



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:55 PM EDT

PDB ID : 1LDK
Title : Structure of the Cul1-Rbx1-Skp1-F boxSkp2 SCF Ubiquitin Ligase Complex
Authors : Zheng, N.; Schulman, B.A.; Song, L.; Miller, J.J.; Jeffrey, P.D.; Wang, P.;
Chu, C.; Koepp, D.M.; Elledge, S.J.; Pagano, M.; Conaway, R.C.; Conaway,
J.W.; Harper, J.W.; Pavletich, N.P.
Deposited on : 2002-04-08
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

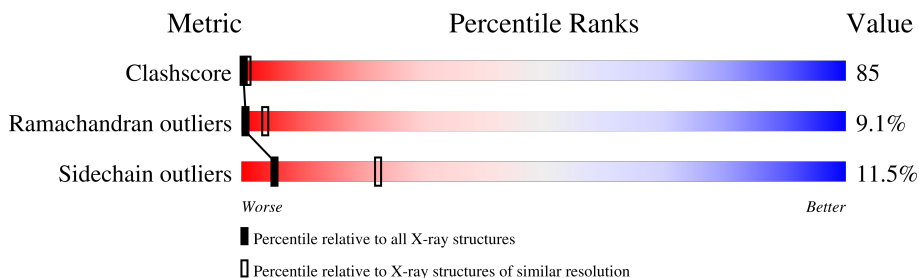
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	14% 56% 18% • 10%
2	B	366	21% 62% 14% •
3	C	90	56% 39% ••
4	D	133	18% 57% 11% • 11%
5	E	41	20% 59% 20% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7922 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 CULLIN HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	358	2950	1870	508	558	14	0	0	0

- Molecule 2 is a protein called CULLIN HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	366	2981	1894	503	569	15	0	0	0

- Molecule 3 is a protein called ring-box protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	88	731	464	133	125	9	574	0	0

- Molecule 4 is a protein called CYCLIN A/CDK2-ASSOCIATED PROTEIN P19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	118	926	594	149	178	5	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	deletion	UNP P63208
D	?	-	ASP	deletion	UNP P63208
D	?	-	GLU	deletion	UNP P63208
D	?	-	GLY	deletion	UNP P63208
D	?	-	ASP	deletion	UNP P63208
D	?	-	ASP	deletion	UNP P63208

- Molecule 5 is a protein called SKP2-like protein type gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	41	331	218	52	58	3	0	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

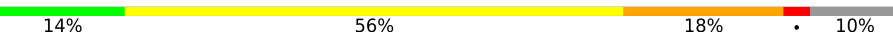
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	C	3	3	3	0	0

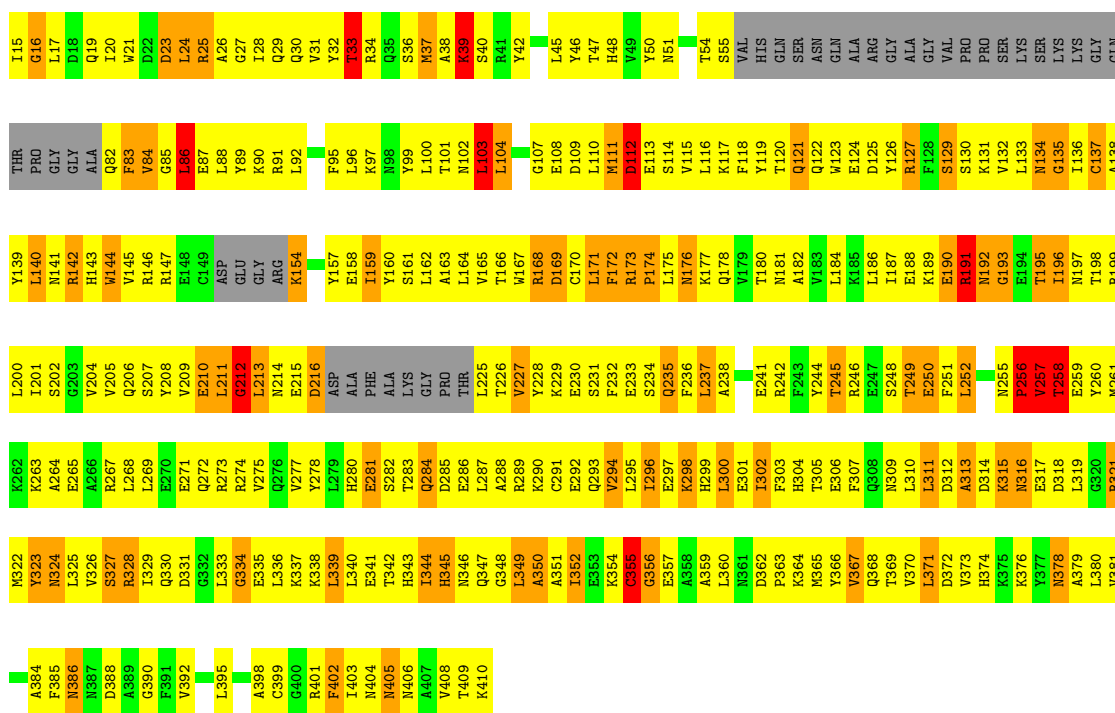
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

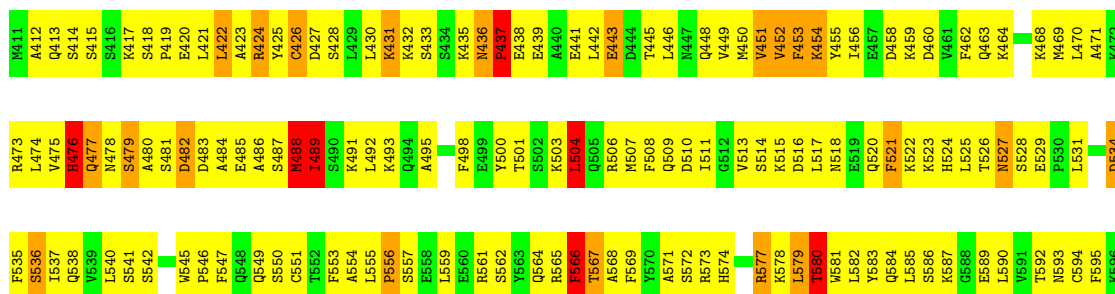
- Molecule 1: CULLIN HOMOLOG

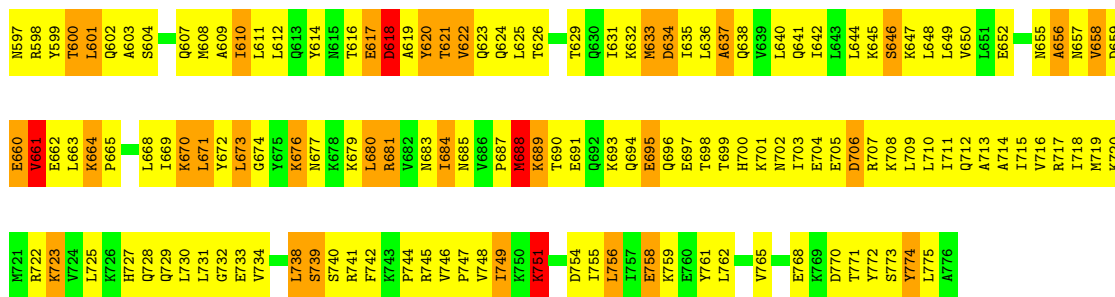
Chain A: 



- Molecule 2: CULLIN HOMOLOG

Chain B: 

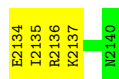
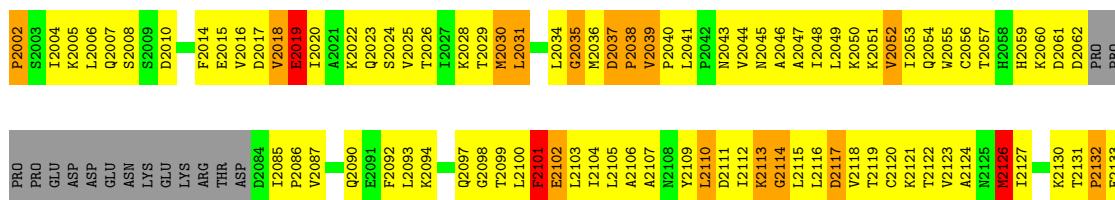




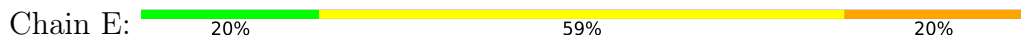
• Molecule 3: ring-box protein 1



• Molecule 4: CYCLIN A/CDK2-ASSOCIATED PROTEIN P19



• Molecule 5: SKP2-like protein type gamma



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	219.38Å 50.53Å 158.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.289 , 0.331	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7922	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.78	7/2999 (0.2%)	1.22	32/4039 (0.8%)
2	B	0.75	8/3027 (0.3%)	1.12	28/4069 (0.7%)
3	C	0.32	0/752	0.64	1/1020 (0.1%)
4	D	0.84	3/940 (0.3%)	1.07	7/1271 (0.6%)
5	E	0.76	1/340 (0.3%)	1.14	4/461 (0.9%)
All	All	0.74	19/8058 (0.2%)	1.12	72/10860 (0.7%)

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	A	0	5
2	B	0	3
4	D	0	1
All	All	0	9

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2102	GLU	N-CA	18.23	1.82	1.46
1	A	135	GLY	N-CA	10.90	1.62	1.46
2	B	453	PHE	N-CA	9.67	1.65	1.46
2	B	489	ILE	N-CA	9.53	1.65	1.46
1	A	210	GLU	N-CA	8.53	1.63	1.46
2	B	443	GLU	C-N	8.50	1.53	1.34
1	A	367	VAL	N-CA	8.43	1.63	1.46
2	B	426	CYS	N-CA	6.88	1.60	1.46
1	A	344	ILE	N-CA	6.87	1.60	1.46
2	B	523	LYS	N-CA	6.84	1.60	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	3149	TRP	C-OXT	6.80	1.36	1.23
4	D	2110	LEU	N-CA	6.64	1.59	1.46
1	A	216	ASP	C-O	-6.61	1.10	1.23
1	A	196	ILE	CG1-CD1	6.08	1.92	1.50
2	B	637	ALA	N-CA	5.96	1.58	1.46
2	B	580	THR	N-CA	-5.80	1.34	1.46
2	B	661	VAL	C-N	-5.46	1.21	1.34
1	A	296	ILE	CG1-CD1	5.04	1.85	1.50
4	D	2126	MET	N-CA	5.02	1.56	1.46

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ASP	O-C-N	-16.77	95.86	122.70
1	A	213	LEU	CA-C-N	-14.28	85.80	117.20
3	C	1023	GLU	N-CA-CB	-12.15	88.73	110.60
5	E	3146	GLU	N-CA-C	-11.82	79.08	111.00
1	A	212	GLY	C-N-CA	-11.81	92.19	121.70
4	D	2102	GLU	N-CA-C	10.59	139.58	111.00
1	A	112	ASP	C-N-CA	10.50	147.95	121.70
4	D	2102	GLU	N-CA-CB	-10.50	91.70	110.60
1	A	16	GLY	N-CA-C	-10.15	87.71	113.10
2	B	706	ASP	N-CA-CB	-9.75	93.06	110.60
1	A	196	ILE	CB-CG1-CD1	-9.65	86.89	113.90
1	A	135	GLY	N-CA-C	-9.55	89.22	113.10
4	D	2110	LEU	N-CA-C	-9.49	85.37	111.00
1	A	213	LEU	CA-C-O	9.02	139.05	120.10
1	A	256	PRO	CA-N-CD	-8.70	99.32	111.50
2	B	476	HIS	N-CA-C	-8.66	87.61	111.00
1	A	213	LEU	C-N-CA	8.51	142.98	121.70
4	D	2101	PHE	C-N-CA	-8.40	100.70	121.70
2	B	706	ASP	N-CA-C	8.23	133.21	111.00
2	B	523	LYS	N-CA-C	-8.12	89.09	111.00
1	A	296	ILE	CB-CG1-CD1	-8.06	91.33	113.90
2	B	437	PRO	CA-N-CD	-7.73	100.67	111.50
5	E	3113	PRO	CA-N-CD	-7.66	100.78	111.50
1	A	33	THR	N-CA-C	-7.65	90.34	111.00
2	B	521	PHE	N-CA-CB	-7.62	96.89	110.60
1	A	213	LEU	O-C-N	7.43	134.59	122.70
2	B	479	SER	CB-CA-C	-7.35	96.14	110.10
1	A	367	VAL	N-CA-C	-7.34	91.19	111.00
2	B	664	LYS	C-N-CD	-7.31	104.51	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	566	PHE	CB-CG-CD2	6.97	125.68	120.80
2	B	646	SER	N-CA-C	-6.89	92.38	111.00
2	B	633	MET	C-N-CA	-6.80	104.71	121.70
4	D	2002	PRO	N-CA-CB	6.74	111.39	103.30
1	A	195	THR	N-CA-C	6.71	129.12	111.00
2	B	618	ASP	CB-CA-C	6.70	123.80	110.40
2	B	566	PHE	CB-CG-CD1	-6.63	116.16	120.80
1	A	134	ASN	C-N-CA	-6.54	108.56	122.30
2	B	495	ALA	N-CA-C	6.42	128.34	111.00
1	A	190	GLU	N-CA-C	-6.41	93.69	111.00
1	A	344	ILE	N-CA-C	-6.36	93.83	111.00
1	A	127	ARG	N-CA-C	-6.33	93.91	111.00
2	B	424	ARG	N-CA-C	-6.26	94.09	111.00
1	A	112	ASP	CA-C-N	6.25	130.96	117.20
2	B	701	LYS	N-CA-C	-6.10	94.53	111.00
2	B	688	MET	CB-CA-C	6.06	122.51	110.40
1	A	313	ALA	N-CA-C	-6.00	94.81	111.00
2	B	436	ASN	CA-CB-CG	-5.93	100.35	113.40
2	B	637	ALA	N-CA-C	-5.92	95.01	111.00
2	B	489	ILE	N-CA-C	5.90	126.92	111.00
1	A	99	TYR	N-CA-CB	-5.82	100.12	110.60
1	A	355	CYS	CA-C-N	5.79	127.78	116.20
4	D	2126	MET	N-CA-C	5.79	126.62	111.00
5	E	3147	SER	N-CA-C	5.78	126.60	111.00
1	A	172	PHE	CB-CG-CD1	5.70	124.79	120.80
1	A	257	VAL	C-N-CA	5.62	135.76	121.70
2	B	774	TYR	CA-C-N	-5.54	105.00	117.20
2	B	504	LEU	CB-CA-C	5.54	120.73	110.20
2	B	660	GLU	C-N-CA	-5.50	107.96	121.70
1	A	129	SER	N-CA-C	-5.39	96.44	111.00
4	D	2105	LEU	C-N-CA	-5.36	108.30	121.70
2	B	412	ALA	N-CA-C	-5.36	96.54	111.00
1	A	191	ARG	N-CA-C	-5.31	96.66	111.00
1	A	350	ALA	N-CA-C	-5.24	96.86	111.00
5	E	3114	ASP	CB-CA-C	-5.22	99.95	110.40
2	B	426	CYS	N-CA-C	-5.18	97.02	111.00
2	B	488	MET	C-N-CA	-5.11	108.93	121.70
2	B	436	ASN	C-N-CD	-5.11	109.36	120.60
1	A	172	PHE	CB-CG-CD2	-5.06	117.26	120.80
1	A	296	ILE	CA-C-N	5.04	128.29	117.20
1	A	356	GLY	N-CA-C	5.03	125.68	113.10
2	B	528	SER	N-CA-C	-5.01	97.47	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASN	CB-CA-C	5.01	120.42	110.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	MET	Mainchain
1	A	112	ASP	Peptide,Mainchain
1	A	113	GLU	Mainchain
1	A	323	TYR	Sidechain
2	B	443	GLU	Mainchain
2	B	452	VAL	Peptide
2	B	488	MET	Peptide
4	D	2101	PHE	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	2950	0	2915	537	1
2	B	2981	0	3049	548	3
3	C	731	0	689	28	1
4	D	926	0	944	170	0
5	E	331	0	331	43	0
6	C	3	0	0	0	0
All	All	7922	0	7928	1256	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 85.

All (1256) 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:A:409:THR:CG2	2:B:415:SER:HA	1.32	1.58
2:B:555:LEU:CD2	2:B:559:LEU:HD22	1.11	1.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ILE:CD1	1:A:296:ILE:CG1	1.85	1.55
2:B:553:PHE:CD1	2:B:631:ILE:HG12	1.37	1.53
4:D:2002:PRO:CB	4:D:2018:VAL:HG13	1.41	1.47
4:D:2038:PRO:O	4:D:2040:PRO:CD	1.63	1.47
1:A:196:ILE:CD1	1:A:196:ILE:CG1	1.92	1.46
4:D:2102:GLU:N	4:D:2102:GLU:CA	1.82	1.41
1:A:409:THR:CG2	2:B:415:SER:CA	1.88	1.40
1:A:144:TRP:O	1:A:144:TRP:CE3	1.72	1.40
2:B:555:LEU:HD23	2:B:559:LEU:CD2	0.91	1.39
1:A:196:ILE:CD1	1:A:196:ILE:CG2	2.04	1.35
1:A:409:THR:HG21	2:B:415:SER:CA	1.40	1.34
2:B:712:GLN:HB3	2:B:756:LEU:CD2	1.60	1.30
1:A:107:GLY:O	1:A:110:LEU:HG	1.10	1.28
2:B:555:LEU:CD2	2:B:559:LEU:CD2	1.77	1.27
2:B:577:ARG:O	2:B:577:ARG:HD3	1.32	1.26
4:D:2038:PRO:O	4:D:2040:PRO:HD3	1.14	1.25
2:B:578:LYS:O	2:B:579:LEU:HD23	1.24	1.25
1:A:196:ILE:CD1	1:A:196:ILE:HG21	1.61	1.25
1:A:297:GLU:O	1:A:300:LEU:HB2	1.32	1.23
1:A:142:ARG:O	1:A:146:ARG:NH2	1.71	1.23
1:A:211:LEU:O	1:A:213:LEU:HD23	1.07	1.22
2:B:553:PHE:CD1	2:B:631:ILE:CG1	2.24	1.21
4:D:2002:PRO:CB	4:D:2018:VAL:CG1	2.21	1.19
1:A:293:GLN:HG3	1:A:297:GLU:OE2	1.42	1.18
1:A:111:MET:HB2	1:A:114:SER:OG	1.41	1.18
2:B:553:PHE:CE1	2:B:631:ILE:HD11	1.80	1.16
2:B:712:GLN:HB3	2:B:756:LEU:HD21	1.23	1.15
1:A:402:PHE:O	1:A:406:ASN:ND2	1.81	1.14
1:A:30:GLN:O	1:A:33:THR:O	1.62	1.14
1:A:211:LEU:O	1:A:213:LEU:CD2	1.96	1.14
2:B:569:PHE:O	2:B:572:SER:OG	1.66	1.13
2:B:620:TYR:CD2	2:B:624:GLN:HG2	1.82	1.13
2:B:551:CYS:SG	2:B:632:LYS:HD2	1.89	1.12
2:B:719:MET:HE1	2:B:774:TYR:HB2	1.28	1.12
2:B:521:PHE:O	2:B:525:LEU:HB2	1.50	1.11
2:B:619:ALA:HB2	2:B:670:LYS:CB	1.80	1.11
1:A:100:LEU:HA	1:A:103:LEU:HD23	1.30	1.11
1:A:296:ILE:HG12	1:A:325:LEU:HD22	1.31	1.10
1:A:196:ILE:HG21	1:A:196:ILE:HD12	1.24	1.10
2:B:727:HIS:O	2:B:727:HIS:ND1	1.85	1.10
2:B:637:ALA:HB1	2:B:663:LEU:HD12	1.34	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:LEU:O	2:B:476:HIS:O	1.71	1.09
2:B:638:GLN:OE1	2:B:688:MET:CE	1.99	1.09
1:A:186:LEU:HD21	1:A:197:ASN:HD22	0.96	1.09
1:A:297:GLU:O	1:A:300:LEU:N	1.86	1.09
2:B:555:LEU:HD21	2:B:559:LEU:HD22	1.27	1.09
5:E:3145:ASP:OD2	5:E:3146:GLU:O	1.71	1.08
1:A:196:ILE:CG2	1:A:196:ILE:HD13	1.73	1.08
2:B:553:PHE:HD1	2:B:631:ILE:CG1	1.60	1.08
2:B:469:MET:HB3	2:B:473:ARG:HH12	1.12	1.07
2:B:574:HIS:HB2	2:B:577:ARG:HG3	1.31	1.07
1:A:39:LYS:HE2	4:D:2037:ASP:H	1.12	1.06
1:A:107:GLY:O	1:A:110:LEU:CG	2.02	1.06
2:B:566:PHE:O	2:B:569:PHE:N	1.89	1.06
2:B:553:PHE:CE1	2:B:629:THR:HB	1.91	1.06
2:B:712:GLN:CB	2:B:756:LEU:HD21	1.85	1.05
1:A:107:GLY:HA2	1:A:110:LEU:HD11	1.36	1.05
1:A:168:ARG:HH11	1:A:213:LEU:HD22	1.20	1.04
1:A:186:LEU:HD21	1:A:197:ASN:ND2	1.69	1.04
1:A:404:ASN:O	1:A:405:ASN:OD1	1.76	1.03
1:A:144:TRP:O	1:A:144:TRP:CD2	2.11	1.03
1:A:297:GLU:O	1:A:300:LEU:CB	2.07	1.03
4:D:2038:PRO:O	4:D:2040:PRO:HD2	1.50	1.03
2:B:555:LEU:HD23	2:B:559:LEU:HD23	1.09	1.02
2:B:553:PHE:CE1	2:B:631:ILE:CD1	2.41	1.02
2:B:619:ALA:CB	2:B:670:LYS:HB3	1.90	1.02
2:B:660:GLU:O	2:B:661:VAL:O	1.76	1.02
1:A:112:ASP:HB3	1:A:182:ALA:HA	1.39	1.02
1:A:173:ARG:H	1:A:174:PRO:HD2	1.26	1.01
1:A:142:ARG:O	1:A:146:ARG:CZ	2.09	1.01
1:A:158:GLU:HG3	1:A:159:ILE:H	1.24	1.01
1:A:196:ILE:CD1	1:A:196:ILE:CB	2.39	1.00
1:A:409:THR:HG21	2:B:415:SER:C	1.82	0.99
1:A:186:LEU:CD1	1:A:197:ASN:HB3	1.93	0.99
1:A:196:ILE:HD13	1:A:196:ILE:HG23	1.39	0.98
2:B:553:PHE:CE1	2:B:631:ILE:CG1	2.46	0.98
2:B:758:GLU:OE1	2:B:759:LYS:HG3	1.63	0.98
2:B:453:PHE:HA	2:B:456:ILE:HD13	1.46	0.98
2:B:477:GLN:O	2:B:477:GLN:HG2	1.63	0.98
1:A:186:LEU:HD13	1:A:197:ASN:HB3	1.47	0.97
1:A:118:PHE:O	1:A:122:GLN:HG2	1.65	0.96
1:A:296:ILE:CD1	1:A:296:ILE:CB	2.43	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:474:LEU:C	2:B:476:HIS:O	2.04	0.96
1:A:197:ASN:CB	1:A:200:LEU:HD12	1.97	0.95
2:B:577:ARG:O	2:B:577:ARG:CD	2.15	0.95
1:A:256:PRO:HB2	1:A:259:GLU:HB2	1.49	0.95
2:B:571:ALA:CA	2:B:577:ARG:HH21	1.80	0.94
2:B:719:MET:SD	2:B:774:TYR:CG	2.60	0.94
4:D:2100:LEU:HA	4:D:2103:LEU:HD12	1.47	0.94
1:A:100:LEU:HD12	1:A:166:THR:HG22	1.48	0.94
1:A:142:ARG:O	1:A:146:ARG:NE	2.00	0.94
4:D:2040:PRO:O	4:D:2041:LEU:HD23	1.68	0.94
2:B:719:MET:SD	2:B:774:TYR:CB	2.56	0.94
2:B:553:PHE:CE1	2:B:631:ILE:HG12	2.04	0.93
2:B:553:PHE:HE1	2:B:631:ILE:HD11	1.17	0.93
1:A:111:MET:HB2	1:A:114:SER:HG	1.18	0.92
1:A:17:LEU:HA	1:A:20:ILE:HB	1.51	0.92
2:B:610:ILE:HD13	2:B:610:ILE:H	1.34	0.91
1:A:39:LYS:HE2	4:D:2037:ASP:N	1.84	0.91
2:B:719:MET:SD	2:B:774:TYR:HB3	2.10	0.91
1:A:409:THR:C	2:B:414:SER:O	2.03	0.91
1:A:352:ILE:HD11	1:A:406:ASN:HB3	1.52	0.90
1:A:235:GLN:H	1:A:235:GLN:NE2	1.68	0.90
2:B:430:LEU:O	2:B:431:LYS:O	1.89	0.90
5:E:3126:LEU:HD12	5:E:3126:LEU:H	1.35	0.90
1:A:100:LEU:HA	1:A:103:LEU:CD2	2.01	0.90
1:A:15:ILE:HG22	1:A:20:ILE:HG13	1.50	0.90
1:A:257:VAL:O	1:A:260:TYR:HB3	1.72	0.90
2:B:719:MET:CE	2:B:774:TYR:CD1	2.55	0.89
4:D:2031:LEU:HA	4:D:2035:GLY:HA2	1.52	0.89
2:B:712:GLN:HB3	2:B:756:LEU:HD22	1.53	0.89
2:B:577:ARG:HD3	2:B:577:ARG:C	1.90	0.89
1:A:197:ASN:CG	1:A:200:LEU:HD12	1.91	0.89
4:D:2102:GLU:H	4:D:2102:GLU:HG3	1.37	0.88
2:B:719:MET:HE3	2:B:774:TYR:CD1	2.08	0.88
1:A:409:THR:HG22	2:B:415:SER:HA	1.34	0.88
2:B:638:GLN:OE1	2:B:688:MET:SD	2.31	0.88
2:B:574:HIS:HB2	2:B:577:ARG:CG	2.04	0.88
2:B:722:ARG:O	2:B:774:TYR:CE2	2.25	0.88
2:B:727:HIS:HB3	2:B:770:ASP:HB3	1.56	0.88
1:A:296:ILE:CG1	1:A:325:LEU:HD22	2.03	0.87
2:B:427:ASP:OD1	2:B:431:LYS:HD2	1.75	0.87
2:B:711:ILE:HG22	2:B:711:ILE:O	1.74	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2014:PHE:O	4:D:2016:VAL:HG23	1.72	0.87
2:B:711:ILE:HA	2:B:714:ALA:HB3	1.57	0.87
1:A:366:TYR:CD2	1:A:408:VAL:HG21	2.10	0.87
1:A:54:THR:HG23	5:E:3113:PRO:HG3	1.55	0.87
2:B:582:LEU:HD21	3:C:1032:LEU:HG	1.58	0.86
1:A:321:ARG:HH11	1:A:321:ARG:HG2	1.41	0.86
2:B:578:LYS:HG3	2:B:579:LEU:N	1.90	0.86
2:B:578:LYS:HG3	2:B:579:LEU:H	1.37	0.86
4:D:2018:VAL:HG23	4:D:2019:GLU:H	1.40	0.86
1:A:157:TYR:C	1:A:157:TYR:CD2	2.45	0.86
1:A:187:ILE:O	1:A:190:GLU:HB2	1.76	0.86
1:A:107:GLY:HA2	1:A:110:LEU:CD1	2.06	0.85
2:B:660:GLU:O	2:B:661:VAL:C	2.11	0.85
2:B:619:ALA:CB	2:B:670:LYS:CB	2.49	0.85
4:D:2048:ILE:O	4:D:2052:VAL:HG23	1.75	0.85
2:B:730:LEU:HD12	2:B:733:GLU:HB2	1.57	0.85
4:D:2038:PRO:C	4:D:2040:PRO:HD3	1.95	0.85
1:A:235:GLN:N	1:A:235:GLN:HE21	1.74	0.85
1:A:158:GLU:HG3	1:A:159:ILE:N	1.89	0.85
1:A:326:VAL:HG21	1:A:336:LEU:HD11	1.59	0.85
1:A:355:CYS:O	1:A:359:ALA:HB3	1.76	0.85
4:D:2101:PHE:C	4:D:2102:GLU:CA	2.45	0.84
2:B:719:MET:HE1	2:B:774:TYR:CB	2.05	0.84
1:A:197:ASN:OD1	1:A:200:LEU:CD1	2.25	0.84
1:A:297:GLU:C	1:A:300:LEU:HB2	1.97	0.84
1:A:111:MET:CB	1:A:114:SER:OG	2.23	0.84
2:B:578:LYS:C	2:B:579:LEU:HD23	1.96	0.84
2:B:661:VAL:HG12	2:B:662:GLU:O	1.78	0.84
1:A:235:GLN:H	1:A:235:GLN:HE21	1.21	0.84
2:B:708:LYS:HD2	2:B:708:LYS:N	1.94	0.83
2:B:719:MET:CE	2:B:774:TYR:HB2	2.08	0.83
1:A:39:LYS:HB2	1:A:39:LYS:NZ	1.94	0.83
2:B:578:LYS:O	2:B:579:LEU:CD2	2.19	0.83
2:B:534:ASP:HB2	3:C:1026:LYS:HG3	1.57	0.83
2:B:571:ALA:HA	2:B:577:ARG:NH2	1.92	0.83
2:B:660:GLU:C	2:B:661:VAL:O	2.17	0.82
4:D:2102:GLU:N	4:D:2102:GLU:HG3	1.94	0.82
1:A:157:TYR:CD2	1:A:157:TYR:O	2.33	0.82
2:B:542:SER:HA	3:C:1032:LEU:HD22	1.60	0.82
2:B:620:TYR:CD2	2:B:624:GLN:CG	2.62	0.82
4:D:2102:GLU:N	4:D:2102:GLU:CB	2.42	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2107:ALA:HB2	4:D:2115:LEU:HD22	1.60	0.82
1:A:300:LEU:HD13	1:A:304:HIS:NE2	1.94	0.81
1:A:168:ARG:HH11	1:A:213:LEU:CD2	1.93	0.81
1:A:168:ARG:NH1	1:A:213:LEU:HD22	1.94	0.81
2:B:553:PHE:HE1	2:B:631:ILE:CD1	1.85	0.81
2:B:571:ALA:HA	2:B:577:ARG:HH21	1.42	0.81
1:A:147:ARG:HH22	5:E:3146:GLU:HG2	1.46	0.81
2:B:616:THR:HG22	2:B:617:GLU:H	1.43	0.81
2:B:765:VAL:HG22	2:B:773:SER:HB2	1.63	0.81
1:A:209:VAL:O	1:A:212:GLY:N	2.12	0.81
2:B:620:TYR:CD1	2:B:624:GLN:OE1	2.34	0.80
2:B:662:GLU:O	2:B:663:LEU:HD23	1.81	0.80
1:A:101:THR:C	1:A:102:ASN:HD22	1.83	0.80
1:A:107:GLY:C	1:A:110:LEU:HG	2.01	0.80
2:B:641:GLN:HA	2:B:644:LEU:HD12	1.61	0.80
1:A:244:TYR:HB3	1:A:295:LEU:HD21	1.63	0.80
2:B:432:LYS:HD2	2:B:480:ALA:HB2	1.62	0.80
2:B:566:PHE:O	2:B:567:THR:C	2.19	0.80
2:B:430:LEU:O	2:B:431:LYS:C	2.18	0.80
2:B:571:ALA:HB2	2:B:577:ARG:NH2	1.97	0.80
2:B:574:HIS:CB	2:B:577:ARG:HG3	2.09	0.80
1:A:363:PRO:HA	2:B:421:LEU:HD12	1.64	0.79
1:A:110:LEU:HB2	1:A:115:VAL:HG23	1.63	0.79
2:B:469:MET:HB3	2:B:473:ARG:NH1	1.94	0.79
2:B:547:PHE:CE1	2:B:585:LEU:HD21	2.17	0.79
2:B:719:MET:CE	2:B:774:TYR:CG	2.65	0.79
1:A:409:THR:HG21	2:B:415:SER:HA	0.84	0.79
2:B:573:ARG:O	2:B:574:HIS:CG	2.36	0.79
2:B:571:ALA:CB	2:B:577:ARG:NH2	2.46	0.78
2:B:712:GLN:CG	2:B:756:LEU:HD21	2.13	0.78
1:A:356:GLY:HA2	1:A:359:ALA:HB3	1.64	0.78
2:B:619:ALA:HB2	2:B:670:LYS:HB2	1.65	0.78
1:A:296:ILE:CD1	1:A:296:ILE:HB	2.11	0.78
2:B:464:LYS:HZ2	2:B:703:ILE:HA	1.48	0.78
1:A:144:TRP:CD2	1:A:144:TRP:C	2.56	0.78
1:A:134:ASN:O	1:A:138:ALA:N	2.16	0.78
2:B:637:ALA:HB1	2:B:663:LEU:CD1	2.12	0.77
4:D:2131:THR:H	4:D:2134:GLU:HB3	1.47	0.77
2:B:541:SER:H	2:B:545:TRP:HE1	1.27	0.77
1:A:409:THR:HG22	2:B:415:SER:CA	1.90	0.77
2:B:719:MET:CE	2:B:774:TYR:CB	2.62	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ARG:N	1:A:174:PRO:HD2	1.99	0.77
1:A:197:ASN:HB3	1:A:200:LEU:HD12	1.63	0.77
2:B:522:LYS:NZ	2:B:525:LEU:HD23	2.00	0.77
1:A:286:GLU:O	1:A:289:ARG:N	2.18	0.77
2:B:551:CYS:SG	2:B:632:LYS:CD	2.72	0.77
1:A:186:LEU:CD2	1:A:197:ASN:HD22	1.88	0.77
2:B:640:LEU:HD11	2:B:669:ILE:HG12	1.65	0.77
2:B:582:LEU:HB2	3:C:1030:VAL:HG23	1.66	0.77
5:E:3109:TRP:HA	5:E:3138:ARG:HH22	1.50	0.77
1:A:231:SER:O	1:A:235:GLN:OE1	2.04	0.76
1:A:100:LEU:CA	1:A:103:LEU:HD23	2.12	0.76
2:B:473:ARG:HB3	2:B:479:SER:OG	1.86	0.76
2:B:708:LYS:HD2	2:B:708:LYS:H	1.48	0.76
1:A:188:GLU:C	1:A:190:GLU:H	1.88	0.76
2:B:427:ASP:O	2:B:431:LYS:HG3	1.86	0.76
1:A:211:LEU:O	1:A:214:ASN:ND2	2.18	0.76
2:B:547:PHE:CD1	2:B:585:LEU:HD21	2.21	0.76
1:A:171:LEU:O	1:A:176:ASN:HB2	1.86	0.76
1:A:293:GLN:CG	1:A:297:GLU:OE2	2.29	0.76
2:B:716:VAL:HG22	2:B:719:MET:HE2	1.67	0.76
2:B:638:GLN:OE1	2:B:688:MET:HE1	1.84	0.75
2:B:620:TYR:CG	2:B:624:GLN:OE1	2.39	0.75
2:B:671:LEU:HD22	2:B:672:TYR:N	2.01	0.75
1:A:175:LEU:O	1:A:178:GLN:HB3	1.86	0.75
1:A:292:GLU:O	1:A:296:ILE:HD12	1.86	0.75
2:B:604:SER:O	2:B:608:MET:HG2	1.85	0.75
2:B:436:ASN:OD1	2:B:437:PRO:O	2.03	0.75
1:A:212:GLY:O	1:A:214:ASN:ND2	2.20	0.75
1:A:197:ASN:HA	1:A:200:LEU:HG	1.67	0.75
2:B:712:GLN:OE1	2:B:756:LEU:HD21	1.87	0.75
1:A:34:ARG:C	1:A:36:SER:H	1.90	0.75
2:B:695:GLU:O	2:B:699:THR:HG22	1.87	0.75
2:B:566:PHE:O	2:B:568:ALA:N	2.20	0.75
1:A:197:ASN:OD1	1:A:200:LEU:HD12	1.86	0.74
2:B:716:VAL:HA	2:B:719:MET:HB3	1.67	0.74
1:A:132:VAL:HG23	4:D:2034:LEU:HD21	1.68	0.74
1:A:296:ILE:HG21	1:A:325:LEU:O	1.86	0.74
1:A:211:LEU:C	1:A:214:ASN:HD21	1.91	0.74
2:B:620:TYR:CE2	2:B:624:GLN:HG2	2.23	0.74
2:B:638:GLN:OE1	2:B:688:MET:HE3	1.87	0.74
2:B:587:LYS:HD3	2:B:587:LYS:N	2.03	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2024:SER:HA	4:D:2112:ILE:HG12	1.68	0.74
1:A:111:MET:HE3	1:A:114:SER:HB3	1.70	0.74
1:A:157:TYR:O	1:A:157:TYR:HD2	1.70	0.74
2:B:642:ILE:HD11	2:B:688:MET:N	2.01	0.74
2:B:711:ILE:O	2:B:715:ILE:HG13	1.88	0.74
1:A:111:MET:O	1:A:115:VAL:HB	1.87	0.74
2:B:538:GLN:HB2	3:C:1030:VAL:HG12	1.69	0.73
2:B:722:ARG:HD3	2:B:725:LEU:HD23	1.70	0.73
2:B:520:GLN:OE1	2:B:573:ARG:NH2	2.22	0.73
4:D:2119:THR:O	4:D:2122:THR:OG1	2.01	0.73
1:A:177:LYS:O	1:A:181:ASN:OD1	2.06	0.73
1:A:307:PHE:CD1	1:A:336:LEU:HD22	2.24	0.73
1:A:348:GLY:O	1:A:352:ILE:HG23	1.88	0.73
1:A:24:LEU:HD23	1:A:45:LEU:HD22	1.71	0.73
2:B:745:ARG:O	2:B:749:ILE:HG12	1.88	0.73
1:A:159:ILE:HG22	1:A:160:TYR:N	2.04	0.73
1:A:212:GLY:O	1:A:214:ASN:CG	2.26	0.73
1:A:257:VAL:HG11	1:A:306:GLU:CG	2.18	0.73
1:A:108:GLU:O	1:A:109:ASP:HB2	1.87	0.73
1:A:327:SER:HA	1:A:333:LEU:HD11	1.71	0.73
2:B:442:LEU:O	2:B:446:LEU:CD2	2.36	0.73
2:B:676:LYS:HE3	2:B:676:LYS:N	2.04	0.73
1:A:186:LEU:HD11	1:A:197:ASN:HB3	1.69	0.72
2:B:555:LEU:HD22	2:B:559:LEU:CD2	2.14	0.72
1:A:257:VAL:HG13	1:A:258:THR:H	1.54	0.72
1:A:234:SER:HB3	1:A:235:GLN:NE2	2.04	0.72
2:B:491:LYS:H	2:B:491:LYS:HD2	1.54	0.72
1:A:186:LEU:CD1	1:A:197:ASN:CB	2.65	0.72
4:D:2102:GLU:N	4:D:2102:GLU:CG	2.52	0.72
1:A:32:TYR:OH	1:A:130:SER:HA	1.89	0.72
1:A:54:THR:HG23	5:E:3113:PRO:CG	2.19	0.72
2:B:460:ASP:O	2:B:463:GLN:HB3	1.90	0.72
5:E:3111:SER:O	5:E:3113:PRO:HD3	1.89	0.72
1:A:39:LYS:HG2	4:D:2036:MET:HB3	1.72	0.72
1:A:197:ASN:OD1	1:A:200:LEU:HD11	1.89	0.72
2:B:727:HIS:O	2:B:727:HIS:CG	2.43	0.71
4:D:2005:LYS:O	4:D:2006:LEU:HD22	1.90	0.71
1:A:168:ARG:NH1	1:A:213:LEU:HD13	2.05	0.71
1:A:404:ASN:O	1:A:405:ASN:CG	2.28	0.71
4:D:2038:PRO:C	4:D:2040:PRO:CD	2.56	0.71
2:B:589:GLU:HA	2:B:602:GLN:HA	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:603:ALA:HA	2:B:685:ASN:OD1	1.91	0.71
1:A:227:VAL:HA	1:A:230:GLU:HG2	1.72	0.71
2:B:762:LEU:HD13	2:B:772:TYR:HD2	1.55	0.71
2:B:696:GLN:O	2:B:700:HIS:N	2.24	0.71
2:B:742:PHE:O	2:B:744:PRO:HD3	1.90	0.71
1:A:86:LEU:HD11	1:A:90:LYS:HE3	1.73	0.71
2:B:599:TYR:CE2	2:B:677:ASN:HB3	2.25	0.71
2:B:668:LEU:C	2:B:669:ILE:HD12	2.11	0.71
2:B:761:TYR:O	2:B:775:LEU:HD12	1.91	0.71
4:D:2037:ASP:HB3	4:D:2038:PRO:HD2	1.72	0.71
2:B:427:ASP:CG	2:B:431:LYS:HD2	2.12	0.70
1:A:154:LYS:HD2	1:A:154:LYS:N	2.05	0.70
1:A:257:VAL:HG11	1:A:306:GLU:CD	2.11	0.70
4:D:2118:VAL:HG13	4:D:2119:THR:H	1.56	0.70
1:A:145:VAL:CG1	1:A:157:TYR:HD2	2.04	0.70
1:A:211:LEU:C	1:A:214:ASN:ND2	2.45	0.70
1:A:297:GLU:C	1:A:300:LEU:H	1.94	0.70
1:A:378:ASN:HA	1:A:395:LEU:HD11	1.72	0.70
2:B:626:THR:HG23	2:B:636:LEU:HD22	1.72	0.70
2:B:619:ALA:HB2	2:B:670:LYS:HB3	1.55	0.70
4:D:2037:ASP:HB3	4:D:2038:PRO:CD	2.21	0.70
1:A:241:GLU:HG3	1:A:290:LYS:HD2	1.73	0.70
5:E:3126:LEU:HB3	5:E:3149:TRP:CZ3	2.27	0.70
1:A:257:VAL:CG1	1:A:306:GLU:OE2	2.40	0.70
1:A:376:LYS:O	1:A:379:ALA:HB3	1.91	0.70
1:A:207:SER:O	1:A:211:LEU:HB2	1.91	0.70
1:A:245:THR:O	1:A:249:THR:HG22	1.92	0.69
2:B:696:GLN:O	2:B:700:HIS:HB2	1.92	0.69
1:A:281:GLU:HG2	1:A:282:SER:N	2.07	0.69
1:A:246:ARG:HG3	1:A:246:ARG:HH11	1.57	0.69
1:A:293:GLN:O	1:A:297:GLU:HG2	1.91	0.69
2:B:506:ARG:HA	2:B:509:GLN:HG2	1.74	0.69
4:D:2023:GLN:HE22	4:D:2056:CYS:HA	1.57	0.69
2:B:571:ALA:CA	2:B:577:ARG:NH2	2.48	0.69
4:D:2031:LEU:HD23	4:D:2031:LEU:O	1.93	0.69
1:A:111:MET:CB	1:A:114:SER:HG	2.02	0.69
2:B:592:THR:HG21	2:B:599:TYR:HB2	1.73	0.69
2:B:714:ALA:HA	2:B:717:ARG:HD2	1.73	0.69
2:B:427:ASP:OD1	2:B:431:LYS:CD	2.41	0.69
2:B:487:SER:OG	2:B:491:LYS:HE2	1.93	0.69
1:A:144:TRP:CE3	1:A:144:TRP:C	2.64	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LEU:HD11	1:A:137:CYS:SG	2.33	0.68
1:A:15:ILE:CG2	1:A:20:ILE:HG13	2.21	0.68
2:B:711:ILE:O	2:B:711:ILE:CG2	2.41	0.68
1:A:173:ARG:H	1:A:174:PRO:CD	2.04	0.68
2:B:515:LYS:HA	2:B:518:ASN:HD22	1.57	0.68
2:B:577:ARG:CD	2:B:577:ARG:C	2.61	0.68
1:A:205:VAL:HG13	1:A:228:TYR:CE2	2.28	0.68
2:B:577:ARG:H	2:B:577:ARG:HD2	1.57	0.68
2:B:571:ALA:CB	2:B:577:ARG:HH21	2.05	0.68
2:B:592:THR:CG2	2:B:599:TYR:HB2	2.24	0.68
1:A:300:LEU:O	1:A:304:HIS:CD2	2.47	0.67
2:B:473:ARG:HD2	2:B:479:SER:OG	1.94	0.67
2:B:645:LYS:O	2:B:647:LYS:HD2	1.94	0.67
2:B:431:LYS:HA	2:B:479:SER:HA	1.75	0.67
2:B:540:LEU:HB2	3:C:1032:LEU:HD23	1.75	0.67
2:B:633:MET:SD	2:B:634:ASP:HA	2.34	0.67
2:B:555:LEU:CD2	2:B:559:LEU:HD21	2.13	0.67
2:B:619:ALA:HB2	2:B:670:LYS:CA	2.24	0.67
1:A:104:LEU:HD22	1:A:108:GLU:HG3	1.77	0.67
5:E:3109:TRP:HA	5:E:3138:ARG:NH2	2.09	0.67
2:B:633:MET:SD	2:B:634:ASP:CA	2.83	0.67
2:B:719:MET:HA	2:B:722:ARG:HB2	1.76	0.67
4:D:2017:ASP:HB3	4:D:2020:ILE:CG1	2.25	0.67
1:A:50:TYR:CE2	4:D:2109:TYR:HA	2.30	0.66
1:A:297:GLU:O	1:A:300:LEU:CA	2.43	0.66
2:B:574:HIS:O	2:B:577:ARG:HG3	1.96	0.66
2:B:433:SER:O	2:B:435:LYS:O	2.14	0.66
4:D:2005:LYS:C	4:D:2006:LEU:HD22	2.16	0.66
1:A:145:VAL:CG1	1:A:157:TYR:CD2	2.79	0.66
2:B:537:ILE:HG13	3:C:1029:ALA:C	2.16	0.66
2:B:553:PHE:CD1	2:B:631:ILE:CD1	2.71	0.66
2:B:577:ARG:HD2	2:B:577:ARG:N	2.11	0.66
1:A:186:LEU:HD13	1:A:197:ASN:CB	2.24	0.66
2:B:574:HIS:HB3	2:B:577:ARG:HB3	1.77	0.66
2:B:586:SER:C	2:B:587:LYS:HD3	2.16	0.66
2:B:642:ILE:HD11	2:B:688:MET:CA	2.26	0.66
4:D:2049:LEU:CD2	4:D:2053:ILE:HB	2.25	0.66
1:A:168:ARG:NH1	1:A:215:GLU:HG3	2.11	0.66
1:A:188:GLU:C	1:A:190:GLU:N	2.49	0.66
2:B:723:LYS:HB3	2:B:774:TYR:HE2	1.59	0.66
2:B:633:MET:SD	2:B:633:MET:C	2.74	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:705:GLU:O	2:B:709:LEU:HB2	1.96	0.66
1:A:111:MET:CE	1:A:114:SER:HB3	2.26	0.65
1:A:261:MET:HB3	1:A:325:LEU:HD12	1.78	0.65
2:B:590:LEU:HB2	2:B:601:LEU:HB2	1.77	0.65
4:D:2004:ILE:HG12	4:D:2031:LEU:HD11	1.77	0.65
4:D:2049:LEU:HD23	4:D:2049:LEU:O	1.96	0.65
1:A:399:CYS:O	1:A:403:ILE:HG13	1.96	0.65
4:D:2044:VAL:HG21	4:D:2106:ALA:HB1	1.77	0.65
1:A:401:ARG:HG3	1:A:401:ARG:HH11	1.62	0.65
2:B:442:LEU:O	2:B:446:LEU:HD23	1.96	0.65
1:A:285:ASP:O	1:A:288:ALA:HB3	1.96	0.65
2:B:476:HIS:N	2:B:476:HIS:CD2	2.64	0.65
2:B:516:ASP:O	2:B:520:GLN:HG3	1.97	0.65
2:B:707:ARG:NH1	2:B:742:PHE:HB2	2.11	0.65
2:B:503:LYS:O	2:B:504:LEU:C	2.34	0.65
4:D:2017:ASP:OD2	4:D:2018:VAL:HG22	1.97	0.65
4:D:2024:SER:OG	4:D:2110:LEU:HB3	1.96	0.65
2:B:640:LEU:CD1	2:B:644:LEU:HD11	2.27	0.65
2:B:683:ASN:OD1	2:B:684:ILE:N	2.29	0.65
2:B:541:SER:HA	3:C:1033:TRP:CZ2	2.31	0.64
1:A:144:TRP:O	1:A:144:TRP:HE3	1.69	0.64
1:A:366:TYR:CE2	1:A:408:VAL:HG21	2.31	0.64
2:B:640:LEU:O	2:B:644:LEU:HG	1.96	0.64
5:E:3117:LEU:HD22	5:E:3142:LEU:HD13	1.79	0.64
1:A:364:LYS:O	1:A:367:VAL:N	2.29	0.64
1:A:409:THR:CG2	2:B:415:SER:C	2.54	0.64
2:B:525:LEU:O	2:B:529:GLU:HB2	1.97	0.64
2:B:756:LEU:HA	2:B:759:LYS:HE2	1.77	0.64
1:A:355:CYS:O	1:A:359:ALA:CB	2.46	0.64
2:B:644:LEU:O	2:B:646:SER:O	2.15	0.64
2:B:723:LYS:HD3	2:B:723:LYS:N	2.12	0.64
1:A:132:VAL:O	1:A:136:ILE:HG13	1.98	0.64
2:B:635:ILE:HG13	2:B:638:GLN:NE2	2.13	0.64
2:B:684:ILE:O	2:B:685:ASN:OD1	2.16	0.64
2:B:729:GLN:O	2:B:733:GLU:HG3	1.98	0.64
1:A:130:SER:O	1:A:133:LEU:HB3	1.98	0.64
1:A:296:ILE:HG12	1:A:325:LEU:CD2	2.19	0.64
2:B:579:LEU:C	2:B:580:THR:HG22	2.17	0.64
1:A:294:VAL:HG12	1:A:295:LEU:HG	1.78	0.63
2:B:595:PHE:CE2	2:B:671:LEU:HD21	2.33	0.63
4:D:2045:ASN:OD1	4:D:2048:ILE:HG13	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HD21	1:A:159:ILE:HB	1.63	0.63
2:B:620:TYR:CE2	2:B:624:GLN:CG	2.81	0.63
1:A:27:GLY:O	1:A:31:VAL:HG12	1.97	0.63
1:A:142:ARG:C	1:A:146:ARG:HH21	1.99	0.63
1:A:244:TYR:HE2	1:A:267:ARG:HD2	1.64	0.63
2:B:442:LEU:HG	2:B:446:LEU:HD21	1.80	0.63
2:B:522:LYS:HZ2	2:B:522:LYS:HB3	1.62	0.63
1:A:366:TYR:HD2	1:A:408:VAL:HG21	1.60	0.63
2:B:723:LYS:HA	2:B:774:TYR:CE2	2.34	0.63
2:B:762:LEU:HD22	2:B:772:TYR:HB3	1.81	0.63
4:D:2085:ILE:HD12	4:D:2085:ILE:H	1.63	0.63
1:A:297:GLU:CA	1:A:300:LEU:HB2	2.29	0.62
2:B:756:LEU:HD23	2:B:759:LYS:NZ	2.14	0.62
1:A:306:GLU:O	1:A:309:ASN:HB2	1.99	0.62
2:B:468:LYS:HE2	2:B:699:THR:HB	1.79	0.62
1:A:258:THR:O	1:A:258:THR:OG1	2.11	0.62
2:B:619:ALA:CB	2:B:670:LYS:HA	2.29	0.62
2:B:758:GLU:OE1	2:B:759:LYS:CG	2.43	0.62
4:D:2019:GLU:N	4:D:2019:GLU:OE2	2.31	0.62
1:A:248:SER:HB2	1:A:299:HIS:NE2	2.14	0.62
2:B:578:LYS:CG	2:B:579:LEU:N	2.63	0.62
2:B:690:THR:O	2:B:693:LYS:HB3	2.00	0.62
5:E:3129:LEU:HA	5:E:3132:VAL:HG22	1.81	0.62
1:A:168:ARG:HH12	1:A:215:GLU:HG3	1.64	0.62
1:A:283:THR:HG22	1:A:283:THR:O	1.99	0.62
1:A:311:LEU:HD12	1:A:343:HIS:CG	2.35	0.62
1:A:111:MET:O	1:A:115:VAL:CB	2.48	0.62
1:A:173:ARG:N	1:A:174:PRO:CD	2.60	0.62
2:B:417:LYS:O	2:B:420:GLU:HB3	2.00	0.62
2:B:453:PHE:C	2:B:455:TYR:H	2.03	0.62
4:D:2107:ALA:CB	4:D:2115:LEU:HD22	2.30	0.62
2:B:450:MET:HB3	2:B:454:LYS:HE3	1.82	0.61
2:B:622:VAL:O	2:B:626:THR:N	2.33	0.61
2:B:730:LEU:O	2:B:732:GLY:N	2.33	0.61
4:D:2054:GLN:HA	4:D:2057:THR:OG1	2.00	0.61
1:A:176:ASN:O	1:A:177:LYS:C	2.34	0.61
1:A:323:TYR:O	1:A:323:TYR:CD2	2.53	0.61
2:B:427:ASP:OD1	2:B:431:LYS:CG	2.49	0.61
2:B:559:LEU:HD11	3:C:1027:TRP:CE3	2.35	0.61
1:A:39:LYS:HB2	1:A:39:LYS:HZ3	1.64	0.61
1:A:39:LYS:HE3	4:D:2037:ASP:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:VAL:HG12	1:A:295:LEU:N	2.14	0.61
2:B:746:VAL:CG2	2:B:747:PRO:HD3	2.30	0.61
1:A:371:LEU:HD11	2:B:448:GLN:HB3	1.82	0.61
2:B:619:ALA:CB	2:B:670:LYS:CA	2.79	0.61
4:D:2049:LEU:HA	4:D:2052:VAL:CG2	2.30	0.61
2:B:569:PHE:O	2:B:572:SER:CB	2.48	0.61
2:B:712:GLN:CD	2:B:756:LEU:HD21	2.21	0.61
1:A:118:PHE:O	1:A:122:GLN:CG	2.42	0.61
1:A:145:VAL:HG12	1:A:157:TYR:CD2	2.36	0.61
1:A:208:TYR:HB3	1:A:228:TYR:HA	1.82	0.61
2:B:453:PHE:O	2:B:455:TYR:N	2.34	0.61
1:A:386:ASN:O	1:A:386:ASN:ND2	2.34	0.61
2:B:586:SER:OG	3:C:1028:ASN:O	2.18	0.61
2:B:609:ALA:HB1	2:B:629:THR:HG21	1.81	0.61
2:B:723:LYS:CB	2:B:774:TYR:HE2	2.13	0.61
1:A:337:LYS:HD3	1:A:338:LYS:N	2.15	0.61
1:A:21:TRP:CZ2	1:A:25:ARG:HG3	2.36	0.61
1:A:311:LEU:HD11	1:A:340:LEU:HD13	1.83	0.61
2:B:586:SER:OG	3:C:1029:ALA:HA	2.01	0.61
2:B:442:LEU:O	2:B:446:LEU:HD22	1.99	0.60
1:A:39:LYS:CE	4:D:2037:ASP:H	2.01	0.60
2:B:551:CYS:HG	2:B:632:LYS:HD2	1.61	0.60
2:B:745:ARG:HB2	2:B:748:VAL:HG22	1.83	0.60
1:A:233:GLU:O	1:A:237:LEU:HB2	2.01	0.60
2:B:498:PHE:CZ	2:B:501:THR:HG21	2.36	0.60
2:B:521:PHE:O	2:B:525:LEU:CB	2.38	0.60
5:E:3111:SER:O	5:E:3113:PRO:CD	2.48	0.60
2:B:689:LYS:HA	2:B:689:LYS:HE2	1.83	0.60
2:B:697:GLU:HA	2:B:700:HIS:HB3	1.83	0.60
2:B:746:VAL:HG23	2:B:747:PRO:HD3	1.83	0.60
2:B:491:LYS:HD2	2:B:491:LYS:N	2.16	0.60
2:B:522:LYS:HZ3	2:B:525:LEU:HD23	1.64	0.60
1:A:209:VAL:O	1:A:212:GLY:CA	2.49	0.60
1:A:360:LEU:C	1:A:360:LEU:HD12	2.22	0.60
2:B:430:LEU:HD13	2:B:442:LEU:HD11	1.83	0.60
4:D:2031:LEU:CA	4:D:2035:GLY:HA2	2.28	0.60
4:D:2090:GLN:O	4:D:2094:LYS:HB2	2.02	0.60
1:A:186:LEU:HD11	1:A:197:ASN:CB	2.30	0.60
1:A:252:LEU:HD13	1:A:302:ILE:CD1	2.32	0.60
1:A:388:ASP:O	1:A:392:VAL:HG23	2.01	0.60
2:B:723:LYS:CA	2:B:774:TYR:HE2	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HG3	1:A:242:ARG:HH11	1.65	0.60
1:A:311:LEU:CD2	1:A:319:LEU:HD21	2.32	0.60
2:B:718:ILE:N	2:B:718:ILE:HD12	2.17	0.60
2:B:723:LYS:HB3	2:B:774:TYR:CE2	2.36	0.60
4:D:2109:TYR:HD2	4:D:2110:LEU:HD23	1.67	0.60
5:E:3113:PRO:HB3	5:E:3115:GLU:OE1	2.02	0.60
1:A:344:ILE:HA	1:A:347:GLN:HB2	1.84	0.60
2:B:424:ARG:HG3	2:B:424:ARG:HH11	1.66	0.60
2:B:595:PHE:CZ	2:B:671:LEU:HD21	2.37	0.60
2:B:511:ILE:O	2:B:515:LYS:HG3	2.02	0.59
2:B:746:VAL:HA	2:B:749:ILE:HD11	1.84	0.59
4:D:2127:ILE:HD12	4:D:2135:ILE:HD12	1.84	0.59
1:A:378:ASN:HA	1:A:395:LEU:CD1	2.32	0.59
4:D:2131:THR:O	4:D:2134:GLU:HB3	2.02	0.59
2:B:579:LEU:C	2:B:580:THR:CG2	2.69	0.59
4:D:2025:VAL:HG22	4:D:2111:ASP:O	2.02	0.59
4:D:2085:ILE:HD12	4:D:2085:ILE:N	2.18	0.59
1:A:294:VAL:HA	1:A:298:LYS:HD2	1.82	0.59
2:B:524:HIS:O	2:B:527:ASN:HB2	2.01	0.59
4:D:2017:ASP:HB3	4:D:2020:ILE:HG13	1.85	0.59
1:A:24:LEU:HD22	1:A:28:ILE:HG13	1.83	0.59
1:A:197:ASN:O	1:A:200:LEU:HB2	2.03	0.59
1:A:201:ILE:HG21	1:A:278:TYR:CE1	2.38	0.59
1:A:202:SER:HB3	1:A:278:TYR:HB2	1.83	0.59
1:A:246:ARG:HG3	1:A:246:ARG:NH1	2.15	0.59
1:A:248:SER:HB2	1:A:299:HIS:HE2	1.65	0.59
1:A:15:ILE:HG22	1:A:16:GLY:N	2.17	0.59
2:B:635:ILE:O	2:B:638:GLN:HB2	2.03	0.59
4:D:2133:GLU:N	4:D:2136:ARG:HH21	2.01	0.59
1:A:39:LYS:HB2	1:A:39:LYS:HZ2	1.68	0.59
1:A:299:HIS:O	1:A:302:ILE:HG13	2.02	0.59
1:A:112:ASP:CB	1:A:182:ALA:HA	2.25	0.59
1:A:157:TYR:C	1:A:157:TYR:HD2	2.04	0.59
1:A:274:ARG:HD2	1:A:278:TYR:CE2	2.37	0.58
2:B:620:TYR:CE2	2:B:624:GLN:CD	2.77	0.58
1:A:19:GLN:O	1:A:23:ASP:OD1	2.21	0.58
1:A:24:LEU:O	1:A:28:ILE:HG13	2.02	0.58
2:B:739:SER:C	2:B:741:ARG:H	2.07	0.58
1:A:87:GLU:OE2	1:A:87:GLU:HA	2.03	0.58
1:A:310:LEU:O	1:A:313:ALA:O	2.21	0.58
2:B:537:ILE:HG13	3:C:1030:VAL:N	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:668:LEU:N	2:B:668:LEU:HD12	2.19	0.58
1:A:335:GLU:O	1:A:339:LEU:HB2	2.03	0.58
2:B:696:GLN:O	2:B:700:HIS:CB	2.51	0.58
1:A:51:ASN:HD21	4:D:2043:ASN:HD21	1.52	0.58
1:A:274:ARG:NH1	1:A:278:TYR:OH	2.35	0.58
4:D:2087:VAL:O	4:D:2090:GLN:HB2	2.03	0.58
1:A:213:LEU:HG	1:A:227:VAL:CG2	2.33	0.58
2:B:515:LYS:HA	2:B:518:ASN:ND2	2.19	0.58
2:B:553:PHE:HD1	2:B:631:ILE:HG12	0.66	0.58
2:B:677:ASN:ND2	2:B:679:LYS:O	2.37	0.58
1:A:205:VAL:O	1:A:209:VAL:HG23	2.03	0.58
1:A:286:GLU:HG3	1:A:289:ARG:NH1	2.19	0.58
2:B:614:TYR:CD1	2:B:671:LEU:HB2	2.38	0.58
4:D:2118:VAL:HG13	4:D:2119:THR:N	2.18	0.58
1:A:197:ASN:HA	1:A:200:LEU:CG	2.32	0.58
2:B:599:TYR:HE2	2:B:677:ASN:HB3	1.69	0.58
2:B:712:GLN:CB	2:B:756:LEU:CD2	2.49	0.58
2:B:607:GLN:O	2:B:610:ILE:HD13	2.04	0.57
2:B:610:ILE:HD13	2:B:610:ILE:N	2.12	0.57
2:B:649:LEU:HA	2:B:670:LYS:O	2.03	0.57
2:B:703:ILE:HG12	2:B:707:ARG:HH21	1.68	0.57
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.67	0.57
1:A:158:GLU:CG	1:A:159:ILE:H	2.10	0.57
1:A:175:LEU:O	1:A:178:GLN:CB	2.52	0.57
2:B:578:LYS:C	2:B:579:LEU:CD2	2.68	0.57
2:B:717:ARG:O	2:B:720:LYS:HD3	2.04	0.57
2:B:453:PHE:HA	2:B:456:ILE:CD1	2.29	0.57
1:A:159:ILE:O	1:A:160:TYR:C	2.43	0.57
1:A:244:TYR:CE2	1:A:267:ARG:HD2	2.38	0.57
1:A:34:ARG:C	1:A:36:SER:N	2.55	0.57
4:D:2023:GLN:NE2	4:D:2056:CYS:HA	2.20	0.57
4:D:2115:LEU:HD23	4:D:2115:LEU:C	2.25	0.57
4:D:2130:LYS:H	5:E:3131:LYS:NZ	2.03	0.57
1:A:197:ASN:O	1:A:200:LEU:N	2.38	0.57
1:A:213:LEU:HG	1:A:227:VAL:HG23	1.86	0.57
1:A:50:TYR:HA	1:A:139:TYR:CD2	2.39	0.56
1:A:143:HIS:ND1	1:A:146:ARG:NH2	2.53	0.56
2:B:483:ASP:O	2:B:486:ALA:HB3	2.05	0.56
2:B:719:MET:HE1	2:B:774:TYR:CD1	2.39	0.56
4:D:2002:PRO:CB	4:D:2018:VAL:HG11	2.31	0.56
4:D:2123:VAL:CG1	5:E:3120:ILE:HD13	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:O	1:A:184:LEU:HD23	2.05	0.56
1:A:257:VAL:HG13	1:A:258:THR:HG22	1.88	0.56
1:A:306:GLU:O	1:A:309:ASN:N	2.36	0.56
1:A:326:VAL:O	1:A:328:ARG:N	2.39	0.56
1:A:378:ASN:CA	1:A:395:LEU:HD11	2.35	0.56
4:D:2014:PHE:O	4:D:2016:VAL:N	2.39	0.56
1:A:42:TYR:HD2	4:D:2030:MET:SD	2.28	0.56
1:A:226:THR:O	1:A:229:LYS:N	2.39	0.56
2:B:555:LEU:HD23	2:B:559:LEU:HD22	0.64	0.56
2:B:622:VAL:HG21	2:B:664:LYS:O	2.05	0.56
1:A:380:LEU:O	1:A:384:ALA:HB3	2.06	0.56
2:B:545:TRP:HB3	2:B:547:PHE:CD2	2.40	0.56
2:B:545:TRP:HB3	2:B:547:PHE:CE2	2.41	0.56
2:B:704:GLU:OE1	2:B:707:ARG:HG3	2.06	0.56
2:B:662:GLU:O	2:B:663:LEU:CD2	2.53	0.56
1:A:287:LEU:CD2	1:A:291:CYS:SG	2.93	0.56
2:B:765:VAL:CG2	2:B:773:SER:HB2	2.35	0.56
1:A:251:PHE:CE2	1:A:255:ASN:HB2	2.41	0.56
4:D:2017:ASP:HB3	4:D:2020:ILE:HG12	1.86	0.56
5:E:3126:LEU:H	5:E:3126:LEU:CD1	2.13	0.56
2:B:562:SER:HA	2:B:565:ARG:HB3	1.88	0.56
4:D:2044:VAL:HG22	4:D:2106:ALA:CB	2.36	0.56
1:A:311:LEU:HD22	1:A:319:LEU:HD21	1.88	0.55
2:B:423:ALA:HA	2:B:462:PHE:CE1	2.40	0.55
2:B:517:LEU:O	2:B:520:GLN:HB2	2.06	0.55
1:A:37:MET:O	1:A:37:MET:HG2	2.07	0.55
2:B:601:LEU:HD11	2:B:648:LEU:HD21	1.87	0.55
2:B:728:GLN:HE21	2:B:728:GLN:HA	1.70	0.55
1:A:348:GLY:HA2	1:A:373:VAL:HG21	1.88	0.55
1:A:403:ILE:HD12	2:B:455:TYR:HB3	1.87	0.55
2:B:745:ARG:HH21	2:B:748:VAL:HG11	1.71	0.55
4:D:2121:LYS:O	4:D:2124:ALA:HB3	2.06	0.55
2:B:751:LYS:NZ	2:B:755:ILE:HD11	2.22	0.55
4:D:2044:VAL:CG2	4:D:2106:ALA:HB1	2.36	0.55
1:A:104:LEU:CD2	1:A:108:GLU:HG3	2.36	0.55
4:D:2044:VAL:CG2	4:D:2106:ALA:CB	2.84	0.55
4:D:2133:GLU:O	4:D:2137:LYS:HG3	2.07	0.55
2:B:553:PHE:CE1	2:B:629:THR:CB	2.80	0.55
2:B:566:PHE:C	2:B:568:ALA:N	2.60	0.55
2:B:722:ARG:O	2:B:774:TYR:HE2	1.89	0.55
1:A:307:PHE:CG	1:A:336:LEU:HD22	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:LEU:N	2:B:601:LEU:O	2.40	0.55
2:B:610:ILE:H	2:B:610:ILE:CD1	2.13	0.55
1:A:96:LEU:HD23	1:A:163:ALA:HA	1.87	0.55
1:A:131:LYS:O	1:A:134:ASN:HB2	2.07	0.55
1:A:350:ALA:O	1:A:354:LYS:HG3	2.07	0.55
2:B:485:GLU:O	2:B:489:ILE:HG12	2.07	0.55
2:B:542:SER:HB2	3:C:1032:LEU:HB3	1.89	0.55
2:B:704:GLU:OE1	2:B:708:LYS:HE2	2.06	0.55
4:D:2044:VAL:HG22	4:D:2106:ALA:HB2	1.88	0.55
2:B:442:LEU:HD23	2:B:484:ALA:HB1	1.89	0.54
2:B:619:ALA:HB2	2:B:670:LYS:HA	1.89	0.54
4:D:2017:ASP:OD2	4:D:2018:VAL:N	2.40	0.54
1:A:115:VAL:HG13	1:A:116:LEU:N	2.22	0.54
2:B:540:LEU:HD12	2:B:582:LEU:HD11	1.87	0.54
2:B:559:LEU:HD11	3:C:1027:TRP:CD2	2.41	0.54
2:B:535:PHE:O	2:B:536:SER:HB2	2.05	0.54
2:B:730:LEU:HA	2:B:733:GLU:HB2	1.90	0.54
4:D:2131:THR:O	4:D:2135:ILE:HG12	2.08	0.54
5:E:3125:CYS:O	5:E:3128:GLU:N	2.39	0.54
1:A:180:THR:HG22	1:A:184:LEU:HD23	1.90	0.54
1:A:380:LEU:CD1	1:A:384:ALA:HB2	2.38	0.54
2:B:745:ARG:NH2	2:B:748:VAL:HG11	2.22	0.54
1:A:115:VAL:O	1:A:118:PHE:HB3	2.08	0.54
1:A:257:VAL:HG11	1:A:306:GLU:HG2	1.87	0.54
2:B:432:LYS:HD2	2:B:480:ALA:CB	2.34	0.54
2:B:458:ASP:C	2:B:460:ASP:H	2.11	0.54
2:B:475:VAL:C	2:B:476:HIS:O	2.33	0.54
4:D:2123:VAL:HG11	5:E:3120:ILE:HD13	1.88	0.54
2:B:424:ARG:HG3	2:B:424:ARG:NH1	2.22	0.54
4:D:2133:GLU:HA	4:D:2136:ARG:HE	1.73	0.54
1:A:39:LYS:HE2	4:D:2037:ASP:CA	2.38	0.54
4:D:2019:GLU:HA	4:D:2022:LYS:HB2	1.88	0.54
1:A:86:LEU:HD23	1:A:87:GLU:N	2.23	0.54
1:A:272:GLN:HG3	1:A:284:GLN:HE22	1.73	0.54
1:A:275:VAL:HG21	1:A:284:GLN:HG2	1.88	0.54
2:B:756:LEU:HA	2:B:759:LYS:CE	2.38	0.54
1:A:96:LEU:CD2	1:A:163:ALA:HA	2.38	0.54
1:A:321:ARG:HH11	1:A:321:ARG:CG	2.18	0.54
2:B:616:THR:HG22	2:B:617:GLU:N	2.19	0.53
2:B:719:MET:SD	2:B:774:TYR:CD2	3.01	0.53
1:A:159:ILE:CG2	1:A:160:TYR:N	2.71	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:NE2	1:A:235:GLN:N	2.41	0.53
2:B:476:HIS:CD2	2:B:476:HIS:H	2.26	0.53
2:B:593:ASN:OD1	2:B:598:ARG:NH1	2.41	0.53
2:B:604:SER:OG	2:B:607:GLN:HG3	2.07	0.53
2:B:734:VAL:HG12	2:B:738:LEU:HD23	1.90	0.53
1:A:129:SER:HA	1:A:132:VAL:HG12	1.90	0.53
1:A:340:LEU:HD22	1:A:385:PHE:CE2	2.43	0.53
2:B:449:VAL:O	2:B:452:VAL:HB	2.08	0.53
2:B:621:THR:O	2:B:625:LEU:N	2.41	0.53
2:B:719:MET:HE1	2:B:774:TYR:CG	2.41	0.53
5:E:3113:PRO:CB	5:E:3115:GLU:OE1	2.56	0.53
5:E:3140:TYR:C	5:E:3140:TYR:CD2	2.82	0.53
1:A:142:ARG:HB2	1:A:146:ARG:HH21	1.73	0.53
2:B:522:LYS:HZ3	2:B:522:LYS:HA	1.74	0.53
2:B:526:THR:O	2:B:527:ASN:C	2.45	0.53
2:B:727:HIS:HB3	2:B:770:ASP:CB	2.35	0.53
2:B:418:SER:N	2:B:419:PRO:HD2	2.23	0.53
2:B:474:LEU:HD13	2:B:507:MET:O	2.08	0.53
2:B:623:GLN:HA	2:B:626:THR:HB	1.90	0.53
1:A:269:LEU:O	1:A:272:GLN:HB3	2.09	0.53
1:A:360:LEU:C	1:A:362:ASP:H	2.12	0.53
2:B:589:GLU:HG2	2:B:602:GLN:HG2	1.90	0.53
4:D:2118:VAL:HA	4:D:2121:LYS:HD3	1.91	0.53
1:A:82:GLN:O	1:A:82:GLN:HG2	2.09	0.53
1:A:173:ARG:HB3	1:A:174:PRO:HD3	1.90	0.53
2:B:707:ARG:HB2	2:B:708:LYS:HD2	1.89	0.53
4:D:2127:ILE:CD1	4:D:2135:ILE:HD12	2.39	0.53
1:A:257:VAL:HG11	1:A:306:GLU:OE2	2.07	0.53
1:A:271:GLU:O	1:A:275:VAL:HG23	2.09	0.53
2:B:573:ARG:O	2:B:574:HIS:CD2	2.61	0.53
2:B:640:LEU:HD12	2:B:644:LEU:HD11	1.91	0.53
2:B:714:ALA:HB1	2:B:738:LEU:CD2	2.38	0.53
4:D:2049:LEU:O	4:D:2053:ILE:HG22	2.09	0.53
1:A:110:LEU:CD1	1:A:118:PHE:CG	2.91	0.52
1:A:135:GLY:C	1:A:137:CYS:N	2.62	0.52
1:A:17:LEU:C	1:A:19:GLN:H	2.12	0.52
1:A:24:LEU:HD22	1:A:24:LEU:O	2.09	0.52
1:A:297:GLU:HA	1:A:300:LEU:HB2	1.92	0.52
1:A:321:ARG:HG2	1:A:321:ARG:NH1	2.14	0.52
2:B:442:LEU:HG	2:B:446:LEU:CD2	2.40	0.52
2:B:464:LYS:NZ	2:B:703:ILE:HA	2.22	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:LYS:NZ	2:B:522:LYS:HB3	2.24	0.52
2:B:706:ASP:O	2:B:710:LEU:HB2	2.09	0.52
2:B:727:HIS:ND1	2:B:727:HIS:C	2.62	0.52
1:A:39:LYS:HG3	4:D:2036:MET:HE2	1.92	0.52
2:B:644:LEU:C	2:B:646:SER:O	2.48	0.52
2:B:738:LEU:C	2:B:740:SER:H	2.12	0.52
1:A:45:LEU:O	1:A:46:TYR:C	2.48	0.52
1:A:214:ASN:O	1:A:215:GLU:C	2.44	0.52
1:A:171:LEU:O	1:A:172:PHE:C	2.47	0.52
1:A:244:TYR:HE2	1:A:267:ARG:CD	2.23	0.52
2:B:458:ASP:O	2:B:460:ASP:N	2.42	0.52
1:A:100:LEU:HD13	1:A:167:TRP:HA	1.91	0.52
1:A:227:VAL:HA	1:A:230:GLU:CG	2.38	0.52
2:B:592:THR:OG1	2:B:599:TYR:N	2.42	0.52
4:D:2043:ASN:HB2	4:D:2109:TYR:CE1	2.44	0.52
4:D:2131:THR:HB	4:D:2132:PRO:HD2	1.91	0.52
5:E:3146:GLU:O	5:E:3148:LEU:N	2.42	0.52
1:A:234:SER:HB3	1:A:235:GLN:HE22	1.73	0.52
2:B:484:ALA:O	2:B:487:SER:HB3	2.09	0.52
2:B:620:TYR:CD2	2:B:624:GLN:CD	2.82	0.52
1:A:234:SER:CB	1:A:235:GLN:NE2	2.73	0.52
2:B:475:VAL:HG13	3:C:1030:VAL:HG11	1.92	0.52
2:B:427:ASP:OD2	2:B:431:LYS:HD2	2.10	0.52
2:B:501:THR:O	2:B:501:THR:HG22	2.09	0.52
1:A:111:MET:O	1:A:115:VAL:N	2.40	0.52
1:A:115:VAL:CG1	1:A:116:LEU:N	2.73	0.52
2:B:707:ARG:HH11	2:B:742:PHE:HB2	1.74	0.52
4:D:2099:THR:HA	4:D:2102:GLU:OE1	2.10	0.52
1:A:260:TYR:OH	1:A:295:LEU:O	2.26	0.51
4:D:2086:PRO:O	4:D:2090:GLN:HG3	2.10	0.51
4:D:2131:THR:N	4:D:2134:GLU:HB3	2.20	0.51
1:A:117:LYS:O	1:A:121:GLN:CB	2.58	0.51
1:A:314:ASP:O	1:A:316:ASN:N	2.43	0.51
2:B:633:MET:SD	2:B:634:ASP:N	2.83	0.51
4:D:2016:VAL:CG1	4:D:2053:ILE:HD11	2.40	0.51
1:A:304:HIS:CE1	1:A:335:GLU:HB3	2.45	0.51
2:B:438:GLU:O	2:B:441:GLU:HB3	2.10	0.51
4:D:2104:ILE:HG21	5:E:3112:LEU:HD11	1.92	0.51
2:B:513:VAL:HG13	2:B:514:SER:N	2.26	0.51
4:D:2031:LEU:O	4:D:2031:LEU:CD2	2.59	0.51
1:A:39:LYS:CE	4:D:2037:ASP:N	2.67	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2010:ASP:CG	4:D:2046:ALA:H	2.13	0.51
1:A:47:THR:O	1:A:48:HIS:C	2.47	0.51
1:A:100:LEU:CD1	1:A:166:THR:HG22	2.31	0.51
1:A:233:GLU:HG2	1:A:237:LEU:HD12	1.93	0.51
2:B:574:HIS:CB	2:B:577:ARG:HB3	2.41	0.51
4:D:2117:ASP:O	4:D:2120:CYS:HB3	2.10	0.51
1:A:177:LYS:C	1:A:181:ASN:OD1	2.48	0.51
2:B:470:LEU:O	2:B:474:LEU:HG	2.11	0.51
4:D:2055:TRP:CD2	4:D:2115:LEU:HD12	2.46	0.51
1:A:225:LEU:O	1:A:229:LYS:HB2	2.10	0.51
1:A:275:VAL:HG11	1:A:284:GLN:HG2	1.93	0.51
2:B:510:ASP:O	2:B:513:VAL:HG12	2.10	0.51
2:B:717:ARG:C	2:B:720:LYS:HD3	2.32	0.51
4:D:2025:VAL:HG22	4:D:2111:ASP:HB3	1.91	0.51
1:A:351:ALA:HA	1:A:354:LYS:HE2	1.93	0.50
2:B:445:THR:O	2:B:448:GLN:HB2	2.12	0.50
2:B:554:ALA:O	2:B:556:PRO:HD2	2.11	0.50
2:B:680:LEU:HD12	2:B:680:LEU:H	1.75	0.50
2:B:756:LEU:HB3	2:B:761:TYR:CG	2.46	0.50
1:A:158:GLU:CG	1:A:159:ILE:N	2.68	0.50
1:A:158:GLU:HB3	1:A:161:SER:OG	2.11	0.50
2:B:587:LYS:N	2:B:587:LYS:CD	2.74	0.50
1:A:92:LEU:O	1:A:95:PHE:HB3	2.11	0.50
1:A:180:THR:HG23	1:A:232:PHE:CD1	2.47	0.50
1:A:275:VAL:HG11	1:A:284:GLN:CG	2.41	0.50
1:A:300:LEU:CD1	1:A:304:HIS:NE2	2.70	0.50
1:A:323:TYR:HB2	1:A:385:PHE:HD1	1.76	0.50
1:A:352:ILE:HA	1:A:369:THR:HG21	1.92	0.50
2:B:430:LEU:C	2:B:431:LYS:O	2.49	0.50
2:B:657:ASN:O	2:B:659:ASP:N	2.45	0.50
4:D:2050:LYS:O	4:D:2054:GLN:HG2	2.11	0.50
4:D:2093:LEU:HD13	4:D:2119:THR:HA	1.93	0.50
1:A:159:ILE:O	1:A:162:LEU:N	2.44	0.50
2:B:522:LYS:HZ1	2:B:525:LEU:HD23	1.75	0.50
2:B:616:THR:HG22	2:B:617:GLU:HG3	1.93	0.50
1:A:145:VAL:HG12	1:A:157:TYR:CE2	2.47	0.50
2:B:474:LEU:HD12	2:B:507:MET:HB3	1.93	0.50
4:D:2018:VAL:O	4:D:2020:ILE:N	2.45	0.50
4:D:2029:THR:O	4:D:2031:LEU:N	2.45	0.50
1:A:256:PRO:HB3	1:A:258:THR:HG23	1.94	0.50
1:A:323:TYR:O	1:A:323:TYR:CG	2.65	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:ARG:HA	2:B:720:LYS:HE3	1.93	0.50
4:D:2087:VAL:HA	4:D:2090:GLN:NE2	2.27	0.50
1:A:117:LYS:O	1:A:121:GLN:HB2	2.11	0.50
2:B:645:LYS:C	2:B:646:SER:O	2.38	0.50
2:B:768:GLU:HB2	2:B:771:THR:HG23	1.94	0.50
4:D:2117:ASP:O	4:D:2121:LYS:HG3	2.10	0.50
2:B:430:LEU:HD12	2:B:442:LEU:HD21	1.93	0.50
1:A:360:LEU:HD22	1:A:408:VAL:HA	1.94	0.50
2:B:595:PHE:HB3	2:B:674:GLY:O	2.12	0.50
4:D:2131:THR:H	4:D:2134:GLU:CB	2.20	0.50
1:A:21:TRP:O	1:A:24:LEU:N	2.44	0.49
1:A:234:SER:CB	1:A:235:GLN:HE21	2.24	0.49
1:A:248:SER:CB	1:A:299:HIS:HE2	2.26	0.49
2:B:690:THR:HG23	2:B:691:GLU:N	2.27	0.49
4:D:2131:THR:OG1	4:D:2134:GLU:HB2	2.12	0.49
5:E:3129:LEU:HA	5:E:3132:VAL:CG2	2.41	0.49
2:B:476:HIS:N	2:B:476:HIS:HD2	2.08	0.49
4:D:2018:VAL:HG23	4:D:2019:GLU:N	2.19	0.49
1:A:108:GLU:O	1:A:109:ASP:CB	2.60	0.49
4:D:2085:ILE:H	4:D:2085:ILE:CD1	2.24	0.49
1:A:286:GLU:CD	1:A:289:ARG:HH22	2.15	0.49
2:B:442:LEU:HD23	2:B:484:ALA:CB	2.43	0.49
4:D:2051:LYS:HE3	4:D:2092:PHE:CZ	2.48	0.49
1:A:38:ALA:C	1:A:40:SER:N	2.66	0.49
1:A:204:VAL:O	1:A:207:SER:N	2.45	0.49
1:A:227:VAL:CA	1:A:230:GLU:HG2	2.40	0.49
2:B:608:MET:CE	3:C:1024:VAL:HG13	2.42	0.49
4:D:2118:VAL:CG1	4:D:2119:THR:H	2.25	0.49
1:A:39:LYS:HE2	4:D:2037:ASP:C	2.32	0.49
1:A:107:GLY:HA3	1:A:118:PHE:CE2	2.47	0.49
1:A:260:TYR:O	1:A:264:ALA:N	2.42	0.49
2:B:621:THR:O	2:B:622:VAL:C	2.50	0.49
3:C:1020:LYS:O	3:C:1021:ARG:HB2	2.13	0.49
4:D:2119:THR:O	4:D:2120:CYS:C	2.52	0.49
4:D:2131:THR:O	4:D:2135:ILE:N	2.45	0.49
4:D:2101:PHE:O	4:D:2102:GLU:CA	2.61	0.48
1:A:17:LEU:C	1:A:20:ILE:H	2.17	0.48
1:A:97:LYS:O	1:A:101:THR:HG23	2.13	0.48
1:A:147:ARG:HH22	5:E:3146:GLU:CG	2.21	0.48
1:A:186:LEU:HD11	1:A:200:LEU:HD12	1.95	0.48
1:A:196:ILE:C	1:A:198:THR:N	2.64	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:THR:O	1:A:230:GLU:N	2.44	0.48
4:D:2055:TRP:CG	4:D:2115:LEU:HD12	2.48	0.48
1:A:92:LEU:HD12	1:A:159:ILE:HD11	1.95	0.48
4:D:2119:THR:OG1	4:D:2120:CYS:N	2.46	0.48
5:E:3109:TRP:O	5:E:3110:ASP:C	2.51	0.48
5:E:3125:CYS:C	5:E:3127:PRO:HD2	2.34	0.48
1:A:17:LEU:C	1:A:19:GLN:N	2.66	0.48
1:A:268:LEU:HD11	1:A:296:ILE:HD11	1.95	0.48
2:B:458:ASP:HB3	2:B:460:ASP:OD1	2.13	0.48
2:B:691:GLU:O	2:B:695:GLU:HB2	2.14	0.48
1:A:352:ILE:CD1	1:A:406:ASN:HB3	2.33	0.48
2:B:716:VAL:HG13	2:B:719:MET:HE3	1.95	0.48
4:D:2008:SER:OG	4:D:2049:LEU:CD1	2.61	0.48
4:D:2097:GLN:O	4:D:2100:LEU:N	2.47	0.48
1:A:195:THR:O	1:A:195:THR:CG2	2.61	0.48
2:B:427:ASP:OD1	2:B:431:LYS:HG3	2.14	0.48
2:B:578:LYS:C	2:B:579:LEU:CG	2.82	0.48
2:B:717:ARG:HA	2:B:720:LYS:CE	2.44	0.48
4:D:2133:GLU:HA	4:D:2136:ARG:NE	2.27	0.48
1:A:189:LYS:HB3	1:A:193:GLY:HA2	1.95	0.48
1:A:333:LEU:O	1:A:334:GLY:C	2.51	0.48
2:B:571:ALA:HB2	2:B:577:ARG:HH21	1.67	0.48
5:E:3117:LEU:CD2	5:E:3142:LEU:HD13	2.43	0.48
1:A:371:LEU:HD22	2:B:448:GLN:NE2	2.28	0.48
2:B:712:GLN:OE1	2:B:756:LEU:CD2	2.59	0.48
1:A:257:VAL:O	1:A:260:TYR:CB	2.54	0.48
1:A:362:ASP:OD1	1:A:362:ASP:O	2.32	0.48
2:B:611:LEU:CD2	2:B:648:LEU:HD23	2.44	0.47
2:B:620:TYR:CE1	2:B:624:GLN:OE1	2.65	0.47
4:D:2004:ILE:CG1	4:D:2031:LEU:HD11	2.43	0.47
2:B:482:ASP:HB3	2:B:508:PHE:HZ	1.79	0.47
2:B:652:GLU:HG3	2:B:668:LEU:HB2	1.96	0.47
4:D:2052:VAL:HG12	4:D:2056:CYS:SG	2.54	0.47
2:B:584:GLN:C	2:B:585:LEU:HD12	2.34	0.47
1:A:257:VAL:CG1	1:A:258:THR:H	2.26	0.47
2:B:688:MET:H	2:B:688:MET:HG3	1.32	0.47
4:D:2008:SER:OG	4:D:2049:LEU:HD12	2.14	0.47
4:D:2037:ASP:O	4:D:2038:PRO:C	2.52	0.47
4:D:2037:ASP:CB	4:D:2038:PRO:CD	2.91	0.47
1:A:280:HIS:CE1	1:A:282:SER:HG	2.29	0.47
2:B:442:LEU:C	2:B:446:LEU:HD23	2.34	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:MET:O	2:B:453:PHE:N	2.44	0.47
2:B:587:LYS:HB3	2:B:603:ALA:O	2.15	0.47
2:B:671:LEU:HD22	2:B:672:TYR:H	1.77	0.47
4:D:2037:ASP:O	4:D:2039:VAL:N	2.47	0.47
2:B:514:SER:O	2:B:517:LEU:HB3	2.15	0.47
2:B:756:LEU:HD23	2:B:759:LYS:HZ3	1.79	0.47
1:A:38:ALA:C	1:A:40:SER:H	2.18	0.47
1:A:39:LYS:CG	4:D:2036:MET:HE2	2.44	0.47
1:A:83:PHE:O	1:A:84:VAL:C	2.53	0.47
1:A:207:SER:OG	1:A:211:LEU:HD22	2.14	0.47
1:A:296:ILE:HA	1:A:303:PHE:HE2	1.79	0.47
1:A:345:HIS:CE1	1:A:401:ARG:O	2.68	0.47
2:B:488:MET:HE3	2:B:492:LEU:HD11	1.97	0.47
2:B:525:LEU:HD12	2:B:529:GLU:HB3	1.97	0.47
2:B:540:LEU:HD22	2:B:545:TRP:CH2	2.49	0.47
2:B:559:LEU:C	2:B:561:ARG:H	2.17	0.47
2:B:571:ALA:HA	2:B:577:ARG:CZ	2.44	0.47
2:B:574:HIS:O	2:B:577:ARG:CG	2.63	0.47
2:B:756:LEU:HB3	2:B:761:TYR:HB2	1.96	0.47
4:D:2049:LEU:HD23	4:D:2053:ILE:H	1.80	0.47
4:D:2113:LYS:O	4:D:2114:GLY:C	2.53	0.47
1:A:261:MET:O	1:A:265:GLU:N	2.41	0.47
2:B:491:LYS:H	2:B:491:LYS:CD	2.24	0.47
2:B:671:LEU:HD12	3:C:1020:LYS:HE2	1.95	0.47
2:B:697:GLU:HG3	2:B:698:THR:N	2.29	0.47
2:B:765:VAL:HB	2:B:771:THR:CB	2.44	0.47
1:A:257:VAL:O	1:A:260:TYR:N	2.43	0.47
1:A:292:GLU:OE1	1:A:328:ARG:HB3	2.15	0.47
1:A:326:VAL:O	1:A:329:ILE:N	2.36	0.47
2:B:553:PHE:CZ	2:B:629:THR:HB	2.43	0.47
2:B:765:VAL:HB	2:B:771:THR:HB	1.96	0.47
1:A:120:THR:O	1:A:123:TRP:HB3	2.15	0.47
1:A:233:GLU:HG3	1:A:283:THR:HG23	1.96	0.47
1:A:372:ASP:O	1:A:373:VAL:C	2.53	0.47
2:B:422:LEU:CD2	2:B:449:VAL:HG13	2.45	0.47
2:B:432:LYS:HB2	2:B:478:ASN:OD1	2.15	0.47
1:A:102:ASN:HD22	1:A:102:ASN:N	2.10	0.46
1:A:160:TYR:OH	1:A:210:GLU:OE2	2.23	0.46
2:B:611:LEU:HD21	2:B:648:LEU:HD23	1.97	0.46
2:B:716:VAL:O	2:B:719:MET:N	2.48	0.46
2:B:723:LYS:HA	2:B:774:TYR:HE2	1.71	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:734:VAL:O	2:B:738:LEU:HB3	2.15	0.46
1:A:215:GLU:O	1:A:216:ASP:O	2.33	0.46
2:B:421:LEU:O	2:B:424:ARG:N	2.45	0.46
2:B:471:ALA:O	2:B:475:VAL:HG23	2.16	0.46
2:B:607:GLN:HA	2:B:610:ILE:HD11	1.97	0.46
4:D:2016:VAL:HG21	4:D:2053:ILE:CD1	2.45	0.46
5:E:3140:TYR:C	5:E:3140:TYR:HD2	2.17	0.46
1:A:129:SER:O	1:A:132:VAL:HG12	2.14	0.46
1:A:173:ARG:HB3	1:A:174:PRO:CD	2.45	0.46
2:B:671:LEU:HD12	3:C:1020:LYS:CE	2.45	0.46
4:D:2025:VAL:CG2	4:D:2111:ASP:HB3	2.45	0.46
4:D:2049:LEU:O	4:D:2053:ILE:N	2.45	0.46
1:A:147:ARG:NH2	5:E:3146:GLU:HG2	2.24	0.46
1:A:227:VAL:O	1:A:228:TYR:C	2.52	0.46
2:B:537:ILE:HG12	2:B:538:GLN:N	2.30	0.46
2:B:540:LEU:HD13	2:B:545:TRP:CE3	2.51	0.46
1:A:180:THR:HG23	1:A:232:PHE:HD1	1.80	0.46
3:C:1033:TRP:HE3	3:C:1033:TRP:C	2.19	0.46
1:A:167:TRP:HD1	1:A:211:LEU:HD21	1.80	0.46
1:A:364:LYS:HG3	2:B:425:TYR:CE2	2.51	0.46
2:B:765:VAL:HB	2:B:771:THR:OG1	2.16	0.46
1:A:401:ARG:HG3	1:A:401:ARG:NH1	2.26	0.46
2:B:427:ASP:CG	2:B:431:LYS:CD	2.84	0.46
2:B:534:ASP:CB	3:C:1026:LYS:HG3	2.39	0.46
2:B:756:LEU:HB3	2:B:761:TYR:CB	2.45	0.46
5:E:3136:CYS:SG	5:E:3139:TRP:CD1	3.08	0.46
1:A:371:LEU:CD1	2:B:448:GLN:HB3	2.45	0.46
2:B:540:LEU:HD13	2:B:545:TRP:CD2	2.51	0.46
2:B:765:VAL:HG23	2:B:772:TYR:C	2.36	0.46
1:A:196:ILE:C	1:A:198:THR:H	2.19	0.46
1:A:280:HIS:CE1	1:A:282:SER:H	2.34	0.46
1:A:284:GLN:O	1:A:285:ASP:C	2.54	0.46
1:A:303:PHE:HA	1:A:322:MET:HE1	1.97	0.46
2:B:632:LYS:HB3	2:B:635:ILE:CG2	2.46	0.46
2:B:672:TYR:O	2:B:674:GLY:N	2.48	0.46
2:B:704:GLU:OE1	2:B:704:GLU:HA	2.16	0.46
1:A:260:TYR:O	1:A:263:LYS:N	2.49	0.46
1:A:333:LEU:O	1:A:335:GLU:N	2.48	0.46
2:B:683:ASN:O	2:B:684:ILE:HG23	2.16	0.46
1:A:140:LEU:HG	1:A:144:TRP:HD1	1.81	0.45
1:A:173:ARG:CB	1:A:174:PRO:HD3	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:VAL:HG12	1:A:295:LEU:CG	2.46	0.45
2:B:436:ASN:OD1	2:B:436:ASN:C	2.51	0.45
2:B:553:PHE:HZ	2:B:609:ALA:HB2	1.81	0.45
2:B:730:LEU:HD11	2:B:734:VAL:CG2	2.46	0.45
5:E:3117:LEU:C	5:E:3117:LEU:HD23	2.36	0.45
1:A:54:THR:O	1:A:55:SER:OG	2.32	0.45
1:A:135:GLY:O	1:A:137:CYS:N	2.49	0.45
1:A:230:GLU:HG3	1:A:231:SER:N	2.31	0.45
1:A:297:GLU:C	1:A:299:HIS:N	2.70	0.45
1:A:402:PHE:CD1	1:A:402:PHE:C	2.89	0.45
2:B:629:THR:OG1	2:B:631:ILE:HG13	2.15	0.45
1:A:119:TYR:O	1:A:120:THR:C	2.54	0.45
4:D:2098:GLY:O	4:D:2102:GLU:HG3	2.17	0.45
1:A:229:LYS:HG3	1:A:233:GLU:OE1	2.17	0.45
2:B:460:ASP:OD2	2:B:703:ILE:HD11	2.16	0.45
2:B:524:HIS:O	2:B:527:ASN:N	2.48	0.45
1:A:26:ALA:O	1:A:30:GLN:HG3	2.15	0.45
1:A:116:LEU:O	1:A:117:LYS:C	2.54	0.45
1:A:226:THR:O	1:A:227:VAL:C	2.54	0.45
1:A:345:HIS:CE1	1:A:401:ARG:HG2	2.51	0.45
2:B:537:ILE:CG1	2:B:538:GLN:N	2.79	0.45
2:B:620:TYR:HD2	2:B:624:GLN:HG2	1.65	0.45
2:B:633:MET:O	2:B:633:MET:CG	2.63	0.45
2:B:703:ILE:HG23	2:B:704:GLU:N	2.32	0.45
1:A:232:PHE:CZ	1:A:236:PHE:HB2	2.51	0.45
1:A:242:ARG:HG3	1:A:242:ARG:NH1	2.30	0.45
1:A:256:PRO:O	1:A:257:VAL:C	2.54	0.45
1:A:340:LEU:O	1:A:340:LEU:HD12	2.16	0.45
2:B:583:TYR:C	2:B:585:LEU:H	2.20	0.45
2:B:652:GLU:OE1	2:B:652:GLU:N	2.37	0.45
2:B:668:LEU:N	2:B:668:LEU:CD1	2.80	0.45
2:B:751:LYS:HZ1	2:B:755:ILE:HD11	1.80	0.45
1:A:127:ARG:O	1:A:130:SER:HB2	2.16	0.45
2:B:648:LEU:O	2:B:672:TYR:N	2.41	0.45
1:A:296:ILE:O	1:A:303:PHE:CE2	2.70	0.45
1:A:371:LEU:O	1:A:374:HIS:HB3	2.16	0.45
2:B:442:LEU:CD2	2:B:484:ALA:HB1	2.47	0.45
2:B:584:GLN:HB2	2:B:585:LEU:HD12	1.98	0.45
2:B:649:LEU:N	2:B:649:LEU:HD12	2.31	0.45
2:B:758:GLU:O	2:B:758:GLU:HG2	2.16	0.45
4:D:2022:LYS:HA	4:D:2028:LYS:HG3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LYS:N	1:A:154:LYS:CD	2.79	0.45
1:A:286:GLU:HA	1:A:289:ARG:HB2	1.99	0.45
1:A:342:THR:HG22	1:A:346:ASN:ND2	2.32	0.45
2:B:652:GLU:CG	2:B:668:LEU:HB2	2.46	0.45
2:B:714:ALA:HB1	2:B:738:LEU:HD22	1.99	0.45
4:D:2044:VAL:O	4:D:2044:VAL:HG12	2.16	0.45
4:D:2099:THR:O	4:D:2103:LEU:HG	2.16	0.45
1:A:212:GLY:O	1:A:214:ASN:OD1	2.35	0.45
1:A:296:ILE:HG21	1:A:325:LEU:C	2.37	0.45
2:B:423:ALA:HA	2:B:462:PHE:HE1	1.82	0.45
2:B:522:LYS:NZ	2:B:522:LYS:CB	2.80	0.45
2:B:632:LYS:HB3	2:B:635:ILE:HG22	1.98	0.45
1:A:127:ARG:NE	1:A:210:GLU:OE1	2.49	0.44
1:A:205:VAL:O	1:A:206:GLN:C	2.53	0.44
2:B:475:VAL:HG21	2:B:547:PHE:CE2	2.52	0.44
2:B:751:LYS:HE2	2:B:751:LYS:O	2.17	0.44
4:D:2116:LEU:O	4:D:2119:THR:OG1	2.35	0.44
1:A:97:LYS:HD2	1:A:101:THR:HG21	1.99	0.44
1:A:286:GLU:HG3	1:A:289:ARG:CZ	2.46	0.44
1:A:368:GLN:O	1:A:371:LEU:N	2.45	0.44
2:B:540:LEU:HB3	2:B:545:TRP:CE2	2.52	0.44
1:A:54:THR:O	1:A:54:THR:HG22	2.17	0.44
1:A:145:VAL:HG13	1:A:157:TYR:HD2	1.81	0.44
1:A:287:LEU:HD23	1:A:287:LEU:O	2.17	0.44
1:A:402:PHE:C	1:A:404:ASN:N	2.71	0.44
2:B:464:LYS:NZ	2:B:702:ASN:O	2.50	0.44
2:B:513:VAL:CG1	2:B:514:SER:N	2.81	0.44
1:A:173:ARG:CB	1:A:174:PRO:CD	2.93	0.44
1:A:181:ASN:O	1:A:182:ALA:C	2.56	0.44
2:B:475:VAL:HG12	2:B:476:HIS:HD2	1.82	0.44
2:B:590:LEU:O	2:B:600:THR:HA	2.18	0.44
2:B:756:LEU:CB	2:B:761:TYR:HB2	2.47	0.44
4:D:2104:ILE:HG22	5:E:3116:LEU:HD13	2.00	0.44
5:E:3125:CYS:O	5:E:3126:LEU:C	2.55	0.44
1:A:21:TRP:CD1	1:A:91:ARG:HD3	2.53	0.44
1:A:227:VAL:O	1:A:230:GLU:N	2.51	0.44
1:A:227:VAL:O	1:A:229:LYS:N	2.51	0.44
1:A:248:SER:O	1:A:251:PHE:HB3	2.18	0.44
1:A:286:GLU:O	1:A:287:LEU:C	2.56	0.44
1:A:399:CYS:HA	1:A:402:PHE:CE2	2.53	0.44
2:B:475:VAL:HG12	2:B:476:HIS:CD2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:655:ASN:O	2:B:656:ALA:HB2	2.16	0.44
2:B:712:GLN:O	2:B:761:TYR:CE2	2.71	0.44
1:A:24:LEU:CD1	1:A:28:ILE:HD11	2.48	0.44
2:B:545:TRP:CD1	2:B:545:TRP:N	2.86	0.44
2:B:619:ALA:HB1	2:B:670:LYS:HA	2.00	0.44
1:A:335:GLU:O	1:A:339:LEU:N	2.40	0.44
1:A:360:LEU:HB2	1:A:408:VAL:HG13	1.99	0.44
2:B:430:LEU:N	2:B:430:LEU:HD22	2.32	0.44
2:B:507:MET:HG2	2:B:545:TRP:CE2	2.53	0.44
2:B:641:GLN:HA	2:B:644:LEU:CD1	2.40	0.44
1:A:257:VAL:HG13	1:A:258:THR:N	2.28	0.44
2:B:511:ILE:HD11	2:B:538:GLN:HE21	1.83	0.44
2:B:694:GLN:O	2:B:695:GLU:C	2.56	0.44
4:D:2059:HIS:CD2	4:D:2062:ASP:OD2	2.71	0.44
4:D:2046:ALA:O	4:D:2047:ALA:C	2.56	0.44
5:E:3130:LEU:O	5:E:3133:SER:HB3	2.18	0.44
1:A:167:TRP:CD1	1:A:211:LEU:HD21	2.53	0.43
2:B:506:ARG:HA	2:B:509:GLN:HE21	1.83	0.43
4:D:2101:PHE:O	4:D:2102:GLU:HA	2.17	0.43
2:B:542:SER:CB	3:C:1032:LEU:HB3	2.48	0.43
2:B:703:ILE:CG2	2:B:704:GLU:N	2.80	0.43
2:B:481:SER:O	2:B:484:ALA:HB3	2.18	0.43
2:B:631:ILE:HB	2:B:636:LEU:CD1	2.48	0.43
1:A:27:GLY:HA3	1:A:45:LEU:HD21	2.00	0.43
2:B:689:LYS:HE2	2:B:689:LYS:CA	2.46	0.43
1:A:170:CYS:O	1:A:170:CYS:SG	2.77	0.43
1:A:228:TYR:O	1:A:232:PHE:HB3	2.18	0.43
1:A:380:LEU:HD12	1:A:384:ALA:HB2	2.00	0.43
1:A:171:LEU:O	1:A:173:ARG:N	2.52	0.43
2:B:450:MET:HG3	2:B:491:LYS:HB3	1.99	0.43
2:B:590:LEU:HD21	2:B:608:MET:SD	2.58	0.43
2:B:708:LYS:O	2:B:709:LEU:C	2.56	0.43
2:B:730:LEU:HD11	2:B:734:VAL:HG23	2.01	0.43
1:A:235:GLN:O	1:A:238:ALA:HB3	2.19	0.43
1:A:306:GLU:O	1:A:307:PHE:C	2.56	0.43
2:B:725:LEU:HD12	2:B:725:LEU:C	2.38	0.43
4:D:2010:ASP:OD2	4:D:2010:ASP:N	2.52	0.43
1:A:321:ARG:CG	1:A:321:ARG:NH1	2.80	0.43
1:A:371:LEU:O	1:A:372:ASP:C	2.57	0.43
2:B:508:PHE:C	2:B:511:ILE:HG22	2.39	0.43
2:B:553:PHE:CZ	2:B:609:ALA:HB2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASN:O	1:A:193:GLY:O	2.36	0.43
1:A:297:GLU:HA	1:A:300:LEU:CB	2.48	0.43
1:A:388:ASP:OD1	1:A:390:GLY:N	2.47	0.43
2:B:540:LEU:HB3	2:B:545:TRP:CD1	2.53	0.43
2:B:541:SER:N	2:B:545:TRP:NE1	2.51	0.43
1:A:38:ALA:O	1:A:40:SER:N	2.51	0.43
1:A:107:GLY:CA	1:A:110:LEU:CD1	2.86	0.43
1:A:204:VAL:O	1:A:205:VAL:C	2.58	0.43
1:A:273:ARG:O	1:A:277:VAL:HG23	2.18	0.43
1:A:287:LEU:HD23	1:A:291:CYS:SG	2.58	0.43
1:A:293:GLN:HG2	1:A:298:LYS:HE3	2.00	0.43
1:A:322:MET:C	1:A:324:ASN:N	2.70	0.43
2:B:430:LEU:CD1	2:B:442:LEU:HD21	2.49	0.43
2:B:432:LYS:HD2	2:B:480:ALA:CA	2.48	0.43
2:B:450:MET:C	2:B:453:PHE:H	2.22	0.43
2:B:745:ARG:HB3	2:B:747:PRO:HD2	2.00	0.43
4:D:2131:THR:HB	4:D:2132:PRO:CD	2.48	0.43
1:A:110:LEU:CD1	1:A:118:PHE:CD2	3.02	0.42
1:A:249:THR:O	1:A:250:GLU:C	2.55	0.42
2:B:590:LEU:HB2	2:B:601:LEU:CB	2.47	0.42
2:B:711:ILE:HB	2:B:712:GLN:HE21	1.84	0.42
1:A:116:LEU:HD21	1:A:182:ALA:HB3	2.00	0.42
1:A:208:TYR:CD1	1:A:232:PHE:HB2	2.54	0.42
1:A:310:LEU:O	1:A:313:ALA:N	2.52	0.42
2:B:668:LEU:O	2:B:669:ILE:HD12	2.19	0.42
4:D:2024:SER:CA	4:D:2112:ILE:HG12	2.45	0.42
5:E:3126:LEU:N	5:E:3127:PRO:HD2	2.34	0.42
5:E:3132:VAL:HG23	5:E:3133:SER:N	2.34	0.42
1:A:32:TYR:HE2	1:A:126:TYR:CE1	2.37	0.42
1:A:121:GLN:HB2	1:A:121:GLN:HE21	1.61	0.42
1:A:381:VAL:HG21	1:A:395:LEU:HD12	2.00	0.42
1:A:409:THR:HG23	2:B:415:SER:CA	2.16	0.42
2:B:712:GLN:OE1	2:B:756:LEU:HD11	2.20	0.42
2:B:734:VAL:HG12	2:B:734:VAL:O	2.19	0.42
2:B:738:LEU:O	2:B:740:SER:N	2.52	0.42
4:D:2119:THR:O	4:D:2122:THR:N	2.53	0.42
1:A:86:LEU:HD23	1:A:87:GLU:CD	2.40	0.42
1:A:304:HIS:ND1	1:A:335:GLU:HB3	2.33	0.42
1:A:330:GLN:O	1:A:330:GLN:HG3	2.19	0.42
1:A:343:HIS:CD2	1:A:347:GLN:HG3	2.55	0.42
2:B:468:LYS:CE	2:B:699:THR:HB	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:672:TYR:O	2:B:673:LEU:C	2.57	0.42
4:D:2017:ASP:O	4:D:2020:ILE:HB	2.18	0.42
4:D:2114:GLY:O	4:D:2117:ASP:HB2	2.19	0.42
5:E:3120:ILE:C	5:E:3122:SER:H	2.22	0.42
2:B:458:ASP:C	2:B:460:ASP:N	2.73	0.42
2:B:617:GLU:O	2:B:618:ASP:O	2.38	0.42
1:A:37:MET:HG2	1:A:42:TYR:CE1	2.54	0.42
1:A:323:TYR:CG	1:A:385:PHE:HA	2.55	0.42
2:B:620:TYR:CD2	2:B:624:GLN:OE1	2.72	0.42
4:D:2006:LEU:O	4:D:2008:SER:N	2.53	0.42
4:D:2043:ASN:HB2	4:D:2109:TYR:CZ	2.54	0.42
5:E:3136:CYS:O	5:E:3137:LYS:C	2.57	0.42
1:A:287:LEU:HD21	1:A:291:CYS:SG	2.60	0.42
1:A:326:VAL:C	1:A:328:ARG:N	2.72	0.42
2:B:728:GLN:HA	2:B:728:GLN:NE2	2.33	0.42
1:A:191:ARG:O	1:A:193:GLY:N	2.51	0.42
1:A:261:MET:O	1:A:264:ALA:HB3	2.19	0.42
1:A:297:GLU:HG3	1:A:298:LYS:N	2.34	0.42
2:B:619:ALA:HB1	2:B:670:LYS:CA	2.50	0.42
2:B:746:VAL:HG22	2:B:747:PRO:HD3	2.02	0.42
4:D:2016:VAL:CG2	4:D:2053:ILE:HD11	2.50	0.42
1:A:26:ALA:O	1:A:29:GLN:HB3	2.20	0.42
1:A:134:ASN:OD1	1:A:159:ILE:HG22	2.19	0.42
1:A:366:TYR:O	1:A:370:VAL:HG23	2.20	0.42
1:A:409:THR:O	1:A:410:LYS:C	2.58	0.42
2:B:432:LYS:HA	2:B:480:ALA:H	1.84	0.42
1:A:310:LEU:O	1:A:313:ALA:C	2.58	0.42
1:A:370:VAL:HG13	1:A:402:PHE:CE1	2.55	0.42
4:D:2026:THR:HB	4:D:2110:LEU:CA	2.50	0.42
1:A:39:LYS:HG2	4:D:2036:MET:CB	2.44	0.41
1:A:167:TRP:O	1:A:170:CYS:HB3	2.19	0.41
1:A:286:GLU:O	1:A:289:ARG:HB2	2.19	0.41
1:A:315:LYS:HD3	1:A:318:ASP:OD2	2.20	0.41
1:A:357:GLU:H	1:A:359:ALA:H	1.68	0.41
4:D:2054:GLN:O	4:D:2057:THR:HB	2.20	0.41
1:A:84:VAL:HG23	1:A:84:VAL:O	2.20	0.41
1:A:88:LEU:HD12	1:A:88:LEU:O	2.20	0.41
1:A:129:SER:CA	1:A:132:VAL:HG12	2.50	0.41
1:A:244:TYR:HE2	1:A:267:ARG:CG	2.32	0.41
1:A:307:PHE:HD1	1:A:322:MET:SD	2.43	0.41
1:A:322:MET:C	1:A:324:ASN:H	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:LYS:HB2	2:B:478:ASN:CG	2.41	0.41
2:B:485:GLU:C	2:B:487:SER:N	2.73	0.41
2:B:489:ILE:N	2:B:489:ILE:HD13	2.35	0.41
2:B:622:VAL:HB	2:B:665:PRO:HA	2.02	0.41
4:D:2022:LYS:CB	4:D:2028:LYS:HG3	2.50	0.41
1:A:95:PHE:CD2	1:A:95:PHE:C	2.92	0.41
1:A:168:ARG:HH12	1:A:215:GLU:CG	2.32	0.41
1:A:306:GLU:OE1	1:A:309:ASN:ND2	2.47	0.41
2:B:714:ALA:HB1	2:B:738:LEU:HD21	2.01	0.41
4:D:2124:ALA:HB1	5:E:3124:LEU:HD21	2.02	0.41
4:D:2130:LYS:O	5:E:3131:LYS:HD2	2.21	0.41
5:E:3116:LEU:O	5:E:3119:GLY:N	2.39	0.41
2:B:571:ALA:HB2	2:B:577:ARG:HH22	1.77	0.41
2:B:650:VAL:O	2:B:670:LYS:HD3	2.20	0.41
2:B:723:LYS:CB	2:B:774:TYR:CE2	2.97	0.41
5:E:3109:TRP:HB2	5:E:3110:ASP:H	1.66	0.41
2:B:489:ILE:O	2:B:493:LYS:HG3	2.20	0.41
3:C:1024:VAL:O	3:C:1025:LYS:C	2.58	0.41
4:D:2053:ILE:HG23	4:D:2054:GLN:N	2.36	0.41
4:D:2126:MET:O	4:D:2127:ILE:HD13	2.21	0.41
2:B:422:LEU:HD22	2:B:449:VAL:HG13	2.02	0.41
2:B:477:GLN:O	2:B:477:GLN:CG	2.47	0.41
2:B:537:ILE:HG13	3:C:1030:VAL:CA	2.50	0.41
2:B:707:ARG:NH1	2:B:742:PHE:CB	2.82	0.41
1:A:104:LEU:HD13	1:A:108:GLU:CD	2.41	0.41
1:A:104:LEU:HD13	1:A:108:GLU:OE1	2.21	0.41
1:A:297:GLU:CG	1:A:298:LYS:N	2.83	0.41
1:A:341:GLU:HG3	1:A:398:ALA:HB2	2.03	0.41
2:B:513:VAL:O	2:B:517:LEU:N	2.52	0.41
2:B:545:TRP:HE3	2:B:547:PHE:HE2	1.69	0.41
2:B:573:ARG:C	2:B:574:HIS:CG	2.90	0.41
2:B:608:MET:HE3	3:C:1024:VAL:HG13	2.02	0.41
2:B:691:GLU:HA	2:B:694:GLN:HB2	2.02	0.41
4:D:2118:VAL:CG1	4:D:2119:THR:N	2.82	0.41
1:A:96:LEU:HD22	1:A:162:LEU:HD22	2.03	0.41
1:A:197:ASN:O	1:A:201:ILE:N	2.49	0.41
1:A:250:GLU:HG3	1:A:251:PHE:N	2.36	0.41
1:A:281:GLU:C	1:A:283:THR:N	2.73	0.41
1:A:368:GLN:O	1:A:369:THR:C	2.59	0.41
2:B:648:LEU:C	2:B:649:LEU:HD12	2.41	0.41
2:B:762:LEU:CD2	2:B:772:TYR:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LEU:O	1:A:89:TYR:N	2.54	0.41
1:A:164:LEU:O	1:A:165:VAL:C	2.59	0.41
1:A:196:ILE:O	1:A:196:ILE:HG22	2.20	0.41
1:A:316:ASN:O	1:A:319:LEU:HB3	2.20	0.41
1:A:347:GLN:C	1:A:349:LEU:N	2.75	0.41
1:A:364:LYS:O	1:A:365:MET:C	2.59	0.41
1:A:401:ARG:O	1:A:401:ARG:HG2	2.21	0.41
2:B:414:SER:HB3	2:B:417:LYS:HB2	2.01	0.41
2:B:431:LYS:CA	2:B:479:SER:HA	2.46	0.41
2:B:436:ASN:OD1	2:B:437:PRO:N	2.54	0.41
2:B:581:TRP:HA	3:C:1031:ALA:HB2	2.03	0.41
4:D:2110:LEU:HD12	4:D:2112:ILE:HD11	2.02	0.41
1:A:50:TYR:HD1	1:A:51:ASN:HD22	1.69	0.41
1:A:166:THR:C	1:A:168:ARG:N	2.71	0.41
1:A:343:HIS:CD2	1:A:347:GLN:CG	3.04	0.41
1:A:362:ASP:OD1	1:A:362:ASP:C	2.60	0.41
2:B:590:LEU:HD23	3:C:1024:VAL:HA	2.03	0.41
2:B:746:VAL:HG23	2:B:747:PRO:CD	2.51	0.41
3:C:1021:ARG:HG3	3:C:1022:PHE:N	2.35	0.41
4:D:2049:LEU:HD22	4:D:2053:ILE:HB	2.01	0.41
4:D:2085:ILE:HG13	4:D:2121:LYS:HE3	2.03	0.41
4:D:2130:LYS:H	5:E:3131:LYS:HZ2	1.68	0.41
1:A:37:MET:HG2	1:A:42:TYR:HE1	1.85	0.40
1:A:39:LYS:CG	4:D:2036:MET:HG2	2.51	0.40
1:A:335:GLU:HG3	1:A:339:LEU:HD22	2.03	0.40
1:A:367:VAL:HG13	2:B:422:LEU:HD23	2.02	0.40
2:B:451:VAL:HG12	2:B:452:VAL:N	2.36	0.40
2:B:553:PHE:HE1	2:B:631:ILE:CG1	2.09	0.40
2:B:578:LYS:C	2:B:579:LEU:HG	2.42	0.40
2:B:644:LEU:HA	2:B:649:LEU:O	2.20	0.40
2:B:739:SER:C	2:B:741:ARG:N	2.72	0.40
4:D:2004:ILE:HD11	4:D:2039:VAL:CG2	2.51	0.40
4:D:2034:LEU:O	4:D:2034:LEU:HG	2.21	0.40
1:A:111:MET:O	1:A:115:VAL:CG1	2.69	0.40
1:A:186:LEU:HD22	1:A:197:ASN:HB2	2.03	0.40
1:A:251:PHE:CE2	1:A:255:ASN:CB	3.04	0.40
1:A:402:PHE:C	1:A:404:ASN:H	2.24	0.40
2:B:425:TYR:O	2:B:428:SER:HB3	2.21	0.40
2:B:612:LEU:C	2:B:614:TYR:H	2.24	0.40
1:A:45:LEU:HB3	1:A:136:ILE:CG2	2.52	0.40
1:A:209:VAL:O	1:A:212:GLY:HA3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:ASP:C	1:A:313:ALA:O	2.57	0.40
2:B:637:ALA:CB	2:B:663:LEU:HD12	2.26	0.40
2:B:669:ILE:HD12	2:B:669:ILE:N	2.36	0.40
2:B:723:LYS:HA	2:B:774:TYR:CD2	2.55	0.40
4:D:2004:ILE:HG13	4:D:2005:LYS:N	2.36	0.40
4:D:2022:LYS:CA	4:D:2028:LYS:HG3	2.51	0.40
1:A:124:GLU:O	1:A:126:TYR:N	2.54	0.40
1:A:162:LEU:O	1:A:166:THR:N	2.38	0.40
1:A:316:ASN:CG	1:A:380:LEU:HD13	2.41	0.40
1:A:316:ASN:OD1	1:A:380:LEU:HD13	2.21	0.40
2:B:426:CYS:O	2:B:427:ASP:C	2.59	0.40
2:B:524:HIS:O	2:B:529:GLU:OE1	2.39	0.40
2:B:633:MET:O	2:B:633:MET:HG2	2.21	0.40
2:B:691:GLU:HA	2:B:694:GLN:CG	2.51	0.40
4:D:2051:LYS:HA	4:D:2054:GLN:OE1	2.20	0.40
1:A:268:LEU:HD13	1:A:328:ARG:NH2	2.37	0.40
1:A:299:HIS:C	1:A:301:GLU:N	2.75	0.40
1:A:318:ASP:O	1:A:319:LEU:C	2.60	0.40
1:A:326:VAL:O	1:A:327:SER:C	2.59	0.40
2:B:500:TYR:HB3	2:B:504:LEU:HD12	2.03	0.40
2:B:642:ILE:HD11	2:B:687:PRO:C	2.39	0.40
2:B:681:ARG:NH1	2:B:681:ARG:HG2	2.36	0.40
2:B:709:LEU:HD23	2:B:709:LEU:HA	1.95	0.40
4:D:2024:SER:OG	4:D:2110:LEU:CB	2.66	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH2	1:A:305:THR:OG1[3_546]	1.76	0.44
2:B:597:ASN:OD1	2:B:659:ASP:OD2[3_547]	2.00	0.20
2:B:572:SER:O	3:C:1061:ALA:CB[1_545]	2.04	0.16
2:B:660:GLU:OE1	2:B:676:LYS:CB[3_557]	2.04	0.16

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	350/396 (88%)	236 (67%)	92 (26%)	22 (6%)	1	8
2	B	364/366 (100%)	261 (72%)	75 (21%)	28 (8%)	1	5
3	C	86/90 (96%)	44 (51%)	24 (28%)	18 (21%)	0	0
4	D	114/133 (86%)	68 (60%)	31 (27%)	15 (13%)	0	1
5	E	39/41 (95%)	26 (67%)	9 (23%)	4 (10%)	0	3
All	All	953/1026 (93%)	635 (67%)	231 (24%)	87 (9%)	1	4

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	PHE
1	A	174	PRO
1	A	176	ASN
1	A	192	ASN
1	A	193	GLY
2	B	431	LYS
2	B	454	LYS
2	B	527	ASN
2	B	536	SER
2	B	557	SER
2	B	594	CYS
2	B	618	ASP
2	B	622	VAL
2	B	661	VAL
2	B	688	MET
2	B	731	LEU
3	C	1088	LEU
3	C	1104	GLN
4	D	2015	GLU
4	D	2018	VAL
4	D	2037	ASP
4	D	2038	PRO
5	E	3147	SER
1	A	212	GLY
1	A	227	VAL
1	A	298	LYS
1	A	327	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	331	ASP
1	A	334	GLY
2	B	459	LYS
2	B	601	LEU
2	B	658	VAL
2	B	673	LEU
2	B	680	LEU
2	B	684	ILE
2	B	738	LEU
2	B	739	SER
3	C	1098	ASN
4	D	2007	GLN
4	D	2019	GLU
4	D	2114	GLY
4	D	2126	MET
5	E	3137	LYS
1	A	86	LEU
1	A	315	LYS
1	A	317	GLU
1	A	405	ASN
2	B	439	GLU
2	B	504	LEU
2	B	713	ALA
3	C	1021	ARG
3	C	1047	ASN
3	C	1076	ASN
3	C	1078	ALA
3	C	1089	LYS
2	B	531	LEU
2	B	546	PRO
2	B	556	PRO
2	B	567	THR
2	B	751	LYS
3	C	1080	HIS
3	C	1105	LYS
4	D	2060	LYS
1	A	103	LEU
1	A	169	ASP
1	A	173	ARG
2	B	656	ALA
3	C	1054	ILE
3	C	1069	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	1099	ARG
3	C	1103	PHE
4	D	2030	MET
4	D	2035	GLY
4	D	2039	VAL
4	D	2052	VAL
5	E	3110	ASP
1	A	39	LYS
1	A	84	VAL
1	A	85	GLY
1	A	258	THR
3	C	1090	THR
3	C	1091	ARG
4	D	2113	LYS
3	C	1024	VAL
3	C	1038	VAL
4	D	2132	PRO
5	E	3126	LEU

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	321/347 (92%)	272 (85%)	49 (15%)	2 12
2	B	338/338 (100%)	301 (89%)	37 (11%)	6 25
3	C	78/79 (99%)	70 (90%)	8 (10%)	7 27
4	D	105/122 (86%)	101 (96%)	4 (4%)	33 66
5	E	37/38 (97%)	34 (92%)	3 (8%)	11 39
All	All	879/924 (95%)	778 (88%)	101 (12%)	5 22

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	24	LEU
1	A	25	ARG
1	A	33	THR
1	A	37	MET
1	A	39	LYS
1	A	86	LEU
1	A	103	LEU
1	A	104	LEU
1	A	121	GLN
1	A	125	ASP
1	A	137	CYS
1	A	140	LEU
1	A	142	ARG
1	A	144	TRP
1	A	154	LYS
1	A	159	ILE
1	A	168	ARG
1	A	169	ASP
1	A	171	LEU
1	A	191	ARG
1	A	211	LEU
1	A	235	GLN
1	A	237	LEU
1	A	245	THR
1	A	249	THR
1	A	250	GLU
1	A	252	LEU
1	A	256	PRO
1	A	257	VAL
1	A	258	THR
1	A	281	GLU
1	A	284	GLN
1	A	294	VAL
1	A	300	LEU
1	A	302	ILE
1	A	311	LEU
1	A	321	ARG
1	A	324	ASN
1	A	328	ARG
1	A	339	LEU
1	A	345	HIS
1	A	349	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	352	ILE
1	A	355	CYS
1	A	371	LEU
1	A	378	ASN
1	A	386	ASN
1	A	402	PHE
2	B	413	GLN
2	B	422	LEU
2	B	437	PRO
2	B	451	VAL
2	B	476	HIS
2	B	477	GLN
2	B	482	ASP
2	B	488	MET
2	B	489	ILE
2	B	534	ASP
2	B	549	GLN
2	B	550	SER
2	B	564	GLN
2	B	566	PHE
2	B	577	ARG
2	B	579	LEU
2	B	580	THR
2	B	600	THR
2	B	610	ILE
2	B	617	GLU
2	B	620	TYR
2	B	621	THR
2	B	634	ASP
2	B	658	VAL
2	B	670	LYS
2	B	671	LEU
2	B	676	LYS
2	B	681	ARG
2	B	688	MET
2	B	689	LYS
2	B	695	GLU
2	B	723	LYS
2	B	749	ILE
2	B	751	LYS
2	B	754	ASP
2	B	756	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	758	GLU
3	C	1019	LYS
3	C	1033	TRP
3	C	1035	TRP
3	C	1037	ILE
3	C	1057	GLN
3	C	1079	PHE
3	C	1097	ASP
3	C	1100	GLU
4	D	2019	GLU
4	D	2031	LEU
4	D	2061	ASP
4	D	2117	ASP
5	E	3113	PRO
5	E	3115	GLU
5	E	3140	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	48	HIS
1	A	51	ASN
1	A	102	ASN
1	A	121	GLN
1	A	141	ASN
1	A	214	ASN
1	A	235	GLN
1	A	276	GLN
1	A	284	GLN
1	A	316	ASN
1	A	324	ASN
1	A	346	ASN
1	A	368	GLN
1	A	378	ASN
1	A	386	ASN
2	B	448	GLN
2	B	476	HIS
2	B	477	GLN
2	B	509	GLN
2	B	574	HIS
2	B	602	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	615	ASN
2	B	630	GLN
2	B	657	ASN
2	B	677	ASN
2	B	692	GLN
2	B	728	GLN
2	B	737	GLN
4	D	2023	GLN
4	D	2059	HIS
4	D	2090	GLN
4	D	2097	GLN
4	D	2125	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.