.40
1:H:278:GLY:HA3	1:H:384:GLY:O	2.21	0.40

All (27) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:SER:CB	1:H:354:ASP:O[2_545]	0.79	1.41
1:B:356:LYS:NZ	1:F:341:GLU:CB[2_454]	0.88	1.32
1:B:356:LYS:NZ	1:F:341:GLU:CA[2_454]	0.92	1.28
1:A:478:ASP:OD2	1:H:423:LYS:CE[2_445]	1.10	1.10
1:B:393:SER:OG	1:H:354:ASP:O[2_545]	1.14	1.06
1:A:478:ASP:OD2	1:H:423:LYS:CD[2_445]	1.51	0.69
1:B:356:LYS:NZ	1:F:341:GLU:C[2_454]	1.58	0.62
1:B:356:LYS:CE	1:F:341:GLU:CB[2_454]	1.59	0.61
1:B:393:SER:OG	1:H:354:ASP:C[2_545]	1.63	0.57
1:B:292:ASP:OD1	1:H:354:ASP:OD2[2_545]	1.68	0.52
1:B:393:SER:OG	1:H:356:LYS:N[2_545]	1.70	0.50
1:B:393:SER:OG	1:H:355:ASP:CA[2_545]	1.88	0.32
1:E:300:ARG:NH1	1:F:396:GLU:OE2[2_454]	1.90	0.30
1:D:8:ASP:O	1:F:1:MET:N[1_565]	1.92	0.28

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:SER:OG	1:H:355:ASP:N[2_545]	1.94	0.26
1:B:393:SER:CB	1:H:354:ASP:C[2_545]	1.96	0.24
1:B:393:SER:OG	1:H:355:ASP:C[2_545]	1.96	0.24
1:C:486:LYS:NZ	1:E:195:LYS:CE[1_545]	1.98	0.22
1:C:33:ARG:CD	2:A:517:HOH:O[2_555]	2.01	0.19
1:A:376:ARG:NH2	1:H:17:GLY:O[2_545]	2.02	0.18
1:B:356:LYS:CE	1:F:341:GLU:CA[2_454]	2.02	0.18
1:B:356:LYS:CD	1:F:341:GLU:CB[2_454]	2.03	0.17
1:B:393:SER:O	1:H:355:ASP:CA[2_545]	2.05	0.15
1:A:478:ASP:CG	1:H:423:LYS:CE[2_445]	2.06	0.14
1:D:10:ARG:NH2	1:F:4:GLN:OE1[1_565]	2.13	0.07
1:B:356:LYS:NZ	1:F:341:GLU:N[2_454]	2.15	0.05
1:B:397:GLU:OE1	1:H:356:LYS:CG[2_545]	2.17	0.03

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	485/495 (98%)	452 (93%)	31 (6%)	2 (0%)	34 60
1	B	486/495 (98%)	452 (93%)	30 (6%)	4 (1%)	19 43
1	C	486/495 (98%)	440 (90%)	41 (8%)	5 (1%)	15 37
1	D	485/495 (98%)	453 (93%)	31 (6%)	1 (0%)	47 73
1	E	483/495 (98%)	446 (92%)	35 (7%)	2 (0%)	34 60
1	F	485/495 (98%)	443 (91%)	40 (8%)	2 (0%)	34 60
1	G	485/495 (98%)	432 (89%)	45 (9%)	8 (2%)	9 24
1	H	485/495 (98%)	453 (93%)	29 (6%)	3 (1%)	25 50
All	All	3880/3960 (98%)	3571 (92%)	282 (7%)	27 (1%)	22 46

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	178	PRO
1	A	356	LYS
1	C	178	PRO
1	G	341	GLU
1	G	357	ALA
1	F	178	PRO
1	G	296	GLN
1	G	459	MET
1	B	39	ALA
1	B	356	LYS
1	B	404	ASN
1	C	175	GLU
1	E	313	PRO
1	E	459	MET
1	B	351	LYS
1	C	353	PRO
1	C	366	PRO
1	C	419	ALA
1	F	235	GLU
1	H	356	LYS
1	H	419	ALA
1	D	459	MET
1	A	408	GLY
1	G	366	PRO
1	G	338	ILE
1	G	293	ILE
1	H	178	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	376/383 (98%)	308 (82%)	68 (18%)	1 4
1	B	377/383 (98%)	308 (82%)	69 (18%)	1 4
1	C	377/383 (98%)	307 (81%)	70 (19%)	1 4
1	D	376/383 (98%)	308 (82%)	68 (18%)	1 4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	374/383 (98%)	306 (82%)	68 (18%)	1 4
1	F	376/383 (98%)	304 (81%)	72 (19%)	1 4
1	G	376/383 (98%)	303 (81%)	73 (19%)	1 3
1	H	376/383 (98%)	307 (82%)	69 (18%)	1 4
All	All	3008/3064 (98%)	2451 (82%)	557 (18%)	1 4

All (557) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	10	ARG
1	A	19	THR
1	A	34	ILE
1	A	59	LEU
1	A	63	GLU
1	A	66	ARG
1	A	79	SER
1	A	87	SER
1	A	89	ASN
1	A	90	THR
1	A	92	HIS
1	A	94	ILE
1	A	95	ARG
1	A	98	ARG
1	A	102	VAL
1	A	118	LYS
1	A	122	SER
1	A	127	ASP
1	A	167	ASN
1	A	171	ILE
1	A	174	SER
1	A	175	GLU
1	A	176	ILE
1	A	180	SER
1	A	184	ILE
1	A	185	VAL
1	A	187	LEU
1	A	189	THR
1	A	190	GLU
1	A	191	VAL
1	A	207	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	210	GLN
1	A	212	LEU
1	A	215	HIS
1	A	221	ILE
1	A	229	THR
1	A	232	ARG
1	A	238	LYS
1	A	242	LYS
1	A	243	ARG
1	A	247	GLU
1	A	258	GLU
1	A	273	ILE
1	A	291	LYS
1	A	309	ARG
1	A	324	THR
1	A	327	LEU
1	A	328	ARG
1	A	338	ILE
1	A	342	GLN
1	A	351	LYS
1	A	356	LYS
1	A	358	LEU
1	A	374	GLN
1	A	376	ARG
1	A	377	VAL
1	A	387	VAL
1	A	393	SER
1	A	399	LEU
1	A	415	THR
1	A	416	GLN
1	A	440	ARG
1	A	458	GLU
1	A	469	GLU
1	A	477	VAL
1	A	480	LYS
1	A	481	ILE
1	B	1	MET
1	B	2	GLN
1	B	10	ARG
1	B	15	VAL
1	B	19	THR
1	B	34	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	ASP
1	B	50	LYS
1	B	63	GLU
1	B	66	ARG
1	B	74	ARG
1	B	79	SER
1	B	81	GLU
1	B	92	HIS
1	B	94	ILE
1	B	95	ARG
1	B	118	LYS
1	B	122	SER
1	B	136	ARG
1	B	137	LYS
1	B	172	LYS
1	B	175	GLU
1	B	184	ILE
1	B	189	THR
1	B	191	VAL
1	B	195	LYS
1	B	212	LEU
1	B	220	LYS
1	B	221	ILE
1	B	242	LYS
1	B	243	ARG
1	B	247	GLU
1	B	251	LYS
1	B	258	GLU
1	B	262	ILE
1	B	276	ASN
1	B	299	GLU
1	B	300	ARG
1	B	324	THR
1	B	327	LEU
1	B	328	ARG
1	B	329	ARG
1	B	338	ILE
1	B	341	GLU
1	B	345	LYS
1	B	351	LYS
1	B	358	LEU
1	B	372	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	374	GLN
1	B	376	ARG
1	B	377	VAL
1	B	380	GLU
1	B	381	GLU
1	B	387	VAL
1	B	393	SER
1	B	399	LEU
1	B	406	GLU
1	B	415	THR
1	B	423	LYS
1	B	426	ASN
1	B	432	MET
1	B	440	ARG
1	B	452	GLN
1	B	457	ARG
1	B	458	GLU
1	B	477	VAL
1	B	480	LYS
1	B	481	ILE
1	B	487	ARG
1	C	1	MET
1	C	2	GLN
1	C	15	VAL
1	C	19	THR
1	C	23	VAL
1	C	24	SER
1	C	30	LEU
1	C	43	ASP
1	C	79	SER
1	C	84	GLN
1	C	87	SER
1	C	90	THR
1	C	92	HIS
1	C	98	ARG
1	C	122	SER
1	C	135	GLN
1	C	136	ARG
1	C	142	VAL
1	C	156	SER
1	C	172	LYS
1	C	175	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	180	SER
1	C	184	ILE
1	C	189	THR
1	C	191	VAL
1	C	212	LEU
1	C	220	LYS
1	C	221	ILE
1	C	227	THR
1	C	235	GLU
1	C	237	SER
1	C	244	ILE
1	C	258	GLU
1	C	263	GLU
1	C	271	TRP
1	C	309	ARG
1	C	327	LEU
1	C	328	ARG
1	C	329	ARG
1	C	334	SER
1	C	338	ILE
1	C	340	ILE
1	C	345	LYS
1	C	351	LYS
1	C	354	ASP
1	C	356	LYS
1	C	374	GLN
1	C	377	VAL
1	C	378	CYS
1	C	380	GLU
1	C	383	PHE
1	C	388	THR
1	C	391	ARG
1	C	393	SER
1	C	399	LEU
1	C	401	ILE
1	C	404	ASN
1	C	416	GLN
1	C	423	LYS
1	C	432	MET
1	C	440	ARG
1	C	445	SER
1	C	458	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	466	ASP
1	C	469	GLU
1	C	471	ARG
1	C	478	ASP
1	C	480	LYS
1	C	481	ILE
1	C	487	ARG
1	D	10	ARG
1	D	12	VAL
1	D	24	SER
1	D	43	ASP
1	D	63	GLU
1	D	66	ARG
1	D	70	LYS
1	D	74	ARG
1	D	81	GLU
1	D	89	ASN
1	D	92	HIS
1	D	95	ARG
1	D	97	SER
1	D	118	LYS
1	D	122	SER
1	D	136	ARG
1	D	159	MET
1	D	172	LYS
1	D	174	SER
1	D	180	SER
1	D	184	ILE
1	D	191	VAL
1	D	212	LEU
1	D	220	LYS
1	D	221	ILE
1	D	233	ILE
1	D	238	LYS
1	D	242	LYS
1	D	243	ARG
1	D	247	GLU
1	D	258	GLU
1	D	263	GLU
1	D	273	ILE
1	D	291	LYS
1	D	299	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	300	ARG
1	D	309	ARG
1	D	317	GLU
1	D	320	MET
1	D	323	LEU
1	D	324	THR
1	D	327	LEU
1	D	328	ARG
1	D	329	ARG
1	D	331	ARG
1	D	338	ILE
1	D	342	GLN
1	D	345	LYS
1	D	354	ASP
1	D	358	LEU
1	D	374	GLN
1	D	376	ARG
1	D	380	GLU
1	D	387	VAL
1	D	393	SER
1	D	399	LEU
1	D	404	ASN
1	D	413	LEU
1	D	415	THR
1	D	416	GLN
1	D	423	LYS
1	D	432	MET
1	D	445	SER
1	D	457	ARG
1	D	468	THR
1	D	477	VAL
1	D	486	LYS
1	D	487	ARG
1	E	1	MET
1	E	2	GLN
1	E	8	ASP
1	E	10	ARG
1	E	15	VAL
1	E	34	ILE
1	E	74	ARG
1	E	79	SER
1	E	87	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	89	ASN
1	E	92	HIS
1	E	94	ILE
1	E	95	ARG
1	E	124	ILE
1	E	135	GLN
1	E	137	LYS
1	E	153	MET
1	E	172	LYS
1	E	175	GLU
1	E	178	PRO
1	E	180	SER
1	E	184	ILE
1	E	189	THR
1	E	191	VAL
1	E	195	LYS
1	E	201	VAL
1	E	207	THR
1	E	212	LEU
1	E	214	GLU
1	E	220	LYS
1	E	229	THR
1	E	232	ARG
1	E	233	ILE
1	E	238	LYS
1	E	242	LYS
1	E	243	ARG
1	E	247	GLU
1	E	258	GLU
1	E	262	ILE
1	E	273	ILE
1	E	304	LEU
1	E	309	ARG
1	E	324	THR
1	E	327	LEU
1	E	328	ARG
1	E	338	ILE
1	E	351	LYS
1	E	355	ASP
1	E	356	LYS
1	E	358	LEU
1	E	374	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	386	PHE
1	E	387	VAL
1	E	388	THR
1	E	391	ARG
1	E	393	SER
1	E	399	LEU
1	E	405	THR
1	E	415	THR
1	E	416	GLN
1	E	423	LYS
1	E	426	ASN
1	E	432	MET
1	E	439	LYS
1	E	440	ARG
1	E	458	GLU
1	E	480	LYS
1	E	481	ILE
1	F	1	MET
1	F	10	ARG
1	F	19	THR
1	F	30	LEU
1	F	34	ILE
1	F	44	LEU
1	F	51	ARG
1	F	59	LEU
1	F	66	ARG
1	F	70	LYS
1	F	77	GLU
1	F	79	SER
1	F	80	GLU
1	F	84	GLN
1	F	87	SER
1	F	89	ASN
1	F	94	ILE
1	F	95	ARG
1	F	122	SER
1	F	127	ASP
1	F	136	ARG
1	F	172	LYS
1	F	174	SER
1	F	175	GLU
1	F	176	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	186	GLU
1	F	195	LYS
1	F	201	VAL
1	F	212	LEU
1	F	214	GLU
1	F	221	ILE
1	F	226	SER
1	F	229	THR
1	F	238	LYS
1	F	243	ARG
1	F	245	GLN
1	F	247	GLU
1	F	251	LYS
1	F	258	GLU
1	F	263	GLU
1	F	289	LEU
1	F	291	LYS
1	F	293	ILE
1	F	299	GLU
1	F	309	ARG
1	F	323	LEU
1	F	324	THR
1	F	327	LEU
1	F	328	ARG
1	F	329	ARG
1	F	330	ASP
1	F	340	ILE
1	F	345	LYS
1	F	351	LYS
1	F	354	ASP
1	F	374	GLN
1	F	376	ARG
1	F	379	GLN
1	F	381	GLU
1	F	390	VAL
1	F	393	SER
1	F	399	LEU
1	F	415	THR
1	F	432	MET
1	F	445	SER
1	F	458	GLU
1	F	468	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	471	ARG
1	F	478	ASP
1	F	480	LYS
1	F	481	ILE
1	F	487	ARG
1	G	8	ASP
1	G	10	ARG
1	G	15	VAL
1	G	19	THR
1	G	20	ILE
1	G	21	ASP
1	G	30	LEU
1	G	34	ILE
1	G	43	ASP
1	G	66	ARG
1	G	70	LYS
1	G	74	ARG
1	G	75	ILE
1	G	79	SER
1	G	87	SER
1	G	89	ASN
1	G	98	ARG
1	G	118	LYS
1	G	122	SER
1	G	136	ARG
1	G	148	TRP
1	G	149	ASN
1	G	159	MET
1	G	174	SER
1	G	175	GLU
1	G	177	THR
1	G	183	ARG
1	G	184	ILE
1	G	195	LYS
1	G	201	VAL
1	G	214	GLU
1	G	221	ILE
1	G	238	LYS
1	G	243	ARG
1	G	247	GLU
1	G	251	LYS
1	G	258	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	271	TRP
1	G	289	LEU
1	G	293	ILE
1	G	299	GLU
1	G	300	ARG
1	G	320	MET
1	G	323	LEU
1	G	328	ARG
1	G	331	ARG
1	G	334	SER
1	G	337	ASP
1	G	338	ILE
1	G	340	ILE
1	G	345	LYS
1	G	351	LYS
1	G	355	ASP
1	G	358	LEU
1	G	376	ARG
1	G	377	VAL
1	G	380	GLU
1	G	387	VAL
1	G	388	THR
1	G	390	VAL
1	G	393	SER
1	G	399	LEU
1	G	404	ASN
1	G	415	THR
1	G	416	GLN
1	G	432	MET
1	G	445	SER
1	G	447	PHE
1	G	453	SER
1	G	457	ARG
1	G	468	THR
1	G	481	ILE
1	G	486	LYS
1	H	1	MET
1	H	4	GLN
1	H	8	ASP
1	H	19	THR
1	H	24	SER
1	H	59	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	66	ARG
1	H	74	ARG
1	H	79	SER
1	H	87	SER
1	H	89	ASN
1	H	92	HIS
1	H	95	ARG
1	H	100	LEU
1	H	118	LYS
1	H	122	SER
1	H	124	ILE
1	H	127	ASP
1	H	146	VAL
1	H	147	PRO
1	H	155	THR
1	H	168	THR
1	H	175	GLU
1	H	180	SER
1	H	184	ILE
1	H	195	LYS
1	H	212	LEU
1	H	214	GLU
1	H	221	ILE
1	H	229	THR
1	H	233	ILE
1	H	238	LYS
1	H	242	LYS
1	H	243	ARG
1	H	244	ILE
1	H	247	GLU
1	H	258	GLU
1	H	263	GLU
1	H	271	TRP
1	H	273	ILE
1	H	299	GLU
1	H	304	LEU
1	H	306	LYS
1	H	309	ARG
1	H	325	SER
1	H	327	LEU
1	H	328	ARG
1	H	329	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	338	ILE
1	H	354	ASP
1	H	355	ASP
1	H	356	LYS
1	H	358	LEU
1	H	362	PHE
1	H	363	TYR
1	H	380	GLU
1	H	387	VAL
1	H	399	LEU
1	H	404	ASN
1	H	415	THR
1	H	416	GLN
1	H	423	LYS
1	H	432	MET
1	H	450	VAL
1	H	458	GLU
1	H	471	ARG
1	H	478	ASP
1	H	480	LYS
1	H	481	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	92	HIS
1	A	132	ASN
1	A	167	ASN
1	A	215	HIS
1	A	277	GLN
1	A	290	HIS
1	A	342	GLN
1	A	404	ASN
1	A	417	ASN
1	B	2	GLN
1	B	4	GLN
1	B	84	GLN
1	B	132	ASN
1	B	277	GLN
1	B	290	HIS
1	B	417	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	465	HIS
1	C	2	GLN
1	C	132	ASN
1	C	135	GLN
1	C	215	HIS
1	C	277	GLN
1	C	290	HIS
1	C	416	GLN
1	C	417	ASN
1	C	429	HIS
1	D	2	GLN
1	D	84	GLN
1	D	132	ASN
1	D	206	HIS
1	D	276	ASN
1	D	277	GLN
1	D	290	HIS
1	D	404	ASN
1	D	416	GLN
1	D	417	ASN
1	D	429	HIS
1	E	2	GLN
1	E	84	GLN
1	E	132	ASN
1	E	277	GLN
1	E	290	HIS
1	E	342	GLN
1	E	374	GLN
1	E	417	ASN
1	E	426	ASN
1	F	2	GLN
1	F	144	GLN
1	F	277	GLN
1	F	290	HIS
1	F	296	GLN
1	F	417	ASN
1	F	429	HIS
1	F	465	HIS
1	G	2	GLN
1	G	132	ASN
1	G	144	GLN
1	G	290	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	379	GLN
1	G	426	ASN
1	H	2	GLN
1	H	4	GLN
1	H	84	GLN
1	H	89	ASN
1	H	92	HIS
1	H	132	ASN
1	H	144	GLN
1	H	215	HIS
1	H	277	GLN
1	H	290	HIS
1	H	342	GLN
1	H	379	GLN
1	H	417	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	487/495 (98%)	-0.10	2 (0%)	92	93	14, 34, 61, 93	0
1	B	487/495 (98%)	-0.08	3 (0%)	89	91	16, 36, 61, 102	0
1	C	487/495 (98%)	-0.13	1 (0%)	95	96	12, 37, 62, 145	0
1	D	487/495 (98%)	0.04	5 (1%)	82	83	14, 35, 59, 165	0
1	E	485/495 (97%)	0.06	9 (1%)	66	69	16, 37, 61, 113	0
1	F	487/495 (98%)	0.17	8 (1%)	72	74	11, 44, 76, 131	0
1	G	487/495 (98%)	0.24	21 (4%)	35	33	18, 47, 94, 137	0
1	H	487/495 (98%)	0.39	24 (4%)	29	28	16, 45, 79, 148	0
All	All	3894/3960 (98%)	0.07	73 (1%)	66	69	11, 39, 73, 165	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	376	ARG	5.3
1	H	358	LEU	5.0
1	G	341	GLU	4.2
1	E	482	ALA	4.2
1	F	382	VAL	4.0
1	C	354	ASP	3.8
1	D	356	LYS	3.7
1	G	309	ARG	3.6
1	F	1	MET	3.6
1	E	357	ALA	3.5
1	H	31	ILE	3.4
1	G	83	ALA	3.4
1	E	485	PHE	3.3
1	E	483	PRO	3.2
1	H	359	ALA	3.1
1	E	1	MET	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	325	SER	3.1
1	H	361	GLY	3.1
1	H	340	ILE	3.0
1	H	23	VAL	3.0
1	G	311	GLY	3.0
1	H	354	ASP	3.0
1	H	88	LEU	2.9
1	H	480	LYS	2.9
1	H	1	MET	2.8
1	F	377	VAL	2.8
1	G	331	ARG	2.8
1	G	377	VAL	2.7
1	G	328	ARG	2.7
1	H	87	SER	2.7
1	D	486	LYS	2.7
1	E	257	PHE	2.6
1	F	36	ALA	2.6
1	A	377	VAL	2.6
1	H	12	VAL	2.6
1	B	23	VAL	2.6
1	H	337	ASP	2.5
1	F	378	CYS	2.4
1	H	180	SER	2.4
1	G	384	GLY	2.3
1	A	356	LYS	2.3
1	G	334	SER	2.3
1	F	369	VAL	2.3
1	E	78	CYS	2.3
1	F	299	GLU	2.3
1	E	97	SER	2.3
1	H	26	HIS	2.3
1	G	323	LEU	2.3
1	G	93	PRO	2.2
1	H	83	ALA	2.2
1	B	357	ALA	2.2
1	E	102	VAL	2.2
1	H	191	VAL	2.2
1	G	317	GLU	2.2
1	D	485	PHE	2.2
1	H	364	VAL	2.2
1	G	326	ALA	2.2
1	B	478	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	296	GLN	2.2
1	H	386	PHE	2.2
1	G	362	PHE	2.2
1	G	279	GLN	2.1
1	G	374	GLN	2.1
1	G	36	ALA	2.1
1	H	372	LYS	2.1
1	G	310	LEU	2.1
1	D	1	MET	2.1
1	G	386	PHE	2.1
1	H	86	GLU	2.1
1	G	316	PRO	2.1
1	G	327	LEU	2.0
1	H	85	LEU	2.0
1	D	351	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.