



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:18 pm BST

PDB ID : 1E0K
Title : gp4d helicase from phage T7
Authors : Singleton, M.R.; Sawaya, M.R.; Ellenberger, T.; Wigley, D.B.
Deposited on : 2000-03-30
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

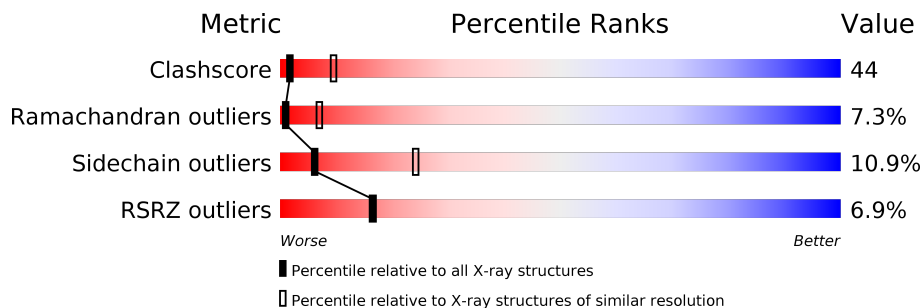
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. 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	289	7% (Poor fit) 36% (0 outliers), 50% (1 outlier), 13% (2 outliers)
1	B	289	4% (Poor fit) 37% (0 outliers), 50% (1 outlier), 12% (2 outliers)
1	C	289	4% (Poor fit) 38% (0 outliers), 51% (1 outlier), 11% (2 outliers)
1	D	289	10% (Poor fit) 35% (0 outliers), 49% (1 outlier), 15% (2 outliers)
1	E	289	9% (Poor fit) 36% (0 outliers), 50% (1 outlier), 13% (2 outliers)
1	F	289	7% (Poor fit) 35% (0 outliers), 54% (1 outlier), 10% (2 outliers)

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13284 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.

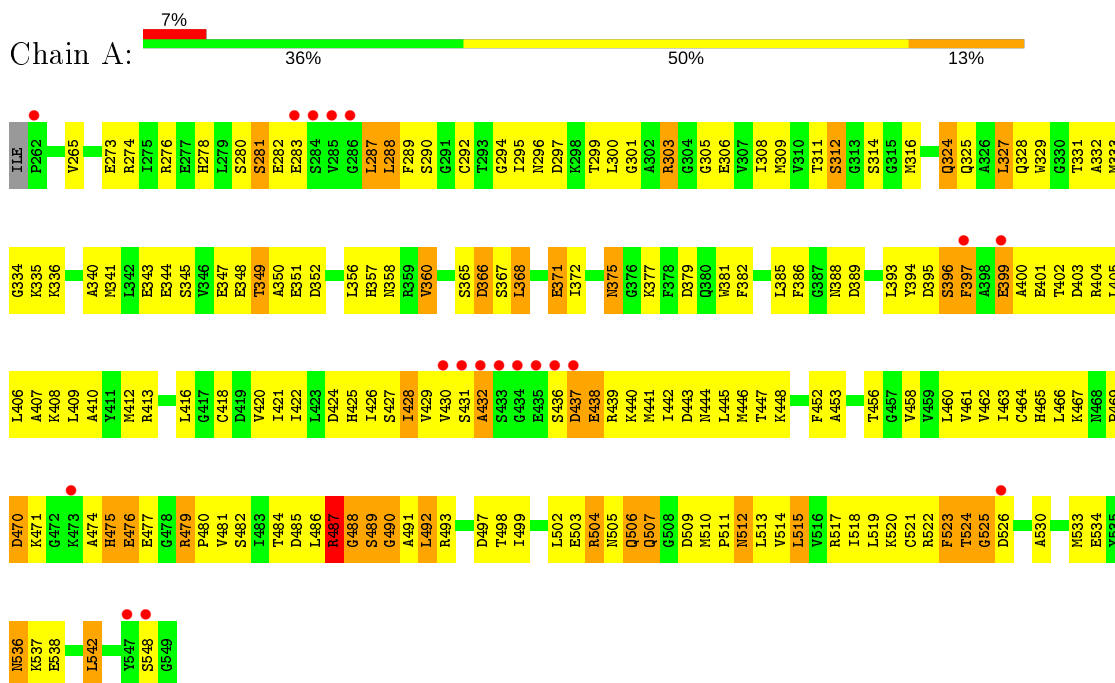
- Molecule 1 is a protein called DNA HELICASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2214	1378	390	433	13	0	0	0
1	B	288	2214	1378	390	433	13	0	0	0
1	C	288	2214	1378	390	433	13	0	0	0
1	D	288	2214	1378	390	433	13	0	0	0
1	E	288	2214	1378	390	433	13	0	0	0
1	F	288	2214	1378	390	433	13	0	0	0

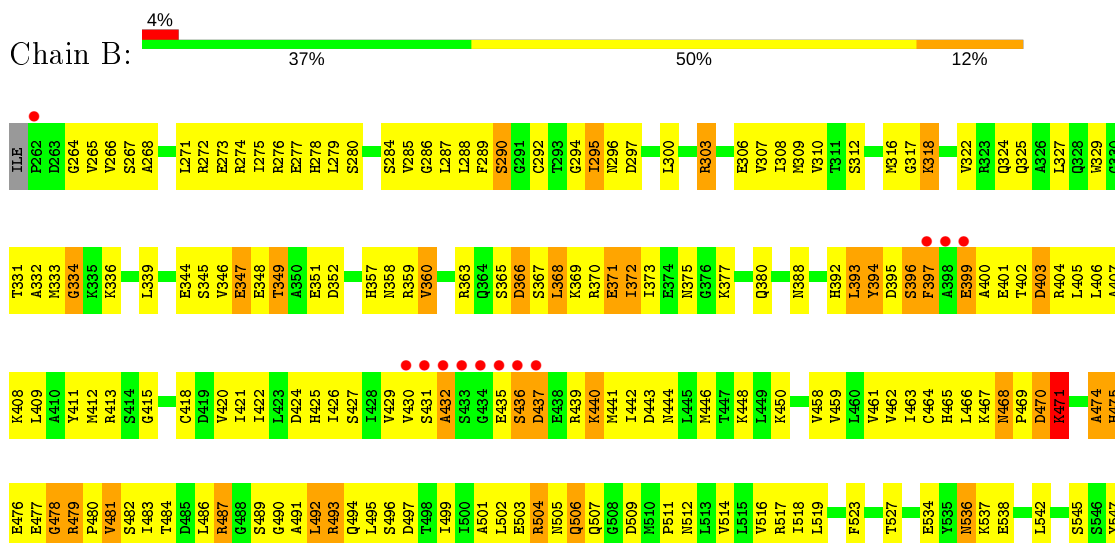
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: DNA HELICASE

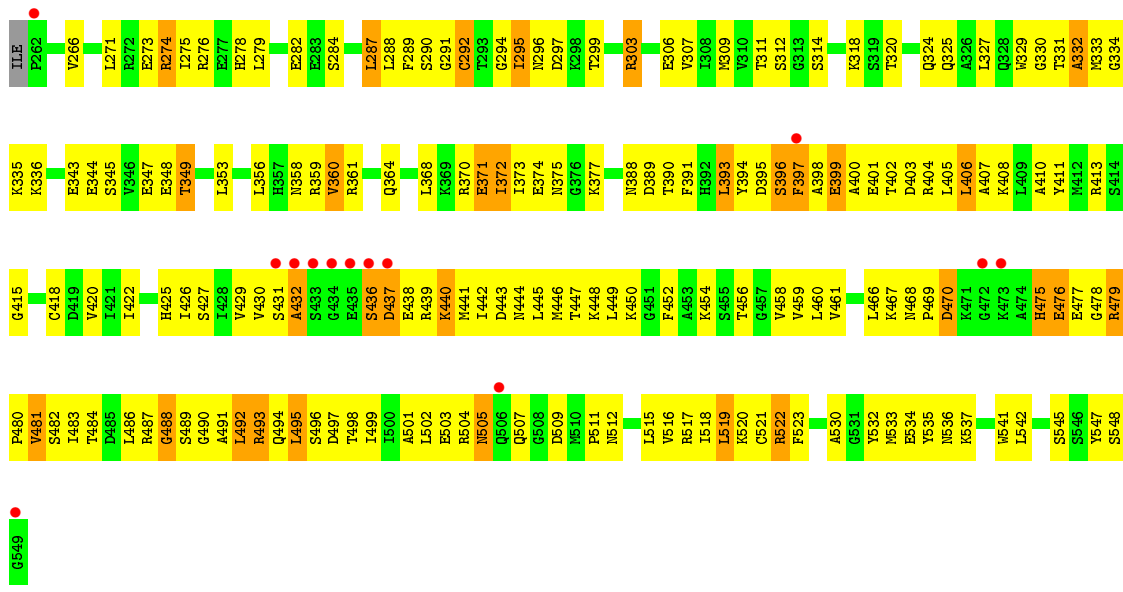


- Molecule 1: DNA HELICASE

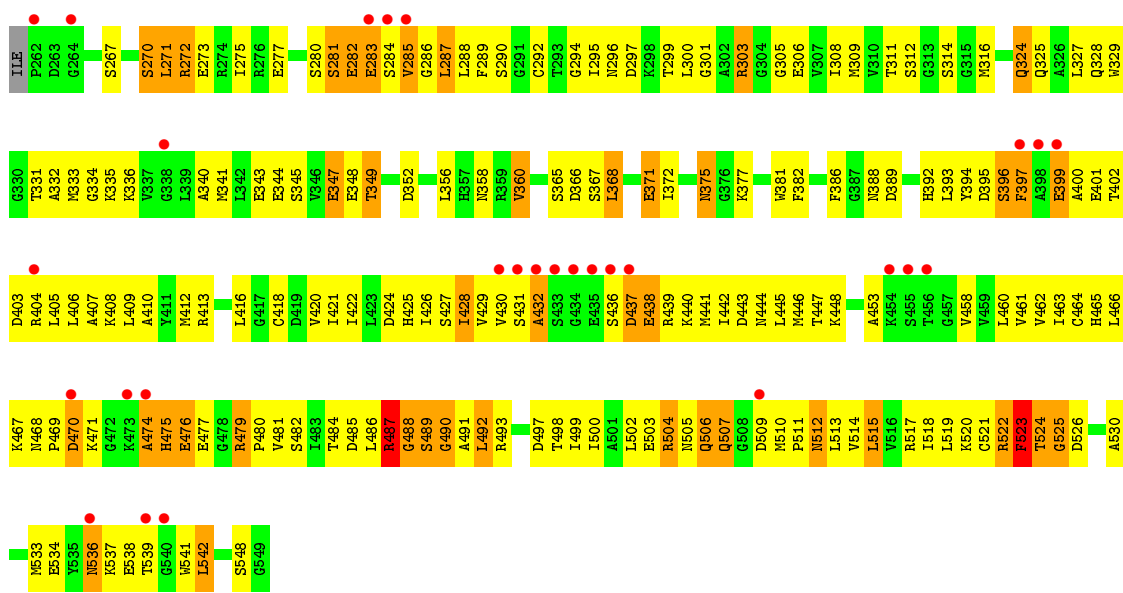




• Molecule 1: DNA HELICASE

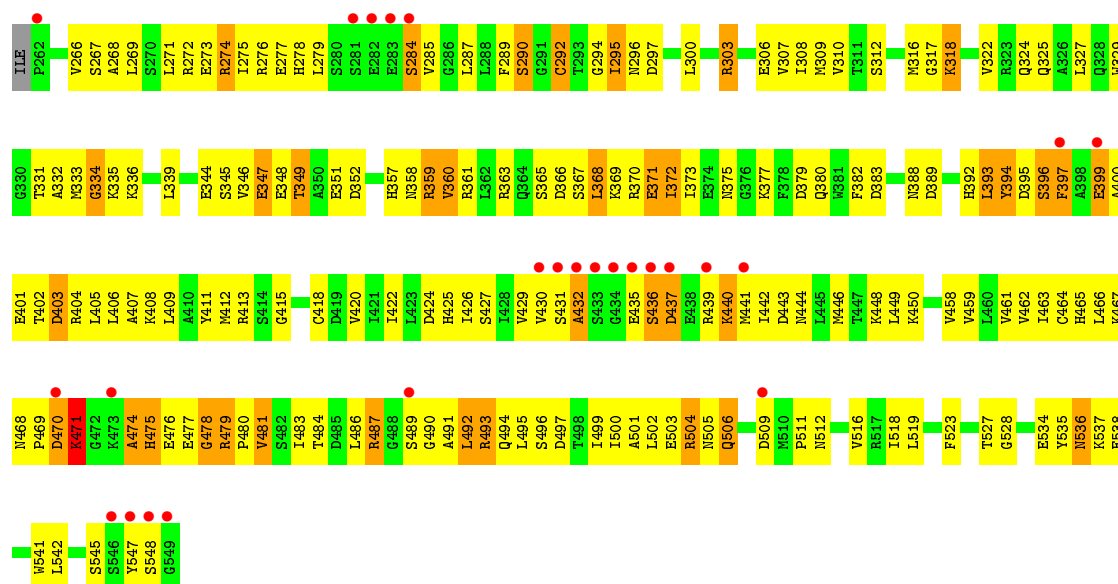


• Molecule 1: DNA HELICASE

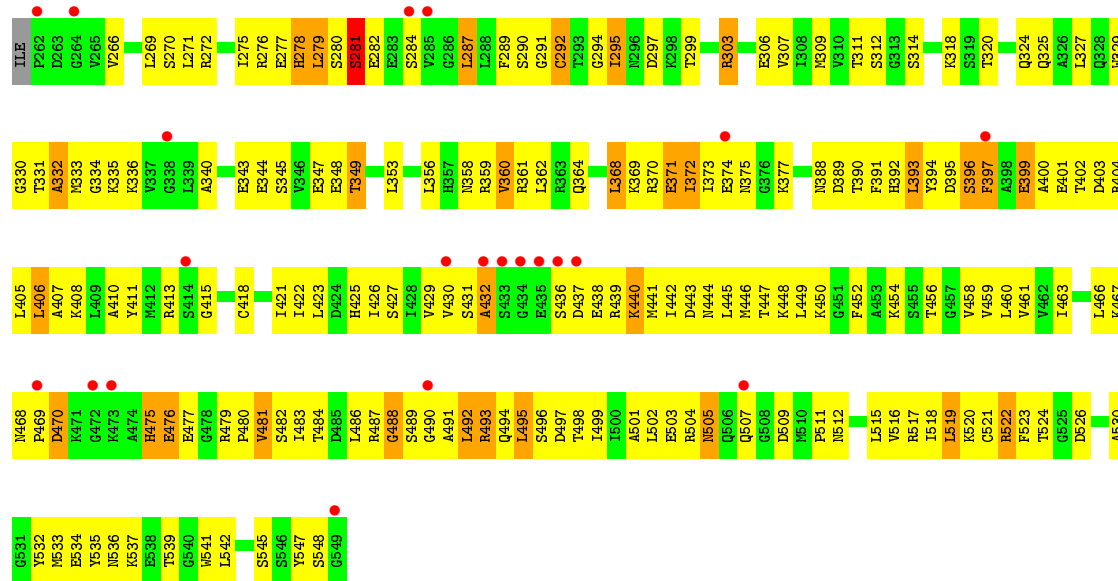


• Molecule 1: DNA HELICASE





• Molecule 1: DNA HELICASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.65Å 120.65Å 284.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 19.83 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-3.30) 94.7 (19.83-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 3.29Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.254 , 0.308 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	96.0	Xtrriage
Anisotropy	0.221	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 90.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13284	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.48	0/2243	0.73	1/3011 (0.0%)
1	B	0.45	0/2244	0.77	3/3014 (0.1%)
1	C	0.47	0/2244	0.75	1/3014 (0.0%)
1	D	1.02	8/2243 (0.4%)	0.78	3/3011 (0.1%)
1	E	0.45	0/2244	0.77	3/3014 (0.1%)
1	F	0.43	0/2244	0.75	1/3014 (0.0%)
All	All	0.59	8/13462 (0.1%)	0.76	12/18078 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	523	PHE	CE1-CZ	19.75	1.74	1.37
1	D	523	PHE	CD1-CE1	19.15	1.77	1.39
1	D	523	PHE	CE2-CZ	19.09	1.73	1.37
1	D	523	PHE	CD2-CE2	15.77	1.70	1.39
1	D	283	GLU	N-CA	14.31	1.75	1.46
1	D	523	PHE	CG-CD1	10.87	1.55	1.38
1	D	523	PHE	CG-CD2	10.25	1.54	1.38
1	D	282	GLU	C-N	6.15	1.48	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	GLU	C-N-CA	10.08	146.91	121.70
1	D	283	GLU	N-CA-C	6.61	128.84	111.00
1	B	295	ILE	N-CA-C	-5.85	95.19	111.00
1	E	474	ALA	N-CA-C	5.80	126.67	111.00
1	B	474	ALA	N-CA-C	5.72	126.46	111.00
1	D	474	ALA	N-CA-C	5.58	126.06	111.00
1	E	295	ILE	N-CA-C	-5.57	95.95	111.00
1	F	295	ILE	N-CA-C	-5.56	96.00	111.00
1	E	478	GLY	N-CA-C	-5.55	99.23	113.10
1	B	478	GLY	N-CA-C	-5.40	99.61	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	474	ALA	N-CA-C	5.36	125.48	111.00
1	C	295	ILE	N-CA-C	-5.29	96.71	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2214	0	2216	184	0
1	B	2214	0	2217	206	0
1	C	2214	0	2217	189	0
1	D	2214	0	2215	239	0
1	E	2214	0	2217	202	0
1	F	2214	0	2217	184	0
All	All	13284	0	13299	1161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (1161) 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:D:523:PHE:CE1	1:D:523:PHE:CD1	1.77	1.66
1:D:523:PHE:CE1	1:D:523:PHE:CZ	1.74	1.65
1:D:283:GLU:N	1:D:523:PHE:CE1	1.70	1.51
1:D:283:GLU:HA	1:D:523:PHE:CE1	1.42	1.50
1:D:283:GLU:CA	1:D:283:GLU:N	1.75	1.50
1:D:283:GLU:CA	1:D:523:PHE:CE1	2.01	1.41
1:D:282:GLU:C	1:D:523:PHE:CE1	2.00	1.32
1:D:283:GLU:N	1:D:523:PHE:CD1	1.83	1.26
1:D:283:GLU:CA	1:D:523:PHE:CD1	2.20	1.24
1:D:282:GLU:C	1:D:523:PHE:CD1	2.11	1.22
1:D:283:GLU:CA	1:D:523:PHE:CZ	2.24	1.18
1:E:290:SER:H	1:E:325:GLN:NE2	1.46	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:477:GLU:HA	1:D:505:ASN:HD22	1.11	1.10
1:A:290:SER:H	1:A:325:GLN:NE2	1.50	1.09
1:A:477:GLU:HA	1:A:505:ASN:HD22	1.14	1.09
1:B:290:SER:H	1:B:325:GLN:NE2	1.50	1.09
1:D:290:SER:H	1:D:325:GLN:NE2	1.52	1.07
1:D:282:GLU:O	1:D:523:PHE:CE1	2.06	1.06
1:F:290:SER:H	1:F:325:GLN:NE2	1.56	1.04
1:C:290:SER:H	1:C:325:GLN:NE2	1.59	1.01
1:F:344:GLU:HG3	1:F:349:THR:HG22	1.43	0.99
1:F:406:LEU:HD21	1:F:448:LYS:HB3	1.43	0.99
1:C:406:LEU:HD21	1:C:448:LYS:HB3	1.46	0.97
1:D:425:HIS:HE1	1:D:427:SER:HB2	1.28	0.96
1:D:283:GLU:HA	1:D:523:PHE:CZ	1.97	0.96
1:C:344:GLU:HG3	1:C:349:THR:HG22	1.44	0.96
1:A:425:HIS:HE1	1:A:427:SER:HB2	1.30	0.94
1:D:283:GLU:C	1:D:523:PHE:CD1	2.40	0.94
1:D:282:GLU:O	1:D:523:PHE:CD1	2.18	0.94
1:A:366:ASP:OD1	1:B:284:SER:HB3	1.68	0.93
1:D:283:GLU:HB2	1:D:303:ARG:HD2	1.47	0.93
1:F:402:THR:HG23	1:F:445:LEU:HD13	1.51	0.92
1:B:440:LYS:HZ2	1:B:444:ASN:HD22	1.17	0.92
1:F:375:ASN:HD21	1:F:377:LYS:HB2	1.34	0.91
1:E:425:HIS:HE1	1:E:427:SER:HB2	1.34	0.91
1:E:440:LYS:HZ2	1:E:444:ASN:HD22	1.16	0.90
1:F:518:ILE:HD13	1:F:530:ALA:HB2	1.53	0.90
1:D:290:SER:H	1:D:325:GLN:HE22	1.14	0.90
1:A:290:SER:H	1:A:325:GLN:HE22	1.07	0.90
1:D:477:GLU:HA	1:D:505:ASN:ND2	1.86	0.89
1:D:283:GLU:CA	1:D:523:PHE:CG	2.54	0.89
1:B:476:GLU:O	1:B:506:GLN:HG2	1.72	0.89
1:C:375:ASN:HD21	1:C:377:LYS:HB2	1.37	0.89
1:C:518:ILE:HD13	1:C:530:ALA:HB2	1.55	0.89
1:E:476:GLU:HG3	1:F:483:ILE:HD12	1.54	0.89
1:F:266:VAL:HG11	1:F:271:LEU:HD21	1.52	0.88
1:A:477:GLU:HA	1:A:505:ASN:ND2	1.88	0.88
1:C:402:THR:HG23	1:C:445:LEU:HD13	1.53	0.88
1:D:283:GLU:CA	1:D:523:PHE:CE2	2.55	0.88
1:E:476:GLU:O	1:E:506:GLN:HG2	1.72	0.88
1:E:367:SER:HA	1:E:370:ARG:HH12	1.38	0.88
1:C:290:SER:H	1:C:325:GLN:HE21	1.17	0.87
1:B:476:GLU:HG3	1:C:483:ILE:HD12	1.54	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:HIS:HE1	1:B:427:SER:HB2	1.38	0.86
1:D:329:TRP:CZ3	1:D:420:VAL:HG11	2.09	0.86
1:E:478:GLY:O	1:E:479:ARG:HB3	1.75	0.86
1:D:425:HIS:CE1	1:D:427:SER:HB2	2.10	0.86
1:E:393:LEU:HD12	1:E:393:LEU:N	1.91	0.86
1:E:477:GLU:OE2	1:F:482:SER:HB2	1.75	0.86
1:E:425:HIS:CE1	1:E:427:SER:HB2	2.10	0.85
1:A:425:HIS:CE1	1:A:427:SER:HB2	2.11	0.85
1:B:367:SER:HA	1:B:370:ARG:HH12	1.39	0.85
1:B:478:GLY:O	1:B:479:ARG:HB3	1.75	0.85
1:B:393:LEU:HD12	1:B:393:LEU:N	1.91	0.85
1:F:429:VAL:HG23	1:F:430:VAL:H	1.41	0.85
1:C:429:VAL:HG23	1:C:430:VAL:H	1.40	0.84
1:B:440:LYS:NZ	1:B:444:ASN:HD22	1.75	0.84
1:F:516:VAL:HG21	1:F:533:MET:HE2	1.60	0.83
1:A:329:TRP:CZ3	1:A:420:VAL:HG11	2.12	0.83
1:B:344:GLU:HG3	1:B:349:THR:HG22	1.59	0.83
1:B:474:ALA:HA	1:B:479:ARG:HD2	1.59	0.83
1:B:290:SER:H	1:B:325:GLN:HE21	1.24	0.83
1:A:429:VAL:HG23	1:A:430:VAL:H	1.44	0.82
1:D:518:ILE:CD1	1:D:530:ALA:HB2	2.08	0.82
1:B:440:LYS:O	1:B:440:LYS:HD3	1.80	0.82
1:D:518:ILE:HD11	1:D:530:ALA:HB2	1.58	0.82
1:B:290:SER:N	1:B:325:GLN:NE2	2.28	0.82
1:D:283:GLU:HG2	1:D:284:SER:O	1.78	0.82
1:E:440:LYS:O	1:E:440:LYS:HD3	1.80	0.82
1:F:290:SER:H	1:F:325:GLN:HE21	1.25	0.82
1:B:425:HIS:CE1	1:B:427:SER:HB2	2.14	0.82
1:E:344:GLU:HG3	1:E:349:THR:HG22	1.60	0.82
1:E:440:LYS:NZ	1:E:444:ASN:HD22	1.78	0.82
1:E:474:ALA:HA	1:E:479:ARG:HD2	1.62	0.80
1:D:358:ASN:O	1:D:360:VAL:HG22	1.82	0.80
1:F:327:LEU:HD13	1:F:353:LEU:HD22	1.63	0.80
1:A:477:GLU:OE2	1:B:482:SER:HB2	1.82	0.80
1:C:425:HIS:CE1	1:C:427:SER:HB2	2.16	0.80
1:E:316:MET:HE1	1:E:503:GLU:HA	1.62	0.80
1:A:507:GLN:HE21	1:B:517:ARG:HH11	1.27	0.80
1:D:429:VAL:HG23	1:D:430:VAL:H	1.47	0.80
1:A:358:ASN:O	1:A:360:VAL:HG22	1.81	0.79
1:D:283:GLU:CA	1:D:523:PHE:CD2	2.66	0.79
1:E:290:SER:H	1:E:325:GLN:HE22	1.29	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:MET:HE1	1:B:503:GLU:HA	1.63	0.79
1:C:266:VAL:HG11	1:C:271:LEU:HD21	1.65	0.79
1:A:518:ILE:CD1	1:A:530:ALA:HB2	2.12	0.78
1:B:477:GLU:HA	1:B:505:ASN:HD22	1.47	0.78
1:E:290:SER:H	1:E:325:GLN:HE21	1.26	0.78
1:F:509:ASP:O	1:F:511:PRO:HD3	1.83	0.78
1:E:285:VAL:HG22	1:E:300:LEU:HD22	1.65	0.78
1:F:358:ASN:O	1:F:360:VAL:HG22	1.83	0.78
1:D:283:GLU:HB2	1:D:303:ARG:CD	2.13	0.78
1:A:375:ASN:HD21	1:A:377:LYS:HG3	1.49	0.78
1:A:518:ILE:HD11	1:A:530:ALA:HB2	1.64	0.78
1:A:288:LEU:HD12	1:A:288:LEU:N	1.99	0.78
1:C:509:ASP:O	1:C:511:PRO:HD3	1.84	0.78
1:F:425:HIS:CE1	1:F:427:SER:HB2	2.18	0.78
1:C:358:ASN:O	1:C:360:VAL:HG22	1.84	0.78
1:A:517:ARG:HD2	1:A:519:LEU:HD11	1.66	0.77
1:B:289:PHE:H	1:B:296:ASN:HD21	1.33	0.77
1:C:278:HIS:O	1:C:282:GLU:HB2	1.85	0.77
1:C:327:LEU:HD13	1:C:353:LEU:HD22	1.66	0.77
1:C:404:ARG:NH1	1:C:408:LYS:HE3	1.99	0.77
1:D:514:VAL:HG13	1:D:533:MET:HB2	1.67	0.77
1:F:280:SER:O	1:F:281:SER:HB2	1.84	0.77
1:F:404:ARG:NH1	1:F:408:LYS:HE3	2.00	0.77
1:A:426:ILE:O	1:A:426:ILE:HG23	1.84	0.76
1:B:429:VAL:HG23	1:B:430:VAL:H	1.50	0.76
1:D:271:LEU:O	1:D:275:ILE:HG13	1.85	0.76
1:D:517:ARG:HD2	1:D:519:LEU:HD11	1.65	0.76
1:A:316:MET:HE3	1:A:504:ARG:H	1.51	0.76
1:D:283:GLU:CB	1:D:303:ARG:HD2	2.15	0.76
1:D:375:ASN:HD21	1:D:377:LYS:HG3	1.49	0.76
1:D:426:ILE:HG23	1:D:426:ILE:O	1.84	0.76
1:D:283:GLU:CB	1:D:523:PHE:CE2	2.70	0.75
1:E:429:VAL:HG23	1:E:430:VAL:H	1.50	0.75
1:E:477:GLU:HA	1:E:505:ASN:HD22	1.49	0.75
1:D:283:GLU:HG3	1:D:523:PHE:CZ	2.21	0.75
1:D:465:HIS:O	1:D:487:ARG:HB2	1.85	0.75
1:F:287:LEU:HD11	1:F:335:LYS:HG3	1.67	0.75
1:C:287:LEU:HD11	1:C:335:LYS:HG3	1.66	0.75
1:D:282:GLU:C	1:D:523:PHE:CG	2.37	0.75
1:A:446:MET:HG3	1:A:492:LEU:HB3	1.69	0.75
1:A:292:CYS:O	1:A:295:ILE:HD13	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:CE	1:A:504:ARG:H	2.00	0.74
1:B:324:GLN:HE22	1:B:542:LEU:H	1.32	0.73
1:D:446:MET:HG3	1:D:492:LEU:HB3	1.70	0.73
1:D:316:MET:HE3	1:D:504:ARG:H	1.53	0.73
1:E:324:GLN:HE22	1:E:542:LEU:H	1.34	0.73
1:A:290:SER:N	1:A:325:GLN:NE2	2.34	0.73
1:A:514:VAL:HG13	1:A:533:MET:HB2	1.70	0.73
1:D:272:ARG:HG2	1:D:273:GLU:N	2.02	0.73
1:D:289:PHE:H	1:D:296:ASN:HD21	1.34	0.73
1:A:465:HIS:O	1:A:487:ARG:HB2	1.87	0.73
1:B:470:ASP:OD2	1:C:467:LYS:NZ	2.23	0.72
1:E:309:MET:HE3	1:E:462:VAL:O	1.88	0.72
1:E:489:SER:O	1:E:491:ALA:N	2.23	0.72
1:C:404:ARG:HH12	1:C:408:LYS:CE	2.03	0.72
1:B:290:SER:H	1:B:325:GLN:HE22	1.37	0.72
1:B:431:SER:HB3	1:B:441:MET:CE	2.21	0.71
1:B:489:SER:O	1:B:491:ALA:N	2.23	0.71
1:C:429:VAL:HG23	1:C:430:VAL:N	2.05	0.71
1:E:431:SER:HB3	1:E:441:MET:CE	2.21	0.71
1:F:404:ARG:HH12	1:F:408:LYS:HE3	1.56	0.71
1:E:426:ILE:O	1:E:426:ILE:HG12	1.91	0.70
1:A:476:GLU:HG3	1:B:483:ILE:HD12	1.73	0.70
1:F:404:ARG:HH12	1:F:408:LYS:CE	2.04	0.70
1:C:475:HIS:HB2	1:C:476:GLU:OE2	1.92	0.70
1:E:290:SER:N	1:E:325:GLN:NE2	2.31	0.70
1:F:429:VAL:HG23	1:F:430:VAL:N	2.07	0.70
1:F:290:SER:N	1:F:325:GLN:NE2	2.38	0.70
1:F:516:VAL:HG21	1:F:533:MET:CE	2.21	0.70
1:C:290:SER:N	1:C:325:GLN:NE2	2.37	0.70
1:C:404:ARG:HH12	1:C:408:LYS:HE3	1.55	0.69
1:F:475:HIS:HB2	1:F:476:GLU:OE2	1.92	0.69
1:C:444:ASN:OD1	1:C:448:LYS:HE2	1.93	0.69
1:B:316:MET:CE	1:B:503:GLU:HA	2.23	0.69
1:B:271:LEU:CD2	1:B:274:ARG:HH21	2.06	0.69
1:D:480:PRO:HA	1:D:503:GLU:CD	2.14	0.69
1:D:329:TRP:HZ3	1:D:420:VAL:HG11	1.57	0.68
1:D:316:MET:CE	1:D:504:ARG:H	2.05	0.68
1:B:309:MET:HE3	1:B:462:VAL:O	1.93	0.68
1:C:516:VAL:HG21	1:C:533:MET:CE	2.23	0.68
1:D:292:CYS:O	1:D:295:ILE:HD13	1.94	0.68
1:E:275:ILE:O	1:E:278:HIS:HB3	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:401:GLU:HB3	1:F:404:ARG:HB2	1.74	0.68
1:E:367:SER:HA	1:E:370:ARG:NH1	2.08	0.68
1:E:316:MET:CE	1:E:503:GLU:HA	2.23	0.68
1:C:284:SER:HB2	1:C:523:PHE:CZ	2.29	0.68
1:E:444:ASN:OD1	1:E:448:LYS:HE2	1.93	0.68
1:F:444:ASN:OD1	1:F:448:LYS:HE2	1.94	0.68
1:B:271:LEU:HD21	1:B:274:ARG:HH21	1.59	0.68
1:C:399:GLU:HB3	1:C:430:VAL:HG11	1.75	0.68
1:E:345:SER:O	1:E:349:THR:HG23	1.92	0.68
1:C:438:GLU:HA	1:C:441:MET:HG2	1.76	0.68
1:B:367:SER:HA	1:B:370:ARG:NH1	2.09	0.67
1:C:401:GLU:HB3	1:C:404:ARG:HB2	1.75	0.67
1:C:516:VAL:HG21	1:C:533:MET:HE3	1.75	0.67
1:D:282:GLU:CD	1:D:523:PHE:HA	2.14	0.67
1:D:282:GLU:HG3	1:D:282:GLU:O	1.94	0.67
1:F:336:LYS:HB3	1:F:418:CYS:HA	1.76	0.67
1:F:375:ASN:HD21	1:F:377:LYS:CB	2.04	0.67
1:F:438:GLU:HA	1:F:441:MET:HG2	1.77	0.67
1:C:476:GLU:H	1:C:476:GLU:CD	1.98	0.67
1:D:401:GLU:HA	1:D:430:VAL:O	1.95	0.67
1:F:401:GLU:HA	1:F:430:VAL:O	1.94	0.67
1:E:406:LEU:HD21	1:E:448:LYS:HB3	1.75	0.67
1:F:344:GLU:CG	1:F:349:THR:HG22	2.23	0.67
1:F:452:PHE:CE1	1:F:456:THR:HG21	2.30	0.67
1:C:401:GLU:HA	1:C:430:VAL:O	1.94	0.67
1:F:399:GLU:HB3	1:F:430:VAL:HG11	1.77	0.67
1:C:284:SER:HB2	1:C:523:PHE:HZ	1.59	0.67
1:E:284:SER:HB2	1:E:523:PHE:HZ	1.60	0.66
1:D:402:THR:HG23	1:D:445:LEU:HD13	1.78	0.66
1:E:450:LYS:HD3	1:E:495:LEU:O	1.96	0.66
1:B:534:GLU:HG3	1:B:545:SER:HB2	1.77	0.66
1:C:294:GLY:HA2	1:C:297:ASP:HB2	1.77	0.66
1:B:444:ASN:OD1	1:B:448:LYS:HE2	1.95	0.66
1:E:331:THR:HG22	1:E:332:ALA:N	2.11	0.66
1:C:375:ASN:HD21	1:C:377:LYS:CB	2.07	0.66
1:E:344:GLU:HB2	1:E:348:GLU:OE1	1.95	0.66
1:F:476:GLU:CD	1:F:476:GLU:H	1.98	0.66
1:F:481:VAL:HG12	1:F:503:GLU:HG2	1.78	0.66
1:B:426:ILE:O	1:B:426:ILE:HG12	1.95	0.65
1:C:288:LEU:H	1:C:288:LEU:HD12	1.62	0.65
1:D:477:GLU:CA	1:D:505:ASN:HD22	1.99	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LEU:HD21	1:B:448:LYS:HB3	1.76	0.65
1:A:437:ASP:C	1:A:439:ARG:H	2.00	0.65
1:D:476:GLU:HG3	1:E:483:ILE:HD12	1.77	0.65
1:E:327:LEU:HD21	1:E:357:HIS:HA	1.79	0.65
1:A:480:PRO:HA	1:A:503:GLU:CD	2.16	0.65
1:C:481:VAL:HG12	1:C:503:GLU:HG2	1.78	0.65
1:D:402:THR:HG21	1:D:448:LYS:NZ	2.12	0.65
1:D:437:ASP:C	1:D:439:ARG:H	2.00	0.65
1:C:290:SER:N	1:C:325:GLN:HE21	1.93	0.65
1:D:300:LEU:HD12	1:D:524:THR:HG21	1.78	0.65
1:F:294:GLY:HA2	1:F:297:ASP:HB2	1.78	0.65
1:B:331:THR:HG22	1:B:332:ALA:N	2.11	0.64
1:D:476:GLU:O	1:D:506:GLN:HG2	1.97	0.64
1:C:336:LYS:HB3	1:C:418:CYS:HA	1.79	0.64
1:B:290:SER:N	1:B:325:GLN:HE22	1.94	0.64
1:D:524:THR:C	1:D:526:ASP:H	2.00	0.64
1:A:401:GLU:HA	1:A:430:VAL:O	1.96	0.64
1:A:476:GLU:O	1:A:506:GLN:HG2	1.97	0.64
1:E:534:GLU:HG3	1:E:545:SER:HB2	1.78	0.64
1:B:481:VAL:HG11	1:B:501:ALA:HB1	1.78	0.64
1:D:372:ILE:HG21	1:D:381:TRP:CZ3	2.33	0.64
1:E:467:LYS:HE3	1:E:486:LEU:O	1.98	0.64
1:A:402:THR:HG23	1:A:445:LEU:HD13	1.80	0.64
1:E:358:ASN:O	1:E:360:VAL:HG22	1.98	0.64
1:F:344:GLU:HG3	1:F:349:THR:CG2	2.24	0.64
1:B:450:LYS:HD3	1:B:495:LEU:O	1.99	0.63
1:B:309:MET:HB3	1:B:499:ILE:HA	1.80	0.63
1:E:481:VAL:HG11	1:E:501:ALA:HB1	1.78	0.63
1:A:524:THR:C	1:A:526:ASP:H	2.02	0.63
1:D:394:TYR:CE1	1:D:408:LYS:HD2	2.34	0.63
1:B:411:TYR:O	1:B:415:GLY:N	2.31	0.63
1:E:394:TYR:CE2	1:E:408:LYS:HD2	2.34	0.63
1:A:329:TRP:HZ3	1:A:420:VAL:HG11	1.60	0.63
1:B:347:GLU:OE1	1:C:274:ARG:HD2	1.97	0.63
1:B:465:HIS:O	1:B:487:ARG:HB2	1.99	0.63
1:C:344:GLU:CG	1:C:349:THR:HG22	2.23	0.63
1:C:375:ASN:ND2	1:C:377:LYS:HB2	2.12	0.63
1:E:316:MET:HG2	1:E:504:ARG:HH11	1.64	0.63
1:A:280:SER:O	1:A:281:SER:HB2	1.99	0.62
1:B:316:MET:HG2	1:B:504:ARG:HG2	1.80	0.62
1:B:316:MET:HG2	1:B:504:ARG:HH11	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:TYR:CE1	1:A:408:LYS:HD2	2.34	0.62
1:E:470:ASP:OD2	1:F:467:LYS:NZ	2.33	0.62
1:A:309:MET:HB3	1:A:499:ILE:HG12	1.82	0.62
1:C:425:HIS:HE1	1:C:427:SER:HB2	1.63	0.62
1:B:345:SER:O	1:B:349:THR:HG23	1.99	0.62
1:C:452:PHE:CE1	1:C:456:THR:HG21	2.34	0.62
1:E:309:MET:HB3	1:E:499:ILE:HA	1.81	0.62
1:F:425:HIS:HE1	1:F:427:SER:HB2	1.64	0.62
1:A:477:GLU:CA	1:A:505:ASN:HD22	2.01	0.62
1:A:518:ILE:N	1:A:518:ILE:HD12	2.15	0.62
1:B:468:ASN:HD21	1:C:493:ARG:CZ	2.11	0.62
1:F:290:SER:N	1:F:325:GLN:HE21	1.96	0.62
1:D:280:SER:O	1:D:281:SER:HB2	2.00	0.62
1:D:290:SER:N	1:D:325:GLN:HE22	1.93	0.62
1:B:273:GLU:OE2	1:B:276:ARG:NH1	2.32	0.62
1:B:394:TYR:CE2	1:B:408:LYS:HD2	2.35	0.62
1:E:466:LEU:HD21	1:E:486:LEU:HD23	1.81	0.62
1:D:347:GLU:OE1	1:E:274:ARG:HB3	1.99	0.62
1:D:476:GLU:OE1	1:D:476:GLU:N	2.34	0.61
1:D:327:LEU:HD22	1:D:356:LEU:HG	1.82	0.61
1:E:294:GLY:HA2	1:E:297:ASP:HB2	1.82	0.61
1:E:536:ASN:C	1:E:536:ASN:HD22	2.02	0.61
1:F:467:LYS:HE3	1:F:486:LEU:O	2.00	0.61
1:B:344:GLU:HB2	1:B:348:GLU:OE1	1.99	0.61
1:E:465:HIS:O	1:E:487:ARG:HB2	2.00	0.61
1:F:375:ASN:ND2	1:F:377:LYS:HB2	2.10	0.61
1:F:402:THR:HG23	1:F:445:LEU:CD1	2.27	0.61
1:A:290:SER:N	1:A:325:GLN:HE22	1.88	0.61
1:B:358:ASN:O	1:B:360:VAL:HG22	2.01	0.61
1:D:309:MET:HB3	1:D:499:ILE:HG12	1.82	0.61
1:C:467:LYS:HE3	1:C:486:LEU:O	1.99	0.61
1:D:311:THR:HG21	1:D:486:LEU:HD21	1.83	0.61
1:E:411:TYR:O	1:E:415:GLY:N	2.32	0.61
1:B:327:LEU:HD21	1:B:357:HIS:HA	1.81	0.61
1:C:344:GLU:HG3	1:C:349:THR:CG2	2.24	0.61
1:A:422:ILE:HD13	1:A:461:VAL:HB	1.82	0.60
1:A:311:THR:HG21	1:A:486:LEU:HD21	1.83	0.60
1:A:300:LEU:HD12	1:A:524:THR:HG21	1.81	0.60
1:E:394:TYR:CD2	1:E:408:LYS:HD2	2.36	0.60
1:F:320:THR:HG22	1:F:324:GLN:NE2	2.16	0.60
1:A:372:ILE:HG21	1:A:381:TRP:CZ3	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:THR:HG21	1:A:448:LYS:NZ	2.16	0.60
1:E:292:CYS:HB3	1:E:295:ILE:CD1	2.30	0.60
1:F:284:SER:O	1:F:303:ARG:HD2	2.00	0.60
1:B:466:LEU:HD21	1:B:486:LEU:HD23	1.81	0.60
1:B:285:VAL:HG12	1:B:286:GLY:N	2.17	0.60
1:F:312:SER:OG	1:F:318:LYS:HG3	2.00	0.60
1:A:372:ILE:HD13	1:A:381:TRP:CZ3	2.36	0.60
1:D:524:THR:O	1:D:526:ASP:N	2.34	0.60
1:E:316:MET:HE2	1:E:502:LEU:O	2.02	0.60
1:A:476:GLU:OE1	1:A:476:GLU:N	2.34	0.60
1:C:278:HIS:O	1:C:282:GLU:CB	2.49	0.60
1:E:316:MET:HG2	1:E:504:ARG:HG2	1.84	0.60
1:A:350:ALA:HB1	1:B:275:ILE:HD11	1.84	0.60
1:B:371:GLU:O	1:B:373:ILE:N	2.34	0.60
1:C:344:GLU:OE2	1:C:349:THR:HB	2.01	0.60
1:C:484:THR:HA	1:C:493:ARG:NH2	2.16	0.60
1:D:329:TRP:CE3	1:D:420:VAL:HG11	2.36	0.60
1:D:367:SER:O	1:D:371:GLU:HG2	2.01	0.60
1:F:295:ILE:HD11	1:F:516:VAL:HG11	1.84	0.60
1:D:466:LEU:HD13	1:D:475:HIS:CE1	2.37	0.60
1:E:371:GLU:O	1:E:373:ILE:N	2.34	0.60
1:C:312:SER:OG	1:C:318:LYS:HG3	2.01	0.59
1:B:402:THR:HG21	1:B:448:LYS:NZ	2.17	0.59
1:D:394:TYR:HE1	1:D:408:LYS:HD2	1.67	0.59
1:D:518:ILE:HD12	1:D:518:ILE:N	2.16	0.59
1:E:408:LYS:O	1:E:411:TYR:HB3	2.02	0.59
1:A:329:TRP:CE3	1:A:420:VAL:HG11	2.37	0.59
1:D:372:ILE:HD13	1:D:381:TRP:CZ3	2.37	0.59
1:A:515:LEU:C	1:A:515:LEU:HD23	2.23	0.59
1:B:344:GLU:CG	1:B:349:THR:HG22	2.32	0.59
1:E:366:ASP:OD1	1:F:284:SER:HB3	2.02	0.59
1:E:446:MET:SD	1:E:492:LEU:HB3	2.42	0.59
1:E:478:GLY:O	1:E:479:ARG:CB	2.49	0.59
1:B:294:GLY:HA2	1:B:297:ASP:HB2	1.85	0.59
1:B:288:LEU:HB3	1:B:296:ASN:OD1	2.03	0.59
1:C:404:ARG:HH12	1:C:408:LYS:NZ	2.01	0.59
1:D:512:ASN:O	1:D:534:GLU:HA	2.02	0.59
1:A:305:GLY:HA2	1:A:453:ALA:O	2.02	0.59
1:D:422:ILE:HD13	1:D:461:VAL:HB	1.84	0.59
1:B:370:ARG:HB3	1:B:370:ARG:HH11	1.67	0.59
1:B:477:GLU:OE2	1:C:482:SER:HB2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:LEU:O	1:E:409:LEU:HG	2.03	0.59
1:A:395:ASP:O	1:A:396:SER:HB2	2.02	0.59
1:B:467:LYS:HE3	1:B:486:LEU:O	2.02	0.59
1:E:370:ARG:HB3	1:E:370:ARG:HH11	1.67	0.59
1:F:336:LYS:CB	1:F:418:CYS:HA	2.32	0.59
1:F:484:THR:HA	1:F:493:ARG:NH2	2.17	0.59
1:A:479:ARG:HG2	1:A:479:ARG:O	2.02	0.59
1:B:316:MET:HE2	1:B:502:LEU:O	2.03	0.59
1:E:402:THR:HG21	1:E:448:LYS:NZ	2.17	0.59
1:F:404:ARG:HH12	1:F:408:LYS:NZ	2.00	0.59
1:A:524:THR:O	1:A:526:ASP:N	2.36	0.58
1:B:394:TYR:CD2	1:B:408:LYS:HD2	2.37	0.58
1:A:488:GLY:O	1:A:490:GLY:N	2.36	0.58
1:A:352:ASP:O	1:A:356:LEU:HB2	2.03	0.58
1:D:316:MET:CE	1:D:503:GLU:HA	2.34	0.58
1:E:365:SER:O	1:E:369:LYS:HG3	2.04	0.58
1:A:475:HIS:H	1:A:479:ARG:HD2	1.69	0.58
1:B:466:LEU:CD2	1:B:486:LEU:HD23	2.33	0.58
1:D:352:ASP:O	1:D:356:LEU:HB2	2.03	0.58
1:D:536:ASN:O	1:D:538:GLU:N	2.36	0.58
1:A:340:ALA:H	1:A:341:MET:HE3	1.69	0.58
1:A:367:SER:O	1:A:371:GLU:HG2	2.04	0.58
1:C:393:LEU:HD12	1:C:393:LEU:N	2.19	0.58
1:D:340:ALA:H	1:D:341:MET:HE3	1.69	0.58
1:D:340:ALA:N	1:D:341:MET:HE3	2.19	0.58
1:D:515:LEU:HD23	1:D:515:LEU:C	2.23	0.58
1:B:478:GLY:O	1:B:479:ARG:CB	2.49	0.58
1:E:466:LEU:CD2	1:E:486:LEU:HD23	2.33	0.58
1:A:340:ALA:N	1:A:341:MET:HE3	2.19	0.58
1:D:290:SER:N	1:D:325:GLN:NE2	2.37	0.58
1:A:399:GLU:HB3	1:A:430:VAL:HG21	1.86	0.57
1:B:408:LYS:O	1:B:411:TYR:HB3	2.03	0.57
1:B:493:ARG:HG3	1:B:493:ARG:O	2.04	0.57
1:D:395:ASP:O	1:D:396:SER:HB2	2.03	0.57
1:D:399:GLU:HB3	1:D:430:VAL:HG21	1.86	0.57
1:E:266:VAL:HG11	1:E:271:LEU:HD21	1.85	0.57
1:E:344:GLU:CG	1:E:349:THR:HG22	2.32	0.57
1:E:536:ASN:ND2	1:E:538:GLU:H	2.02	0.57
1:B:405:LEU:O	1:B:409:LEU:HG	2.04	0.57
1:C:371:GLU:O	1:C:374:GLU:N	2.36	0.57
1:C:458:VAL:HG22	1:C:459:VAL:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:425:HIS:H	1:D:463:ILE:HB	1.69	0.57
1:A:536:ASN:O	1:A:538:GLU:N	2.37	0.57
1:F:394:TYR:CE1	1:F:408:LYS:HD2	2.39	0.57
1:A:316:MET:HE3	1:A:504:ARG:N	2.18	0.57
1:A:327:LEU:HD22	1:A:356:LEU:HG	1.84	0.57
1:A:466:LEU:HD13	1:A:475:HIS:CE1	2.40	0.57
1:F:343:GLU:C	1:F:397:PHE:HE1	2.07	0.57
1:F:476:GLU:N	1:F:476:GLU:CD	2.57	0.57
1:A:394:TYR:HE1	1:A:408:LYS:HD2	1.68	0.57
1:A:425:HIS:H	1:A:463:ILE:HB	1.70	0.57
1:C:292:CYS:SG	1:C:295:ILE:CD1	2.92	0.57
1:D:282:GLU:N	1:D:523:PHE:CE2	2.72	0.57
1:E:273:GLU:OE2	1:E:276:ARG:NH1	2.37	0.57
1:E:351:GLU:OE1	1:F:278:HIS:NE2	2.37	0.57
1:B:292:CYS:HB3	1:B:295:ILE:CD1	2.35	0.57
1:F:345:SER:OG	1:F:348:GLU:HB2	2.04	0.57
1:B:278:HIS:O	1:B:280:SER:N	2.38	0.57
1:D:488:GLY:O	1:D:490:GLY:N	2.37	0.57
1:F:443:ASP:O	1:F:447:THR:HG23	2.05	0.57
1:F:446:MET:SD	1:F:492:LEU:HB3	2.44	0.57
1:B:285:VAL:HG22	1:B:300:LEU:HD22	1.86	0.56
1:C:476:GLU:CD	1:C:476:GLU:N	2.57	0.56
1:D:412:MET:HE3	1:D:421:ILE:HG23	1.87	0.56
1:D:475:HIS:H	1:D:479:ARG:HD2	1.69	0.56
1:B:446:MET:SD	1:B:492:LEU:HB3	2.45	0.56
1:D:312:SER:HB2	1:D:502:LEU:O	2.05	0.56
1:D:506:GLN:HB2	1:E:527:THR:OG1	2.04	0.56
1:A:489:SER:O	1:A:491:ALA:N	2.37	0.56
1:B:536:ASN:HD22	1:B:536:ASN:C	2.07	0.56
1:C:266:VAL:CG1	1:C:271:LEU:HD21	2.35	0.56
1:D:283:GLU:HB2	1:D:523:PHE:CE2	2.40	0.56
1:E:289:PHE:H	1:E:296:ASN:HD21	1.52	0.56
1:A:283:GLU:HB3	1:A:303:ARG:HG2	1.88	0.56
1:B:440:LYS:HZ2	1:B:444:ASN:ND2	1.98	0.56
1:C:509:ASP:C	1:C:511:PRO:HD3	2.25	0.56
1:F:371:GLU:O	1:F:374:GLU:N	2.37	0.56
1:A:412:MET:HE3	1:A:421:ILE:HG23	1.86	0.56
1:A:429:VAL:HG23	1:A:430:VAL:N	2.16	0.56
1:B:395:ASP:O	1:B:396:SER:HB2	2.06	0.56
1:C:372:ILE:HA	1:C:375:ASN:OD1	2.06	0.56
1:D:479:ARG:O	1:D:479:ARG:HG2	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:ILE:HA	1:E:375:ASN:OD1	2.06	0.56
1:E:399:GLU:HB3	1:E:430:VAL:HG11	1.88	0.56
1:D:489:SER:O	1:D:491:ALA:N	2.38	0.56
1:D:480:PRO:HB3	1:D:517:ARG:NH2	2.20	0.56
1:F:320:THR:CG2	1:F:324:GLN:HE21	2.18	0.56
1:F:422:ILE:HD13	1:F:461:VAL:HB	1.87	0.56
1:C:402:THR:HG23	1:C:445:LEU:CD1	2.29	0.56
1:D:288:LEU:HB3	1:D:296:ASN:OD1	2.05	0.56
1:D:305:GLY:HA2	1:D:453:ALA:O	2.06	0.56
1:D:509:ASP:C	1:D:511:PRO:HD3	2.26	0.56
1:E:477:GLU:CA	1:E:505:ASN:HD22	2.18	0.56
1:B:509:ASP:C	1:B:511:PRO:HD3	2.25	0.56
1:C:345:SER:OG	1:C:348:GLU:HB2	2.06	0.56
1:B:436:SER:O	1:B:437:ASP:O	2.23	0.56
1:E:436:SER:O	1:E:437:ASP:O	2.24	0.56
1:E:316:MET:HE3	1:E:504:ARG:N	2.21	0.56
1:F:290:SER:H	1:F:325:GLN:HE22	1.50	0.55
1:F:344:GLU:OE2	1:F:349:THR:HB	2.06	0.55
1:F:518:ILE:HD13	1:F:530:ALA:CB	2.34	0.55
1:C:394:TYR:CE1	1:C:408:LYS:HD2	2.41	0.55
1:F:327:LEU:HD22	1:F:356:LEU:HD23	1.87	0.55
1:B:483:ILE:HG21	1:B:493:ARG:HD3	1.88	0.55
1:D:375:ASN:ND2	1:D:377:LYS:HG3	2.19	0.55
1:A:316:MET:CE	1:A:503:GLU:HA	2.37	0.55
1:B:375:ASN:HD21	1:B:377:LYS:HD2	1.72	0.55
1:B:536:ASN:ND2	1:B:538:GLU:H	2.05	0.55
1:C:426:ILE:O	1:C:426:ILE:HG12	2.06	0.55
1:E:375:ASN:HD21	1:E:377:LYS:HD2	1.72	0.55
1:E:413:ARG:CD	1:E:458:VAL:HB	2.37	0.55
1:E:484:THR:HA	1:E:493:ARG:NH2	2.21	0.55
1:F:426:ILE:O	1:F:426:ILE:HG12	2.07	0.55
1:A:480:PRO:HB3	1:A:517:ARG:NH2	2.21	0.55
1:A:303:ARG:NH2	1:A:523:PHE:CB	2.69	0.55
1:D:294:GLY:HA2	1:D:297:ASP:HB2	1.88	0.55
1:E:290:SER:N	1:E:325:GLN:HE22	1.99	0.55
1:F:372:ILE:HA	1:F:375:ASN:OD1	2.07	0.55
1:A:316:MET:CE	1:A:504:ARG:N	2.70	0.55
1:C:336:LYS:CB	1:C:418:CYS:HA	2.37	0.55
1:D:442:ILE:HG23	1:D:443:ASP:N	2.22	0.55
1:E:352:ASP:OD2	1:E:363:ARG:NH2	2.39	0.55
1:F:393:LEU:HD12	1:F:393:LEU:N	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ALA:CB	1:B:275:ILE:HD11	2.37	0.55
1:B:316:MET:HE3	1:B:504:ARG:N	2.22	0.55
1:B:372:ILE:HA	1:B:375:ASN:OD1	2.07	0.55
1:B:477:GLU:CA	1:B:505:ASN:HD22	2.17	0.55
1:E:360:VAL:HG11	1:E:368:LEU:HD11	1.89	0.55
1:D:440:LYS:O	1:D:440:LYS:HD3	2.07	0.55
1:E:493:ARG:HG3	1:E:493:ARG:O	2.06	0.55
1:F:320:THR:CG2	1:F:324:GLN:NE2	2.69	0.55
1:F:458:VAL:HG22	1:F:459:VAL:N	2.22	0.55
1:B:365:SER:O	1:B:369:LYS:HG3	2.07	0.55
1:B:413:ARG:CD	1:B:458:VAL:HB	2.37	0.55
1:C:429:VAL:CG2	1:C:430:VAL:H	2.16	0.55
1:D:386:PHE:CD1	1:E:268:ALA:HB1	2.42	0.55
1:D:429:VAL:HG23	1:D:430:VAL:N	2.19	0.55
1:E:483:ILE:HG21	1:E:493:ARG:HD3	1.89	0.55
1:F:509:ASP:C	1:F:511:PRO:HD3	2.26	0.55
1:A:509:ASP:C	1:A:511:PRO:HD3	2.27	0.54
1:B:400:ALA:O	1:B:430:VAL:HB	2.07	0.54
1:C:295:ILE:HD11	1:C:516:VAL:HG11	1.87	0.54
1:C:343:GLU:C	1:C:397:PHE:HE1	2.10	0.54
1:F:429:VAL:CG2	1:F:430:VAL:H	2.17	0.54
1:A:375:ASN:ND2	1:A:377:LYS:HG3	2.19	0.54
1:F:292:CYS:SG	1:F:295:ILE:CD1	2.95	0.54
1:C:370:ARG:O	1:C:374:GLU:HG3	2.07	0.54
1:C:449:LEU:HD22	1:C:460:LEU:HD21	1.90	0.54
1:D:303:ARG:NH2	1:D:523:PHE:CB	2.70	0.54
1:D:282:GLU:CA	1:D:523:PHE:CD2	2.87	0.54
1:E:395:ASP:O	1:E:396:SER:HB2	2.07	0.54
1:E:307:VAL:HB	1:E:496:SER:HA	1.88	0.54
1:E:401:GLU:HA	1:E:430:VAL:O	2.08	0.54
1:A:512:ASN:O	1:A:534:GLU:HA	2.08	0.54
1:B:370:ARG:CB	1:B:370:ARG:NH1	2.71	0.54
1:C:282:GLU:O	1:C:282:GLU:HG3	2.07	0.54
1:E:509:ASP:C	1:E:511:PRO:HD3	2.28	0.54
1:A:401:GLU:HB3	1:A:404:ARG:HB2	1.90	0.54
1:C:516:VAL:CG2	1:C:533:MET:HE3	2.37	0.54
1:A:438:GLU:HA	1:A:441:MET:HG2	1.90	0.54
1:B:413:ARG:HD3	1:B:458:VAL:HB	1.90	0.54
1:E:471:LYS:O	1:E:471:LYS:HD3	2.07	0.54
1:D:343:GLU:HG3	1:D:428:ILE:HD11	1.90	0.53
1:E:400:ALA:O	1:E:430:VAL:HB	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:THR:HG22	1:C:324:GLN:NE2	2.24	0.53
1:C:405:LEU:O	1:C:406:LEU:C	2.46	0.53
1:E:393:LEU:CD1	1:E:393:LEU:N	2.63	0.53
1:E:467:LYS:HG3	1:E:487:ARG:HA	1.90	0.53
1:E:346:VAL:HB	1:E:393:LEU:HD22	1.91	0.53
1:B:399:GLU:HB3	1:B:430:VAL:HG21	1.89	0.53
1:C:405:LEU:O	1:C:407:ALA:N	2.41	0.53
1:C:443:ASP:O	1:C:447:THR:HG23	2.07	0.53
1:D:272:ARG:CG	1:D:273:GLU:N	2.72	0.53
1:F:331:THR:HG22	1:F:332:ALA:N	2.24	0.53
1:F:452:PHE:HE1	1:F:456:THR:HG21	1.74	0.53
1:B:307:VAL:HB	1:B:496:SER:HA	1.90	0.53
1:B:399:GLU:HB3	1:B:430:VAL:HG11	1.91	0.53
1:D:524:THR:OG1	1:D:526:ASP:HB3	2.09	0.53
1:A:442:ILE:HG23	1:A:443:ASP:N	2.23	0.53
1:C:345:SER:O	1:C:349:THR:HG23	2.09	0.53
1:D:283:GLU:CB	1:D:523:PHE:CZ	2.92	0.53
1:E:370:ARG:NH1	1:E:370:ARG:CB	2.72	0.53
1:A:343:GLU:HG3	1:A:428:ILE:HD11	1.90	0.53
1:B:471:LYS:O	1:B:471:LYS:HD3	2.08	0.53
1:D:316:MET:HE3	1:D:504:ARG:N	2.21	0.53
1:D:507:GLN:NE2	1:E:528:GLY:HA2	2.23	0.53
1:A:440:LYS:HD3	1:A:440:LYS:O	2.08	0.53
1:E:370:ARG:CB	1:E:370:ARG:HH11	2.22	0.53
1:B:392:HIS:C	1:B:393:LEU:HD12	2.29	0.52
1:C:422:ILE:HD13	1:C:461:VAL:HB	1.90	0.52
1:D:514:VAL:CG1	1:D:533:MET:HB2	2.38	0.52
1:F:345:SER:O	1:F:349:THR:HG23	2.09	0.52
1:A:312:SER:HB2	1:A:502:LEU:O	2.10	0.52
1:B:370:ARG:CB	1:B:370:ARG:HH11	2.21	0.52
1:B:404:ARG:O	1:B:408:LYS:HG3	2.09	0.52
1:E:317:GLY:O	1:E:318:LYS:C	2.48	0.52
1:E:413:ARG:HD3	1:E:458:VAL:HB	1.90	0.52
1:E:399:GLU:HB3	1:E:430:VAL:HG21	1.90	0.52
1:F:401:GLU:O	1:F:404:ARG:HB3	2.09	0.52
1:B:440:LYS:NZ	1:B:444:ASN:ND2	2.54	0.52
1:D:327:LEU:CD2	1:D:356:LEU:HG	2.38	0.52
1:D:401:GLU:HB3	1:D:404:ARG:HB2	1.91	0.52
1:D:438:GLU:HA	1:D:441:MET:HG2	1.91	0.52
1:B:352:ASP:OD2	1:B:363:ARG:NH2	2.40	0.52
1:A:379:ASP:OD1	1:B:276:ARG:NH2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:THR:HG22	1:C:332:ALA:N	2.25	0.52
1:D:283:GLU:O	1:D:303:ARG:NH1	2.43	0.52
1:F:449:LEU:HD22	1:F:460:LEU:HD21	1.91	0.52
1:B:499:ILE:HB	1:B:519:LEU:HB3	1.92	0.52
1:B:303:ARG:O	1:B:306:GLU:HB2	2.09	0.52
1:D:282:GLU:HA	1:D:523:PHE:CD2	2.44	0.52
1:D:372:ILE:HG21	1:D:381:TRP:CH2	2.44	0.52
1:F:489:SER:O	1:F:491:ALA:N	2.43	0.52
1:A:288:LEU:CD1	1:A:288:LEU:N	2.70	0.52
1:A:294:GLY:HA2	1:A:297:ASP:HB2	1.92	0.52
1:B:401:GLU:HA	1:B:430:VAL:O	2.09	0.52
1:C:446:MET:SD	1:C:492:LEU:HB3	2.50	0.52
1:D:375:ASN:ND2	1:D:375:ASN:O	2.43	0.52
1:D:412:MET:HE3	1:D:421:ILE:HD12	1.92	0.52
1:B:484:THR:HA	1:B:493:ARG:NH2	2.25	0.52
1:B:536:ASN:HD21	1:B:538:GLU:HB2	1.75	0.52
1:D:524:THR:C	1:D:526:ASP:N	2.64	0.52
1:E:303:ARG:O	1:E:306:GLU:HB2	2.10	0.52
1:B:467:LYS:HG3	1:B:487:ARG:HA	1.91	0.51
1:D:490:GLY:O	1:D:493:ARG:HG2	2.10	0.51
1:E:499:ILE:HB	1:E:519:LEU:HB3	1.92	0.51
1:E:536:ASN:HD21	1:E:538:GLU:HB2	1.75	0.51
1:B:360:VAL:HG11	1:B:368:LEU:HD11	1.92	0.51
1:B:396:SER:O	1:B:397:PHE:CB	2.59	0.51
1:B:324:GLN:NE2	1:B:542:LEU:H	2.07	0.51
1:C:515:LEU:HD12	1:C:532:TYR:CE2	2.45	0.51
1:F:287:LEU:CD1	1:F:335:LYS:HE3	2.40	0.51
1:A:282:GLU:HG3	1:A:282:GLU:O	2.11	0.51
1:C:404:ARG:HH12	1:C:408:LYS:HZ2	1.59	0.51
1:C:517:ARG:HD2	1:C:519:LEU:HD11	1.92	0.51
1:E:518:ILE:HG22	1:E:527:THR:HA	1.92	0.51
1:B:351:GLU:OE1	1:C:278:HIS:NE2	2.42	0.51
1:C:327:LEU:HD22	1:C:356:LEU:HD23	1.90	0.51
1:C:492:LEU:HD12	1:C:492:LEU:H	1.76	0.51
1:E:442:ILE:HG23	1:E:443:ASP:N	2.26	0.51
1:B:492:LEU:C	1:B:494:GLN:H	2.14	0.51
1:C:489:SER:O	1:C:491:ALA:N	2.43	0.51
1:C:480:PRO:HA	1:C:503:GLU:CD	2.31	0.51
1:E:404:ARG:O	1:E:408:LYS:HG3	2.11	0.51
1:F:395:ASP:O	1:F:396:SER:HB2	2.10	0.51
1:A:504:ARG:NE	1:A:511:PRO:O	2.33	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:LEU:HD21	1:B:274:ARG:NH2	2.24	0.51
1:A:333:MET:O	1:A:335:LYS:HG2	2.10	0.51
1:A:510:MET:HB3	1:A:513:LEU:HB2	1.93	0.51
1:C:288:LEU:HB3	1:C:296:ASN:CG	2.31	0.51
1:A:524:THR:OG1	1:A:526:ASP:HB3	2.10	0.51
1:C:371:GLU:O	1:C:373:ILE:N	2.44	0.51
1:F:394:TYR:HE1	1:F:408:LYS:HD2	1.75	0.51
1:F:359:ARG:NH1	1:F:541:TRP:CE2	2.79	0.51
1:C:288:LEU:HB3	1:C:296:ASN:OD1	2.10	0.51
1:E:536:ASN:C	1:E:536:ASN:ND2	2.63	0.51
1:F:370:ARG:O	1:F:374:GLU:HG3	2.10	0.51
1:F:492:LEU:HD12	1:F:492:LEU:H	1.75	0.51
1:A:412:MET:HE3	1:A:421:ILE:HD12	1.94	0.50
1:B:317:GLY:O	1:B:318:LYS:C	2.48	0.50
1:B:370:ARG:HB2	1:B:370:ARG:NH1	2.26	0.50
1:D:536:ASN:C	1:D:538:GLU:N	2.65	0.50
1:E:284:SER:HB2	1:E:523:PHE:CZ	2.43	0.50
1:F:411:TYR:CE1	1:F:415:GLY:HA3	2.46	0.50
1:F:406:LEU:CD2	1:F:448:LYS:HB3	2.28	0.50
1:A:265:VAL:HG12	1:A:265:VAL:O	2.11	0.50
1:A:399:GLU:HB3	1:A:430:VAL:HG11	1.94	0.50
1:A:521:CYS:O	1:A:525:GLY:N	2.41	0.50
1:B:431:SER:HB3	1:B:441:MET:HE3	1.93	0.50
1:C:288:LEU:HA	1:C:296:ASN:HD21	1.75	0.50
1:D:283:GLU:CD	1:D:303:ARG:HD2	2.32	0.50
1:F:517:ARG:HD2	1:F:519:LEU:HD11	1.92	0.50
1:B:324:GLN:HE22	1:B:542:LEU:N	2.06	0.50
1:E:375:ASN:HD21	1:E:377:LYS:CG	2.24	0.50
1:F:440:LYS:C	1:F:440:LYS:HD3	2.31	0.50
1:F:480:PRO:HA	1:F:503:GLU:CD	2.31	0.50
1:B:442:ILE:HG23	1:B:443:ASP:N	2.26	0.50
1:B:346:VAL:HB	1:B:393:LEU:HD22	1.94	0.50
1:E:469:PRO:O	1:E:470:ASP:C	2.50	0.50
1:C:394:TYR:HE1	1:C:408:LYS:HD2	1.77	0.50
1:C:401:GLU:O	1:C:404:ARG:HB3	2.11	0.50
1:C:518:ILE:HD13	1:C:530:ALA:CB	2.34	0.50
1:B:265:VAL:HG12	1:B:265:VAL:O	2.12	0.50
1:C:395:ASP:O	1:C:396:SER:HB2	2.12	0.50
1:E:440:LYS:HZ2	1:E:444:ASN:ND2	1.98	0.50
1:F:371:GLU:O	1:F:373:ILE:N	2.44	0.50
1:D:283:GLU:HG2	1:D:284:SER:C	2.32	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:392:HIS:C	1:E:393:LEU:HD12	2.31	0.50
1:F:359:ARG:NH1	1:F:541:TRP:CZ2	2.80	0.50
1:B:271:LEU:CD2	1:B:274:ARG:NH2	2.74	0.50
1:C:426:ILE:O	1:C:426:ILE:HG23	2.12	0.50
1:F:306:GLU:HA	1:F:497:ASP:OD2	2.12	0.50
1:B:396:SER:O	1:B:397:PHE:HB3	2.12	0.49
1:D:283:GLU:CG	1:D:523:PHE:CZ	2.93	0.49
1:F:411:TYR:CD1	1:F:415:GLY:HA3	2.47	0.49
1:A:327:LEU:CD2	1:A:356:LEU:HG	2.42	0.49
1:C:440:LYS:C	1:C:440:LYS:HD3	2.31	0.49
1:E:394:TYR:CD1	1:E:394:TYR:C	2.85	0.49
1:A:490:GLY:O	1:A:493:ARG:HG2	2.11	0.49
1:D:267:SER:O	1:D:270:SER:OG	2.22	0.49
1:D:300:LEU:HD12	1:D:524:THR:CG2	2.41	0.49
1:A:536:ASN:C	1:A:538:GLU:N	2.65	0.49
1:A:538:GLU:HA	1:A:538:GLU:OE1	2.11	0.49
1:B:375:ASN:HD21	1:B:377:LYS:CG	2.25	0.49
1:C:405:LEU:O	1:C:408:LYS:N	2.43	0.49
1:A:303:ARG:NH2	1:A:523:PHE:HB3	2.28	0.49
1:B:483:ILE:CG2	1:B:493:ARG:HD3	2.42	0.49
1:C:320:THR:CG2	1:C:324:GLN:HE21	2.26	0.49
1:C:396:SER:O	1:C:397:PHE:CB	2.61	0.49
1:D:413:ARG:NH1	1:D:418:CYS:O	2.42	0.49
1:E:396:SER:O	1:E:397:PHE:CB	2.59	0.49
1:F:271:LEU:O	1:F:275:ILE:HG13	2.13	0.49
1:B:294:GLY:C	1:B:296:ASN:N	2.64	0.49
1:B:289:PHE:CD2	1:B:295:ILE:HG22	2.48	0.49
1:C:399:GLU:HB3	1:C:430:VAL:CG1	2.43	0.49
1:D:467:LYS:HG3	1:D:487:ARG:HA	1.94	0.49
1:D:538:GLU:HA	1:D:538:GLU:OE1	2.13	0.49
1:F:266:VAL:HG11	1:F:271:LEU:CD2	2.35	0.49
1:F:440:LYS:O	1:F:440:LYS:HD3	2.13	0.49
1:A:303:ARG:HH21	1:A:523:PHE:HB2	1.78	0.49
1:A:324:GLN:HE22	1:A:542:LEU:N	2.10	0.49
1:A:518:ILE:N	1:A:518:ILE:CD1	2.76	0.49
1:B:394:TYR:C	1:B:394:TYR:CD1	2.85	0.49
1:B:424:ASP:C	1:B:424:ASP:OD1	2.51	0.49
1:B:307:VAL:N	1:B:497:ASP:OD2	2.39	0.49
1:D:299:THR:O	1:D:300:LEU:HB2	2.12	0.49
1:D:510:MET:N	1:D:511:PRO:HD3	2.28	0.49
1:E:308:ILE:HB	1:E:461:VAL:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:396:SER:O	1:E:397:PHE:HB3	2.13	0.49
1:F:431:SER:O	1:F:432:ALA:C	2.51	0.49
1:A:358:ASN:ND2	1:A:381:TRP:NE1	2.60	0.49
1:A:467:LYS:HG3	1:A:487:ARG:HA	1.94	0.49
1:C:406:LEU:CD2	1:C:448:LYS:HB3	2.32	0.49
1:A:299:THR:O	1:A:300:LEU:HB2	2.12	0.49
1:E:492:LEU:C	1:E:494:GLN:H	2.15	0.49
1:F:426:ILE:O	1:F:426:ILE:HG23	2.12	0.49
1:B:475:HIS:CD2	1:B:479:ARG:HD3	2.47	0.48
1:C:449:LEU:O	1:C:452:PHE:HB3	2.13	0.48
1:E:440:LYS:NZ	1:E:444:ASN:ND2	2.56	0.48
1:E:483:ILE:CG2	1:E:493:ARG:HD3	2.43	0.48
1:A:300:LEU:HD12	1:A:524:THR:CG2	2.43	0.48
1:B:393:LEU:CD1	1:B:393:LEU:N	2.62	0.48
1:C:287:LEU:HG	1:C:329:TRP:CD1	2.48	0.48
1:D:283:GLU:HB2	1:D:303:ARG:NE	2.27	0.48
1:D:437:ASP:C	1:D:439:ARG:N	2.67	0.48
1:F:405:LEU:O	1:F:406:LEU:C	2.51	0.48
1:F:517:ARG:HD2	1:F:519:LEU:CD1	2.43	0.48
1:A:437:ASP:C	1:A:439:ARG:N	2.67	0.48
1:B:429:VAL:HG23	1:B:430:VAL:N	2.24	0.48
1:C:327:LEU:HD13	1:C:353:LEU:CD2	2.41	0.48
1:D:303:ARG:NH2	1:D:523:PHE:HB3	2.28	0.48
1:E:429:VAL:HG23	1:E:430:VAL:N	2.23	0.48
1:F:501:ALA:C	1:F:502:LEU:HD12	2.34	0.48
1:A:283:GLU:O	1:A:306:GLU:OE2	2.30	0.48
1:B:268:ALA:O	1:B:271:LEU:HB2	2.13	0.48
1:B:344:GLU:HG3	1:B:349:THR:CG2	2.39	0.48
1:C:306:GLU:HA	1:C:497:ASP:OD2	2.13	0.48
1:C:517:ARG:HD2	1:C:519:LEU:CD1	2.43	0.48
1:D:316:MET:HE1	1:D:503:GLU:HA	1.95	0.48
1:D:480:PRO:HB3	1:D:517:ARG:HH21	1.79	0.48
1:F:292:CYS:SG	1:F:295:ILE:HD13	2.53	0.48
1:A:506:GLN:HB2	1:B:527:THR:OG1	2.14	0.48
1:C:291:GLY:O	1:C:292:CYS:HB2	2.13	0.48
1:C:359:ARG:NH1	1:C:541:TRP:CE2	2.82	0.48
1:E:480:PRO:HA	1:E:503:GLU:CD	2.33	0.48
1:A:372:ILE:HG21	1:A:381:TRP:CH2	2.48	0.48
1:B:492:LEU:C	1:B:494:GLN:N	2.67	0.48
1:C:440:LYS:O	1:C:440:LYS:HD3	2.14	0.48
1:C:452:PHE:HE1	1:C:456:THR:HG21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:PRO:HA	1:D:503:GLU:OE2	2.14	0.48
1:E:370:ARG:NH1	1:E:370:ARG:HB2	2.28	0.48
1:E:426:ILE:O	1:E:426:ILE:CG1	2.61	0.48
1:F:396:SER:O	1:F:397:PHE:CB	2.61	0.48
1:F:405:LEU:O	1:F:407:ALA:N	2.47	0.48
1:D:316:MET:CE	1:D:504:ARG:N	2.73	0.48
1:E:467:LYS:CG	1:E:487:ARG:HA	2.44	0.48
1:A:510:MET:N	1:A:511:PRO:HD3	2.29	0.48
1:B:310:VAL:HG11	1:B:322:VAL:HG23	1.95	0.48
1:B:316:MET:CG	1:B:504:ARG:HH11	2.27	0.48
1:D:324:GLN:HE22	1:D:542:LEU:N	2.11	0.48
1:D:413:ARG:HD3	1:D:458:VAL:HB	1.96	0.48
1:D:477:GLU:CA	1:D:505:ASN:ND2	2.68	0.48
1:D:510:MET:HB3	1:D:513:LEU:HB2	1.95	0.48
1:C:361:ARG:HB3	1:C:364:GLN:OE1	2.14	0.48
1:D:399:GLU:HB3	1:D:430:VAL:HG11	1.95	0.48
1:D:468:ASN:HD21	1:E:493:ARG:HD2	1.79	0.48
1:E:310:VAL:HG11	1:E:322:VAL:HG23	1.94	0.48
1:E:492:LEU:C	1:E:494:GLN:N	2.68	0.48
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.47	0.47
1:A:524:THR:C	1:A:526:ASP:N	2.65	0.47
1:B:439:ARG:O	1:B:442:ILE:HG22	2.14	0.47
1:B:480:PRO:HA	1:B:503:GLU:CD	2.34	0.47
1:C:320:THR:CG2	1:C:324:GLN:NE2	2.77	0.47
1:D:283:GLU:C	1:D:523:PHE:CG	2.86	0.47
1:D:437:ASP:O	1:D:439:ARG:N	2.47	0.47
1:E:327:LEU:HD21	1:E:357:HIS:CA	2.43	0.47
1:A:289:PHE:HA	1:A:325:GLN:HE21	1.79	0.47
1:B:435:GLU:O	1:B:436:SER:O	2.33	0.47
1:C:411:TYR:CE1	1:C:415:GLY:HA3	2.49	0.47
1:E:439:ARG:O	1:E:442:ILE:HG22	2.14	0.47
1:E:324:GLN:NE2	1:E:542:LEU:H	2.08	0.47
1:B:308:ILE:HB	1:B:461:VAL:HA	1.96	0.47
1:B:469:PRO:O	1:B:470:ASP:C	2.51	0.47
1:D:502:LEU:HD23	1:D:514:VAL:HG21	1.96	0.47
1:D:389:ASP:HB2	1:E:269:LEU:HD12	1.97	0.47
1:E:401:GLU:HB3	1:E:404:ARG:HB2	1.96	0.47
1:F:275:ILE:O	1:F:278:HIS:HB3	2.14	0.47
1:A:375:ASN:O	1:A:375:ASN:ND2	2.45	0.47
1:D:284:SER:O	1:D:285:VAL:HG23	2.14	0.47
1:D:498:THR:HG23	1:D:520:LYS:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:TRP:CZ3	1:E:420:VAL:HG11	2.49	0.47
1:F:405:LEU:O	1:F:408:LYS:N	2.45	0.47
1:F:307:VAL:HB	1:F:496:SER:HA	1.96	0.47
1:F:518:ILE:HG22	1:F:518:ILE:O	2.14	0.47
1:B:346:VAL:CG2	1:C:271:LEU:HD13	2.44	0.47
1:D:482:SER:OG	1:D:484:THR:OG1	2.32	0.47
1:E:435:GLU:O	1:E:436:SER:O	2.32	0.47
1:B:467:LYS:CG	1:B:487:ARG:HA	2.45	0.47
1:C:331:THR:O	1:C:334:GLY:N	2.39	0.47
1:D:425:HIS:CD2	1:D:465:HIS:HE2	2.33	0.47
1:B:370:ARG:O	1:B:373:ILE:HB	2.15	0.47
1:C:292:CYS:SG	1:C:295:ILE:HD13	2.55	0.47
1:E:333:MET:O	1:E:335:LYS:HG2	2.15	0.47
1:F:299:THR:O	1:F:303:ARG:NH1	2.40	0.47
1:F:399:GLU:HB3	1:F:430:VAL:HG21	1.96	0.47
1:A:278:HIS:O	1:A:282:GLU:HB2	2.15	0.47
1:B:401:GLU:HB3	1:B:404:ARG:HB2	1.97	0.47
1:C:359:ARG:NH1	1:C:541:TRP:CZ2	2.83	0.47
1:D:402:THR:HG21	1:D:448:LYS:HZ1	1.79	0.47
1:B:507:GLN:HE21	1:C:517:ARG:HH11	1.63	0.47
1:D:407:ALA:O	1:D:410:ALA:HB3	2.14	0.47
1:D:518:ILE:CD1	1:D:518:ILE:N	2.78	0.47
1:E:294:GLY:C	1:E:296:ASN:N	2.66	0.47
1:E:492:LEU:HD12	1:E:493:ARG:H	1.79	0.47
1:C:491:ALA:O	1:C:495:LEU:HD22	2.15	0.47
1:E:324:GLN:HE22	1:E:542:LEU:N	2.07	0.47
1:E:475:HIS:CD2	1:E:479:ARG:HD3	2.49	0.47
1:F:289:PHE:CD2	1:F:295:ILE:CG2	2.98	0.47
1:A:396:SER:O	1:A:397:PHE:CB	2.62	0.47
1:B:536:ASN:ND2	1:B:536:ASN:C	2.67	0.47
1:C:431:SER:O	1:C:432:ALA:C	2.52	0.47
1:E:382:PHE:CE2	1:F:272:ARG:HG3	2.50	0.47
1:F:492:LEU:C	1:F:494:GLN:N	2.67	0.47
1:A:437:ASP:O	1:A:439:ARG:N	2.48	0.46
1:B:492:LEU:HD12	1:B:493:ARG:H	1.79	0.46
1:D:283:GLU:O	1:D:299:THR:O	2.32	0.46
1:E:316:MET:CE	1:E:504:ARG:H	2.27	0.46
1:A:514:VAL:CG1	1:A:533:MET:HB2	2.43	0.46
1:D:396:SER:O	1:D:397:PHE:CB	2.63	0.46
1:A:502:LEU:HD23	1:A:514:VAL:HG21	1.97	0.46
1:D:375:ASN:HD21	1:D:377:LYS:CG	2.23	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:ASN:O	1:D:447:THR:OG1	2.26	0.46
1:C:399:GLU:HB3	1:C:430:VAL:HG21	1.96	0.46
1:D:521:CYS:O	1:D:525:GLY:N	2.41	0.46
1:E:289:PHE:CD2	1:E:295:ILE:HG22	2.50	0.46
1:E:303:ARG:NH2	1:E:523:PHE:HB3	2.31	0.46
1:A:336:LYS:CB	1:A:418:CYS:HA	2.46	0.46
1:C:521:CYS:O	1:C:522:ARG:C	2.53	0.46
1:E:287:LEU:HD11	1:E:335:LYS:HE2	1.96	0.46
1:E:339:LEU:O	1:E:393:LEU:HA	2.14	0.46
1:F:515:LEU:HD12	1:F:532:TYR:CE2	2.50	0.46
1:A:331:THR:HG22	1:A:332:ALA:N	2.29	0.46
1:A:480:PRO:HB3	1:A:517:ARG:HH21	1.81	0.46
1:E:383:ASP:CG	1:F:272:ARG:HH22	2.19	0.46
1:F:399:GLU:HB3	1:F:430:VAL:CG1	2.44	0.46
1:F:413:ARG:HD3	1:F:458:VAL:HB	1.98	0.46
1:B:351:GLU:HG3	1:C:279:LEU:HD21	1.98	0.46
1:D:308:ILE:HD13	1:D:308:ILE:N	2.30	0.46
1:D:358:ASN:ND2	1:D:381:TRP:NE1	2.63	0.46
1:D:394:TYR:OH	1:D:400:ALA:HB2	2.16	0.46
1:D:412:MET:CE	1:D:421:ILE:HD12	2.45	0.46
1:D:506:GLN:H	1:D:506:GLN:HG2	1.56	0.46
1:D:507:GLN:HE22	1:E:528:GLY:HA2	1.81	0.46
1:A:295:ILE:HD12	1:A:295:ILE:N	2.30	0.46
1:A:444:ASN:O	1:A:447:THR:OG1	2.26	0.46
1:A:477:GLU:CA	1:A:505:ASN:ND2	2.70	0.46
1:B:285:VAL:CG1	1:B:286:GLY:N	2.79	0.46
1:D:345:SER:OG	1:D:348:GLU:HG3	2.16	0.46
1:D:405:LEU:HD11	1:D:409:LEU:HD21	1.97	0.46
1:D:426:ILE:HG22	1:D:464:CYS:HB3	1.97	0.46
1:D:392:HIS:ND1	1:E:267:SER:HB2	2.31	0.46
1:E:370:ARG:O	1:E:373:ILE:HB	2.16	0.46
1:E:316:MET:CG	1:E:504:ARG:HH11	2.28	0.46
1:D:282:GLU:N	1:D:523:PHE:CZ	2.84	0.46
1:B:346:VAL:HG21	1:C:271:LEU:HD13	1.99	0.45
1:B:295:ILE:HG13	1:B:516:VAL:HG11	1.98	0.45
1:C:492:LEU:C	1:C:494:GLN:N	2.68	0.45
1:D:295:ILE:HD12	1:D:295:ILE:N	2.32	0.45
1:D:399:GLU:OE1	1:D:430:VAL:HG22	2.16	0.45
1:E:344:GLU:HG3	1:E:349:THR:CG2	2.39	0.45
1:F:361:ARG:HB3	1:F:364:GLN:OE1	2.16	0.45
1:B:339:LEU:O	1:B:393:LEU:HA	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:ALA:O	1:C:430:VAL:HB	2.16	0.45
1:C:534:GLU:HG3	1:C:545:SER:HB2	1.99	0.45
1:D:368:LEU:HA	1:D:371:GLU:HG3	1.98	0.45
1:D:536:ASN:C	1:D:538:GLU:H	2.19	0.45
1:E:401:GLU:HG2	1:E:402:THR:H	1.81	0.45
1:F:502:LEU:HD12	1:F:502:LEU:N	2.31	0.45
1:F:503:GLU:OE1	1:F:515:LEU:HD22	2.16	0.45
1:A:336:LYS:HB2	1:A:418:CYS:HA	1.98	0.45
1:A:421:ILE:HB	1:A:460:LEU:HD12	1.98	0.45
1:B:425:HIS:H	1:B:463:ILE:HB	1.82	0.45
1:D:336:LYS:HB2	1:D:418:CYS:HA	1.98	0.45
1:D:504:ARG:NE	1:D:511:PRO:O	2.34	0.45
1:F:535:TYR:HD1	1:F:542:LEU:HD12	1.81	0.45
1:A:351:GLU:OE1	1:B:278:HIS:NE2	2.46	0.45
1:A:412:MET:CE	1:A:421:ILE:HD12	2.46	0.45
1:C:503:GLU:OE1	1:C:515:LEU:HD22	2.16	0.45
1:D:303:ARG:HH21	1:D:523:PHE:HB2	1.81	0.45
1:E:272:ARG:HG2	1:E:273:GLU:N	2.31	0.45
1:D:466:LEU:HD23	1:D:486:LEU:HA	1.99	0.45
1:F:266:VAL:CG1	1:F:270:SER:OG	2.65	0.45
1:F:400:ALA:O	1:F:430:VAL:HB	2.16	0.45
1:A:344:GLU:HG3	1:A:349:THR:HG22	1.99	0.45
1:B:329:TRP:CZ3	1:B:420:VAL:HG11	2.51	0.45
1:C:446:MET:HA	1:C:446:MET:CE	2.47	0.45
1:C:467:LYS:O	1:C:469:PRO:HD3	2.16	0.45
1:D:306:GLU:HG2	1:D:497:ASP:HB2	1.98	0.45
1:D:344:GLU:HG3	1:D:349:THR:HG22	1.97	0.45
1:E:402:THR:HG21	1:E:448:LYS:HZ1	1.80	0.45
1:B:468:ASN:OD1	1:C:493:ARG:NH2	2.49	0.45
1:C:535:TYR:HD1	1:C:542:LEU:HD12	1.82	0.45
1:E:348:GLU:O	1:E:351:GLU:HB3	2.16	0.45
1:E:422:ILE:HD13	1:E:461:VAL:HB	1.98	0.45
1:F:450:LYS:O	1:F:450:LYS:HD2	2.16	0.45
1:F:537:LYS:HB3	1:F:537:LYS:HE2	1.76	0.45
1:B:266:VAL:HG12	1:B:267:SER:N	2.32	0.45
1:B:422:ILE:HD13	1:B:461:VAL:HB	1.98	0.45
1:B:316:MET:CE	1:B:504:ARG:H	2.29	0.45
1:F:466:LEU:HB3	1:F:475:HIS:HE1	1.82	0.45
1:A:375:ASN:HD21	1:A:377:LYS:CG	2.23	0.45
1:C:276:ARG:HB2	1:C:276:ARG:NH1	2.32	0.45
1:C:330:GLY:HA3	1:C:391:PHE:CZ	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:HD3	1:C:458:VAL:HB	1.99	0.45
1:D:336:LYS:CB	1:D:418:CYS:HA	2.45	0.45
1:D:421:ILE:HB	1:D:460:LEU:HD12	1.99	0.45
1:A:308:ILE:N	1:A:308:ILE:HD13	2.32	0.45
1:B:466:LEU:HD23	1:B:486:LEU:HA	1.98	0.45
1:F:411:TYR:O	1:F:415:GLY:N	2.45	0.45
1:A:426:ILE:O	1:A:426:ILE:CG2	2.56	0.44
1:A:466:LEU:CD2	1:A:486:LEU:HD23	2.47	0.44
1:A:466:LEU:HD23	1:A:486:LEU:HA	1.99	0.44
1:A:306:GLU:HG2	1:A:497:ASP:HB2	1.99	0.44
1:B:518:ILE:HG22	1:B:527:THR:HA	1.99	0.44
1:D:426:ILE:O	1:D:426:ILE:CG2	2.57	0.44
1:E:295:ILE:HG13	1:E:516:VAL:HG11	1.99	0.44
1:F:330:GLY:HA3	1:F:391:PHE:CZ	2.53	0.44
1:A:536:ASN:C	1:A:538:GLU:H	2.20	0.44
1:B:404:ARG:O	1:B:407:ALA:HB3	2.17	0.44
1:C:505:ASN:HD22	1:C:505:ASN:C	2.20	0.44
1:D:303:ARG:HB2	1:D:306:GLU:OE2	2.17	0.44
1:E:440:LYS:C	1:E:440:LYS:HD3	2.36	0.44
1:F:469:PRO:O	1:F:470:ASP:C	2.56	0.44
1:F:492:LEU:CD1	1:F:492:LEU:H	2.29	0.44
1:B:275:ILE:O	1:B:275:ILE:CG2	2.64	0.44
1:B:401:GLU:HG2	1:B:402:THR:H	1.83	0.44
1:D:519:LEU:O	1:D:520:LYS:HB2	2.17	0.44
1:E:409:LEU:HD23	1:E:412:MET:HE2	1.99	0.44
1:F:309:MET:HB3	1:F:499:ILE:HA	2.00	0.44
1:F:491:ALA:O	1:F:495:LEU:HD22	2.18	0.44
1:A:413:ARG:NH1	1:A:418:CYS:O	2.41	0.44
1:B:440:LYS:C	1:B:440:LYS:HD3	2.37	0.44
1:C:375:ASN:HD21	1:C:377:LYS:CG	2.31	0.44
1:C:492:LEU:CD1	1:C:492:LEU:H	2.31	0.44
1:E:466:LEU:HD23	1:E:486:LEU:HA	1.99	0.44
1:F:375:ASN:HD21	1:F:377:LYS:CG	2.29	0.44
1:A:399:GLU:OE1	1:A:430:VAL:HG22	2.16	0.44
1:B:367:SER:O	1:B:371:GLU:HG2	2.18	0.44
1:F:289:PHE:CD2	1:F:295:ILE:HG22	2.52	0.44
1:F:392:HIS:C	1:F:393:LEU:HD12	2.38	0.44
1:F:439:ARG:O	1:F:442:ILE:HG22	2.17	0.44
1:F:534:GLU:HG3	1:F:545:SER:HB2	1.99	0.44
1:C:501:ALA:C	1:C:502:LEU:HD12	2.38	0.44
1:D:365:SER:OG	1:D:368:LEU:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:ARG:O	1:E:407:ALA:HB3	2.17	0.44
1:F:289:PHE:HA	1:F:325:GLN:HE21	1.82	0.44
1:F:331:THR:O	1:F:334:GLY:N	2.38	0.44
1:A:482:SER:OG	1:A:484:THR:OG1	2.32	0.44
1:B:289:PHE:N	1:B:296:ASN:HD21	2.09	0.44
1:D:542:LEU:HA	1:D:542:LEU:HD12	1.81	0.44
1:F:442:ILE:HG21	1:F:488:GLY:CA	2.48	0.44
1:F:547:TYR:CG	1:F:548:SER:N	2.86	0.44
1:A:288:LEU:HB3	1:A:296:ASN:OD1	2.17	0.44
1:C:450:LYS:HD2	1:C:450:LYS:O	2.18	0.44
1:D:405:LEU:O	1:D:409:LEU:HG	2.17	0.44
1:A:287:LEU:HD11	1:A:335:LYS:HG3	1.99	0.44
1:A:368:LEU:HA	1:A:371:GLU:HG3	2.00	0.44
1:A:498:THR:HG23	1:A:520:LYS:O	2.18	0.44
1:B:409:LEU:HD23	1:B:412:MET:HE2	1.99	0.44
1:C:289:PHE:H	1:C:296:ASN:HD21	1.65	0.44
1:C:411:TYR:CD1	1:C:415:GLY:HA3	2.53	0.44
1:D:367:SER:O	1:D:371:GLU:CG	2.66	0.44
1:D:466:LEU:CD2	1:D:486:LEU:HD23	2.47	0.44
1:A:385:LEU:HD23	1:A:386:PHE:CE2	2.53	0.43
1:A:405:LEU:HD11	1:A:409:LEU:HD21	1.99	0.43
1:B:393:LEU:HD12	1:B:393:LEU:H	1.79	0.43
1:B:440:LYS:HZ2	1:B:444:ASN:HB2	1.83	0.43
1:C:275:ILE:O	1:C:278:HIS:HB3	2.18	0.43
1:C:309:MET:HB3	1:C:499:ILE:HA	2.00	0.43
1:E:275:ILE:O	1:E:279:LEU:HG	2.17	0.43
1:F:309:MET:HB3	1:F:499:ILE:HG12	2.00	0.43
1:A:401:GLU:HG2	1:A:402:THR:H	1.82	0.43
1:C:331:THR:O	1:C:333:MET:N	2.51	0.43
1:E:367:SER:O	1:E:371:GLU:HG2	2.17	0.43
1:F:449:LEU:O	1:F:452:PHE:HB3	2.18	0.43
1:F:359:ARG:HB3	1:F:539:THR:HG22	2.00	0.43
1:B:267:SER:O	1:B:268:ALA:C	2.57	0.43
1:C:478:GLY:O	1:C:479:ARG:O	2.36	0.43
1:E:290:SER:N	1:E:325:GLN:HE21	2.05	0.43
1:E:379:ASP:OD2	1:F:276:ARG:NH2	2.51	0.43
1:F:311:THR:O	1:F:312:SER:HB3	2.18	0.43
1:F:467:LYS:O	1:F:469:PRO:HD3	2.18	0.43
1:F:505:ASN:C	1:F:505:ASN:HD22	2.20	0.43
1:A:519:LEU:O	1:A:520:LYS:HB2	2.18	0.43
1:B:403:ASP:O	1:B:407:ALA:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:GLU:HA	1:C:282:GLU:OE1	2.18	0.43
1:D:287:LEU:O	1:D:301:GLY:HA3	2.18	0.43
1:D:309:MET:O	1:D:500:ILE:N	2.49	0.43
1:D:405:LEU:HG	1:D:409:LEU:HD11	2.00	0.43
1:E:312:SER:OG	1:E:318:LYS:HG3	2.18	0.43
1:E:403:ASP:O	1:E:407:ALA:HB2	2.18	0.43
1:B:404:ARG:HG3	1:B:404:ARG:HH11	1.83	0.43
1:C:312:SER:OG	1:C:318:LYS:CG	2.67	0.43
1:C:492:LEU:O	1:C:494:GLN:N	2.51	0.43
1:D:439:ARG:O	1:D:443:ASP:OD2	2.36	0.43
1:E:309:MET:O	1:E:500:ILE:N	2.41	0.43
1:E:547:TYR:CG	1:E:548:SER:N	2.87	0.43
1:F:413:ARG:CD	1:F:458:VAL:HB	2.47	0.43
1:F:498:THR:HA	1:F:520:LYS:O	2.19	0.43
1:A:394:TYR:OH	1:A:400:ALA:HB2	2.18	0.43
1:B:468:ASN:HD21	1:C:493:ARG:NE	2.15	0.43
1:B:547:TYR:CG	1:B:548:SER:N	2.86	0.43
1:C:505:ASN:HD22	1:C:507:GLN:H	1.66	0.43
1:E:518:ILE:HG22	1:E:518:ILE:O	2.19	0.43
1:F:327:LEU:HD13	1:F:353:LEU:CD2	2.40	0.43
1:F:446:MET:CE	1:F:446:MET:HA	2.48	0.43
1:A:367:SER:O	1:A:371:GLU:CG	2.67	0.43
1:A:427:SER:O	1:A:429:VAL:N	2.52	0.43
1:A:426:ILE:HG22	1:A:464:CYS:HB3	2.00	0.43
1:B:303:ARG:NH2	1:B:523:PHE:HB3	2.33	0.43
1:B:492:LEU:O	1:B:494:GLN:N	2.52	0.43
1:D:331:THR:HG22	1:D:332:ALA:N	2.33	0.43
1:D:388:ASN:O	1:D:389:ASP:C	2.56	0.43
1:D:401:GLU:HG2	1:D:402:THR:H	1.83	0.43
1:D:466:LEU:HB3	1:D:475:HIS:HE1	1.84	0.43
1:D:498:THR:HG22	1:D:499:ILE:N	2.33	0.43
1:E:404:ARG:HG3	1:E:404:ARG:HH11	1.82	0.43
1:F:303:ARG:NH2	1:F:523:PHE:CB	2.81	0.43
1:C:307:VAL:HB	1:C:496:SER:HA	2.00	0.43
1:C:547:TYR:CG	1:C:548:SER:N	2.87	0.43
1:D:431:SER:O	1:D:432:ALA:C	2.56	0.43
1:D:309:MET:HE3	1:D:462:VAL:HB	2.00	0.43
1:E:309:MET:HE1	1:E:464:CYS:HB3	2.01	0.43
1:F:291:GLY:O	1:F:292:CYS:HB2	2.18	0.43
1:F:521:CYS:O	1:F:522:ARG:C	2.57	0.43
1:A:407:ALA:O	1:A:410:ALA:HB3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:HE2	1:A:503:GLU:HA	2.00	0.43
1:B:458:VAL:HG22	1:B:459:VAL:N	2.34	0.43
1:B:309:MET:HE1	1:B:464:CYS:HB3	1.99	0.43
1:D:283:GLU:O	1:D:303:ARG:CZ	2.67	0.43
1:D:333:MET:O	1:D:335:LYS:HG2	2.18	0.43
1:F:289:PHE:CA	1:F:325:GLN:HE21	2.32	0.43
1:F:450:LYS:HE2	1:F:454:LYS:HD2	2.01	0.43
1:A:439:ARG:O	1:A:443:ASP:OD2	2.37	0.43
1:A:480:PRO:HA	1:A:503:GLU:OE2	2.18	0.43
1:C:296:ASN:HD22	1:C:296:ASN:HA	1.68	0.43
1:B:327:LEU:HD21	1:B:357:HIS:CA	2.47	0.42
1:E:492:LEU:O	1:E:494:GLN:N	2.52	0.42
1:F:505:ASN:HD22	1:F:507:GLN:H	1.66	0.42
1:A:357:HIS:ND1	1:A:385:LEU:HB2	2.34	0.42
1:A:388:ASN:O	1:A:389:ASP:C	2.57	0.42
1:C:288:LEU:HB3	1:C:296:ASN:ND2	2.33	0.42
1:C:469:PRO:O	1:C:470:ASP:C	2.56	0.42
1:D:283:GLU:HB2	1:D:523:PHE:CD2	2.53	0.42
1:E:375:ASN:HD21	1:E:377:LYS:CD	2.31	0.42
1:A:303:ARG:HB2	1:A:306:GLU:OE2	2.19	0.42
1:B:375:ASN:HD21	1:B:377:LYS:CD	2.32	0.42
1:C:477:GLU:HA	1:C:505:ASN:ND2	2.34	0.42
1:E:424:ASP:C	1:E:424:ASP:OD1	2.57	0.42
1:F:331:THR:O	1:F:333:MET:N	2.52	0.42
1:F:388:ASN:O	1:F:389:ASP:C	2.58	0.42
1:A:431:SER:O	1:A:432:ALA:C	2.56	0.42
1:B:344:GLU:OE2	1:B:349:THR:HG22	2.19	0.42
1:C:398:ALA:O	1:C:399:GLU:C	2.58	0.42
1:F:266:VAL:HG12	1:F:270:SER:OG	2.19	0.42
1:F:312:SER:OG	1:F:318:LYS:CG	2.66	0.42
1:B:506:GLN:H	1:B:506:GLN:HG2	1.61	0.42
1:E:458:VAL:HG22	1:E:459:VAL:N	2.34	0.42
1:F:429:VAL:CG2	1:F:430:VAL:N	2.77	0.42
1:F:492:LEU:HD12	1:F:492:LEU:N	2.34	0.42
1:A:424:ASP:O	1:A:425:HIS:HB3	2.19	0.42
1:A:316:MET:HE1	1:A:503:GLU:HA	2.01	0.42
1:C:282:GLU:O	1:C:282:GLU:CG	2.66	0.42
1:C:299:THR:O	1:C:303:ARG:NH1	2.40	0.42
1:E:431:SER:HB3	1:E:441:MET:HE3	1.98	0.42
1:F:368:LEU:HA	1:F:368:LEU:HD23	1.82	0.42
1:A:413:ARG:HD3	1:A:458:VAL:HB	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:SER:OG	1:B:318:LYS:HG3	2.19	0.42
1:C:287:LEU:HD21	1:C:420:VAL:HG21	2.01	0.42
1:C:439:ARG:O	1:C:442:ILE:HG22	2.20	0.42
1:C:466:LEU:HB3	1:C:475:HIS:HE1	1.85	0.42
1:D:425:HIS:CE1	1:D:427:SER:CB	2.93	0.42
1:D:316:MET:HE2	1:D:503:GLU:HA	2.01	0.42
1:E:518:ILE:CG2	1:E:527:THR:HA	2.50	0.42
1:F:401:GLU:HB3	1:F:404:ARG:CB	2.47	0.42
1:F:458:VAL:HG22	1:F:459:VAL:H	1.85	0.42
1:B:336:LYS:HB2	1:B:418:CYS:HA	2.02	0.42
1:B:366:ASP:OD1	1:C:284:SER:OG	2.33	0.42
1:B:409:LEU:HA	1:B:412:MET:HE3	2.02	0.42
1:C:442:ILE:HG21	1:C:488:GLY:CA	2.49	0.42
1:D:468:ASN:HA	1:D:469:PRO:HD2	1.84	0.42
1:E:312:SER:HB2	1:E:502:LEU:O	2.20	0.42
1:E:336:LYS:HB2	1:E:418:CYS:HA	2.02	0.42
1:E:446:MET:O	1:E:449:LEU:N	2.53	0.42
1:E:425:HIS:H	1:E:463:ILE:HB	1.84	0.42
1:F:492:LEU:O	1:F:494:GLN:N	2.52	0.42
1:F:524:THR:C	1:F:526:ASP:H	2.23	0.42
1:B:371:GLU:C	1:B:373:ILE:N	2.73	0.42
1:C:288:LEU:CA	1:C:296:ASN:HD21	2.32	0.42
1:C:388:ASN:O	1:C:389:ASP:C	2.57	0.42
1:C:450:LYS:HE2	1:C:454:LYS:HD2	2.02	0.42
1:D:426:ILE:CG2	1:D:464:CYS:HB3	2.50	0.42
1:F:325:GLN:HB3	1:F:329:TRP:CZ3	2.55	0.42
1:A:289:PHE:CD2	1:A:295:ILE:HG22	2.55	0.42
1:A:303:ARG:NH2	1:A:523:PHE:HB2	2.35	0.42
1:C:276:ARG:C	1:C:278:HIS:N	2.73	0.42
1:C:405:LEU:C	1:C:407:ALA:N	2.73	0.42
1:D:375:ASN:C	1:D:375:ASN:ND2	2.73	0.42
1:E:393:LEU:HD12	1:E:393:LEU:H	1.79	0.42
1:E:316:MET:CE	1:E:504:ARG:N	2.83	0.42
1:F:362:LEU:O	1:F:369:LYS:HE2	2.20	0.42
1:A:372:ILE:HD13	1:A:381:TRP:HZ3	1.83	0.41
1:A:466:LEU:HB3	1:A:475:HIS:HE1	1.85	0.41
1:A:382:PHE:CZ	1:B:272:ARG:HB2	2.55	0.41
1:B:312:SER:HB2	1:B:502:LEU:O	2.20	0.41
1:C:401:GLU:HB3	1:C:404:ARG:CB	2.47	0.41
1:C:309:MET:HB3	1:C:499:ILE:HG12	2.02	0.41
1:D:309:MET:O	1:D:499:ILE:HA	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:ILE:HD13	1:D:530:ALA:HB2	1.98	0.41
1:D:513:LEU:HD12	1:D:533:MET:O	2.21	0.41
1:B:377:LYS:O	1:B:380:GLN:HB2	2.20	0.41
1:C:458:VAL:HG22	1:C:459:VAL:H	1.85	0.41
1:E:377:LYS:O	1:E:380:GLN:HB2	2.20	0.41
1:F:477:GLU:HA	1:F:505:ASN:ND2	2.35	0.41
1:D:427:SER:O	1:D:429:VAL:N	2.52	0.41
1:D:539:THR:OG1	1:D:541:TRP:HB2	2.20	0.41
1:E:345:SER:OG	1:E:347:GLU:HG2	2.20	0.41
1:F:421:ILE:HB	1:F:460:LEU:HD12	2.01	0.41
1:F:463:ILE:HG21	1:F:463:ILE:HD13	1.87	0.41
1:A:405:LEU:O	1:A:409:LEU:HG	2.20	0.41
1:A:416:LEU:HD23	1:A:416:LEU:N	2.35	0.41
1:B:440:LYS:NZ	1:B:444:ASN:HB2	2.35	0.41
1:C:498:THR:HA	1:C:520:LYS:O	2.21	0.41
1:D:283:GLU:CG	1:D:523:PHE:CE2	3.03	0.41
1:D:416:LEU:N	1:D:416:LEU:HD23	2.35	0.41
1:D:515:LEU:HD21	1:D:517:ARG:HB2	2.03	0.41
1:E:371:GLU:C	1:E:373:ILE:N	2.73	0.41
1:A:446:MET:CG	1:A:492:LEU:HB3	2.45	0.41
1:D:286:GLY:O	1:D:287:LEU:O	2.39	0.41
1:D:289:PHE:N	1:D:296:ASN:HD21	2.09	0.41
1:D:382:PHE:CE1	1:E:275:ILE:HD12	2.55	0.41
1:E:506:GLN:HG2	1:E:506:GLN:H	1.61	0.41
1:A:287:LEU:O	1:A:301:GLY:HA3	2.20	0.41
1:B:348:GLU:O	1:B:351:GLU:HB3	2.20	0.41
1:C:401:GLU:OE1	1:C:404:ARG:N	2.50	0.41
1:D:282:GLU:OE2	1:D:522:ARG:O	2.39	0.41
1:D:340:ALA:H	1:D:341:MET:CE	2.32	0.41
1:D:515:LEU:CD2	1:D:515:LEU:C	2.89	0.41
1:E:431:SER:O	1:E:432:ALA:C	2.59	0.41
1:B:431:SER:O	1:B:432:ALA:C	2.59	0.41
1:C:436:SER:O	1:C:437:ASP:O	2.39	0.41
1:C:468:ASN:HA	1:C:469:PRO:HD2	1.85	0.41
1:D:327:LEU:HD12	1:D:327:LEU:HA	1.83	0.41
1:D:343:GLU:HG3	1:D:428:ILE:CD1	2.50	0.41
1:E:373:ILE:HD11	1:F:279:LEU:CB	2.51	0.41
1:A:365:SER:OG	1:A:368:LEU:HB2	2.21	0.41
1:A:452:PHE:CE1	1:A:456:THR:HG21	2.55	0.41
1:C:518:ILE:HG22	1:C:518:ILE:O	2.20	0.41
1:C:537:LYS:HB3	1:C:537:LYS:HE2	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:LEU:HA	1:E:412:MET:HE3	2.03	0.41
1:E:479:ARG:HA	1:E:480:PRO:HD2	1.92	0.41
1:A:309:MET:O	1:A:499:ILE:HA	2.21	0.41
1:A:345:SER:OG	1:A:348:GLU:HG3	2.21	0.41
1:A:405:LEU:HG	1:A:409:LEU:HD11	2.03	0.41
1:B:287:LEU:HG	1:B:329:TRP:NE1	2.36	0.41
1:B:333:MET:O	1:B:334:GLY:C	2.59	0.41
1:C:287:LEU:HG	1:C:329:TRP:NE1	2.36	0.41
1:C:325:GLN:HB3	1:C:329:TRP:CZ3	2.56	0.41
1:E:369:LYS:NZ	1:F:282:GLU:HG3	2.36	0.41
1:E:359:ARG:HD3	1:E:541:TRP:NE1	2.35	0.41
1:F:289:PHE:HB3	1:F:325:GLN:NE2	2.36	0.41
1:F:406:LEU:O	1:F:410:ALA:HB2	2.20	0.41
1:A:469:PRO:O	1:A:470:ASP:C	2.59	0.41
1:C:311:THR:O	1:C:312:SER:HB3	2.21	0.41
1:C:324:GLN:HE22	1:C:542:LEU:HB2	1.85	0.41
1:D:424:ASP:OD1	1:D:425:HIS:N	2.54	0.41
1:A:340:ALA:H	1:A:341:MET:CE	2.34	0.41
1:B:316:MET:CE	1:B:504:ARG:N	2.84	0.41
1:C:413:ARG:CD	1:C:458:VAL:HB	2.51	0.41
1:F:440:LYS:HZ3	1:F:444:ASN:HB2	1.85	0.41
1:B:412:MET:HE3	1:B:421:ILE:HD12	2.02	0.40
1:C:411:TYR:O	1:C:415:GLY:N	2.51	0.40
1:D:445:LEU:HA	1:D:448:LYS:HE3	2.03	0.40
1:E:344:GLU:OE2	1:E:349:THR:HG22	2.20	0.40
1:F:468:ASN:HA	1:F:469:PRO:HD2	1.86	0.40
1:D:303:ARG:N	1:D:303:ARG:HD3	2.36	0.40
1:E:361:ARG:NH1	1:E:535:TYR:OH	2.54	0.40
1:A:324:GLN:HE22	1:A:542:LEU:HB2	1.86	0.40
1:D:424:ASP:O	1:D:425:HIS:HB3	2.21	0.40
1:F:404:ARG:NH1	1:F:408:LYS:CE	2.72	0.40
1:A:309:MET:HE3	1:A:462:VAL:O	2.21	0.40
1:B:402:THR:HG21	1:B:448:LYS:HZ2	1.84	0.40
1:B:519:LEU:HD12	1:B:519:LEU:HA	1.78	0.40
1:E:310:VAL:HG22	1:E:500:ILE:HB	2.04	0.40
1:F:340:ALA:HB3	1:F:423:LEU:HA	2.02	0.40
1:B:502:LEU:HD23	1:B:514:VAL:HG21	2.02	0.40
1:C:407:ALA:O	1:C:410:ALA:HB3	2.21	0.40
1:D:469:PRO:O	1:D:470:ASP:C	2.59	0.40
1:D:474:ALA:O	1:D:476:GLU:N	2.54	0.40
1:E:333:MET:O	1:E:334:GLY:C	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:307:VAL:N	1:E:497:ASP:OD2	2.39	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/289 (98%)	225 (79%)	34 (12%)	25 (9%)	1	5
1	B	286/289 (99%)	226 (79%)	42 (15%)	18 (6%)	1	9
1	C	286/289 (99%)	225 (79%)	45 (16%)	16 (6%)	2	11
1	D	284/289 (98%)	223 (78%)	34 (12%)	27 (10%)	0	4
1	E	286/289 (99%)	231 (81%)	37 (13%)	18 (6%)	1	9
1	F	286/289 (99%)	225 (79%)	40 (14%)	21 (7%)	1	7
All	All	1712/1734 (99%)	1355 (79%)	232 (14%)	125 (7%)	1	7

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	SER
1	A	436	SER
1	A	437	ASP
1	A	475	HIS
1	A	489	SER
1	A	490	GLY
1	B	279	LEU
1	B	371	GLU
1	B	372	ILE
1	B	396	SER
1	B	399	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	432	ALA
1	B	436	SER
1	B	437	ASP
1	B	475	HIS
1	B	490	GLY
1	C	292	CYS
1	C	371	GLU
1	C	436	SER
1	C	437	ASP
1	C	475	HIS
1	C	479	ARG
1	C	490	GLY
1	D	281	SER
1	D	396	SER
1	D	436	SER
1	D	437	ASP
1	D	475	HIS
1	D	489	SER
1	D	490	GLY
1	E	371	GLU
1	E	372	ILE
1	E	396	SER
1	E	399	GLU
1	E	432	ALA
1	E	436	SER
1	E	437	ASP
1	E	475	HIS
1	E	490	GLY
1	F	371	GLU
1	F	436	SER
1	F	437	ASP
1	F	475	HIS
1	F	479	ARG
1	F	490	GLY
1	A	399	GLU
1	A	432	ALA
1	A	438	GLU
1	A	525	GLY
1	A	537	LYS
1	B	334	GLY
1	C	332	ALA
1	C	372	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	396	SER
1	C	399	GLU
1	C	432	ALA
1	C	488	GLY
1	C	522	ARG
1	D	272	ARG
1	D	287	LEU
1	D	371	GLU
1	D	399	GLU
1	D	432	ALA
1	D	438	GLU
1	D	525	GLY
1	D	537	LYS
1	E	334	GLY
1	E	388	ASN
1	F	292	CYS
1	F	332	ALA
1	F	372	ILE
1	F	396	SER
1	F	399	GLU
1	F	432	ALA
1	A	281	SER
1	A	371	GLU
1	A	485	ASP
1	B	388	ASN
1	B	397	PHE
1	B	479	ARG
1	C	397	PHE
1	C	406	LEU
1	D	271	LEU
1	D	285	VAL
1	D	485	ASP
1	E	479	ARG
1	E	537	LYS
1	F	269	LEU
1	F	279	LEU
1	F	281	SER
1	F	287	LEU
1	F	397	PHE
1	F	406	LEU
1	F	488	GLY
1	F	522	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	334	GLY
1	A	397	PHE
1	A	479	ARG
1	A	487	ARG
1	A	548	SER
1	B	318	LYS
1	B	471	LYS
1	B	537	LYS
1	D	397	PHE
1	D	479	ARG
1	D	487	ARG
1	D	548	SER
1	E	318	LYS
1	E	397	PHE
1	E	471	LYS
1	A	327	LEU
1	A	471	LYS
1	A	523	PHE
1	D	334	GLY
1	D	471	LYS
1	E	292	CYS
1	E	389	ASP
1	F	278	HIS
1	A	287	LEU
1	D	523	PHE
1	B	264	GLY
1	A	428	ILE
1	A	488	GLY
1	D	428	ILE
1	D	488	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	241/242 (100%)	211 (88%)	30 (12%)	4 19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	241/242 (100%)	217 (90%)	24 (10%)	7	27
1	C	241/242 (100%)	216 (90%)	25 (10%)	7	25
1	D	241/242 (100%)	212 (88%)	29 (12%)	5	20
1	E	241/242 (100%)	216 (90%)	25 (10%)	7	25
1	F	241/242 (100%)	217 (90%)	24 (10%)	7	27
All	All	1446/1452 (100%)	1289 (89%)	157 (11%)	6	24

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	274	ARG
1	A	288	LEU
1	A	303	ARG
1	A	312	SER
1	A	314	SER
1	A	324	GLN
1	A	328	GLN
1	A	347	GLU
1	A	349	THR
1	A	360	VAL
1	A	366	ASP
1	A	368	LEU
1	A	375	ASN
1	A	393	LEU
1	A	403	ASP
1	A	406	LEU
1	A	470	ASP
1	A	476	GLU
1	A	481	VAL
1	A	487	ARG
1	A	492	LEU
1	A	504	ARG
1	A	506	GLN
1	A	507	GLN
1	A	512	ASN
1	A	515	LEU
1	A	522	ARG
1	A	524	THR
1	A	536	ASN
1	A	542	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	277	GLU
1	B	290	SER
1	B	303	ARG
1	B	347	GLU
1	B	349	THR
1	B	359	ARG
1	B	360	VAL
1	B	366	ASP
1	B	368	LEU
1	B	393	LEU
1	B	394	TYR
1	B	403	ASP
1	B	440	LYS
1	B	468	ASN
1	B	470	ASP
1	B	471	LYS
1	B	481	VAL
1	B	487	ARG
1	B	492	LEU
1	B	493	ARG
1	B	504	ARG
1	B	506	GLN
1	B	512	ASN
1	B	536	ASN
1	C	273	GLU
1	C	274	ARG
1	C	287	LEU
1	C	303	ARG
1	C	314	SER
1	C	347	GLU
1	C	349	THR
1	C	360	VAL
1	C	368	LEU
1	C	390	THR
1	C	393	LEU
1	C	403	ASP
1	C	440	LYS
1	C	470	ASP
1	C	476	GLU
1	C	481	VAL
1	C	487	ARG
1	C	492	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	493	ARG
1	C	495	LEU
1	C	504	ARG
1	C	505	ASN
1	C	512	ASN
1	C	519	LEU
1	C	536	ASN
1	D	270	SER
1	D	277	GLU
1	D	303	ARG
1	D	314	SER
1	D	324	GLN
1	D	328	GLN
1	D	347	GLU
1	D	349	THR
1	D	360	VAL
1	D	366	ASP
1	D	368	LEU
1	D	375	ASN
1	D	393	LEU
1	D	403	ASP
1	D	406	LEU
1	D	470	ASP
1	D	476	GLU
1	D	481	VAL
1	D	487	ARG
1	D	492	LEU
1	D	504	ARG
1	D	506	GLN
1	D	507	GLN
1	D	512	ASN
1	D	515	LEU
1	D	522	ARG
1	D	524	THR
1	D	536	ASN
1	D	542	LEU
1	E	274	ARG
1	E	277	GLU
1	E	284	SER
1	E	290	SER
1	E	303	ARG
1	E	347	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	349	THR
1	E	359	ARG
1	E	360	VAL
1	E	368	LEU
1	E	393	LEU
1	E	394	TYR
1	E	403	ASP
1	E	440	LYS
1	E	468	ASN
1	E	470	ASP
1	E	471	LYS
1	E	481	VAL
1	E	487	ARG
1	E	492	LEU
1	E	493	ARG
1	E	504	ARG
1	E	506	GLN
1	E	512	ASN
1	E	536	ASN
1	F	277	GLU
1	F	281	SER
1	F	303	ARG
1	F	314	SER
1	F	347	GLU
1	F	349	THR
1	F	360	VAL
1	F	368	LEU
1	F	390	THR
1	F	393	LEU
1	F	403	ASP
1	F	440	LYS
1	F	470	ASP
1	F	476	GLU
1	F	481	VAL
1	F	487	ARG
1	F	492	LEU
1	F	493	ARG
1	F	495	LEU
1	F	504	ARG
1	F	505	ASN
1	F	512	ASN
1	F	519	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	536	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	324	GLN
1	A	325	GLN
1	A	358	ASN
1	A	375	ASN
1	A	392	HIS
1	A	425	HIS
1	A	475	HIS
1	A	494	GLN
1	A	505	ASN
1	A	507	GLN
1	A	536	ASN
1	B	296	ASN
1	B	324	GLN
1	B	325	GLN
1	B	358	ASN
1	B	375	ASN
1	B	392	HIS
1	B	444	ASN
1	B	505	ASN
1	B	507	GLN
1	B	536	ASN
1	C	296	ASN
1	C	324	GLN
1	C	325	GLN
1	C	358	ASN
1	C	375	ASN
1	C	475	HIS
1	C	494	GLN
1	C	505	ASN
1	C	536	ASN
1	D	278	HIS
1	D	296	ASN
1	D	324	GLN
1	D	325	GLN
1	D	358	ASN
1	D	375	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	425	HIS
1	D	475	HIS
1	D	494	GLN
1	D	505	ASN
1	D	507	GLN
1	D	536	ASN
1	E	296	ASN
1	E	324	GLN
1	E	325	GLN
1	E	358	ASN
1	E	375	ASN
1	E	444	ASN
1	E	505	ASN
1	E	507	GLN
1	E	536	ASN
1	F	296	ASN
1	F	324	GLN
1	F	325	GLN
1	F	358	ASN
1	F	375	ASN
1	F	392	HIS
1	F	475	HIS
1	F	494	GLN
1	F	505	ASN
1	F	536	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 carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	283:GLU	C	284:SER	N	7.79
1	A	283:GLU	C	284:SER	N	6.86

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/289 (99%)	0.13	19 (6%) 18 18	40, 88, 175, 200	0
1	B	288/289 (99%)	-0.12	13 (4%) 33 32	23, 71, 167, 200	0
1	C	288/289 (99%)	-0.09	13 (4%) 33 32	30, 73, 168, 192	0
1	D	288/289 (99%)	0.41	28 (9%) 7 8	65, 117, 178, 200	0
1	E	288/289 (99%)	0.12	25 (8%) 10 10	47, 103, 176, 200	0
1	F	288/289 (99%)	0.04	21 (7%) 15 15	43, 94, 172, 200	0
All	All	1728/1734 (99%)	0.08	119 (6%) 16 16	23, 92, 175, 200	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	SER	18.5
1	D	284	SER	12.2
1	E	431	SER	10.7
1	A	435	GLU	10.4
1	D	434	GLY	10.3
1	A	434	GLY	9.5
1	A	262	PRO	9.5
1	E	435	GLU	8.8
1	A	285	VAL	8.6
1	B	436	SER	8.3
1	B	397	PHE	8.0
1	F	434	GLY	8.0
1	D	262	PRO	7.5
1	B	431	SER	7.5
1	A	430	VAL	7.3
1	C	436	SER	7.2
1	E	397	PHE	7.1
1	B	433	SER	6.9
1	C	433	SER	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	433	SER	6.5
1	B	434	GLY	6.3
1	D	435	GLU	6.3
1	F	436	SER	5.7
1	F	262	PRO	5.7
1	C	435	GLU	5.4
1	B	435	GLU	5.4
1	B	262	PRO	5.3
1	E	432	ALA	5.3
1	C	473	LYS	5.2
1	A	431	SER	5.2
1	A	436	SER	5.1
1	E	399	GLU	5.1
1	D	433	SER	4.9
1	E	262	PRO	4.8
1	F	397	PHE	4.5
1	F	549	GLY	4.4
1	D	399	GLU	4.4
1	E	283	GLU	4.3
1	D	285	VAL	4.3
1	A	432	ALA	4.3
1	D	431	SER	4.2
1	E	549	GLY	4.2
1	F	433	SER	4.1
1	F	435	GLU	4.0
1	E	473	LYS	4.0
1	C	434	GLY	4.0
1	E	548	SER	3.9
1	D	473	LYS	3.9
1	C	437	ASP	3.8
1	B	437	ASP	3.8
1	D	338	GLY	3.8
1	D	404	ARG	3.7
1	A	283	GLU	3.7
1	E	434	GLY	3.7
1	B	432	ALA	3.7
1	E	509	ASP	3.6
1	F	490	GLY	3.5
1	D	455	SER	3.4
1	A	548	SER	3.4
1	E	436	SER	3.4
1	F	469	PRO	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	549	GLY	3.4
1	C	397	PHE	3.4
1	A	399	GLU	3.3
1	D	436	SER	3.3
1	B	398	ALA	3.2
1	D	470	ASP	3.2
1	A	437	ASP	3.2
1	D	264	GLY	3.2
1	E	284	SER	3.2
1	F	437	ASP	3.2
1	A	397	PHE	3.1
1	F	472	GLY	3.1
1	D	430	VAL	3.1
1	E	430	VAL	3.1
1	C	506	GLN	3.1
1	D	456	THR	3.1
1	A	547	TYR	3.1
1	E	439	ARG	3.0
1	E	437	ASP	3.0
1	B	430	VAL	3.0
1	D	539	THR	3.0
1	E	282	GLU	2.9
1	F	264	GLY	2.9
1	E	489	SER	2.9
1	D	397	PHE	2.9
1	D	283	GLU	2.9
1	D	509	ASP	2.9
1	D	432	ALA	2.8
1	F	473	LYS	2.8
1	A	433	SER	2.8
1	C	472	GLY	2.8
1	C	432	ALA	2.8
1	C	262	PRO	2.7
1	E	441	MET	2.7
1	F	432	ALA	2.7
1	D	454	LYS	2.6
1	F	285	VAL	2.6
1	F	507	GLN	2.6
1	D	437	ASP	2.5
1	B	549	GLY	2.5
1	D	398	ALA	2.4
1	F	338	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	546	SER	2.4
1	B	399	GLU	2.3
1	A	526	ASP	2.3
1	E	281	SER	2.3
1	F	284	SER	2.3
1	F	374	GLU	2.3
1	D	540	GLY	2.2
1	F	430	VAL	2.2
1	D	536	ASN	2.1
1	A	473	LYS	2.1
1	A	286	GLY	2.1
1	E	547	TYR	2.1
1	F	414	SER	2.0
1	C	431	SER	2.0
1	E	470	ASP	2.0
1	D	474	ALA	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 carbohydrates 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.